



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 06:50 PM EDT

PDB ID : 1SMJ / pdb_00001smj
Title : Structure of the A264E mutant of cytochrome P450 BM3 complexed with palmitoleate
Authors : Joyce, M.G.; Girvan, H.M.; Munro, A.W.; Leys, D.
Deposited on : 2004-03-09
Resolution : 2.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

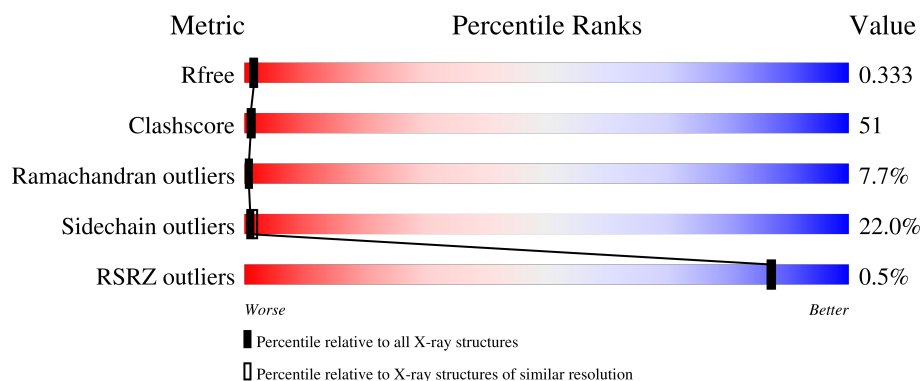
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	471	
1	B	471	
1	C	471	
1	D	471	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14913 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

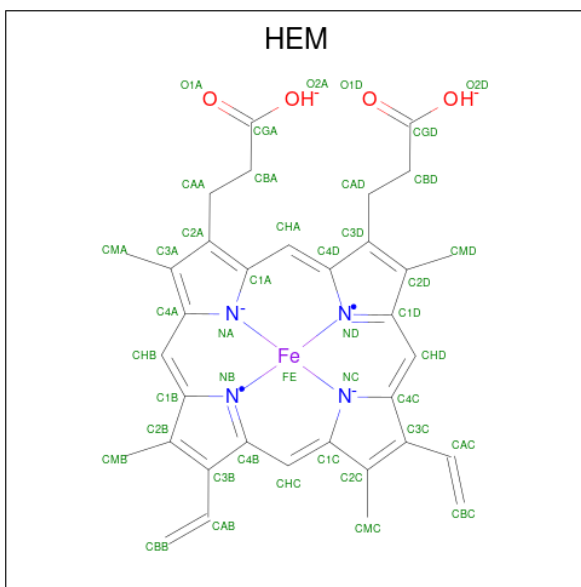
- Molecule 1 is a protein called Bifunctional P-450:NADPH-P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3662	2340	621	684	17			
1	B	455	Total	C	N	O	S	0	0	0
			3670	2344	622	687	17			
1	C	455	Total	C	N	O	S	0	0	0
			3670	2344	622	687	17			
1	D	454	Total	C	N	O	S	0	0	0
			3667	2343	622	685	17			

There are 4 discrepancies between the modelled and reference sequences:

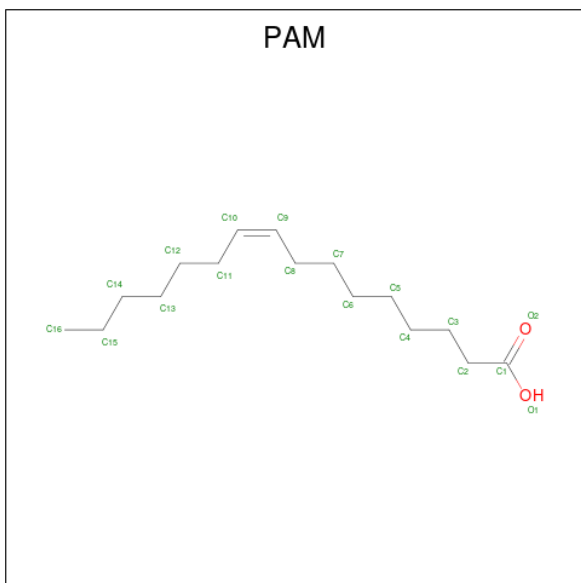
Chain	Residue	Modelled	Actual	Comment	Reference
A	264	GLU	ALA	engineered mutation	UNP P14779
B	264	GLU	ALA	engineered mutation	UNP P14779
C	264	GLU	ALA	engineered mutation	UNP P14779
D	264	GLU	ALA	engineered mutation	UNP P14779

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is PALMITOLEIC ACID (CCD ID: PAM) (formula: $\text{C}_{16}\text{H}_{30}\text{O}_2$).

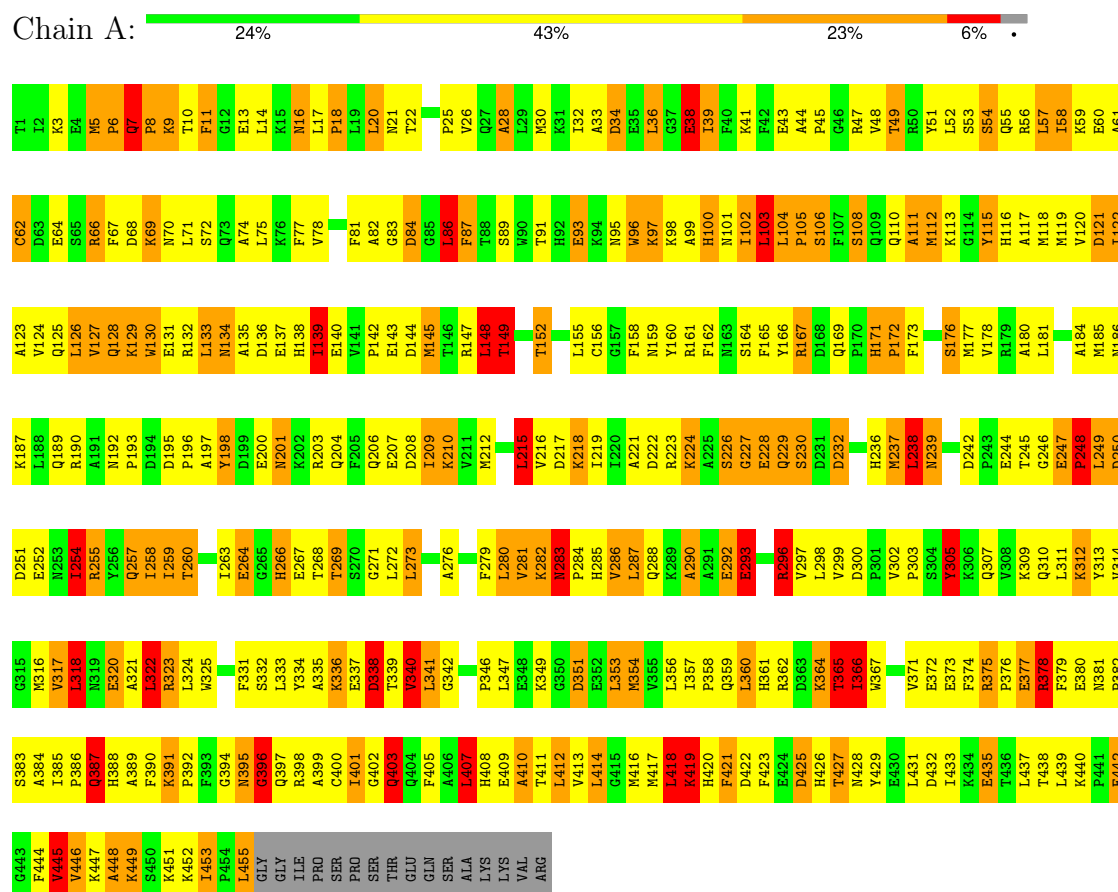


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 18	C 16	O 2	0	0
3	B	1	Total 18	C 16	O 2	0	0
3	C	1	Total 18	C 16	O 2	0	0
3	D	1	Total 18	C 16	O 2	0	0

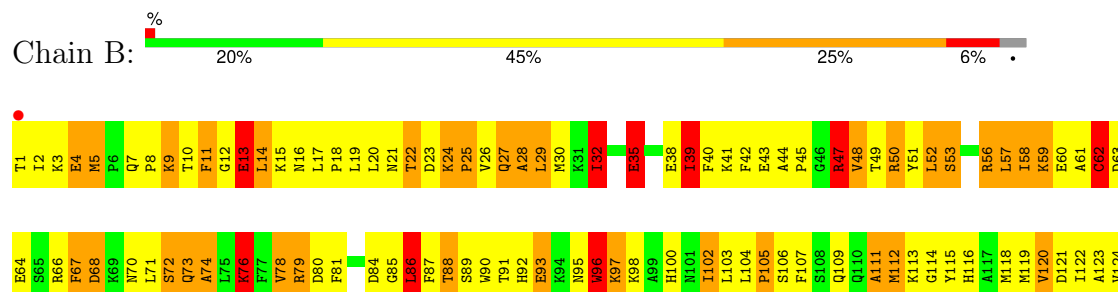
3 Residue-property plots

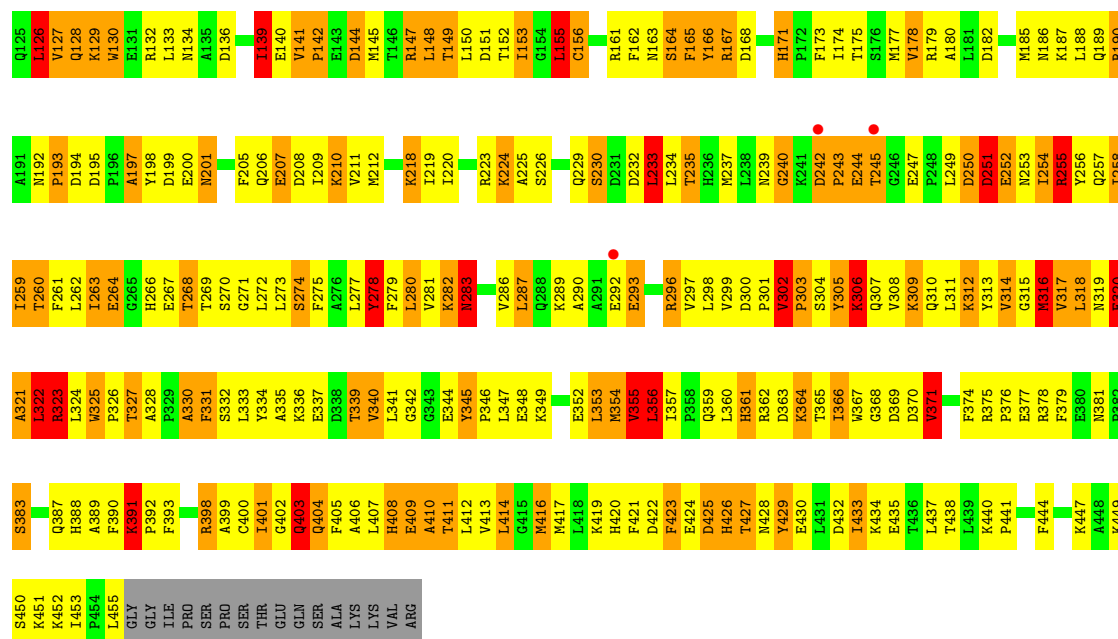
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Bifunctional P-450:NADPH-P450 reductase

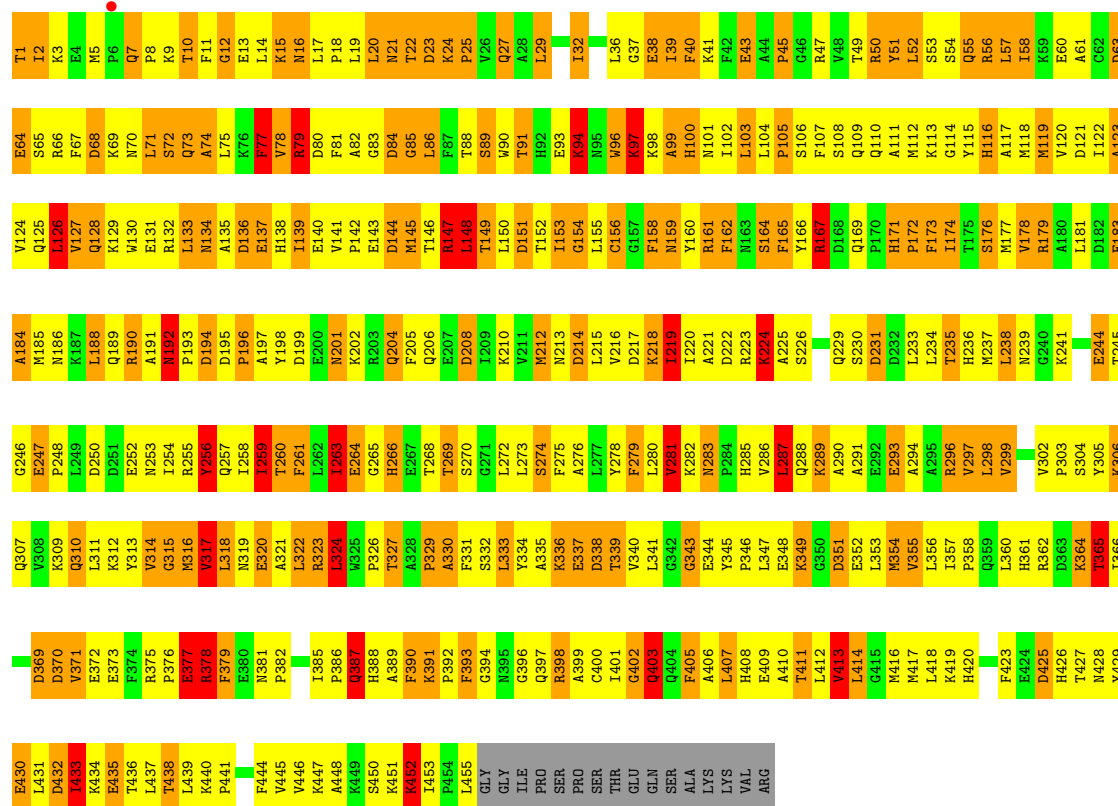
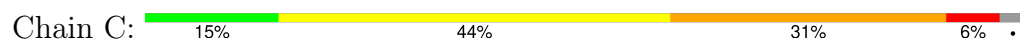


- Molecule 1: Bifunctional P-450:NADPH-P450 reductase

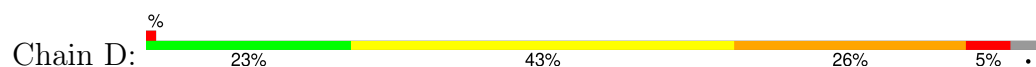




• Molecule 1: Bifunctional P-450:NADPH-P450 reductase



• Molecule 1: Bifunctional P-450:NADPH-P450 reductase



K449	S450	K451	K452	L455	GLY	GLY	ILE	PRO	SER	PRO	SER	THR	C400	I401	G402	GLN	SER	ALA	LYS	LYS	VAL	ARG	
Q387	H388	A389	F390	K391	P392	F393	G394	N395	G396	Q397	R398	R399	C400	I401	G402	GLN	SER	ALA	LYS	LYS	VAL	ARG	
H419	H420	F421	D422	F423	F424	D425	H426	T427	N428	Y429	E430	L431	D432	I433	K434	E435	T436	L437	T438	L439	K440	P441	
K419	H420	F421	D422	F423	F424	D425	H426	T427	N428	Y429	E430	L431	D432	I433	K434	E435	T436	L437	T438	L439	K440	P441	
L324	W325	P326	T327	A328	P329	A330	F331	S332	L333	Y334	A335	K336	E337	T338	F339	G340	V341	G342	G343	E344	Y345	P346	
E264	G265	H266	E267	S270	G271	L272	L273	S274	F275	A276	L277	Y278	F279	T339	G340	V341	G342	G343	E344	Y345	P346		
D185	P186	A187	Y188	D189	E200	R201	K202	R203	Q204	F205	Q206	I209	K210	V211	M212	N213	D214	L215	V216	D217	K218	D222	
K129	W130	E131	R132	L133	N134	A135	D136	E137	T138	T139	V141	P142	E143	D144	M145	T146	R147	L148	T149	L150	D151	T152	
S65	R66	F67	D68	K69	N70	L71	S72	Q73	A74	L75	K76	F77	V78	R79	D80	F81	G82	D83	D84	G85	L86	F87	T88
THR	I2	K3	E4	M5	P6	Q7	P8	F11	G12	E13	L14	K15	N16	L17	P18	L19	L20	K24	P25	V26	Q27	A28	L29
L36	G37	E38	I39	F40	K41	F42	E43	A44	P45	G46	R47	W48	T49	R50	Y51	L52	S53	S54	Q55	R56	L57	I58	K59
M112	Y115	H116	A117	M118	M119	V120	D121	L122	I123	Q125	L126	V127	D128	D129	Y130	V131	Y132	Y133	Y134	Y135	Y136	Y137	Y138
S65	R66	F67	D68	K69	N70	L71	S72	Q73	A74	L75	K76	F77	V78	R79	D80	F81	G82	D83	D84	G85	L86	F87	T88
K129	W130	E131	R132	L133	N134	A135	D136	E137	T138	T139	V141	P142	E143	D144	M145	T146	R147	L148	T149	L150	D151	T152	
D185	P186	A187	Y188	D189	E200	R201	K202	R203	Q204	F205	Q206	I209	K210	V211	M212	N213	D214	L215	V216	D217	K218	D222	
E264	G265	H266	E267	S270	G271	L272	L273	S274	F275	A276	L277	Y278	F279	T339	G340	V341	G342	G343	E344	Y345	P346		
L324	W325	P326	T327	A328	P329	A330	F331	S332	L333	Y334	A335	K336	E337	T338	F339	G340	V341	G342	G343	E344	Y345	P346	
Q387	H388	A389	F390	K391	P392	F393	G394	N395	G396	Q397	R398	R399	C400	I401	G402	GLN	SER	ALA	LYS	LYS	VAL	ARG	
H419	H420	F421	D422	F423	F424	D425	H426	T427	N428	Y429	E430	L431	D432	I433	K434	E435	T436	L437	T438	L439	K440	P441	
K419	H420	F421	D422	F423	F424	D425	H426	T427	N428	Y429	E430	L431	D432	I433	K434	E435	T436	L437	T438	L439	K440	P441	
L324	W325	P326	T327	A328	P329	A330	F331	S332	L333	Y334	A335	K336	E337	T338	F339	G340	V341	G342	G343	E344	Y345	P346	
E264	G265	H266	E267	S270	G271	L272	L273	S274	F275	A276	L277	Y278	F279	T339	G340	V341	G342	G343	E344	Y345	P346		
D185	P186	A187	Y188	D189	E200	R201	K202	R203	Q204	F205	Q206	I209	K210	V211	M212	N213	D214	L215	V216	D217	K218	D222	
K129	W130	E131	R132	L133	N134	A135	D136	E137	T138	T139	V141	P142	E143	D144	M145	T146	R147	L148	T149	L150	D151	T152	
S65	R66	F67	D68	K69	N70	L71	S72	Q73	A74	L75	K76	F77	V78	R79	D80	F81	G82	D83	D84	G85	L86	F87	T88
THR	I2	K3	E4	M5	P6	Q7	P8	F11	G12	E13	L14	K15	N16	L17	P18	L19	L20	K24	P25	V26	Q27	A28	L29

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	107.31Å 166.89Å 224.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.75 15.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-2.75) 98.4 (15.00-2.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.1	Depositor
R, R_{free}	0.253 , 0.338 0.244 , 0.333	Depositor DCC
R_{free} test set	2645 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	64.3	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14913	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, PAM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.04	90/3747 (2.4%)	1.93	117/5068 (2.3%)
1	B	1.90	76/3755 (2.0%)	1.76	65/5078 (1.3%)
1	C	1.95	86/3755 (2.3%)	1.86	96/5078 (1.9%)
1	D	1.81	53/3752 (1.4%)	1.82	81/5072 (1.6%)
All	All	1.93	305/15009 (2.0%)	1.84	359/20296 (1.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	4
1	C	0	1
All	All	0	8

All (305) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	23	ASP	CA-C	13.70	1.71	1.52
1	A	82	ALA	CA-CB	-10.72	1.34	1.53
1	C	74	ALA	CA-CB	-10.09	1.36	1.53
1	A	178	VAL	CA-CB	10.07	1.68	1.54
1	A	339	THR	CA-CB	9.48	1.66	1.53
1	D	428	ASN	CA-C	9.31	1.65	1.52
1	A	273	LEU	N-CA	-9.17	1.35	1.46
1	D	393	PHE	CA-C	-9.02	1.42	1.52
1	C	23	ASP	CG-OD2	8.98	1.42	1.25
1	D	195	ASP	CG-OD2	8.95	1.42	1.25
1	C	263	ILE	CA-CB	-8.89	1.42	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	433	ILE	C-O	8.76	1.33	1.23
1	A	321	ALA	CA-CB	-8.75	1.39	1.53
1	A	305	TYR	CA-C	8.60	1.64	1.52
1	A	26	VAL	CA-CB	-8.58	1.44	1.54
1	B	331	PHE	CA-C	-8.54	1.41	1.52
1	B	393	PHE	CA-C	-8.42	1.42	1.53
1	C	50	ARG	C-O	8.37	1.34	1.24
1	C	25	PRO	C-O	8.36	1.34	1.24
1	C	281	VAL	CA-CB	-8.28	1.43	1.54
1	C	269	THR	CA-C	-8.27	1.45	1.53
1	B	209	ILE	CA-CB	-8.21	1.44	1.54
1	A	250	ASP	CG-OD2	8.19	1.41	1.25
1	B	244	GLU	CD-OE2	8.16	1.40	1.25
1	C	373	GLU	CD-OE2	8.15	1.40	1.25
1	A	249	LEU	C-O	-8.00	1.14	1.24
1	C	255	ARG	NE-CZ	7.99	1.41	1.33
1	C	373	GLU	CD-OE1	7.94	1.40	1.25
1	B	355	VAL	N-CA	-7.90	1.37	1.46
1	B	255	ARG	CZ-NH1	7.90	1.43	1.32
1	B	164	SER	N-CA	-7.87	1.36	1.46
1	B	245	THR	CA-CB	7.83	1.67	1.54
1	C	179	ARG	C-O	7.82	1.33	1.24
1	A	259	ILE	CA-CB	-7.68	1.45	1.54
1	A	216	VAL	CA-CB	-7.65	1.45	1.54
1	D	121	ASP	CA-C	7.65	1.63	1.52
1	A	384	ALA	CA-CB	7.64	1.67	1.53
1	A	6	PRO	CA-C	7.59	1.61	1.52
1	D	120	VAL	CA-CB	7.58	1.63	1.54
1	B	166	TYR	N-CA	7.56	1.55	1.46
1	A	338	ASP	N-CA	7.56	1.55	1.46
1	D	163	ASN	CA-C	7.54	1.63	1.53
1	A	198	TYR	N-CA	-7.46	1.36	1.46
1	A	102	ILE	CA-C	-7.43	1.44	1.52
1	D	58	ILE	CA-CB	7.38	1.63	1.54
1	B	427	THR	CA-CB	7.30	1.65	1.53
1	C	413	VAL	CA-CB	7.22	1.63	1.54
1	B	255	ARG	NE-CZ	7.21	1.41	1.33
1	A	176	SER	CA-C	-7.17	1.43	1.52
1	C	411	THR	C-O	7.16	1.32	1.24
1	A	250	ASP	CA-C	7.13	1.62	1.52
1	B	244	GLU	CD-OE1	7.11	1.38	1.25
1	A	250	ASP	CA-CB	7.10	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	93	GLU	N-CA	7.10	1.55	1.46
1	C	269	THR	N-CA	-7.10	1.38	1.47
1	A	366	ILE	CA-C	-7.10	1.43	1.52
1	C	255	ARG	CZ-NH1	7.08	1.42	1.32
1	B	29	LEU	N-CA	7.04	1.55	1.46
1	B	73	GLN	N-CA	-7.04	1.37	1.46
1	C	85	GLY	C-O	7.04	1.33	1.23
1	B	330	ALA	CA-CB	-7.02	1.41	1.53
1	A	258	ILE	CA-CB	-7.00	1.46	1.54
1	A	139	ILE	CA-CB	6.98	1.63	1.54
1	A	387	GLN	N-CA	-6.97	1.37	1.46
1	D	441	PRO	CA-C	6.97	1.62	1.52
1	C	327	THR	CA-CB	-6.92	1.41	1.53
1	B	205	PHE	CA-CB	-6.91	1.42	1.53
1	A	438	THR	CA-CB	-6.89	1.43	1.53
1	C	21	ASN	N-CA	6.89	1.55	1.46
1	D	146	THR	C-O	-6.88	1.15	1.24
1	C	453	ILE	CA-C	6.82	1.58	1.52
1	C	255	ARG	CZ-NH2	6.79	1.42	1.33
1	A	159	ASN	C-O	6.77	1.32	1.23
1	B	142	PRO	C-O	-6.77	1.15	1.24
1	A	405	PHE	CA-C	6.74	1.61	1.52
1	C	247	GLU	CA-C	6.70	1.60	1.52
1	B	21	ASN	CA-C	6.70	1.60	1.53
1	C	101	ASN	CA-C	-6.70	1.44	1.52
1	D	42	PHE	N-CA	6.69	1.54	1.46
1	D	276	ALA	CA-CB	-6.67	1.43	1.53
1	C	20	LEU	N-CA	-6.67	1.37	1.46
1	D	283	ASN	N-CA	6.66	1.54	1.46
1	A	121	ASP	C-O	6.65	1.31	1.24
1	D	378	ARG	CA-C	6.63	1.61	1.52
1	B	49	THR	CA-C	6.59	1.60	1.52
1	B	67	PHE	CA-C	-6.59	1.44	1.52
1	C	360	LEU	N-CA	-6.58	1.38	1.46
1	D	374	PHE	N-CA	-6.58	1.38	1.46
1	C	265	GLY	C-O	6.57	1.32	1.23
1	A	239	ASN	C-O	-6.56	1.15	1.24
1	B	207	GLU	CA-C	6.53	1.61	1.52
1	B	25	PRO	N-CA	-6.52	1.38	1.47
1	A	87	PHE	C-O	-6.51	1.16	1.24
1	D	222	ASP	CA-C	-6.47	1.43	1.52
1	B	149	THR	CA-C	6.47	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	149	THR	CA-CB	-6.46	1.42	1.53
1	C	214	ASP	N-CA	-6.45	1.38	1.46
1	A	374	PHE	CA-C	-6.43	1.45	1.53
1	D	245	THR	CA-CB	6.42	1.63	1.54
1	B	68	ASP	CA-C	6.40	1.62	1.53
1	C	330	ALA	N-CA	6.36	1.53	1.46
1	C	247	GLU	CD-OE2	6.35	1.37	1.25
1	A	296	ARG	CZ-NH1	6.35	1.41	1.32
1	A	276	ALA	CA-CB	-6.34	1.43	1.53
1	B	58	ILE	CA-CB	-6.33	1.47	1.54
1	B	165	PHE	CA-C	-6.33	1.44	1.52
1	D	139	ILE	CA-CB	6.33	1.61	1.54
1	B	255	ARG	CZ-NH2	6.31	1.41	1.33
1	B	433	ILE	CA-CB	6.28	1.60	1.53
1	D	272	LEU	CA-C	-6.25	1.46	1.53
1	A	268	THR	CA-CB	-6.25	1.43	1.53
1	A	161	ARG	N-CA	-6.24	1.38	1.46
1	D	289	LYS	CA-C	6.24	1.61	1.52
1	C	29	LEU	CA-C	6.23	1.60	1.52
1	C	226	SER	N-CA	6.22	1.54	1.45
1	C	410	ALA	CA-C	6.22	1.61	1.52
1	A	171	HIS	C-O	-6.21	1.16	1.24
1	C	377	GLU	CA-C	6.21	1.61	1.52
1	C	286	VAL	N-CA	6.16	1.54	1.46
1	A	77	PHE	C-O	6.15	1.31	1.24
1	C	430	GLU	CA-C	6.14	1.60	1.52
1	D	273	LEU	CA-C	6.14	1.61	1.52
1	B	197	ALA	CA-CB	-6.12	1.42	1.53
1	A	84	ASP	CA-C	-6.12	1.44	1.52
1	B	167	ARG	CA-C	6.12	1.59	1.52
1	D	259	ILE	CA-CB	-6.10	1.46	1.54
1	B	74	ALA	CA-CB	-6.09	1.44	1.53
1	A	435	GLU	C-O	-6.09	1.16	1.24
1	D	93	GLU	N-CA	6.08	1.53	1.46
1	B	242	ASP	CB-CG	6.08	1.67	1.52
1	B	156	CYS	CA-C	-6.07	1.44	1.52
1	A	321	ALA	C-O	6.06	1.31	1.24
1	C	144	ASP	CA-C	6.06	1.60	1.52
1	C	153	ILE	CA-CB	-6.05	1.46	1.54
1	A	449	LYS	CA-C	6.04	1.60	1.52
1	C	178	VAL	CA-CB	6.01	1.61	1.54
1	B	348	GLU	CA-C	-6.00	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	190	ARG	CA-C	-5.99	1.45	1.52
1	D	33	ALA	CA-CB	-5.99	1.43	1.53
1	D	234	LEU	N-CA	5.96	1.53	1.46
1	D	298	LEU	CA-C	-5.96	1.45	1.53
1	C	27	GLN	N-CA	-5.95	1.38	1.46
1	B	130	TRP	C-O	5.94	1.30	1.24
1	A	442	GLU	N-CA	5.93	1.53	1.46
1	D	392	PRO	CA-C	5.93	1.58	1.52
1	B	354	MET	N-CA	-5.93	1.39	1.46
1	A	242	ASP	CA-C	-5.91	1.45	1.52
1	C	245	THR	N-CA	5.91	1.53	1.46
1	C	431	LEU	C-O	5.88	1.31	1.24
1	C	413	VAL	CA-C	5.88	1.60	1.52
1	D	398	ARG	CA-C	5.87	1.60	1.52
1	B	433	ILE	N-CA	-5.87	1.39	1.46
1	C	438	THR	CA-C	5.87	1.60	1.52
1	A	269	THR	CA-CB	5.86	1.62	1.53
1	B	251	ASP	CA-C	5.84	1.60	1.52
1	A	185	MET	C-O	-5.83	1.17	1.24
1	C	319	ASN	CA-C	-5.83	1.44	1.52
1	A	389	ALA	CA-C	-5.83	1.45	1.52
1	D	422	ASP	N-CA	-5.83	1.39	1.46
1	B	93	GLU	C-O	5.82	1.30	1.24
1	A	36	LEU	N-CA	5.81	1.53	1.45
1	C	245	THR	CA-CB	5.80	1.63	1.53
1	A	248	PRO	N-CA	-5.79	1.40	1.47
1	C	281	VAL	CB-CG1	-5.79	1.33	1.52
1	A	250	ASP	CB-CG	5.76	1.66	1.52
1	C	323	ARG	N-CA	-5.76	1.38	1.46
1	A	438	THR	N-CA	-5.75	1.38	1.45
1	B	316	MET	CA-C	5.75	1.59	1.53
1	B	296	ARG	CZ-NH1	5.74	1.40	1.32
1	A	18	PRO	N-CA	-5.72	1.40	1.47
1	A	360	LEU	C-O	-5.71	1.17	1.24
1	A	251	ASP	C-O	-5.71	1.17	1.24
1	D	68	ASP	CA-C	5.71	1.59	1.52
1	A	405	PHE	C-O	5.69	1.30	1.24
1	D	320	GLU	C-O	5.68	1.30	1.24
1	B	32	ILE	CA-CB	-5.68	1.47	1.54
1	D	359	GLN	CA-C	5.67	1.60	1.52
1	D	328	ALA	N-CA	5.67	1.52	1.46
1	C	403	GLN	CA-C	-5.67	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	120	VAL	CA-CB	5.66	1.62	1.54
1	A	323	ARG	NE-CZ	5.65	1.39	1.33
1	B	182	ASP	CA-C	-5.62	1.45	1.52
1	D	48	VAL	CA-CB	5.62	1.62	1.54
1	A	96	TRP	N-CA	-5.61	1.39	1.46
1	B	180	ALA	C-O	5.60	1.30	1.24
1	A	297	VAL	CA-CB	-5.60	1.46	1.54
1	C	128	GLN	CA-C	5.59	1.60	1.52
1	B	28	ALA	CA-C	-5.57	1.45	1.52
1	C	426	HIS	CA-C	-5.57	1.44	1.52
1	B	233	LEU	CA-C	5.56	1.60	1.52
1	B	47	ARG	CA-C	5.56	1.60	1.52
1	A	290	ALA	CA-CB	-5.55	1.43	1.53
1	A	299	VAL	CA-CB	5.55	1.61	1.54
1	C	123	ALA	CA-CB	-5.54	1.44	1.53
1	A	288	GLN	N-CA	5.53	1.52	1.46
1	B	156	CYS	C-O	-5.53	1.17	1.24
1	A	104	LEU	C-O	-5.52	1.19	1.24
1	A	144	ASP	C-O	-5.51	1.17	1.24
1	B	50	ARG	CA-C	-5.50	1.46	1.52
1	C	164	SER	CA-C	5.50	1.60	1.52
1	A	317	VAL	N-CA	-5.49	1.40	1.46
1	D	167	ARG	N-CA	-5.49	1.39	1.46
1	A	410	ALA	CA-CB	-5.48	1.44	1.53
1	C	40	PHE	N-CA	5.47	1.52	1.45
1	A	230	SER	CA-C	5.47	1.59	1.52
1	C	22	THR	C-O	-5.47	1.17	1.24
1	D	153	ILE	CG1-CD1	5.47	1.73	1.51
1	D	445	VAL	CA-CB	5.45	1.63	1.55
1	C	276	ALA	CA-CB	5.44	1.62	1.53
1	C	68	ASP	CA-C	5.44	1.59	1.52
1	D	437	LEU	N-CA	5.44	1.53	1.46
1	D	398	ARG	N-CA	5.44	1.53	1.46
1	B	45	PRO	N-CA	5.43	1.54	1.47
1	C	24	LYS	C-O	5.43	1.31	1.24
1	B	255	ARG	CA-C	5.42	1.60	1.52
1	A	204	GLN	N-CA	-5.42	1.39	1.46
1	D	54	SER	N-CA	5.42	1.52	1.46
1	C	452	LYS	CA-C	5.40	1.60	1.52
1	A	285	HIS	CA-C	-5.39	1.46	1.52
1	C	261	PHE	C-O	5.39	1.31	1.24
1	C	136	ASP	C-O	5.38	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	93	GLU	CA-C	-5.38	1.46	1.52
1	A	448	ALA	CA-C	-5.36	1.46	1.53
1	B	219	ILE	CA-CB	-5.35	1.48	1.54
1	C	365	THR	CA-C	5.35	1.59	1.52
1	C	426	HIS	N-CA	-5.34	1.39	1.46
1	B	411	THR	CA-CB	-5.33	1.45	1.53
1	C	434	LYS	C-O	5.33	1.30	1.24
1	D	391	LYS	CA-C	5.33	1.59	1.53
1	C	29	LEU	C-O	5.32	1.30	1.24
1	A	354	MET	C-O	-5.31	1.17	1.24
1	B	410	ALA	CA-CB	-5.31	1.44	1.53
1	C	84	ASP	CA-C	5.30	1.59	1.52
1	B	59	LYS	N-CA	5.29	1.52	1.46
1	A	184	ALA	C-O	-5.29	1.17	1.24
1	B	25	PRO	CA-CB	-5.29	1.46	1.53
1	C	409	GLU	N-CA	5.29	1.52	1.46
1	A	217	ASP	N-CA	-5.28	1.40	1.46
1	A	439	LEU	N-CA	5.28	1.52	1.45
1	B	250	ASP	CB-CG	5.27	1.65	1.52
1	C	379	PHE	N-CA	5.27	1.52	1.46
1	D	434	LYS	C-O	5.26	1.30	1.24
1	A	127	VAL	N-CA	-5.25	1.40	1.46
1	D	24	LYS	N-CA	5.25	1.52	1.46
1	A	176	SER	C-O	-5.25	1.17	1.24
1	B	356	LEU	CA-CB	5.24	1.59	1.52
1	D	378	ARG	N-CA	5.24	1.52	1.46
1	B	5	MET	CA-C	5.24	1.58	1.52
1	B	13	GLU	C-O	-5.24	1.17	1.24
1	C	192	ASN	N-CA	5.24	1.52	1.46
1	A	180	ALA	CA-C	5.23	1.59	1.52
1	C	1	THR	CA-CB	5.22	1.68	1.54
1	C	63	ASP	C-O	5.22	1.30	1.23
1	A	102	ILE	CA-CB	5.21	1.60	1.54
1	D	199	ASP	CB-CG	5.21	1.65	1.52
1	A	160	TYR	N-CA	5.20	1.52	1.45
1	C	91	THR	CA-C	5.20	1.59	1.52
1	C	147	ARG	CA-C	5.20	1.59	1.52
1	B	298	LEU	N-CA	5.18	1.53	1.46
1	C	190	ARG	NE-CZ	5.18	1.38	1.33
1	D	174	ILE	CA-CB	5.18	1.61	1.54
1	B	199	ASP	CA-C	-5.18	1.46	1.52
1	C	77	PHE	CD2-CE2	5.17	1.54	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	244	GLU	CA-C	5.17	1.59	1.52
1	C	89	SER	N-CA	5.16	1.52	1.46
1	C	123	ALA	C-O	-5.16	1.17	1.24
1	C	158	PHE	N-CA	5.16	1.52	1.46
1	D	250	ASP	CA-C	5.16	1.60	1.53
1	A	254	ILE	N-CA	-5.16	1.40	1.46
1	C	250	ASP	CA-CB	5.16	1.61	1.53
1	B	225	ALA	CA-C	5.15	1.59	1.52
1	C	23	ASP	CA-CB	5.15	1.62	1.53
1	D	149	THR	CA-CB	-5.15	1.45	1.53
1	C	99	ALA	C-O	5.14	1.30	1.24
1	C	315	GLY	N-CA	-5.14	1.39	1.45
1	A	286	VAL	CA-CB	-5.14	1.48	1.54
1	C	174	ILE	C-O	5.14	1.30	1.24
1	C	445	VAL	CA-CB	-5.13	1.46	1.54
1	B	345	TYR	N-CA	-5.13	1.41	1.46
1	B	208	ASP	C-O	5.13	1.30	1.24
1	C	279	PHE	CA-CB	-5.13	1.45	1.53
1	B	330	ALA	CA-C	5.13	1.59	1.52
1	D	267	GLU	CA-C	5.12	1.59	1.52
1	B	111	ALA	CA-CB	-5.11	1.45	1.53
1	B	261	PHE	C-O	5.10	1.30	1.24
1	A	86	LEU	CG-CD1	-5.08	1.35	1.52
1	A	22	THR	N-CA	5.07	1.53	1.46
1	B	193	PRO	CA-C	5.07	1.59	1.52
1	C	186	ASN	CG-OD1	5.06	1.33	1.23
1	A	397	GLN	N-CA	5.05	1.52	1.46
1	B	424	GLU	C-O	5.05	1.30	1.24
1	A	396	GLY	N-CA	5.05	1.52	1.45
1	C	413	VAL	C-O	5.05	1.29	1.24
1	D	145	MET	C-O	5.05	1.29	1.24
1	A	77	PHE	CA-C	5.04	1.59	1.52
1	B	244	GLU	CA-C	5.04	1.59	1.52
1	A	122	ILE	C-O	5.04	1.30	1.24
1	D	201	ASN	N-CA	5.03	1.52	1.46
1	D	303	PRO	CA-C	5.03	1.59	1.52
1	B	28	ALA	C-O	-5.02	1.18	1.24
1	D	63	ASP	C-O	5.02	1.30	1.24
1	A	49	THR	CA-C	5.01	1.58	1.52
1	A	28	ALA	CA-CB	-5.00	1.45	1.53
1	A	72	SER	C-O	-5.00	1.16	1.23
1	B	292	GLU	CA-C	-5.00	1.47	1.53

All (359) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	MET	N-CA-C	-10.71	99.57	111.14
1	D	222	ASP	N-CA-C	-10.26	100.89	113.41
1	D	28	ALA	N-CA-C	-10.09	100.72	113.23
1	C	360	LEU	N-CA-C	-10.01	100.36	111.07
1	C	247	GLU	N-CA-C	9.72	121.90	109.65
1	A	103	LEU	N-CA-C	9.35	122.67	111.82
1	C	37	GLY	N-CA-C	9.34	120.99	111.56
1	D	299	VAL	N-CA-C	-8.99	103.64	113.43
1	A	185	MET	N-CA-C	-8.96	100.46	111.40
1	B	278	TYR	N-CA-C	-8.72	97.53	111.04
1	A	250	ASP	CB-CA-C	8.67	125.14	109.62
1	B	315	GLY	N-CA-C	-8.62	102.21	115.66
1	C	285	HIS	N-CA-C	-8.52	101.35	112.68
1	C	226	SER	N-CA-C	8.48	121.78	109.14
1	D	329	PRO	N-CA-C	8.28	124.70	114.35
1	A	112	MET	N-CA-C	-8.24	100.97	111.02
1	D	16	ASN	N-CA-C	8.18	123.09	113.20
1	A	181	LEU	N-CA-C	-8.11	101.71	111.69
1	D	273	LEU	N-CA-C	-8.05	102.45	111.71
1	C	396	GLY	N-CA-C	8.03	125.47	111.50
1	A	210	LYS	N-CA-C	8.01	119.70	110.97
1	A	102	ILE	N-CA-C	-8.00	102.54	110.30
1	D	355	VAL	N-CA-C	7.91	118.02	106.55
1	D	223	ARG	N-CA-C	-7.86	102.65	111.14
1	C	135	ALA	N-CA-C	7.70	119.30	111.07
1	C	433	ILE	N-CA-C	7.63	118.48	106.88
1	A	268	THR	CA-C-N	7.59	130.76	120.44
1	A	268	THR	C-N-CA	7.59	130.76	120.44
1	C	419	LYS	N-CA-C	7.59	120.52	111.33
1	A	96	TRP	CA-CB-CG	-7.59	99.18	113.60
1	C	378	ARG	N-CA-C	-7.59	104.16	113.19
1	D	321	ALA	N-CA-C	-7.59	102.95	111.14
1	C	402	GLY	N-CA-C	7.56	125.23	115.32
1	C	171	HIS	N-CA-C	-7.49	100.64	109.93
1	C	314	VAL	CB-CA-C	-7.46	101.16	112.05
1	B	147	ARG	N-CA-C	-7.36	103.19	111.07
1	A	426	HIS	N-CA-C	7.30	121.77	113.01
1	A	255	ARG	N-CA-C	-7.29	104.19	113.23
1	D	217	ASP	N-CA-C	-7.29	103.27	111.14
1	B	171	HIS	N-CA-C	-7.28	100.90	109.93
1	B	28	ALA	N-CA-C	-7.27	103.44	111.36
1	A	129	LYS	N-CA-C	-7.26	103.30	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	TYR	N-CA-C	-7.22	102.81	111.69
1	B	4	GLU	N-CA-C	-7.20	99.37	110.10
1	A	271	GLY	N-CA-C	-7.16	104.14	112.73
1	D	395	ASN	N-CA-C	7.15	120.85	108.76
1	B	40	PHE	N-CA-C	7.15	120.80	109.50
1	A	20	LEU	CA-C-N	-7.14	111.91	122.41
1	A	20	LEU	C-N-CA	-7.14	111.91	122.41
1	B	86	LEU	N-CA-C	7.14	119.06	111.28
1	C	96	TRP	CA-CB-CG	-7.06	100.19	113.60
1	A	257	GLN	CA-C-N	-7.04	111.90	120.70
1	A	257	GLN	C-N-CA	-7.04	111.90	120.70
1	A	322	LEU	CB-CG-CD2	-7.03	89.62	110.70
1	B	348	GLU	N-CA-C	-6.97	99.33	110.14
1	D	281	VAL	N-CA-C	6.90	117.40	110.23
1	D	147	ARG	N-CA-C	-6.89	103.54	112.23
1	D	449	LYS	N-CA-C	-6.89	98.46	109.76
1	C	21	ASN	N-CA-C	6.89	120.08	108.23
1	C	156	CYS	CA-CB-SG	-6.86	98.63	114.40
1	A	446	VAL	CB-CA-C	-6.85	101.74	111.40
1	D	131	GLU	N-CA-C	-6.85	103.89	111.36
1	C	162	PHE	N-CA-C	6.83	121.21	112.34
1	C	355	VAL	N-CA-C	6.82	117.67	107.51
1	A	353	LEU	N-CA-C	-6.82	100.43	110.52
1	D	257	GLN	CB-CA-C	6.79	121.42	110.96
1	A	351	ASP	N-CA-C	6.78	120.21	110.10
1	D	119	MET	CA-C-N	6.75	129.07	120.56
1	D	119	MET	C-N-CA	6.75	129.07	120.56
1	D	279	PHE	N-CA-C	-6.74	103.74	112.23
1	D	54	SER	N-CA-C	6.73	120.80	109.76
1	A	335	ALA	CA-C-N	6.73	129.29	120.28
1	A	335	ALA	C-N-CA	6.73	129.29	120.28
1	B	49	THR	N-CA-C	6.69	118.37	108.60
1	C	113	LYS	N-CA-C	-6.68	104.08	111.82
1	A	148	LEU	N-CA-C	-6.67	103.70	110.97
1	C	420	HIS	CA-C-N	-6.65	112.24	122.62
1	C	420	HIS	C-N-CA	-6.65	112.24	122.62
1	D	255	ARG	N-CA-C	-6.65	103.13	111.11
1	D	447	LYS	N-CA-C	-6.63	99.11	109.72
1	A	178	VAL	N-CA-CB	6.62	121.61	110.56
1	C	161	ARG	CB-CA-C	-6.62	102.63	112.09
1	B	330	ALA	N-CA-C	6.58	117.83	108.74
1	A	176	SER	N-CA-C	-6.54	103.99	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	GLN	N-CA-C	-6.53	104.61	112.58
1	C	405	PHE	N-CA-C	-6.52	103.67	111.69
1	A	38	GLU	N-CA-C	-6.52	105.25	113.72
1	B	287	LEU	N-CA-C	-6.51	102.67	112.04
1	C	45	PRO	N-CD-CG	-6.48	93.49	103.20
1	C	72	SER	N-CA-C	-6.47	100.91	110.48
1	D	211	VAL	CB-CA-C	-6.46	103.70	111.97
1	A	102	ILE	N-CA-CB	6.45	117.66	110.62
1	B	229	GLN	N-CA-C	-6.45	102.34	111.56
1	A	227	GLY	CA-C-N	6.42	129.98	123.04
1	A	227	GLY	C-N-CA	6.42	129.98	123.04
1	A	54	SER	N-CA-C	6.42	118.98	108.52
1	C	40	PHE	CA-C-N	6.41	130.47	121.24
1	C	40	PHE	C-N-CA	6.41	130.47	121.24
1	C	244	GLU	N-CA-C	6.41	120.71	113.02
1	D	205	PHE	N-CA-C	-6.41	103.58	111.40
1	C	140	GLU	N-CA-C	-6.39	98.10	108.52
1	D	380	GLU	N-CA-C	-6.38	102.97	111.96
1	A	419	LYS	CA-C-N	-6.38	112.45	122.65
1	A	419	LYS	C-N-CA	-6.38	112.45	122.65
1	D	38	GLU	N-CA-C	6.37	124.37	110.80
1	B	331	PHE	CA-C-N	-6.35	112.65	122.87
1	B	331	PHE	C-N-CA	-6.35	112.65	122.87
1	D	134	ASN	N-CA-C	6.33	118.19	110.41
1	D	444	PHE	CB-CA-C	6.33	119.97	109.53
1	C	274	SER	CA-C-N	-6.32	111.17	120.28
1	C	274	SER	C-N-CA	-6.32	111.17	120.28
1	A	386	PRO	CA-C-N	-6.29	111.93	120.87
1	A	386	PRO	C-N-CA	-6.29	111.93	120.87
1	A	252	GLU	N-CA-C	-6.28	104.52	111.36
1	A	167	ARG	N-CA-C	6.25	119.69	109.06
1	D	294	ALA	N-CA-C	-6.25	103.03	112.04
1	B	96	TRP	CA-C-N	6.24	128.97	120.54
1	B	96	TRP	C-N-CA	6.24	128.97	120.54
1	B	185	MET	N-CA-C	-6.24	104.02	111.69
1	C	387	GLN	N-CA-C	-6.23	100.14	110.17
1	A	407	LEU	CA-C-N	-6.23	110.84	120.31
1	A	407	LEU	C-N-CA	-6.23	110.84	120.31
1	A	421	PHE	N-CA-C	6.23	119.69	108.48
1	A	16	ASN	N-CA-C	6.22	120.47	113.01
1	C	23	ASP	CB-CG-OD2	6.22	132.70	118.40
1	C	323	ARG	N-CA-C	-6.20	103.83	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	101	ASN	N-CA-C	-6.20	104.07	111.69
1	C	16	ASN	N-CA-C	-6.18	103.81	113.02
1	A	108	SER	N-CA-C	-6.17	101.39	110.52
1	D	244	GLU	N-CA-C	6.16	119.89	112.38
1	D	120	VAL	N-CA-C	6.14	116.31	110.42
1	D	15	LYS	CB-CA-C	-6.13	109.50	116.54
1	B	178	VAL	CB-CA-C	-6.11	103.78	112.22
1	B	35	GLU	N-CA-C	6.08	119.80	112.38
1	D	407	LEU	CB-CA-C	6.07	120.86	110.79
1	C	438	THR	N-CA-C	6.05	118.11	110.24
1	D	112	MET	N-CA-C	6.02	118.61	111.33
1	A	216	VAL	N-CA-C	6.02	116.76	110.62
1	A	302	VAL	N-CA-CB	-6.00	106.01	112.37
1	D	96	TRP	CA-CB-CG	-6.00	102.20	113.60
1	A	152	THR	N-CA-C	6.00	118.34	111.02
1	A	255	ARG	CB-CA-C	6.00	121.72	109.55
1	C	329	PRO	CA-C-N	-6.00	111.55	121.80
1	C	329	PRO	C-N-CA	-6.00	111.55	121.80
1	D	165	PHE	CA-C-N	-5.98	112.27	122.56
1	D	165	PHE	C-N-CA	-5.98	112.27	122.56
1	A	203	ARG	N-CA-C	-5.97	104.11	111.40
1	A	149	THR	OG1-CB-CG2	-5.96	97.38	109.30
1	C	149	THR	OG1-CB-CG2	-5.94	97.42	109.30
1	A	138	HIS	CA-C-N	-5.93	115.45	123.10
1	A	138	HIS	C-N-CA	-5.93	115.45	123.10
1	B	220	ILE	CA-C-O	-5.92	115.25	121.41
1	D	165	PHE	N-CA-C	-5.92	106.06	113.28
1	A	232	ASP	N-CA-C	5.91	117.52	110.19
1	A	215	LEU	CA-C-N	-5.91	112.36	120.46
1	A	215	LEU	C-N-CA	-5.91	112.36	120.46
1	B	47	ARG	N-CA-C	5.91	123.38	110.80
1	A	427	THR	N-CA-C	-5.90	103.63	112.54
1	A	130	TRP	N-CA-C	5.87	117.68	111.28
1	B	72	SER	CA-C-N	-5.87	111.83	120.28
1	B	72	SER	C-N-CA	-5.87	111.83	120.28
1	C	219	ILE	CA-C-N	5.86	128.45	120.77
1	C	219	ILE	C-N-CA	5.86	128.45	120.77
1	A	159	ASN	CB-CA-C	5.86	120.05	111.73
1	B	24	LYS	CG-CD-CE	-5.85	97.85	111.30
1	C	435	GLU	N-CA-C	5.85	118.19	109.59
1	C	204	GLN	N-CA-C	-5.84	104.61	110.97
1	D	212	MET	CG-SD-CE	-5.84	88.06	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	LEU	N-CA-C	-5.80	104.59	111.03
1	A	125	GLN	O-C-N	5.79	128.25	122.12
1	A	186	ASN	N-CA-C	5.78	118.35	111.71
1	B	230	SER	N-CA-C	-5.78	100.26	109.96
1	A	156	CYS	CA-C-N	5.76	127.34	120.14
1	A	156	CYS	C-N-CA	5.76	127.34	120.14
1	D	106	SER	N-CA-C	5.75	119.91	113.01
1	A	455	LEU	CB-CG-CD1	-5.75	93.46	110.70
1	C	276	ALA	N-CA-C	-5.74	103.83	111.24
1	B	150	LEU	N-CA-C	-5.72	104.95	111.07
1	A	210	LYS	CA-CB-CG	-5.72	102.66	114.10
1	A	284	PRO	N-CD-CG	-5.72	94.63	103.20
1	B	335	ALA	CA-C-N	5.72	128.26	120.54
1	B	335	ALA	C-N-CA	5.72	128.26	120.54
1	B	25	PRO	CA-C-N	-5.71	113.91	120.88
1	B	25	PRO	C-N-CA	-5.71	113.91	120.88
1	D	332	SER	N-CA-C	-5.71	101.29	110.14
1	A	242	ASP	N-CA-C	-5.71	99.11	109.44
1	B	219	ILE	N-CA-C	-5.71	105.16	110.53
1	B	430	GLU	N-CA-C	-5.71	100.40	109.59
1	C	291	ALA	CA-C-N	5.70	128.20	120.44
1	C	291	ALA	C-N-CA	5.70	128.20	120.44
1	A	135	ALA	N-CA-C	5.70	120.72	111.37
1	B	27	GLN	CA-CB-CG	-5.70	102.70	114.10
1	C	20	LEU	CA-CB-CG	-5.70	96.37	116.30
1	D	256	TYR	CA-C-N	-5.69	113.14	120.65
1	D	256	TYR	C-N-CA	-5.69	113.14	120.65
1	B	76	LYS	N-CA-CB	5.68	118.24	110.01
1	C	324	LEU	N-CA-C	-5.67	104.48	111.40
1	D	121	ASP	CB-CA-C	5.67	120.15	110.74
1	C	52	LEU	N-CA-C	5.66	118.18	109.07
1	C	10	THR	N-CA-C	5.65	118.69	109.59
1	A	246	GLY	CA-C-N	5.63	129.24	120.68
1	A	246	GLY	C-N-CA	5.63	129.24	120.68
1	B	430	GLU	CA-CB-CG	5.63	125.36	114.10
1	C	250	ASP	CB-CA-C	5.63	119.28	109.65
1	D	58	ILE	N-CA-C	-5.62	104.89	110.62
1	D	451	LYS	N-CA-C	-5.62	106.01	112.92
1	C	389	ALA	N-CA-C	-5.61	106.25	114.39
1	D	328	ALA	CA-C-O	5.61	124.25	119.71
1	A	427	THR	CA-C-N	-5.61	114.05	122.07
1	A	427	THR	C-N-CA	-5.61	114.05	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	186	ASN	N-CA-C	5.60	118.58	111.69
1	A	362	ARG	N-CA-C	-5.60	104.68	113.02
1	C	432	ASP	CA-C-N	-5.60	116.01	122.95
1	C	432	ASP	C-N-CA	-5.60	116.01	122.95
1	B	90	TRP	CA-C-N	-5.59	112.83	120.44
1	B	90	TRP	C-N-CA	-5.59	112.83	120.44
1	D	190	ARG	N-CA-C	5.59	117.41	108.41
1	A	110	GLN	N-CA-C	-5.57	105.21	112.23
1	C	7	GLN	N-CA-C	5.57	118.23	108.82
1	D	429	TYR	N-CA-C	5.57	118.26	109.96
1	B	400	CYS	N-CA-C	5.57	117.80	108.23
1	A	219	ILE	N-CA-C	-5.56	105.19	110.42
1	A	226	SER	N-CA-C	5.56	118.51	109.06
1	A	453	ILE	CB-CA-C	-5.56	104.46	110.85
1	C	193	PRO	N-CA-C	5.55	120.86	114.20
1	A	228	GLU	CB-CA-C	-5.55	109.08	117.07
1	A	340	VAL	CB-CA-C	5.54	118.42	110.33
1	C	373	GLU	N-CA-C	5.54	117.99	109.07
1	A	113	LYS	N-CA-C	5.54	118.03	111.33
1	A	380	GLU	N-CA-C	-5.53	105.33	112.68
1	B	144	ASP	N-CA-C	5.53	116.98	111.07
1	A	250	ASP	CB-CG-OD2	5.52	131.10	118.40
1	A	244	GLU	CA-C-N	-5.52	113.94	122.49
1	A	244	GLU	C-N-CA	-5.52	113.94	122.49
1	A	296	ARG	NE-CZ-NH1	-5.51	115.99	121.50
1	A	387	GLN	CB-CA-C	5.51	119.08	109.65
1	B	393	PHE	CB-CA-C	-5.51	102.57	111.28
1	C	393	PHE	N-CA-CB	5.51	119.37	111.65
1	B	325	TRP	CA-CB-CG	-5.51	103.13	113.60
1	A	166	TYR	CA-C-N	-5.51	112.90	122.37
1	A	166	TYR	C-N-CA	-5.51	112.90	122.37
1	C	167	ARG	N-CA-C	5.51	117.88	108.90
1	A	111	ALA	O-C-N	5.50	128.43	122.15
1	A	445	VAL	CA-C-O	-5.50	116.06	121.67
1	C	63	ASP	N-CA-C	5.50	117.69	108.23
1	A	318	LEU	CA-C-N	-5.49	111.96	120.31
1	A	318	LEU	C-N-CA	-5.49	111.96	120.31
1	D	40	PHE	N-CA-C	5.49	117.45	108.55
1	D	308	VAL	N-CA-C	5.49	116.27	110.72
1	C	297	VAL	N-CA-C	5.49	120.76	109.34
1	C	322	LEU	CA-C-N	-5.49	109.95	121.64
1	C	322	LEU	C-N-CA	-5.49	109.95	121.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	120	VAL	N-CA-CB	-5.49	104.13	110.55
1	C	23	ASP	CB-CG-OD1	-5.49	105.78	118.40
1	D	122	ILE	N-CA-C	5.49	115.93	110.23
1	C	208	ASP	CB-CA-C	-5.47	101.54	110.85
1	A	47	ARG	N-CA-C	5.47	118.84	110.36
1	C	55	GLN	N-CA-C	5.46	117.94	111.33
1	B	27	GLN	CA-C-N	-5.46	112.53	120.29
1	B	27	GLN	C-N-CA	-5.46	112.53	120.29
1	C	445	VAL	CB-CA-C	-5.46	103.71	111.19
1	D	101	ASN	CA-C-N	-5.46	113.68	120.56
1	D	101	ASN	C-N-CA	-5.46	113.68	120.56
1	B	302	VAL	CB-CA-C	5.45	115.42	110.13
1	C	438	THR	OG1-CB-CG2	-5.45	98.39	109.30
1	A	455	LEU	CA-CB-CG	5.45	135.37	116.30
1	B	292	GLU	CB-CA-C	-5.45	102.73	111.39
1	C	144	ASP	OD1-CG-OD2	-5.44	109.83	122.90
1	D	336	LYS	CA-CB-CG	5.44	124.98	114.10
1	D	245	THR	N-CA-CB	5.43	118.15	110.98
1	C	148	LEU	N-CA-C	5.42	118.01	111.40
1	B	47	ARG	CG-CD-NE	5.41	123.91	112.00
1	C	390	PHE	CB-CA-C	-5.41	104.10	111.95
1	D	421	PHE	N-CA-C	5.41	118.37	109.72
1	B	323	ARG	NE-CZ-NH1	-5.41	116.09	121.50
1	D	232	ASP	N-CA-C	5.40	118.23	109.86
1	D	84	ASP	CA-C-N	5.39	126.32	120.44
1	D	84	ASP	C-N-CA	5.39	126.32	120.44
1	D	145	MET	N-CA-C	-5.39	105.32	111.14
1	C	94	LYS	N-CA-C	-5.39	104.64	111.11
1	D	239	ASN	N-CA-C	5.39	119.94	112.45
1	C	212	MET	CG-SD-CE	-5.38	89.05	100.90
1	B	426	HIS	N-CA-C	5.36	122.21	110.80
1	B	255	ARG	N-CA-CB	-5.35	102.03	110.06
1	C	173	PHE	N-CA-C	-5.35	105.34	111.07
1	A	197	ALA	CA-C-N	-5.34	113.37	122.56
1	A	197	ALA	C-N-CA	-5.34	113.37	122.56
1	D	146	THR	N-CA-C	-5.33	105.41	112.34
1	C	138	HIS	CA-C-N	-5.30	115.74	123.06
1	C	138	HIS	C-N-CA	-5.30	115.74	123.06
1	C	255	ARG	CB-CA-C	5.30	120.97	110.42
1	D	403	GLN	N-CA-C	5.28	122.04	110.80
1	D	302	VAL	CB-CA-C	-5.27	101.76	111.36
1	A	184	ALA	N-CA-C	-5.27	105.71	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	354	MET	CB-CA-C	5.24	117.89	110.24
1	C	370	ASP	N-CA-CB	-5.24	103.68	111.43
1	B	306	LYS	N-CA-C	-5.23	106.58	113.12
1	D	145	MET	CG-SD-CE	5.22	112.39	100.90
1	C	351	ASP	N-CA-C	5.20	117.00	110.24
1	C	51	TYR	CA-C-N	-5.20	115.83	123.00
1	C	51	TYR	C-N-CA	-5.20	115.83	123.00
1	A	375	ARG	N-CA-C	5.19	119.87	108.66
1	B	247	GLU	N-CA-C	5.19	117.97	110.14
1	C	256	TYR	N-CA-C	5.18	121.84	110.80
1	B	434	LYS	N-CA-C	5.18	118.00	109.76
1	A	285	HIS	CA-CB-CG	-5.17	108.63	113.80
1	A	438	THR	CA-C-O	-5.17	116.58	122.01
1	C	184	ALA	N-CA-C	-5.16	105.55	111.07
1	D	53	SER	N-CA-C	5.16	119.67	112.90
1	C	261	PHE	N-CA-C	-5.15	107.13	113.41
1	D	234	LEU	N-CA-C	5.15	117.88	111.24
1	C	354	MET	CG-SD-CE	-5.14	89.58	100.90
1	A	66	ARG	NE-CZ-NH1	-5.14	116.36	121.50
1	A	34	ASP	CA-C-N	-5.14	112.50	120.31
1	A	34	ASP	C-N-CA	-5.14	112.50	120.31
1	D	282	LYS	N-CA-C	5.14	119.03	112.87
1	A	238	LEU	N-CA-C	5.13	121.72	110.80
1	B	353	LEU	CA-C-N	-5.13	113.76	121.86
1	B	353	LEU	C-N-CA	-5.13	113.76	121.86
1	D	386	PRO	CA-C-N	-5.13	113.90	122.92
1	D	386	PRO	C-N-CA	-5.13	113.90	122.92
1	D	206	GLN	CA-C-N	5.12	127.41	120.44
1	D	206	GLN	C-N-CA	5.12	127.41	120.44
1	C	105	PRO	CB-CA-C	-5.12	103.11	111.56
1	A	403	GLN	N-CA-C	5.12	121.70	110.80
1	D	255	ARG	CB-CA-C	5.12	119.00	110.81
1	B	105	PRO	CB-CA-C	-5.11	103.72	112.26
1	B	139	ILE	CA-C-N	-5.11	115.74	122.85
1	B	139	ILE	C-N-CA	-5.11	115.74	122.85
1	C	183	GLU	CA-C-N	-5.10	113.81	120.44
1	C	183	GLU	C-N-CA	-5.10	113.81	120.44
1	D	116	HIS	CA-C-N	-5.10	112.56	120.31
1	D	116	HIS	C-N-CA	-5.10	112.56	120.31
1	D	432	ASP	N-CA-C	-5.10	99.36	108.13
1	C	225	ALA	N-CA-C	5.07	117.23	109.62
1	A	395	ASN	N-CA-CB	-5.07	103.45	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	369	ASP	N-CA-C	5.07	121.59	110.80
1	B	398	ARG	CB-CA-C	-5.07	104.35	112.05
1	C	440	LYS	CB-CA-C	5.07	116.81	109.92
1	A	250	ASP	CA-CB-CG	5.06	117.66	112.60
1	C	97	LYS	N-CA-C	-5.06	105.77	111.28
1	C	137	GLU	N-CA-C	-5.05	101.92	109.95
1	D	102	ILE	N-CA-C	-5.05	105.58	110.42
1	A	264	GLU	N-CA-C	5.04	118.20	111.75
1	B	432	ASP	CA-C-N	-5.04	116.08	122.43
1	B	432	ASP	C-N-CA	-5.04	116.08	122.43
1	B	423	PHE	N-CA-C	5.03	116.97	108.96
1	C	435	GLU	O-C-N	-5.03	116.62	122.96
1	D	325	TRP	N-CA-C	5.02	118.11	108.97
1	B	39	ILE	N-CA-C	5.02	119.77	109.34
1	A	433	ILE	N-CA-C	5.01	115.55	107.98
1	C	281	VAL	N-CA-C	5.01	119.77	109.34
1	A	7	GLN	CA-CB-CG	5.01	124.12	114.10
1	A	410	ALA	N-CA-C	-5.01	105.29	111.40
1	B	226	SER	N-CA-C	5.01	116.13	108.52
1	A	102	ILE	CA-C-O	-5.00	115.94	121.29
1	A	111	ALA	CA-C-N	5.00	127.75	120.79
1	A	111	ALA	C-N-CA	5.00	127.75	120.79
1	A	219	ILE	N-CA-CB	5.00	116.30	110.65

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	283	ASN	Peptide
1	A	292	GLU	Peptide
1	A	341	LEU	Peptide
1	B	283	ASN	Peptide
1	B	303	PRO	Peptide
1	B	316	MET	Peptide
1	B	320	GLU	Peptide
1	C	343	GLY	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3662	0	3625	330	2
1	B	3670	0	3635	394	1
1	C	3670	0	3636	420	1
1	D	3667	0	3636	360	0
2	A	43	0	30	14	0
2	B	43	0	30	15	0
2	C	43	0	30	4	0
2	D	43	0	30	13	0
3	A	18	0	29	3	0
3	B	18	0	29	0	0
3	C	18	0	29	6	0
3	D	18	0	29	2	0
All	All	14913	0	14768	1526	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 51.

All (1526) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:PHE:CD2	1:C:401:ILE:HG22	1.45	1.49
1:C:85:GLY:HA2	1:C:257:GLN:NE2	1.50	1.24
1:C:100:HIS:CE1	1:C:104:LEU:HD22	1.72	1.22
1:B:313:TYR:HA	1:B:316:MET:CE	1.71	1.20
1:B:281:VAL:CG1	1:B:425:ASP:HB2	1.71	1.20
1:A:218:LYS:HA	1:A:218:LYS:HE2	1.21	1.17
1:B:118:MET:HB3	1:B:155:LEU:HD23	1.19	1.15
1:C:107:PHE:CE2	1:C:401:ILE:HG22	1.80	1.15
1:B:224:LYS:HE2	1:B:224:LYS:HA	1.26	1.14
1:C:100:HIS:HE1	1:C:104:LEU:HD22	0.98	1.13
1:D:218:LYS:HE3	1:D:218:LYS:HA	1.23	1.13
1:B:242:ASP:HB3	1:B:245:THR:OG1	1.50	1.12
1:A:387:GLN:NE2	1:A:388:HIS:H	1.48	1.11
1:B:272:LEU:HD13	1:B:322:LEU:CD1	1.79	1.11
1:C:212:MET:HE1	1:C:263:ILE:HD11	1.32	1.10
1:C:326:PRO:HG2	1:C:358:PRO:HD3	1.29	1.10
1:B:272:LEU:HD13	1:B:322:LEU:HD12	1.13	1.09
1:A:118:MET:HB3	1:A:155:LEU:HD23	1.34	1.09
1:A:272:LEU:HD13	1:A:322:LEU:HD12	1.34	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:MET:HA	1:C:145:MET:HE2	1.33	1.09
1:C:149:THR:HG21	1:C:266:HIS:O	1.52	1.08
1:C:107:PHE:CD2	1:C:401:ILE:CG2	2.36	1.08
1:B:147:ARG:HG2	1:B:164:SER:HB3	1.36	1.07
1:A:313:TYR:HA	1:A:316:MET:CE	1.82	1.07
1:D:25:PRO:HD2	1:D:435:GLU:OE1	1.53	1.07
1:A:228:GLU:HG3	1:A:229:GLN:H	0.94	1.06
1:C:21:ASN:HA	1:C:189:GLN:OE1	1.55	1.06
1:D:141:VAL:HG12	1:D:142:PRO:HD3	1.34	1.06
1:C:107:PHE:HD2	1:C:401:ILE:CG2	1.71	1.04
1:A:364:LYS:H	1:A:364:LYS:HD2	1.22	1.03
1:A:313:TYR:HA	1:A:316:MET:HE3	1.40	1.03
1:C:272:LEU:HD13	1:C:322:LEU:HD13	1.37	1.03
1:B:147:ARG:CG	1:B:164:SER:HB3	1.88	1.02
1:B:57:LEU:HD12	1:B:341:LEU:HG	1.38	1.01
1:C:11:PHE:CD1	1:C:18:PRO:HG2	1.96	1.01
1:A:177:MET:HA	1:A:212:MET:HE3	1.40	1.01
1:B:242:ASP:CB	1:B:245:THR:OG1	2.09	1.00
1:B:281:VAL:HG11	1:B:425:ASP:HB2	1.06	1.00
1:D:341:LEU:HB3	1:D:345:TYR:HB2	1.41	1.00
1:C:51:TYR:CE2	1:C:354:MET:HG2	1.97	0.99
1:C:272:LEU:HD13	1:C:322:LEU:CD1	1.92	0.99
1:A:147:ARG:HG3	1:A:164:SER:HB3	1.41	0.99
1:A:228:GLU:CG	1:A:229:GLN:H	1.72	0.99
1:A:228:GLU:HG3	1:A:229:GLN:N	1.77	0.98
1:C:64:GLU:OE2	1:C:397:GLN:HG2	1.62	0.98
1:D:147:ARG:HG3	1:D:164:SER:HB3	1.46	0.98
1:C:223:ARG:NH2	1:C:234:LEU:HD23	1.77	0.98
1:D:122:ILE:HG22	1:D:148:LEU:HD12	1.43	0.98
1:B:313:TYR:HA	1:B:316:MET:HE3	1.01	0.97
1:D:201:ASN:N	1:D:201:ASN:HD22	1.60	0.97
1:B:30:MET:HE1	1:B:325:TRP:CH2	1.99	0.97
1:A:272:LEU:HD22	1:A:322:LEU:CD1	1.94	0.97
1:C:39:ILE:HG13	1:C:52:LEU:HD12	1.44	0.97
1:C:149:THR:HG22	1:C:266:HIS:HB2	1.45	0.97
1:A:145:MET:HE2	1:A:145:MET:HA	1.43	0.96
1:C:74:ALA:O	1:C:78:VAL:HG23	1.66	0.96
1:B:201:ASN:N	1:B:201:ASN:HD22	1.58	0.96
1:D:141:VAL:HG11	1:D:444:PHE:CD2	2.00	0.96
1:A:33:ALA:HB3	1:A:359:GLN:NE2	1.82	0.95
1:D:326:PRO:HD2	1:D:358:PRO:HB3	1.49	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ALA:CB	1:A:359:GLN:HE21	1.78	0.95
1:A:296:ARG:HH11	1:A:296:ARG:HG2	1.32	0.94
1:D:66:ARG:NH2	1:D:339:THR:OG1	1.99	0.94
1:B:201:ASN:HD22	1:B:201:ASN:H	1.02	0.94
1:D:201:ASN:HD22	1:D:201:ASN:H	1.09	0.94
1:C:63:ASP:OD2	1:C:66:ARG:HG3	1.66	0.94
1:C:85:GLY:HA2	1:C:257:GLN:HE22	1.07	0.94
1:C:100:HIS:HE1	1:C:104:LEU:CD2	1.81	0.94
1:A:33:ALA:HB3	1:A:359:GLN:HE21	1.32	0.93
1:B:451:LYS:O	1:B:453:ILE:HG13	1.68	0.93
1:D:39:ILE:HG13	1:D:52:LEU:HD12	1.47	0.93
1:A:68:ASP:HB3	1:A:334:TYR:CE1	2.04	0.93
1:A:377:GLU:O	1:A:379:PHE:N	2.02	0.93
1:B:313:TYR:CA	1:B:316:MET:HE3	1.96	0.92
1:B:362:ARG:O	1:B:371:VAL:HG11	1.70	0.92
2:B:472:HEM:HMC2	2:B:472:HEM:HBC2	1.49	0.92
1:C:223:ARG:CZ	1:C:234:LEU:HD23	2.00	0.92
1:C:223:ARG:NE	1:C:234:LEU:HD23	1.85	0.92
1:D:331:PHE:HE2	1:D:394:GLY:HA2	1.35	0.91
1:C:196:PRO:HB3	1:C:199:ASP:OD2	1.70	0.91
1:A:218:LYS:HE2	1:A:218:LYS:CA	1.98	0.91
1:D:86:LEU:HD11	1:D:99:ALA:HB1	1.50	0.91
1:B:10:THR:C	1:B:11:PHE:HD1	1.77	0.90
1:D:331:PHE:CE2	1:D:394:GLY:HA2	2.05	0.90
1:A:139:ILE:HD11	1:A:446:VAL:HG22	1.53	0.90
1:B:78:VAL:HG13	1:B:81:PHE:CZ	2.07	0.90
1:C:279:PHE:O	1:C:283:ASN:ND2	2.05	0.89
1:D:122:ILE:HD13	1:D:122:ILE:N	1.87	0.89
1:D:112:MET:HE1	1:D:405:PHE:HD2	1.37	0.89
1:C:82:ALA:O	1:C:256:TYR:CD1	2.26	0.89
1:D:193:PRO:O	1:D:195:ASP:N	2.05	0.89
1:D:398:ARG:NH2	2:D:472:HEM:O2D	2.06	0.89
1:C:237:MET:HE1	1:C:258:ILE:HG12	1.52	0.89
1:C:436:THR:O	1:C:437:LEU:HB2	1.73	0.89
1:C:18:PRO:O	1:C:21:ASN:N	2.07	0.88
1:A:201:ASN:HD22	1:A:201:ASN:N	1.70	0.88
1:A:320:GLU:OE2	1:A:323:ARG:NE	2.07	0.88
2:B:472:HEM:CMB	2:B:472:HEM:HBB2	2.04	0.88
1:C:94:LYS:HE3	1:C:94:LYS:HA	1.56	0.88
1:B:282:LYS:C	1:B:283:ASN:HD22	1.81	0.88
1:B:10:THR:C	1:B:11:PHE:CD1	2.50	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:ILE:O	1:C:222:ASP:HB3	1.74	0.88
1:A:313:TYR:O	1:A:316:MET:HB2	1.75	0.87
1:A:139:ILE:CD1	1:A:446:VAL:HG22	2.05	0.87
1:C:56:ARG:HG3	1:C:56:ARG:O	1.74	0.87
1:D:61:ALA:HA	1:D:67:PHE:CD2	2.09	0.87
1:A:134:ASN:H	1:A:134:ASN:ND2	1.69	0.87
1:A:139:ILE:CD1	1:A:446:VAL:CG2	2.53	0.87
1:B:58:ILE:HD12	1:B:355:VAL:HG22	1.55	0.87
1:C:223:ARG:HH21	1:C:234:LEU:HD23	1.38	0.86
1:C:201:ASN:H	1:C:201:ASN:HD22	1.23	0.86
1:A:224:LYS:HE2	1:A:224:LYS:HA	1.56	0.86
1:A:139:ILE:HD11	1:A:446:VAL:CG2	2.06	0.86
1:B:282:LYS:HE2	1:B:425:ASP:OD2	1.75	0.86
1:A:177:MET:CA	1:A:212:MET:HE3	2.06	0.85
1:A:310:GLN:O	1:A:312:LYS:HG3	1.76	0.85
1:A:290:ALA:HB2	1:A:313:TYR:CD2	2.12	0.85
1:B:44:ALA:HB3	1:B:47:ARG:HG3	1.57	0.85
1:D:5:MET:HE1	1:D:39:ILE:CD1	2.06	0.85
1:D:296:ARG:O	1:D:299:VAL:HG13	1.76	0.85
1:A:52:LEU:HD23	1:A:58:ILE:HD13	1.58	0.85
1:C:107:PHE:CE2	1:C:401:ILE:CG2	2.57	0.85
1:C:116:HIS:HD2	1:C:408:HIS:NE2	1.74	0.85
1:C:176:SER:HB3	1:C:208:ASP:HB3	1.58	0.84
1:A:377:GLU:C	1:A:379:PHE:H	1.84	0.84
1:D:141:VAL:HG11	1:D:444:PHE:CE2	2.12	0.84
1:D:140:GLU:HB3	1:D:143:GLU:OE1	1.78	0.84
1:C:124:VAL:HG12	1:C:128:GLN:HG3	1.60	0.83
1:A:145:MET:HE2	1:A:145:MET:CA	2.07	0.83
1:C:145:MET:HA	1:C:145:MET:CE	2.07	0.83
1:A:237:MET:HE1	1:A:258:ILE:HG13	1.60	0.83
1:B:281:VAL:HG11	1:B:425:ASP:CB	2.01	0.83
1:D:297:VAL:HG12	1:D:298:LEU:HD23	1.59	0.83
1:B:71:LEU:O	1:B:76:LYS:HE3	1.79	0.83
1:D:141:VAL:HG12	1:D:142:PRO:CD	2.08	0.83
2:D:472:HEM:HBC2	2:D:472:HEM:CMC	2.08	0.83
1:C:149:THR:HG22	1:C:266:HIS:CB	2.08	0.82
1:C:98:LYS:C	1:C:102:ILE:HD12	2.04	0.82
1:A:134:ASN:ND2	1:A:134:ASN:N	2.27	0.82
1:B:313:TYR:O	1:B:316:MET:HB2	1.78	0.82
1:C:10:THR:HA	1:C:15:LYS:O	1.80	0.82
1:D:51:TYR:CE2	1:D:354:MET:HG2	2.15	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ASN:H	1:A:134:ASN:HD22	1.26	0.81
1:C:98:LYS:O	1:C:102:ILE:HD12	1.80	0.81
1:D:179:ARG:HE	1:D:204:GLN:NE2	1.78	0.81
1:B:57:LEU:HD12	1:B:341:LEU:CG	2.11	0.81
1:C:39:ILE:HG13	1:C:52:LEU:CD1	2.11	0.81
1:A:38:GLU:HB3	1:A:54:SER:HB3	1.61	0.81
1:A:313:TYR:HA	1:A:316:MET:HE2	1.61	0.81
1:C:82:ALA:O	1:C:256:TYR:HD1	1.60	0.81
1:D:25:PRO:CD	1:D:435:GLU:OE1	2.28	0.81
1:B:142:PRO:HB2	1:B:440:LYS:HE3	1.62	0.81
1:C:223:ARG:HE	1:C:234:LEU:HD23	1.44	0.81
2:B:472:HEM:HBB2	2:B:472:HEM:HMB2	1.61	0.81
1:C:129:LYS:NZ	1:C:144:ASP:OD1	2.14	0.81
1:B:264:GLU:OE1	1:B:264:GLU:HA	1.81	0.80
1:C:122:ILE:HG22	1:C:148:LEU:HD12	1.62	0.80
1:D:5:MET:HE1	1:D:39:ILE:HD11	1.62	0.80
1:D:218:LYS:HA	1:D:218:LYS:CE	2.07	0.80
1:D:47:ARG:HD3	1:D:73:GLN:HG2	1.63	0.80
1:B:286:VAL:HG13	1:B:313:TYR:OH	1.81	0.80
1:B:5:MET:HE1	1:B:39:ILE:HD11	1.63	0.80
1:A:140:GLU:HA	1:A:445:VAL:HG12	1.64	0.80
1:A:118:MET:HB3	1:A:155:LEU:CD2	2.12	0.80
1:C:258:ILE:O	1:C:259:ILE:C	2.24	0.80
1:D:8:PRO:HD3	1:D:36:LEU:CD1	2.12	0.80
1:D:264:GLU:HB2	3:D:4465:PAM:H141	1.63	0.80
1:A:264:GLU:O	1:A:264:GLU:CD	2.25	0.79
1:C:149:THR:HG22	1:C:266:HIS:HA	1.65	0.79
1:A:38:GLU:CB	1:A:54:SER:HB3	2.12	0.79
1:C:339:THR:O	1:C:340:VAL:HG23	1.82	0.79
2:C:472:HEM:HMC2	2:C:472:HEM:HBC2	1.64	0.79
1:D:62:CYS:HB2	1:D:388:HIS:CE1	2.17	0.79
1:C:331:PHE:CE2	1:C:394:GLY:HA2	2.18	0.79
1:C:147:ARG:HG3	1:C:164:SER:HB3	1.64	0.79
1:B:237:MET:HE1	1:B:258:ILE:HG12	1.64	0.78
1:D:116:HIS:HD2	1:D:408:HIS:NE2	1.81	0.78
1:D:385:ILE:HG22	1:D:386:PRO:O	1.83	0.78
1:B:310:GLN:O	1:B:312:LYS:HG3	1.84	0.78
1:C:107:PHE:HD2	1:C:401:ILE:HG22	0.97	0.78
1:B:321:ALA:O	1:B:323:ARG:N	2.17	0.78
1:D:421:PHE:HB2	1:D:423:PHE:CZ	2.18	0.78
1:B:147:ARG:HG2	1:B:164:SER:CB	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:ASN:O	1:D:195:ASP:HB2	1.83	0.78
1:B:61:ALA:HA	1:B:67:PHE:CE2	2.19	0.77
1:C:83:GLY:HA3	1:C:256:TYR:CE1	2.19	0.77
1:B:30:MET:HE1	1:B:325:TRP:HH2	1.48	0.77
1:A:364:LYS:HD2	1:A:364:LYS:N	1.96	0.77
1:B:171:HIS:HD2	1:B:173:PHE:H	1.30	0.77
1:C:238:LEU:C	1:C:239:ASN:HD22	1.93	0.77
1:D:52:LEU:HB3	1:D:58:ILE:CD1	2.15	0.77
1:B:277:LEU:HD22	1:B:417:MET:HE1	1.67	0.77
1:A:122:ILE:HG22	1:A:148:LEU:HD12	1.67	0.77
1:B:304:SER:OG	1:B:307:GLN:HB2	1.85	0.77
1:D:271:GLY:HA2	1:D:440:LYS:HG3	1.66	0.77
1:A:293:GLU:HA	1:A:296:ARG:NH1	2.00	0.77
1:A:61:ALA:HA	1:A:67:PHE:CD2	2.19	0.76
1:C:244:GLU:O	1:C:244:GLU:CG	2.34	0.76
1:C:90:TRP:HD1	1:C:93:GLU:OE1	1.67	0.76
1:C:326:PRO:CG	1:C:358:PRO:HD3	2.14	0.76
1:C:331:PHE:CD2	1:C:394:GLY:HA2	2.20	0.76
1:A:272:LEU:CD2	1:A:322:LEU:HD13	2.14	0.76
1:D:75:LEU:HD11	1:D:87:PHE:HE1	1.50	0.76
1:A:381:ASN:ND2	1:A:383:SER:HB3	2.01	0.76
1:C:149:THR:HG22	1:C:266:HIS:CA	2.16	0.76
1:B:356:LEU:O	1:B:357:ILE:C	2.29	0.76
1:B:387:GLN:OE1	1:B:388:HIS:CD2	2.39	0.76
1:D:158:PHE:HE1	1:D:258:ILE:HG12	1.50	0.76
1:A:68:ASP:OD2	1:A:91:THR:HB	1.86	0.76
1:A:293:GLU:OE1	1:A:313:TYR:N	2.18	0.75
1:C:126:LEU:O	1:C:129:LYS:N	2.18	0.75
1:A:147:ARG:HG3	1:A:164:SER:CB	2.14	0.75
1:D:134:ASN:ND2	1:D:137:GLU:OE1	2.18	0.75
1:B:89:SER:HB2	1:B:93:GLU:OE1	1.86	0.75
1:A:238:LEU:O	1:A:239:ASN:ND2	2.20	0.75
1:B:16:ASN:HB3	1:B:19:LEU:HD12	1.66	0.75
1:A:98:LYS:HE2	1:A:248:PRO:O	1.85	0.75
2:B:472:HEM:HBC2	2:B:472:HEM:CMC	2.12	0.75
1:A:272:LEU:HD13	1:A:322:LEU:CD1	2.16	0.75
1:A:296:ARG:HG2	1:A:296:ARG:NH1	2.02	0.74
1:D:429:TYR:CE2	1:D:431:LEU:HA	2.21	0.74
1:A:272:LEU:HD22	1:A:322:LEU:HD11	1.69	0.74
1:A:388:HIS:CD2	1:A:391:LYS:HE2	2.22	0.74
1:C:364:LYS:H	1:C:364:LYS:HD2	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:472:HEM:HBC2	2:D:472:HEM:HMC1	1.67	0.74
1:D:62:CYS:CB	1:D:388:HIS:CE1	2.71	0.74
1:C:85:GLY:CA	1:C:257:GLN:HE22	1.95	0.74
1:B:283:ASN:HD22	1:B:283:ASN:N	1.85	0.74
1:C:214:ASP:O	1:C:218:LYS:HG2	1.88	0.74
1:B:304:SER:O	1:B:306:LYS:N	2.21	0.74
1:B:331:PHE:CZ	1:B:355:VAL:HG11	2.23	0.74
1:A:266:HIS:CD2	1:A:267:GLU:H	2.06	0.73
1:B:87:PHE:HE2	1:B:264:GLU:CD	1.96	0.73
1:D:8:PRO:HD3	1:D:36:LEU:HD12	1.69	0.73
1:B:91:THR:OG1	1:B:398:ARG:HD3	1.89	0.73
1:D:162:PHE:HE1	1:D:215:LEU:HD21	1.53	0.73
1:A:298:LEU:CD2	1:A:303:PRO:HB3	2.18	0.73
1:D:370:ASP:OD2	1:D:375:ARG:NH2	2.22	0.73
1:D:26:VAL:O	1:D:29:LEU:N	2.18	0.73
1:D:273:LEU:HD21	1:D:413:VAL:HG12	1.70	0.73
1:B:147:ARG:HG3	1:B:164:SER:HB3	1.70	0.72
1:D:327:THR:O	1:D:329:PRO:HD3	1.89	0.72
1:B:253:ASN:O	1:B:257:GLN:HG2	1.87	0.72
1:D:85:GLY:HA2	1:D:257:GLN:NE2	2.04	0.72
1:A:356:LEU:C	1:A:358:PRO:HD2	2.14	0.72
1:B:212:MET:CE	1:B:263:ILE:HD11	2.20	0.72
1:C:314:VAL:HG23	1:C:315:GLY:N	2.05	0.72
1:B:53:SER:HB3	1:B:359:GLN:CB	2.20	0.72
1:A:162:PHE:HE1	1:A:215:LEU:HD21	1.53	0.72
1:A:282:LYS:HE2	1:A:425:ASP:OD2	1.90	0.72
1:A:272:LEU:CD2	1:A:322:LEU:CD1	2.65	0.71
1:B:87:PHE:CE2	1:B:264:GLU:CD	2.68	0.71
1:B:201:ASN:H	1:B:201:ASN:ND2	1.84	0.71
1:B:416:MET:O	1:B:420:HIS:HD2	1.72	0.71
1:B:124:VAL:O	1:B:128:GLN:HG3	1.90	0.71
1:C:5:MET:CE	1:C:50:ARG:HG2	2.20	0.71
1:C:326:PRO:HG2	1:C:358:PRO:CD	2.15	0.71
1:D:311:LEU:HB3	1:D:314:VAL:HG22	1.73	0.71
1:A:310:GLN:C	1:A:312:LYS:H	1.99	0.71
1:A:376:PRO:O	1:A:377:GLU:C	2.33	0.71
1:B:59:LYS:HG3	1:B:60:GLU:N	2.05	0.71
1:D:149:THR:HG21	1:D:266:HIS:O	1.89	0.71
1:D:293:GLU:OE1	1:D:313:TYR:N	2.23	0.71
1:B:313:TYR:CA	1:B:316:MET:CE	2.62	0.71
1:D:75:LEU:HD11	1:D:87:PHE:CE1	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:296:ARG:HG3	1:D:297:VAL:N	2.05	0.71
1:C:247:GLU:OE1	1:C:248:PRO:HD2	1.90	0.71
1:C:346:PRO:O	1:C:347:LEU:HD23	1.91	0.71
1:C:375:ARG:O	1:C:378:ARG:HG3	1.91	0.71
1:D:102:ILE:HD12	1:D:249:LEU:HG	1.72	0.71
1:D:62:CYS:HB3	1:D:388:HIS:NE2	2.06	0.70
1:D:59:LYS:HA	1:D:388:HIS:ND1	2.07	0.70
1:A:103:LEU:HD11	1:A:237:MET:CG	2.20	0.70
1:A:290:ALA:HB2	1:A:313:TYR:HD2	1.51	0.70
1:B:128:GLN:O	1:B:132:ARG:HG3	1.91	0.70
1:D:5:MET:HE3	1:D:50:ARG:HG2	1.73	0.70
1:A:60:GLU:HG2	1:A:66:ARG:HH12	1.56	0.70
1:B:115:TYR:HA	1:B:118:MET:CE	2.21	0.70
1:D:112:MET:HE1	1:D:405:PHE:CD2	2.25	0.70
1:D:122:ILE:HD13	1:D:122:ILE:H	1.55	0.70
1:A:139:ILE:HD13	1:A:446:VAL:CG2	2.20	0.70
1:A:201:ASN:HD22	1:A:201:ASN:H	1.37	0.70
1:D:335:ALA:O	1:D:349:LYS:HG3	1.92	0.70
1:A:218:LYS:HA	1:A:218:LYS:CE	2.13	0.70
1:C:281:VAL:O	1:C:281:VAL:HG12	1.89	0.70
1:B:61:ALA:HA	1:B:67:PHE:CD2	2.27	0.70
1:D:39:ILE:HG12	1:D:40:PHE:N	2.06	0.70
1:A:103:LEU:HD11	1:A:237:MET:HG3	1.73	0.70
1:B:130:TRP:CH2	1:B:417:MET:HE3	2.27	0.70
1:C:201:ASN:H	1:C:201:ASN:ND2	1.90	0.70
1:A:55:GLN:C	1:A:55:GLN:OE1	2.35	0.69
1:A:298:LEU:HD22	1:A:303:PRO:HB3	1.73	0.69
1:D:218:LYS:HE3	1:D:218:LYS:CA	2.14	0.69
1:A:381:ASN:HD21	1:A:383:SER:HB3	1.57	0.69
1:C:147:ARG:NH1	1:C:167:ARG:O	2.24	0.69
1:C:149:THR:CG2	1:C:266:HIS:HB2	2.22	0.69
1:A:17:LEU:HD13	1:A:44:ALA:HB1	1.74	0.69
1:D:326:PRO:CD	1:D:358:PRO:HB3	2.20	0.69
1:A:201:ASN:N	1:A:201:ASN:ND2	2.39	0.69
1:A:145:MET:HA	1:A:145:MET:CE	2.22	0.69
1:D:86:LEU:HD11	1:D:99:ALA:CB	2.21	0.69
1:B:316:MET:HG2	1:B:379:PHE:HB2	1.74	0.69
1:C:298:LEU:HD21	1:C:311:LEU:HD11	1.74	0.69
1:D:17:LEU:HD22	1:D:45:PRO:HD2	1.75	0.69
1:C:100:HIS:ND1	1:C:100:HIS:C	2.51	0.69
1:C:82:ALA:C	1:C:256:TYR:HD1	2.02	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:THR:CG2	1:C:266:HIS:HA	2.22	0.68
1:C:323:ARG:HG2	1:C:361:HIS:HB3	1.73	0.68
1:B:78:VAL:CG1	1:B:81:PHE:CZ	2.76	0.68
1:D:149:THR:HG22	1:D:266:HIS:HA	1.75	0.68
1:A:423:PHE:CE1	1:A:448:ALA:HB2	2.28	0.68
1:C:112:MET:HB2	1:C:305:TYR:HE2	1.59	0.68
1:A:375:ARG:O	1:A:378:ARG:HG2	1.93	0.68
1:B:84:ASP:O	1:B:89:SER:HB3	1.94	0.68
1:D:56:ARG:O	1:D:59:LYS:HG2	1.93	0.68
1:D:201:ASN:N	1:D:201:ASN:ND2	2.34	0.68
1:B:72:SER:HB3	1:B:354:MET:HE1	1.76	0.68
1:A:97:LYS:HD2	1:A:101:ASN:HD21	1.58	0.68
1:B:272:LEU:CD1	1:B:322:LEU:CD1	2.65	0.68
1:B:130:TRP:CZ2	1:B:139:ILE:HD12	2.28	0.68
1:C:147:ARG:HD3	1:C:164:SER:O	1.94	0.68
1:C:387:GLN:O	1:C:388:HIS:HB2	1.93	0.68
1:C:78:VAL:HG13	1:C:81:PHE:CZ	2.28	0.67
1:A:387:GLN:NE2	1:A:388:HIS:N	2.33	0.67
1:B:296:ARG:HG3	1:B:297:VAL:N	2.09	0.67
1:B:325:TRP:HA	1:B:325:TRP:CE3	2.29	0.67
1:D:66:ARG:HH21	1:D:339:THR:HG1	1.42	0.67
1:B:62:CYS:SG	1:B:391:LYS:HD2	2.35	0.67
1:A:162:PHE:CE1	1:A:215:LEU:HD21	2.30	0.67
1:C:5:MET:HG2	1:C:41:LYS:HB2	1.76	0.67
1:C:91:THR:HG23	1:C:96:TRP:CZ3	2.30	0.67
1:A:206:GLN:O	1:A:210:LYS:HG2	1.94	0.67
1:A:391:LYS:HE3	1:A:395:ASN:OD1	1.95	0.67
1:D:91:THR:OG1	1:D:398:ARG:HD3	1.94	0.67
1:D:370:ASP:O	1:D:373:GLU:HB2	1.94	0.67
1:C:244:GLU:O	1:C:244:GLU:HG2	1.94	0.67
1:C:338:ASP:O	1:C:339:THR:HB	1.94	0.67
1:D:120:VAL:CG2	1:D:412:LEU:HD21	2.24	0.67
1:D:158:PHE:CE1	1:D:258:ILE:HG12	2.29	0.67
1:A:272:LEU:CD1	1:A:322:LEU:HD12	2.19	0.67
1:D:139:ILE:CD1	1:D:446:VAL:CG2	2.73	0.67
1:A:357:ILE:N	1:A:358:PRO:HD2	2.10	0.67
1:B:320:GLU:OE2	1:B:378:ARG:HD2	1.95	0.67
1:C:171:HIS:HD2	1:C:173:PHE:H	1.41	0.67
1:D:85:GLY:HA2	1:D:257:GLN:HE22	1.61	0.67
1:B:3:LYS:HB2	1:B:345:TYR:CE1	2.30	0.66
1:B:7:GLN:HB2	1:B:8:PRO:HD2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:LYS:C	1:B:283:ASN:ND2	2.53	0.66
1:A:272:LEU:O	1:A:273:LEU:C	2.35	0.66
1:D:103:LEU:O	1:D:106:SER:HB2	1.94	0.66
1:D:296:ARG:HG3	1:D:297:VAL:H	1.59	0.66
1:C:82:ALA:C	1:C:256:TYR:CD1	2.74	0.66
1:C:313:TYR:O	1:C:316:MET:N	2.27	0.66
1:C:128:GLN:O	1:C:132:ARG:HG3	1.95	0.66
1:A:310:GLN:O	1:A:312:LYS:N	2.23	0.66
1:B:264:GLU:HG3	2:B:472:HEM:C4C	2.30	0.66
1:B:390:PHE:O	1:B:392:PRO:HD2	1.95	0.66
1:C:111:ALA:O	1:C:114:GLY:N	2.28	0.66
1:D:69:LYS:HB2	1:D:398:ARG:HG3	1.78	0.66
1:B:59:LYS:HG3	1:B:60:GLU:H	1.59	0.66
1:A:414:LEU:HD23	1:A:417:MET:HE2	1.76	0.66
1:C:38:GLU:HB3	1:C:54:SER:HB3	1.77	0.66
1:C:149:THR:CG2	1:C:266:HIS:CA	2.74	0.66
1:D:39:ILE:HG13	1:D:52:LEU:CD1	2.23	0.66
1:D:96:TRP:CZ2	1:D:100:HIS:HD2	2.13	0.66
2:B:472:HEM:HMB2	2:B:472:HEM:CBB	2.25	0.66
1:C:323:ARG:NH2	1:C:324:LEU:HD22	2.10	0.65
1:B:102:ILE:HD12	1:B:249:LEU:CD2	2.26	0.65
1:C:91:THR:CG2	1:C:96:TRP:CZ3	2.80	0.65
1:C:414:LEU:HD23	1:C:417:MET:HE2	1.78	0.65
1:A:281:VAL:HG13	1:A:425:ASP:HB2	1.79	0.65
1:B:289:LYS:HG2	1:B:313:TYR:CE2	2.32	0.65
1:C:176:SER:HB3	1:C:208:ASP:CB	2.26	0.65
1:D:128:GLN:O	1:D:129:LYS:C	2.38	0.65
1:A:177:MET:O	1:A:177:MET:HG2	1.96	0.65
1:B:57:LEU:CD1	1:B:341:LEU:HG	2.22	0.65
1:C:17:LEU:HD22	1:C:45:PRO:HD3	1.79	0.65
1:C:149:THR:HG21	1:C:266:HIS:C	2.20	0.65
1:C:334:TYR:HA	1:C:351:ASP:O	1.96	0.65
1:B:79:ARG:O	1:B:81:PHE:N	2.30	0.65
1:B:97:LYS:O	1:B:98:LYS:C	2.38	0.65
1:C:40:PHE:CE2	1:C:51:TYR:HB2	2.32	0.65
1:B:70:ASN:HB2	1:B:334:TYR:CD1	2.31	0.65
1:D:382:PRO:O	1:D:384:ALA:N	2.30	0.65
1:D:293:GLU:HG3	1:D:313:TYR:CB	2.27	0.64
1:A:139:ILE:HD13	1:A:446:VAL:HG23	1.77	0.64
1:A:357:ILE:N	1:A:358:PRO:CD	2.59	0.64
1:B:112:MET:HB3	1:B:305:TYR:HE2	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:ASN:C	1:B:383:SER:H	2.05	0.64
1:C:38:GLU:CB	1:C:54:SER:HB3	2.27	0.64
1:C:149:THR:OG1	1:C:270:SER:HB3	1.98	0.64
1:A:33:ALA:O	1:A:36:LEU:N	2.29	0.64
1:D:242:ASP:O	1:D:246:GLY:N	2.25	0.64
1:B:210:LYS:N	1:B:210:LYS:HD2	2.12	0.64
1:C:32:ILE:HG22	1:C:36:LEU:HD12	1.78	0.64
1:D:139:ILE:HD13	1:D:446:VAL:HG23	1.78	0.64
1:D:271:GLY:O	1:D:275:PHE:HD2	1.80	0.64
1:A:286:VAL:O	1:A:287:LEU:C	2.41	0.64
1:B:61:ALA:O	1:B:67:PHE:HD2	1.79	0.64
1:D:141:VAL:CG1	1:D:142:PRO:HD3	2.21	0.64
1:D:400:CYS:HB2	2:D:472:HEM:NA	2.12	0.64
1:D:139:ILE:HD11	1:D:446:VAL:CG2	2.27	0.64
1:A:177:MET:HA	1:A:212:MET:CE	2.22	0.64
1:A:418:LEU:N	1:A:418:LEU:HD23	2.09	0.64
1:B:201:ASN:N	1:B:201:ASN:ND2	2.34	0.64
1:C:63:ASP:O	1:C:66:ARG:N	2.30	0.64
1:C:341:LEU:HD22	1:C:353:LEU:HD21	1.79	0.64
1:D:179:ARG:NE	1:D:204:GLN:NE2	2.46	0.64
1:B:264:GLU:HG3	2:B:472:HEM:CHD	2.27	0.64
1:B:272:LEU:HD22	1:B:322:LEU:HD13	1.79	0.64
1:C:142:PRO:HG2	1:C:143:GLU:OE1	1.98	0.64
1:A:38:GLU:HB2	1:A:54:SER:CB	2.28	0.64
1:B:171:HIS:CD2	1:B:173:PHE:H	2.14	0.64
1:D:426:HIS:CD2	1:D:447:LYS:HG3	2.32	0.64
1:B:58:ILE:HG13	1:B:360:LEU:HD22	1.79	0.63
1:B:421:PHE:HB2	1:B:423:PHE:CZ	2.32	0.63
1:C:63:ASP:OD2	1:C:66:ARG:CG	2.44	0.63
1:D:336:LYS:O	1:D:349:LYS:HD2	1.97	0.63
1:B:71:LEU:HD21	1:B:88:THR:O	1.98	0.63
1:B:128:GLN:O	1:B:132:ARG:CG	2.47	0.63
1:B:305:TYR:CD1	1:B:305:TYR:O	2.50	0.63
1:C:167:ARG:HG3	1:C:169:GLN:O	1.97	0.63
1:C:72:SER:O	1:C:73:GLN:C	2.41	0.63
1:D:223:ARG:HH21	1:D:234:LEU:HB3	1.64	0.63
1:A:99:ALA:O	1:A:103:LEU:HB2	1.99	0.63
1:A:62:CYS:HG	1:A:391:LYS:HE3	1.63	0.63
1:B:224:LYS:HE2	1:B:224:LYS:CA	2.14	0.63
1:C:202:LYS:O	1:C:206:GLN:HG2	1.98	0.63
1:A:33:ALA:CB	1:A:359:GLN:NE2	2.51	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:PHE:HE1	1:A:448:ALA:HB2	1.61	0.63
1:B:79:ARG:O	1:B:80:ASP:C	2.37	0.63
1:A:78:VAL:HG11	3:A:1465:PAM:H152	1.80	0.63
1:B:320:GLU:HB3	1:B:374:PHE:CE1	2.33	0.63
1:A:38:GLU:HB2	1:A:54:SER:OG	1.98	0.62
1:A:402:GLY:HA3	2:A:472:HEM:C3C	2.33	0.62
1:C:223:ARG:HH21	1:C:234:LEU:CD2	2.10	0.62
1:C:20:LEU:O	1:C:189:GLN:CD	2.42	0.62
1:C:317:VAL:HG12	1:C:318:LEU:N	2.12	0.62
1:B:212:MET:HE2	1:B:263:ILE:HD11	1.79	0.62
1:C:11:PHE:CE1	1:C:18:PRO:HB2	2.34	0.62
1:D:5:MET:HE1	1:D:39:ILE:HD13	1.81	0.62
1:A:171:HIS:HD2	1:A:173:PHE:H	1.48	0.62
1:C:8:PRO:O	1:C:16:ASN:ND2	2.33	0.62
1:C:223:ARG:HE	1:C:234:LEU:CD2	2.11	0.62
1:D:293:GLU:HG3	1:D:313:TYR:HB3	1.80	0.62
1:C:183:GLU:OE1	1:C:190:ARG:NH2	2.32	0.62
1:D:107:PHE:CD2	1:D:401:ILE:HG22	2.34	0.62
1:B:239:ASN:O	1:B:240:GLY:O	2.18	0.62
1:B:102:ILE:HD12	1:B:249:LEU:HD21	1.81	0.62
1:B:224:LYS:HA	1:B:224:LYS:CE	2.16	0.62
1:C:85:GLY:HA2	1:C:257:GLN:CD	2.23	0.62
1:B:313:TYR:O	1:B:316:MET:N	2.32	0.62
1:A:365:THR:O	1:A:365:THR:OG1	2.16	0.61
1:B:218:LYS:HE2	1:B:218:LYS:HA	1.80	0.61
1:C:72:SER:O	1:C:74:ALA:N	2.34	0.61
3:A:1465:PAM:H42	3:A:1465:PAM:O1	2.00	0.61
1:B:87:PHE:HD2	1:B:264:GLU:HG2	1.65	0.61
1:B:194:ASP:O	1:B:195:ASP:C	2.41	0.61
1:B:330:ALA:HA	1:B:357:ILE:HG13	1.81	0.61
2:A:472:HEM:HBC2	2:A:472:HEM:CMC	2.30	0.61
1:B:321:ALA:C	1:B:323:ARG:H	2.09	0.61
1:D:152:THR:HG21	1:D:409:GLU:OE2	2.01	0.61
1:D:298:LEU:HD21	1:D:311:LEU:HD11	1.83	0.61
1:C:7:GLN:HB3	1:C:41:LYS:HB3	1.82	0.61
1:C:323:ARG:O	1:C:361:HIS:ND1	2.33	0.61
1:D:337:GLU:O	1:D:338:ASP:O	2.19	0.61
1:B:281:VAL:CG1	1:B:425:ASP:CB	2.65	0.61
1:D:215:LEU:O	1:D:216:VAL:C	2.44	0.61
1:D:264:GLU:O	1:D:264:GLU:CG	2.49	0.61
1:D:337:GLU:O	1:D:338:ASP:C	2.44	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:PHE:HE2	1:B:264:GLU:OE2	1.84	0.60
1:C:96:TRP:CZ2	1:C:100:HIS:HD2	2.19	0.60
1:C:332:SER:O	1:C:333:LEU:HD13	2.01	0.60
1:B:419:LYS:HG2	1:B:420:HIS:CD2	2.36	0.60
1:C:212:MET:CE	1:C:263:ILE:HD11	2.20	0.60
1:D:87:PHE:O	1:D:87:PHE:CD1	2.54	0.60
1:D:426:HIS:CG	1:D:447:LYS:HG3	2.37	0.60
1:A:176:SER:HB3	1:A:208:ASP:HB3	1.82	0.60
1:B:12:GLY:O	1:B:14:LEU:N	2.34	0.60
1:B:331:PHE:CE1	1:B:333:LEU:HD21	2.37	0.60
1:C:340:VAL:HG22	1:C:346:PRO:HA	1.82	0.60
1:B:74:ALA:O	1:B:78:VAL:HG23	2.01	0.60
1:A:121:ASP:C	1:A:121:ASP:OD1	2.44	0.60
1:C:273:LEU:HD11	1:C:413:VAL:HG11	1.84	0.60
1:D:377:GLU:O	1:D:380:GLU:HB2	2.01	0.60
1:C:27:GLN:OE1	1:C:433:ILE:HB	2.01	0.60
1:D:279:PHE:O	1:D:283:ASN:ND2	2.35	0.60
1:C:69:LYS:HD3	1:C:398:ARG:NH1	2.16	0.60
1:C:119:MET:HE2	1:C:405:PHE:CZ	2.37	0.60
1:C:223:ARG:HH21	1:C:234:LEU:HB3	1.67	0.60
1:A:293:GLU:HA	1:A:296:ARG:HH12	1.67	0.59
1:B:58:ILE:CD1	1:B:355:VAL:HG22	2.30	0.59
1:B:305:TYR:CE1	1:B:309:LYS:HE2	2.37	0.59
1:C:134:ASN:HD21	1:C:137:GLU:CD	2.10	0.59
1:D:308:VAL:HG13	1:D:411:THR:HG22	1.84	0.59
1:C:77:PHE:CE2	1:C:188:LEU:HD23	2.38	0.59
1:C:337:GLU:O	1:C:338:ASP:C	2.45	0.59
1:D:56:ARG:O	1:D:59:LYS:CG	2.50	0.59
1:D:332:SER:O	1:D:333:LEU:HD13	2.01	0.59
1:A:17:LEU:N	1:A:18:PRO:CD	2.65	0.59
1:B:340:VAL:HG12	1:B:340:VAL:O	2.03	0.59
1:C:289:LYS:HG2	1:C:313:TYR:CE2	2.38	0.59
1:D:11:PHE:O	1:D:12:GLY:O	2.21	0.59
1:D:81:PHE:HB3	1:D:209:ILE:HD13	1.84	0.59
1:A:427:THR:O	1:A:428:ASN:C	2.41	0.59
1:B:242:ASP:HB2	1:B:245:THR:OG1	2.00	0.59
1:D:421:PHE:HB2	1:D:423:PHE:CE2	2.36	0.59
1:A:337:GLU:HA	1:A:349:LYS:HB2	1.84	0.59
1:B:104:LEU:N	1:B:105:PRO:HD2	2.18	0.59
1:B:234:LEU:O	1:B:235:THR:C	2.44	0.59
1:B:275:PHE:CE2	1:B:441:PRO:HD3	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:LEU:CD1	1:C:322:LEU:HD13	2.24	0.59
1:D:16:ASN:O	1:D:42:PHE:CZ	2.56	0.59
1:C:280:LEU:HB3	1:C:287:LEU:HG	1.84	0.59
1:A:69:LYS:HD3	1:A:398:ARG:NH1	2.18	0.59
1:B:331:PHE:HE1	1:B:333:LEU:HD21	1.68	0.59
1:B:319:ASN:O	1:B:323:ARG:HB2	2.02	0.59
1:D:280:LEU:C	1:D:287:LEU:HD12	2.28	0.59
1:B:22:THR:OG1	1:B:23:ASP:N	2.35	0.59
1:B:401:ILE:HG12	2:B:472:HEM:HBD2	1.83	0.59
1:D:39:ILE:HG23	1:D:39:ILE:O	2.03	0.59
1:D:425:ASP:OD2	1:D:428:ASN:HA	2.03	0.59
1:C:24:LYS:N	1:C:25:PRO:HD3	2.18	0.58
1:D:416:MET:O	1:D:420:HIS:HD2	1.86	0.58
1:A:25:PRO:HD2	1:A:435:GLU:OE1	2.03	0.58
1:A:149:THR:HG21	1:A:269:THR:HB	1.84	0.58
1:A:282:LYS:CE	1:A:425:ASP:OD2	2.51	0.58
1:B:314:VAL:O	1:B:317:VAL:HB	2.03	0.58
1:C:263:ILE:HG22	1:C:264:GLU:N	2.17	0.58
1:C:390:PHE:O	1:C:392:PRO:HD2	2.03	0.58
1:A:59:LYS:HA	1:A:388:HIS:ND1	2.17	0.58
1:A:81:PHE:HB3	1:A:209:ILE:HG12	1.84	0.58
1:A:145:MET:HE2	1:A:145:MET:N	2.18	0.58
1:A:413:VAL:HG13	1:A:414:LEU:N	2.19	0.58
1:C:93:GLU:O	1:C:94:LYS:C	2.46	0.58
1:C:126:LEU:O	1:C:127:VAL:C	2.47	0.58
1:A:38:GLU:HB2	1:A:54:SER:HB3	1.86	0.58
1:B:271:GLY:HA3	1:B:327:THR:HG21	1.84	0.58
1:C:145:MET:HE2	1:C:145:MET:CA	2.21	0.58
1:D:120:VAL:HG23	1:D:412:LEU:HD21	1.84	0.58
1:B:56:ARG:HH21	1:B:342:GLY:HA2	1.69	0.58
1:B:62:CYS:SG	1:B:391:LYS:CD	2.92	0.58
1:A:139:ILE:HG12	1:A:139:ILE:O	2.02	0.58
1:B:320:GLU:OE2	1:B:323:ARG:NE	2.36	0.58
1:C:11:PHE:CD1	1:C:18:PRO:CG	2.82	0.58
1:D:30:MET:O	1:D:33:ALA:N	2.37	0.58
1:D:62:CYS:HB3	1:D:388:HIS:CE1	2.38	0.58
1:B:130:TRP:CZ3	1:B:417:MET:HE3	2.39	0.58
1:D:62:CYS:CB	1:D:388:HIS:NE2	2.66	0.58
1:B:171:HIS:HD2	1:B:173:PHE:N	2.01	0.58
1:B:268:THR:HG21	1:B:328:ALA:HB2	1.84	0.58
1:D:63:ASP:OD2	1:D:66:ARG:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:THR:HG22	1:D:266:HIS:HB2	1.84	0.58
1:A:116:HIS:HD2	1:A:408:HIS:HE2	1.52	0.58
1:D:149:THR:HG22	1:D:266:HIS:CA	2.34	0.58
1:D:52:LEU:HB3	1:D:58:ILE:HD11	1.85	0.57
1:B:87:PHE:CD2	1:B:264:GLU:HG2	2.39	0.57
1:C:195:ASP:O	1:C:197:ALA:N	2.37	0.57
1:C:223:ARG:NE	1:C:234:LEU:CD2	2.65	0.57
1:D:39:ILE:HG12	1:D:40:PHE:H	1.68	0.57
1:D:73:GLN:O	1:D:74:ALA:C	2.46	0.57
1:D:323:ARG:HA	1:D:361:HIS:HD1	1.69	0.57
1:A:17:LEU:HD13	1:A:44:ALA:CB	2.34	0.57
1:A:223:ARG:NH2	1:A:232:ASP:OD1	2.38	0.57
1:B:26:VAL:H	1:B:435:GLU:CD	2.12	0.57
1:B:130:TRP:HH2	1:B:417:MET:HE3	1.69	0.57
1:C:22:THR:N	1:C:189:GLN:OE1	2.34	0.57
1:A:266:HIS:CG	1:A:267:GLU:N	2.72	0.57
1:A:419:LYS:O	1:A:419:LYS:HG3	2.04	0.57
1:B:53:SER:HB3	1:B:359:GLN:HB3	1.86	0.57
1:C:84:ASP:CG	1:C:253:ASN:HD22	2.12	0.57
1:C:264:GLU:HB2	3:C:3465:PAM:H141	1.86	0.57
1:C:70:ASN:ND2	1:C:352:GLU:HG2	2.18	0.57
1:C:134:ASN:ND2	1:C:134:ASN:H	2.03	0.57
1:D:150:LEU:HD22	1:D:174:ILE:HD11	1.85	0.57
1:A:305:TYR:O	1:A:309:LYS:HG2	2.05	0.57
1:B:332:SER:HB2	1:B:354:MET:CE	2.35	0.57
1:C:212:MET:O	1:C:215:LEU:N	2.37	0.57
1:D:55:GLN:C	1:D:55:GLN:OE1	2.48	0.57
1:B:272:LEU:O	1:B:273:LEU:C	2.45	0.57
1:B:293:GLU:OE2	1:B:311:LEU:HD23	2.05	0.57
1:C:72:SER:C	1:C:74:ALA:N	2.61	0.57
1:D:273:LEU:CD2	1:D:413:VAL:HG12	2.34	0.57
1:B:321:ALA:N	1:B:374:PHE:HE1	2.02	0.57
1:D:15:LYS:HG3	1:D:43:GLU:HG2	1.87	0.57
1:D:201:ASN:H	1:D:201:ASN:ND2	1.87	0.57
1:A:282:LYS:NZ	1:A:429:TYR:O	2.29	0.57
1:B:60:GLU:O	1:B:67:PHE:HE2	1.88	0.57
1:B:331:PHE:CE2	1:B:355:VAL:HG11	2.40	0.57
1:A:399:ALA:O	1:A:401:ILE:N	2.38	0.57
1:B:301:PRO:HB2	1:B:455:LEU:HA	1.87	0.57
1:C:39:ILE:CG1	1:C:52:LEU:HD12	2.30	0.57
1:C:174:ILE:O	1:C:178:VAL:HG22	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:429:TYR:CZ	1:C:444:PHE:HB2	2.40	0.57
1:D:304:SER:OG	1:D:307:GLN:HG3	2.04	0.57
1:D:420:HIS:N	1:D:420:HIS:CD2	2.72	0.57
1:A:152:THR:CB	1:A:409:GLU:OE2	2.53	0.56
1:C:183:GLU:CD	1:C:190:ARG:HH22	2.11	0.56
1:C:273:LEU:CD1	1:C:413:VAL:HG11	2.35	0.56
1:D:124:VAL:O	1:D:128:GLN:CG	2.53	0.56
1:D:366:ILE:HG23	1:D:386:PRO:HG2	1.87	0.56
1:A:134:ASN:HD22	1:A:137:GLU:CD	2.13	0.56
1:A:334:TYR:HA	1:A:351:ASP:O	2.05	0.56
1:A:400:CYS:HB2	2:A:472:HEM:NA	2.21	0.56
1:A:429:TYR:CE2	1:A:431:LEU:HA	2.40	0.56
1:A:451:LYS:O	1:A:453:ILE:HG13	2.05	0.56
1:B:218:LYS:HE2	1:B:218:LYS:CA	2.35	0.56
1:B:279:PHE:HB3	1:B:374:PHE:CE2	2.41	0.56
1:C:179:ARG:NE	1:C:204:GLN:NE2	2.54	0.56
1:C:337:GLU:O	1:C:338:ASP:O	2.23	0.56
1:D:147:ARG:NH1	1:D:167:ARG:O	2.39	0.56
1:D:400:CYS:SG	1:D:403:GLN:N	2.78	0.56
1:A:266:HIS:CD2	1:A:267:GLU:N	2.73	0.56
1:A:313:TYR:CD1	1:A:316:MET:HE3	2.40	0.56
1:B:155:LEU:HD11	1:B:161:ARG:CZ	2.35	0.56
1:C:179:ARG:HE	1:C:204:GLN:NE2	2.03	0.56
1:C:314:VAL:CG2	1:C:315:GLY:N	2.67	0.56
1:B:218:LYS:HA	1:B:218:LYS:CE	2.35	0.56
1:B:254:ILE:O	1:B:257:GLN:N	2.38	0.56
1:C:219:ILE:HG22	1:C:220:ILE:N	2.20	0.56
1:D:309:LYS:NZ	1:D:404:GLN:NE2	2.54	0.56
1:A:228:GLU:CG	1:A:229:GLN:N	2.43	0.56
1:C:84:ASP:OD1	1:C:253:ASN:ND2	2.37	0.56
1:C:293:GLU:O	1:C:293:GLU:OE2	2.23	0.56
1:C:341:LEU:C	1:C:343:GLY:N	2.63	0.56
1:A:8:PRO:HD2	1:A:16:ASN:ND2	2.19	0.56
1:A:131:GLU:HG2	1:A:421:PHE:HZ	1.71	0.56
1:A:377:GLU:O	1:A:378:ARG:C	2.48	0.56
1:A:387:GLN:OE1	1:A:388:HIS:CD2	2.58	0.56
1:B:52:LEU:HD13	1:B:353:LEU:HD23	1.87	0.56
1:B:304:SER:O	1:B:305:TYR:C	2.47	0.56
1:B:336:LYS:O	1:B:349:LYS:HD2	2.06	0.56
1:B:451:LYS:O	1:B:452:LYS:C	2.48	0.56
1:C:400:CYS:SG	1:C:403:GLN:N	2.78	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:PRO:C	1:D:195:ASP:H	2.13	0.56
1:A:103:LEU:HD11	1:A:237:MET:HG2	1.88	0.56
1:A:281:VAL:CG1	1:A:425:ASP:HB2	2.35	0.56
1:B:148:LEU:HB2	1:B:165:PHE:HZ	1.71	0.56
1:C:269:THR:O	1:C:272:LEU:HB3	2.05	0.56
1:B:7:GLN:CB	1:B:8:PRO:HD2	2.35	0.56
1:C:160:TYR:HE2	1:C:215:LEU:HD11	1.69	0.56
1:B:264:GLU:OE1	1:B:264:GLU:CA	2.50	0.56
1:B:387:GLN:OE1	1:B:388:HIS:N	2.39	0.56
1:C:281:VAL:HG11	1:C:425:ASP:HB2	1.88	0.56
1:A:237:MET:HE1	1:A:258:ILE:CG1	2.34	0.55
1:B:79:ARG:C	1:B:81:PHE:N	2.61	0.55
1:C:107:PHE:HE2	1:C:401:ILE:CG2	2.18	0.55
1:B:316:MET:HG2	1:B:379:PHE:CB	2.37	0.55
1:B:339:THR:OG1	1:B:340:VAL:N	2.34	0.55
1:D:38:GLU:HA	1:D:53:SER:HB2	1.87	0.55
1:A:38:GLU:CB	1:A:54:SER:CB	2.83	0.55
1:A:312:LYS:O	1:A:316:MET:HG3	2.07	0.55
1:C:326:PRO:HG3	1:C:357:ILE:HG22	1.88	0.55
1:D:85:GLY:O	1:D:86:LEU:C	2.50	0.55
1:D:118:MET:HB3	1:D:155:LEU:HD23	1.89	0.55
1:A:68:ASP:HB3	1:A:334:TYR:CZ	2.42	0.55
1:A:177:MET:CB	1:A:212:MET:HE3	2.37	0.55
1:B:68:ASP:OD2	1:B:91:THR:HB	2.05	0.55
1:C:108:SER:O	1:C:111:ALA:N	2.38	0.55
1:D:86:LEU:CD1	1:D:99:ALA:HB1	2.29	0.55
1:D:142:PRO:HG3	1:D:441:PRO:O	2.07	0.55
1:D:293:GLU:OE1	1:D:313:TYR:CB	2.55	0.55
1:B:29:LEU:HD13	1:B:51:TYR:CE2	2.42	0.55
1:B:268:THR:CG2	1:B:328:ALA:HB2	2.37	0.55
1:C:97:LYS:O	1:C:98:LYS:C	2.50	0.55
1:D:17:LEU:O	1:D:20:LEU:N	2.40	0.55
1:D:264:GLU:O	1:D:264:GLU:HG3	2.06	0.55
1:D:323:ARG:NH1	1:D:361:HIS:O	2.39	0.55
1:A:7:GLN:HB2	1:A:41:LYS:O	2.07	0.55
1:C:335:ALA:HB3	1:C:348:GLU:O	2.05	0.55
1:C:341:LEU:C	1:C:343:GLY:H	2.13	0.55
1:C:423:PHE:CE1	1:C:448:ALA:HB2	2.42	0.55
1:A:413:VAL:O	1:A:414:LEU:C	2.49	0.55
1:A:131:GLU:HG2	1:A:421:PHE:CZ	2.42	0.55
1:B:149:THR:HG22	1:B:266:HIS:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:ARG:O	1:C:336:LYS:HB2	2.07	0.55
1:D:38:GLU:O	1:D:53:SER:N	2.35	0.55
1:D:193:PRO:C	1:D:195:ASP:N	2.65	0.55
1:D:273:LEU:CD2	1:D:413:VAL:CG1	2.85	0.55
1:C:147:ARG:HD3	1:C:164:SER:C	2.31	0.55
1:C:212:MET:HE1	1:C:263:ILE:CD1	2.21	0.55
1:C:400:CYS:O	1:C:401:ILE:C	2.48	0.55
1:D:100:HIS:CE1	1:D:104:LEU:HD22	2.42	0.55
1:D:324:LEU:HD12	1:D:362:ARG:NH2	2.21	0.55
1:A:377:GLU:C	1:A:379:PHE:N	2.55	0.55
1:B:272:LEU:HD13	1:B:322:LEU:HD13	1.81	0.55
1:B:444:PHE:CD1	1:B:444:PHE:C	2.81	0.55
1:C:387:GLN:OE1	1:C:388:HIS:CD2	2.60	0.55
1:A:410:ALA:O	1:A:414:LEU:HB2	2.07	0.54
1:B:25:PRO:HD2	1:B:435:GLU:OE1	2.05	0.54
1:C:38:GLU:O	1:C:53:SER:HB2	2.07	0.54
1:A:402:GLY:HA3	2:A:472:HEM:C2C	2.42	0.54
1:C:79:ARG:O	1:C:83:GLY:N	2.40	0.54
1:A:290:ALA:HB2	1:A:313:TYR:CE2	2.43	0.54
1:B:56:ARG:HG3	1:B:57:LEU:HD22	1.90	0.54
1:C:116:HIS:CD2	1:C:408:HIS:NE2	2.65	0.54
1:C:164:SER:O	1:C:167:ARG:HG2	2.08	0.54
1:D:104:LEU:N	1:D:105:PRO:HD2	2.22	0.54
1:A:407:LEU:CD1	1:A:407:LEU:N	2.69	0.54
1:B:66:ARG:O	1:B:336:LYS:HB2	2.07	0.54
1:B:313:TYR:O	1:B:316:MET:CB	2.55	0.54
1:C:223:ARG:NH2	1:C:234:LEU:HB3	2.22	0.54
1:B:5:MET:HE3	1:B:50:ARG:HG2	1.89	0.54
1:B:272:LEU:HD22	1:B:322:LEU:CD1	2.37	0.54
1:B:272:LEU:CD2	1:B:322:LEU:HD13	2.37	0.54
1:A:290:ALA:CB	1:A:313:TYR:HD2	2.20	0.54
1:A:422:ASP:N	1:A:449:LYS:O	2.19	0.54
1:B:98:LYS:O	1:B:102:ILE:HG13	2.08	0.54
1:B:300:ASP:OD2	1:B:307:GLN:NE2	2.41	0.54
1:C:185:MET:O	1:C:185:MET:HG2	2.06	0.54
1:D:185:MET:O	1:D:188:LEU:HB2	2.07	0.54
1:B:58:ILE:O	1:B:61:ALA:HB3	2.07	0.54
1:B:147:ARG:NH1	1:B:167:ARG:O	2.41	0.54
1:C:20:LEU:C	1:C:189:GLN:HG2	2.33	0.54
1:D:297:VAL:HG21	1:D:310:GLN:HB3	1.89	0.54
1:B:155:LEU:O	1:B:156:CYS:C	2.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:TYR:O	1:C:118:MET:N	2.40	0.54
1:C:306:LYS:O	1:C:307:GLN:C	2.51	0.54
1:C:306:LYS:O	1:C:309:LYS:N	2.41	0.54
1:D:281:VAL:HG13	1:D:425:ASP:HB2	1.90	0.54
1:D:337:GLU:C	1:D:338:ASP:O	2.50	0.54
1:A:407:LEU:HD13	1:A:407:LEU:H	1.73	0.54
1:C:115:TYR:O	1:C:116:HIS:C	2.50	0.54
1:C:400:CYS:SG	1:C:402:GLY:N	2.81	0.54
1:D:154:GLY:O	1:D:158:PHE:HB2	2.08	0.54
1:A:62:CYS:SG	1:A:391:LYS:HD2	2.48	0.53
1:A:190:ARG:HG2	1:A:198:TYR:CE2	2.44	0.53
1:A:272:LEU:CD1	1:A:322:LEU:CD1	2.83	0.53
1:A:303:PRO:HA	1:A:307:GLN:OE1	2.08	0.53
1:C:108:SER:O	1:C:110:GLN:N	2.41	0.53
1:A:124:VAL:O	1:A:128:GLN:HG2	2.07	0.53
1:D:322:LEU:HD12	1:D:326:PRO:HA	1.90	0.53
1:A:33:ALA:HB1	1:A:359:GLN:HE21	1.68	0.53
1:C:334:TYR:CA	1:C:351:ASP:O	2.57	0.53
1:D:12:GLY:O	1:D:14:LEU:N	2.42	0.53
1:D:120:VAL:HG22	1:D:412:LEU:HD21	1.89	0.53
1:A:61:ALA:HB2	1:A:353:LEU:HD23	1.91	0.53
1:A:62:CYS:HB3	1:A:388:HIS:CE1	2.43	0.53
1:C:3:LYS:HB2	1:C:345:TYR:CE1	2.44	0.53
1:D:116:HIS:CD2	1:D:408:HIS:NE2	2.70	0.53
1:A:57:LEU:HD12	1:A:341:LEU:HG	1.89	0.53
1:B:9:LYS:HB3	1:B:11:PHE:HE1	1.74	0.53
1:D:87:PHE:O	1:D:87:PHE:HD1	1.92	0.53
1:D:323:ARG:HG2	1:D:361:HIS:HB3	1.89	0.53
1:A:423:PHE:CE1	1:A:448:ALA:CB	2.92	0.53
1:B:11:PHE:CD1	1:B:11:PHE:N	2.75	0.53
1:B:387:GLN:CD	1:B:388:HIS:H	2.17	0.53
1:C:85:GLY:CA	1:C:257:GLN:NE2	2.45	0.53
1:C:194:ASP:HA	1:C:202:LYS:NZ	2.23	0.53
1:C:238:LEU:C	1:C:239:ASN:ND2	2.66	0.53
1:D:410:ALA:O	1:D:411:THR:C	2.50	0.53
1:A:376:PRO:O	1:A:378:ARG:N	2.41	0.53
1:A:419:LYS:HG2	1:A:420:HIS:CD2	2.43	0.53
1:C:171:HIS:CD2	1:C:172:PRO:HD2	2.44	0.53
1:C:171:HIS:CD2	1:C:173:PHE:H	2.23	0.53
1:A:332:SER:C	1:A:333:LEU:HD22	2.34	0.53
1:D:71:LEU:HD22	1:D:90:TRP:CE2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:ILE:N	1:D:122:ILE:CD1	2.60	0.53
1:C:38:GLU:HA	1:C:53:SER:HB2	1.91	0.53
1:D:8:PRO:HD3	1:D:36:LEU:HD11	1.90	0.53
1:A:97:LYS:HD2	1:A:101:ASN:ND2	2.24	0.52
1:A:414:LEU:HA	1:A:417:MET:HE2	1.91	0.52
1:B:56:ARG:NH2	1:B:342:GLY:CA	2.72	0.52
1:B:334:TYR:CD1	1:B:334:TYR:N	2.74	0.52
1:C:235:THR:HA	1:C:238:LEU:HD12	1.89	0.52
1:C:402:GLY:HA3	2:C:472:HEM:C3C	2.44	0.52
1:D:124:VAL:O	1:D:128:GLN:HG2	2.09	0.52
1:D:129:LYS:HE2	1:D:144:ASP:OD1	2.09	0.52
1:A:134:ASN:ND2	1:A:137:GLU:CD	2.67	0.52
1:A:310:GLN:O	1:A:312:LYS:CG	2.55	0.52
1:B:126:LEU:O	1:B:127:VAL:C	2.52	0.52
1:C:139:ILE:HD11	1:C:446:VAL:CG2	2.40	0.52
1:D:318:LEU:CD1	1:D:414:LEU:HD12	2.39	0.52
1:D:402:GLY:HA3	2:D:472:HEM:C4C	2.45	0.52
1:A:371:VAL:HG23	1:A:372:GLU:N	2.23	0.52
1:B:305:TYR:CE1	1:B:309:LYS:CE	2.92	0.52
1:C:253:ASN:O	1:C:254:ILE:C	2.53	0.52
1:D:331:PHE:HE1	1:D:355:VAL:HG21	1.74	0.52
1:B:9:LYS:HB3	1:B:11:PHE:CE1	2.45	0.52
1:B:375:ARG:HB2	1:B:378:ARG:HE	1.73	0.52
1:D:240:GLY:O	1:D:248:PRO:HA	2.10	0.52
1:A:116:HIS:CD2	1:A:408:HIS:HE2	2.27	0.52
1:B:272:LEU:CD1	1:B:322:LEU:HD13	2.38	0.52
1:B:323:ARG:HG3	1:B:390:PHE:CE1	2.44	0.52
1:B:403:GLN:CG	1:B:404:GLN:N	2.70	0.52
1:D:141:VAL:CG1	1:D:444:PHE:CD2	2.85	0.52
1:B:78:VAL:CG1	1:B:81:PHE:CE2	2.93	0.52
1:D:158:PHE:HD1	1:D:234:LEU:HD22	1.75	0.52
1:B:92:HIS:HE1	1:B:336:LYS:HE2	1.74	0.52
1:B:190:ARG:HD3	1:B:198:TYR:CZ	2.45	0.52
1:B:321:ALA:C	1:B:323:ARG:N	2.66	0.52
1:B:368:GLY:O	1:B:370:ASP:N	2.38	0.52
1:C:411:THR:O	1:C:412:LEU:C	2.49	0.52
1:D:209:ILE:HG22	1:D:213:ASN:ND2	2.25	0.52
1:D:306:LYS:HE2	1:D:306:LYS:H	1.74	0.52
2:D:472:HEM:HBB2	2:D:472:HEM:CMB	2.39	0.52
1:B:270:SER:O	1:B:274:SER:HB2	2.10	0.52
1:B:305:TYR:CD1	1:B:305:TYR:C	2.88	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:GLU:OE1	1:C:341:LEU:HD12	2.09	0.52
1:C:231:ASP:CG	1:C:236:HIS:HE1	2.17	0.52
1:C:370:ASP:O	1:C:371:VAL:C	2.53	0.52
1:D:311:LEU:HB3	1:D:314:VAL:CG2	2.39	0.52
1:D:413:VAL:O	1:D:414:LEU:C	2.52	0.52
1:A:340:VAL:HG23	1:A:346:PRO:HA	1.91	0.52
1:B:290:ALA:HB2	1:B:313:TYR:CE2	2.45	0.52
1:C:21:ASN:CA	1:C:189:GLN:OE1	2.44	0.52
1:C:104:LEU:N	1:C:105:PRO:HD2	2.25	0.52
1:D:126:LEU:O	1:D:127:VAL:C	2.53	0.52
1:D:183:GLU:O	1:D:186:ASN:HB2	2.10	0.52
1:D:190:ARG:HD3	1:D:198:TYR:CE2	2.45	0.52
1:A:340:VAL:CG2	1:A:346:PRO:HA	2.41	0.51
1:B:72:SER:O	1:B:73:GLN:C	2.49	0.51
1:C:122:ILE:HG22	1:C:148:LEU:CD1	2.38	0.51
1:C:194:ASP:N	1:C:194:ASP:OD2	2.44	0.51
1:D:29:LEU:O	1:D:30:MET:C	2.52	0.51
1:A:264:GLU:O	1:A:264:GLU:CG	2.56	0.51
1:A:387:GLN:CD	1:A:388:HIS:H	2.17	0.51
1:B:3:LYS:HB2	1:B:345:TYR:HE1	1.74	0.51
1:C:83:GLY:HA3	1:C:256:TYR:CD1	2.46	0.51
1:D:7:GLN:NE2	1:D:41:LYS:O	2.43	0.51
1:D:44:ALA:HB3	1:D:47:ARG:CG	2.40	0.51
1:B:17:LEU:N	1:B:18:PRO:HD2	2.25	0.51
1:B:73:GLN:HA	1:B:76:LYS:HG3	1.92	0.51
1:D:100:HIS:HE1	1:D:104:LEU:HD22	1.75	0.51
1:D:141:VAL:CG1	1:D:142:PRO:CD	2.86	0.51
1:B:289:LYS:HG2	1:B:313:TYR:CZ	2.45	0.51
1:C:145:MET:CE	1:C:145:MET:CA	2.86	0.51
1:D:17:LEU:HD22	1:D:45:PRO:CD	2.39	0.51
1:D:99:ALA:O	1:D:103:LEU:HD22	2.11	0.51
1:D:313:TYR:O	1:D:316:MET:HB2	2.11	0.51
1:A:28:ALA:O	1:A:32:ILE:HG13	2.10	0.51
2:A:472:HEM:HBC2	2:A:472:HEM:HMC1	1.93	0.51
1:B:11:PHE:HD1	1:B:11:PHE:N	2.08	0.51
1:C:160:TYR:CE2	1:C:215:LEU:HD11	2.46	0.51
1:A:280:LEU:HD21	1:A:317:VAL:HG11	1.93	0.51
1:B:78:VAL:HG12	1:B:81:PHE:CE2	2.46	0.51
1:B:118:MET:CB	1:B:155:LEU:HD23	2.13	0.51
1:C:69:LYS:CB	1:C:398:ARG:HG3	2.40	0.51
1:C:79:ARG:HA	1:C:83:GLY:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:ALA:O	1:B:413:VAL:HG12	2.10	0.51
1:D:61:ALA:HB2	1:D:353:LEU:HD23	1.92	0.51
1:B:381:ASN:O	1:B:383:SER:N	2.44	0.51
1:B:5:MET:HE3	1:B:50:ARG:CD	2.41	0.51
1:B:72:SER:CB	1:B:354:MET:HE1	2.41	0.51
1:C:7:GLN:HB2	1:C:8:PRO:HD2	1.93	0.51
1:C:112:MET:CB	1:C:305:TYR:HE2	2.24	0.51
1:C:274:SER:O	1:C:275:PHE:C	2.51	0.51
1:D:169:GLN:O	1:D:170:PRO:C	2.54	0.51
1:A:399:ALA:O	1:A:400:CYS:C	2.49	0.51
1:B:89:SER:CB	1:B:93:GLU:OE1	2.58	0.51
1:B:223:ARG:HH22	1:B:232:ASP:CG	2.19	0.51
1:D:96:TRP:O	1:D:97:LYS:C	2.53	0.51
1:D:273:LEU:HD22	1:D:413:VAL:CG1	2.41	0.51
1:D:291:ALA:O	1:D:295:ALA:HB2	2.11	0.51
1:A:263:ILE:HG22	1:A:264:GLU:N	2.26	0.50
1:B:112:MET:HB3	1:B:305:TYR:CE2	2.45	0.50
1:C:52:LEU:N	1:C:354:MET:O	2.33	0.50
1:D:436:THR:O	1:D:438:THR:N	2.44	0.50
1:B:56:ARG:NH2	1:B:342:GLY:HA2	2.26	0.50
1:B:308:VAL:HG11	1:B:408:HIS:CE1	2.47	0.50
1:C:38:GLU:C	1:C:53:SER:HB2	2.36	0.50
1:C:311:LEU:O	1:C:314:VAL:HG22	2.11	0.50
1:D:177:MET:HB2	1:D:212:MET:HE3	1.93	0.50
1:A:139:ILE:CD1	1:A:446:VAL:HG23	2.35	0.50
1:C:376:PRO:O	1:C:378:ARG:N	2.44	0.50
1:A:381:ASN:CG	1:A:383:SER:HB3	2.36	0.50
1:B:27:GLN:HG3	1:B:435:GLU:OE2	2.11	0.50
1:C:283:ASN:ND2	1:C:283:ASN:N	2.59	0.50
1:C:311:LEU:HB3	1:C:314:VAL:CG2	2.41	0.50
1:D:425:ASP:CG	1:D:425:ASP:O	2.53	0.50
1:A:257:GLN:O	1:A:258:ILE:C	2.48	0.50
1:A:387:GLN:HE22	1:A:388:HIS:H	1.52	0.50
1:A:388:HIS:HD2	1:A:391:LYS:HE2	1.76	0.50
1:B:107:PHE:CZ	1:B:233:LEU:HD11	2.46	0.50
1:B:163:ASN:O	1:B:167:ARG:HD2	2.12	0.50
1:B:262:LEU:O	1:B:266:HIS:HD2	1.95	0.50
1:B:290:ALA:HB2	1:B:313:TYR:CD2	2.47	0.50
1:C:304:SER:O	1:C:305:TYR:C	2.55	0.50
1:D:177:MET:HE1	1:D:266:HIS:CE1	2.46	0.50
1:D:183:GLU:OE1	1:D:190:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:LEU:HD21	1:D:389:ALA:O	2.12	0.50
1:B:107:PHE:HZ	1:B:233:LEU:HD11	1.77	0.50
1:D:5:MET:SD	1:D:6:PRO:HD2	2.52	0.50
1:D:402:GLY:HA3	2:D:472:HEM:C3C	2.46	0.50
1:A:250:ASP:O	1:A:254:ILE:HG13	2.12	0.50
1:B:305:TYR:CZ	1:B:309:LYS:HE2	2.46	0.50
1:C:324:LEU:HD12	1:C:362:ARG:CZ	2.41	0.49
1:D:190:ARG:HD3	1:D:198:TYR:CD2	2.47	0.49
1:A:100:HIS:CE1	1:A:104:LEU:HD22	2.46	0.49
1:A:264:GLU:HG2	2:A:472:HEM:CHD	2.42	0.49
1:B:61:ALA:O	1:B:67:PHE:CD2	2.62	0.49
1:C:58:ILE:CD1	1:C:355:VAL:HG13	2.42	0.49
1:C:72:SER:C	1:C:74:ALA:H	2.20	0.49
1:C:244:GLU:O	1:C:244:GLU:HG3	2.10	0.49
1:C:324:LEU:HD12	1:C:362:ARG:NH2	2.26	0.49
1:D:319:ASN:O	1:D:323:ARG:N	2.45	0.49
1:A:100:HIS:HE1	1:A:104:LEU:HD22	1.77	0.49
1:B:24:LYS:HE2	1:B:433:ILE:O	2.13	0.49
1:B:124:VAL:O	1:B:128:GLN:CG	2.60	0.49
1:B:428:ASN:O	1:B:429:TYR:C	2.55	0.49
1:C:320:GLU:O	1:C:321:ALA:C	2.56	0.49
1:D:120:VAL:HG23	1:D:412:LEU:CD2	2.42	0.49
1:B:95:ASN:O	1:B:96:TRP:C	2.53	0.49
1:B:145:MET:O	1:B:149:THR:N	2.31	0.49
1:B:403:GLN:HG2	1:B:404:GLN:N	2.27	0.49
1:C:5:MET:HE1	1:C:50:ARG:HG2	1.91	0.49
1:C:118:MET:O	1:C:119:MET:C	2.54	0.49
1:C:220:ILE:O	1:C:221:ALA:C	2.52	0.49
1:D:50:ARG:NH2	1:D:351:ASP:HB3	2.28	0.49
1:D:304:SER:O	1:D:305:TYR:C	2.54	0.49
1:D:388:HIS:HD2	1:D:391:LYS:NZ	2.10	0.49
1:A:128:GLN:O	1:A:132:ARG:HG3	2.12	0.49
1:A:280:LEU:HD21	1:A:317:VAL:CG1	2.42	0.49
1:D:431:LEU:HD12	1:D:432:ASP:N	2.27	0.49
1:B:52:LEU:HD21	1:B:57:LEU:HB3	1.94	0.49
1:C:194:ASP:HA	1:C:202:LYS:HZ1	1.78	0.49
1:C:316:MET:HB3	1:C:379:PHE:HB2	1.94	0.49
1:C:339:THR:O	1:C:340:VAL:CG2	2.56	0.49
1:D:431:LEU:HD12	1:D:432:ASP:H	1.78	0.49
1:A:55:GLN:HE22	1:A:59:LYS:HD3	1.77	0.49
1:A:91:THR:OG1	1:A:398:ARG:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:ASP:O	1:A:442:GLU:N	2.42	0.49
1:D:124:VAL:O	1:D:128:GLN:HG3	2.13	0.49
1:A:218:LYS:CA	1:A:218:LYS:CE	2.80	0.49
1:A:272:LEU:HD21	1:A:322:LEU:HD13	1.95	0.49
1:B:86:LEU:HB3	2:B:472:HEM:HMD1	1.94	0.49
1:B:381:ASN:C	1:B:383:SER:N	2.69	0.49
1:C:24:LYS:HA	1:C:435:GLU:HG3	1.94	0.49
1:C:139:ILE:CD1	1:C:446:VAL:HG23	2.43	0.49
1:D:215:LEU:C	1:D:217:ASP:N	2.69	0.49
1:D:258:ILE:O	1:D:259:ILE:C	2.54	0.49
1:A:104:LEU:C	1:A:106:SER:H	2.21	0.49
1:B:297:VAL:HG13	1:B:310:GLN:NE2	2.27	0.49
1:B:403:GLN:HG2	1:B:404:GLN:H	1.78	0.49
1:C:150:LEU:O	1:C:151:ASP:C	2.56	0.49
1:C:403:GLN:O	1:C:406:ALA:HB3	2.13	0.49
1:D:112:MET:HE2	1:D:115:TYR:CD2	2.47	0.49
1:A:62:CYS:SG	1:A:391:LYS:CE	3.01	0.49
1:B:264:GLU:HG2	2:B:472:HEM:C1D	2.47	0.49
2:B:472:HEM:HMC2	2:B:472:HEM:CB	2.32	0.49
1:C:100:HIS:O	1:C:104:LEU:HB2	2.13	0.49
1:D:44:ALA:HB3	1:D:47:ARG:HG3	1.95	0.49
1:A:51:TYR:CE2	1:A:354:MET:HG2	2.48	0.48
1:B:57:LEU:O	1:B:58:ILE:C	2.55	0.48
1:B:86:LEU:HB3	2:B:472:HEM:CMD	2.42	0.48
1:C:86:LEU:CD1	1:C:99:ALA:HB3	2.43	0.48
1:C:86:LEU:O	1:C:398:ARG:NH2	2.45	0.48
1:C:152:THR:O	1:C:153:ILE:C	2.56	0.48
1:C:194:ASP:O	1:C:195:ASP:C	2.56	0.48
1:C:201:ASN:O	1:C:205:PHE:HB2	2.13	0.48
1:D:360:LEU:CD2	1:D:389:ALA:O	2.61	0.48
1:D:361:HIS:CD2	1:D:361:HIS:N	2.80	0.48
1:A:60:GLU:HB3	1:A:341:LEU:HD12	1.94	0.48
1:B:323:ARG:O	1:B:361:HIS:ND1	2.43	0.48
1:D:96:TRP:CZ2	1:D:100:HIS:CD2	2.98	0.48
1:A:61:ALA:HA	1:A:67:PHE:CE2	2.48	0.48
1:B:206:GLN:O	1:B:210:LYS:HG2	2.13	0.48
1:B:403:GLN:O	1:B:406:ALA:HB3	2.13	0.48
1:C:192:ASN:O	1:C:198:TYR:HE2	1.95	0.48
1:A:423:PHE:HE1	1:A:448:ALA:CB	2.25	0.48
1:C:12:GLY:O	1:C:15:LYS:N	2.45	0.48
1:C:96:TRP:CZ2	1:C:100:HIS:CD2	3.00	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:ARG:O	1:C:224:LYS:C	2.57	0.48
1:D:75:LEU:HD21	1:D:87:PHE:CE1	2.48	0.48
1:D:450:SER:OG	1:D:452:LYS:HG3	2.13	0.48
1:B:168:ASP:OD1	1:B:168:ASP:N	2.43	0.48
1:B:173:PHE:CE1	1:B:212:MET:HG2	2.49	0.48
1:C:183:GLU:O	1:C:184:ALA:C	2.51	0.48
1:D:182:ASP:O	1:D:186:ASN:ND2	2.47	0.48
1:A:296:ARG:NH1	1:A:296:ARG:CG	2.71	0.48
1:B:28:ALA:O	1:B:32:ILE:HG13	2.14	0.48
1:B:53:SER:CB	1:B:359:GLN:HB3	2.44	0.48
1:C:51:TYR:OH	3:C:3465:PAM:O1	2.27	0.48
1:C:91:THR:HG23	1:C:96:TRP:CE3	2.48	0.48
1:A:11:PHE:N	1:A:11:PHE:CD1	2.82	0.48
1:B:25:PRO:HD2	1:B:435:GLU:CD	2.39	0.48
1:C:15:LYS:HB2	1:C:43:GLU:O	2.13	0.48
1:A:61:ALA:CB	1:A:353:LEU:HD23	2.44	0.48
3:A:1465:PAM:O1	3:A:1465:PAM:C4	2.61	0.48
1:B:297:VAL:HG13	1:B:310:GLN:HE21	1.78	0.48
1:B:323:ARG:HG3	1:B:390:PHE:CD1	2.49	0.48
1:C:77:PHE:HE2	1:C:188:LEU:HD23	1.78	0.48
1:C:174:ILE:O	1:C:178:VAL:HG13	2.14	0.48
1:D:7:GLN:NE2	1:D:41:LYS:HG2	2.27	0.48
1:D:26:VAL:O	1:D:29:LEU:HB2	2.14	0.48
1:D:115:TYR:O	1:D:116:HIS:C	2.56	0.48
1:A:264:GLU:CG	2:A:472:HEM:CHD	2.91	0.48
1:B:30:MET:CE	1:B:325:TRP:HH2	2.23	0.48
1:C:311:LEU:HA	1:C:311:LEU:HD23	1.48	0.48
1:D:341:LEU:N	1:D:345:TYR:O	2.21	0.48
1:A:171:HIS:CD2	1:A:173:PHE:H	2.31	0.48
1:B:17:LEU:HB3	1:B:18:PRO:HD3	1.95	0.48
1:B:120:VAL:O	1:B:124:VAL:HG23	2.14	0.48
1:B:278:TYR:O	1:B:279:PHE:C	2.57	0.48
1:C:311:LEU:HB3	1:C:314:VAL:HG22	1.95	0.48
1:D:7:GLN:HA	1:D:8:PRO:HD2	1.63	0.48
1:D:271:GLY:HA2	1:D:440:LYS:CG	2.42	0.48
1:A:8:PRO:HD2	1:A:16:ASN:HD21	1.78	0.47
1:A:147:ARG:HD3	1:A:164:SER:O	2.14	0.47
1:B:52:LEU:HD21	1:B:341:LEU:HD21	1.96	0.47
1:B:210:LYS:N	1:B:210:LYS:CD	2.74	0.47
1:B:273:LEU:CD1	1:B:413:VAL:HG11	2.44	0.47
1:D:79:ARG:NH2	1:D:84:ASP:HB3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:MET:O	1:C:120:VAL:N	2.47	0.47
1:C:126:LEU:HB3	1:C:127:VAL:H	1.38	0.47
1:C:223:ARG:NH2	1:C:234:LEU:CD2	2.63	0.47
1:D:11:PHE:O	1:D:12:GLY:C	2.57	0.47
1:D:270:SER:C	1:D:272:LEU:N	2.71	0.47
1:A:264:GLU:HG2	2:A:472:HEM:C1D	2.50	0.47
1:B:356:LEU:HD13	1:B:359:GLN:HG2	1.96	0.47
1:C:210:LYS:N	1:C:210:LYS:HD2	2.29	0.47
1:D:223:ARG:C	1:D:225:ALA:H	2.21	0.47
1:D:232:ASP:O	1:D:233:LEU:C	2.54	0.47
1:A:309:LYS:HA	1:A:309:LYS:HD3	1.73	0.47
1:B:52:LEU:CD2	1:B:57:LEU:HB3	2.43	0.47
1:B:95:ASN:O	1:B:96:TRP:O	2.32	0.47
1:B:149:THR:CG2	1:B:266:HIS:HA	2.45	0.47
1:B:186:ASN:O	1:B:187:LYS:C	2.55	0.47
1:A:300:ASP:CG	1:A:307:GLN:HE22	2.23	0.47
1:B:5:MET:HE3	1:B:50:ARG:HD3	1.97	0.47
1:B:140:GLU:O	1:B:141:VAL:C	2.57	0.47
1:B:282:LYS:HA	1:B:282:LYS:HD3	1.63	0.47
1:C:237:MET:SD	1:C:257:GLN:HB2	2.54	0.47
1:C:306:LYS:HE2	1:C:306:LYS:H	1.78	0.47
1:A:147:ARG:HD2	1:A:165:PHE:CD1	2.50	0.47
1:B:58:ILE:HG21	1:B:360:LEU:HD22	1.95	0.47
1:B:129:LYS:HE3	1:B:144:ASP:OD2	2.15	0.47
1:B:296:ARG:HG3	1:B:297:VAL:H	1.80	0.47
1:C:356:LEU:HD23	1:C:356:LEU:HA	1.80	0.47
1:C:397:GLN:HG3	1:C:398:ARG:N	2.30	0.47
1:D:5:MET:HE3	1:D:50:ARG:CG	2.43	0.47
1:D:264:GLU:O	1:D:264:GLU:CD	2.58	0.47
1:A:20:LEU:O	1:A:189:GLN:HG2	2.13	0.47
1:A:36:LEU:HD23	1:A:36:LEU:HA	1.54	0.47
1:A:411:THR:O	1:A:412:LEU:C	2.58	0.47
1:B:429:TYR:CD1	1:B:444:PHE:HA	2.50	0.47
1:B:451:LYS:O	1:B:453:ILE:CG1	2.52	0.47
1:C:5:MET:HB2	1:C:5:MET:HE2	1.58	0.47
1:C:158:PHE:C	1:C:160:TYR:N	2.71	0.47
1:C:185:MET:HB3	1:C:185:MET:HE2	1.77	0.47
1:C:266:HIS:C	1:C:266:HIS:ND1	2.72	0.47
1:C:337:GLU:C	1:C:338:ASP:O	2.57	0.47
1:C:264:GLU:O	1:C:264:GLU:CD	2.58	0.47
1:C:297:VAL:HG21	1:C:310:GLN:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:ASN:HB3	1:D:332:SER:HB3	1.97	0.47
1:D:387:GLN:HE22	1:D:391:LYS:HZ1	1.61	0.47
1:A:320:GLU:O	1:A:323:ARG:N	2.45	0.47
1:B:35:GLU:O	1:B:35:GLU:CG	2.61	0.47
1:B:263:ILE:HG22	1:B:264:GLU:N	2.30	0.47
1:B:273:LEU:HD11	1:B:413:VAL:HG11	1.97	0.47
1:C:27:GLN:HG3	1:C:435:GLU:OE2	2.15	0.47
1:C:290:ALA:HA	1:C:313:TYR:HD2	1.79	0.47
1:C:377:GLU:C	1:C:379:PHE:H	2.18	0.47
1:D:26:VAL:O	1:D:28:ALA:N	2.48	0.47
1:D:39:ILE:HA	1:D:51:TYR:O	2.15	0.47
1:A:124:VAL:O	1:A:128:GLN:CG	2.63	0.47
1:A:396:GLY:O	1:A:399:ALA:HB2	2.15	0.47
1:B:186:ASN:C	1:B:188:LEU:N	2.71	0.47
1:C:302:VAL:HG12	1:C:303:PRO:O	2.14	0.47
1:C:436:THR:O	1:C:437:LEU:CB	2.49	0.47
1:B:2:ILE:HG12	1:B:346:PRO:CG	2.45	0.46
1:B:39:ILE:HA	1:B:51:TYR:O	2.15	0.46
1:B:332:SER:HB2	1:B:354:MET:HE1	1.97	0.46
1:C:264:GLU:O	1:C:264:GLU:CG	2.62	0.46
1:C:282:LYS:HE2	1:C:425:ASP:OD2	2.14	0.46
1:D:338:ASP:O	1:D:339:THR:HB	2.15	0.46
1:B:8:PRO:HB2	1:B:19:LEU:HD13	1.96	0.46
1:B:390:PHE:CE2	1:B:392:PRO:HG3	2.51	0.46
1:C:79:ARG:HG3	1:C:83:GLY:O	2.14	0.46
1:C:258:ILE:O	1:C:259:ILE:O	2.32	0.46
1:C:38:GLU:HB2	1:C:54:SER:HB3	1.97	0.46
1:A:59:LYS:HB3	1:A:388:HIS:HB2	1.98	0.46
1:A:177:MET:HB2	1:A:212:MET:CE	2.46	0.46
1:B:339:THR:O	1:B:340:VAL:HG23	2.16	0.46
1:C:63:ASP:OD2	1:C:66:ARG:CD	2.63	0.46
1:C:126:LEU:HD11	1:C:145:MET:HE1	1.97	0.46
1:D:193:PRO:O	1:D:194:ASP:C	2.56	0.46
1:D:215:LEU:O	1:D:217:ASP:N	2.48	0.46
1:D:356:LEU:HD23	1:D:356:LEU:HA	1.65	0.46
1:D:364:LYS:HB3	1:D:364:LYS:HE3	1.72	0.46
1:A:126:LEU:O	1:A:127:VAL:C	2.59	0.46
1:C:318:LEU:HD12	1:C:318:LEU:HA	1.80	0.46
1:C:377:GLU:C	1:C:379:PHE:N	2.70	0.46
1:D:149:THR:HG22	1:D:266:HIS:CB	2.44	0.46
1:A:68:ASP:HB3	1:A:334:TYR:HE1	1.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LYS:HG2	1:A:190:ARG:NH1	2.30	0.46
1:B:239:ASN:O	1:B:240:GLY:C	2.58	0.46
1:C:241:LYS:HD3	1:C:246:GLY:O	2.16	0.46
1:C:330:ALA:HB3	3:C:3465:PAM:H42	1.97	0.46
1:C:393:PHE:O	1:C:399:ALA:HB1	2.16	0.46
1:C:403:GLN:HE21	1:C:403:GLN:HB2	1.53	0.46
1:D:17:LEU:N	1:D:18:PRO:CD	2.79	0.46
2:D:472:HEM:CMC	2:D:472:HEM:CBC	2.85	0.46
1:A:210:LYS:HD2	1:A:210:LYS:HA	1.62	0.46
1:B:53:SER:HB3	1:B:359:GLN:HB2	1.94	0.46
1:C:22:THR:OG1	1:C:23:ASP:N	2.46	0.46
1:C:149:THR:CG2	1:C:266:HIS:CB	2.86	0.46
1:D:55:GLN:O	1:D:59:LYS:HG2	2.15	0.46
1:A:7:GLN:NE2	1:A:41:LYS:HG2	2.31	0.46
1:A:84:ASP:OD2	1:A:95:ASN:OD1	2.33	0.46
1:A:338:ASP:HA	1:A:347:LEU:O	2.16	0.46
1:B:130:TRP:CZ3	1:B:417:MET:HG2	2.51	0.46
1:B:278:TYR:O	1:B:281:VAL:N	2.49	0.46
1:C:10:THR:CA	1:C:15:LYS:O	2.59	0.46
1:C:134:ASN:ND2	1:C:134:ASN:N	2.63	0.46
1:D:112:MET:HE2	1:D:115:TYR:HD2	1.81	0.46
1:D:270:SER:C	1:D:272:LEU:H	2.22	0.46
1:B:259:ILE:HG22	1:B:260:THR:N	2.30	0.46
1:B:344:GLU:O	1:B:346:PRO:HD2	2.15	0.46
1:B:425:ASP:OD1	1:B:425:ASP:C	2.56	0.46
1:C:334:TYR:CB	1:C:351:ASP:O	2.64	0.46
1:D:381:ASN:ND2	1:D:384:ALA:HB2	2.31	0.46
1:D:400:CYS:HB2	2:D:472:HEM:C1A	2.50	0.46
1:A:428:ASN:O	1:A:429:TYR:C	2.58	0.46
1:B:212:MET:HE1	1:B:263:ILE:HD11	1.97	0.46
1:B:399:ALA:O	2:B:472:HEM:HBD1	2.15	0.46
1:A:17:LEU:HD22	1:A:45:PRO:CD	2.46	0.45
1:A:309:LYS:NZ	1:A:408:HIS:ND1	2.61	0.45
1:A:401:ILE:HG12	2:A:472:HEM:HBD1	1.98	0.45
1:B:262:LEU:N	1:B:262:LEU:HD23	2.21	0.45
1:B:347:LEU:HD23	1:B:347:LEU:HA	1.62	0.45
1:C:133:LEU:HD21	1:C:139:ILE:HG22	1.98	0.45
1:D:17:LEU:O	1:D:18:PRO:C	2.59	0.45
1:D:400:CYS:HA	2:D:472:HEM:CHA	2.46	0.45
1:B:360:LEU:HD11	1:B:389:ALA:HA	1.98	0.45
1:C:18:PRO:O	1:C:20:LEU:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:MET:HB2	1:C:305:TYR:CE2	2.45	0.45
1:C:195:ASP:C	1:C:197:ALA:H	2.24	0.45
1:C:385:ILE:HG22	1:C:386:PRO:O	2.15	0.45
1:C:407:LEU:HD12	1:C:407:LEU:HA	1.52	0.45
1:D:309:LYS:HZ3	1:D:404:GLN:NE2	2.14	0.45
1:A:139:ILE:HD13	1:A:446:VAL:HG22	1.88	0.45
1:C:134:ASN:C	1:C:134:ASN:HD22	2.25	0.45
1:D:38:GLU:HG3	1:D:39:ILE:HG22	1.99	0.45
1:D:101:ASN:O	1:D:102:ILE:C	2.54	0.45
1:A:142:PRO:HB2	1:A:440:LYS:HE3	1.98	0.45
1:A:414:LEU:HD23	1:A:414:LEU:HA	1.56	0.45
1:C:218:LYS:O	1:C:222:ASP:HB2	2.16	0.45
1:D:400:CYS:C	1:D:402:GLY:H	2.23	0.45
1:A:176:SER:HB3	1:A:208:ASP:CB	2.45	0.45
1:A:375:ARG:O	1:A:378:ARG:CG	2.61	0.45
1:B:11:PHE:O	1:B:14:LEU:HB2	2.16	0.45
1:B:186:ASN:O	1:B:188:LEU:N	2.49	0.45
1:B:192:ASN:O	1:B:198:TYR:HE2	1.99	0.45
1:B:237:MET:CE	1:B:258:ILE:HG12	2.40	0.45
3:C:3465:PAM:H111	3:C:3465:PAM:H81	1.60	0.45
1:D:3:LYS:HG2	1:D:344:GLU:HB3	1.98	0.45
1:D:277:LEU:HD12	1:D:277:LEU:HA	1.64	0.45
1:A:177:MET:HB2	1:A:212:MET:HE3	1.98	0.45
1:B:321:ALA:O	1:B:322:LEU:C	2.60	0.45
1:D:381:ASN:HA	1:D:382:PRO:HD3	1.76	0.45
1:A:108:SER:O	1:A:111:ALA:N	2.45	0.45
1:A:126:LEU:O	1:A:129:LYS:N	2.48	0.45
1:B:390:PHE:C	1:B:392:PRO:CD	2.90	0.45
1:C:75:LEU:HA	1:C:75:LEU:HD23	1.67	0.45
1:C:91:THR:HG22	1:C:96:TRP:CZ3	2.51	0.45
1:C:320:GLU:HG3	1:C:376:PRO:HA	1.97	0.45
1:D:133:LEU:HD12	1:D:133:LEU:HA	1.39	0.45
1:D:194:ASP:HA	1:D:202:LYS:HZ3	1.81	0.45
1:A:116:HIS:O	1:A:117:ALA:C	2.59	0.45
1:A:272:LEU:HD22	1:A:322:LEU:HD13	1.72	0.45
1:B:152:THR:HB	1:B:409:GLU:OE2	2.17	0.45
1:B:177:MET:HG3	1:B:212:MET:HE3	1.97	0.45
1:B:323:ARG:HB2	1:B:390:PHE:HE1	1.82	0.45
1:C:124:VAL:O	1:C:128:GLN:HB2	2.16	0.45
1:C:134:ASN:ND2	1:C:137:GLU:CD	2.75	0.45
1:D:177:MET:HE1	1:D:266:HIS:NE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:LEU:O	1:C:343:GLY:N	2.50	0.45
1:D:97:LYS:HD2	1:D:97:LYS:HA	1.74	0.45
1:D:118:MET:CE	1:D:156:CYS:HA	2.47	0.45
1:D:139:ILE:CD1	1:D:446:VAL:HG23	2.37	0.45
1:D:308:VAL:CG1	1:D:411:THR:HG22	2.47	0.45
1:D:397:GLN:H	1:D:397:GLN:HG3	1.53	0.45
2:D:472:HEM:HBD1	2:D:472:HEM:HHA	1.98	0.45
1:A:6:PRO:O	1:A:7:GLN:HB3	2.17	0.45
1:B:61:ALA:C	1:B:63:ASP:H	2.24	0.45
1:B:175:THR:O	1:B:178:VAL:HG22	2.17	0.45
1:C:153:ILE:HA	1:C:153:ILE:HD12	1.50	0.45
1:D:292:GLU:O	1:D:295:ALA:N	2.50	0.45
1:A:5:MET:SD	1:A:39:ILE:HG12	2.57	0.44
1:A:152:THR:HG21	1:A:409:GLU:OE2	2.17	0.44
1:A:313:TYR:HD1	1:A:316:MET:HE3	1.80	0.44
1:B:84:ASP:C	1:B:89:SER:HB3	2.41	0.44
1:C:338:ASP:O	1:C:339:THR:CB	2.64	0.44
1:C:357:ILE:HB	1:C:358:PRO:CD	2.46	0.44
1:D:204:GLN:O	1:D:204:GLN:HG3	2.15	0.44
1:D:314:VAL:CG2	1:D:411:THR:HG23	2.46	0.44
1:A:236:HIS:O	1:A:237:MET:C	2.60	0.44
1:A:413:VAL:CG1	1:A:414:LEU:N	2.79	0.44
1:B:164:SER:O	1:B:166:TYR:N	2.50	0.44
1:C:61:ALA:HA	1:C:67:PHE:CD2	2.52	0.44
1:C:323:ARG:HA	1:C:361:HIS:ND1	2.31	0.44
1:D:96:TRP:CH2	1:D:100:HIS:HD2	2.34	0.44
1:D:341:LEU:HB3	1:D:345:TYR:CB	2.30	0.44
1:C:115:TYR:O	1:C:117:ALA:N	2.50	0.44
1:D:97:LYS:CE	1:D:101:ASN:HD21	2.30	0.44
1:D:283:ASN:HB3	1:D:286:VAL:HG23	2.00	0.44
1:D:385:ILE:C	1:D:386:PRO:O	2.60	0.44
1:A:323:ARG:HD3	1:A:367:TRP:CZ3	2.53	0.44
1:A:331:PHE:CE2	1:A:394:GLY:HA2	2.51	0.44
1:B:267:GLU:HG2	1:B:438:THR:HG21	2.00	0.44
1:B:306:LYS:O	1:B:307:GLN:C	2.59	0.44
1:B:413:VAL:O	1:B:414:LEU:C	2.59	0.44
1:B:416:MET:HB3	1:B:416:MET:HE2	1.62	0.44
1:C:141:VAL:HG11	1:C:444:PHE:CE2	2.51	0.44
1:C:237:MET:HE1	1:C:258:ILE:CG1	2.34	0.44
1:C:281:VAL:CG1	1:C:425:ASP:HB2	2.48	0.44
1:C:432:ASP:O	1:C:441:PRO:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LEU:O	1:A:87:PHE:C	2.60	0.44
1:A:130:TRP:HA	1:A:133:LEU:HD22	2.00	0.44
1:C:20:LEU:HA	1:C:20:LEU:HD12	1.25	0.44
1:C:51:TYR:HE2	1:C:354:MET:HG2	1.67	0.44
1:C:103:LEU:O	1:C:106:SER:HB2	2.18	0.44
1:C:348:GLU:C	1:C:349:LYS:O	2.56	0.44
2:C:472:HEM:CMB	2:C:472:HEM:HBB2	2.47	0.44
1:D:293:GLU:OE1	1:D:313:TYR:HB3	2.18	0.44
1:D:293:GLU:HG3	1:D:313:TYR:HB2	1.99	0.44
1:A:96:TRP:NE1	2:A:472:HEM:O1D	2.45	0.44
1:C:71:LEU:HD12	1:C:71:LEU:HA	1.81	0.44
1:C:161:ARG:HG2	1:C:161:ARG:HH11	1.82	0.44
1:C:259:ILE:HG22	1:C:260:THR:N	2.32	0.44
1:A:96:TRP:CZ2	1:A:100:HIS:HD2	2.36	0.44
1:A:145:MET:CA	1:A:145:MET:CE	2.87	0.44
1:B:60:GLU:HG2	1:B:66:ARG:HH12	1.82	0.44
1:B:318:LEU:N	1:B:318:LEU:CD1	2.81	0.44
1:C:72:SER:O	1:C:75:LEU:N	2.51	0.44
1:C:126:LEU:HA	1:C:126:LEU:HD23	1.77	0.44
1:C:127:VAL:HG21	1:C:416:MET:HE2	2.00	0.44
1:C:272:LEU:O	1:C:273:LEU:C	2.60	0.44
1:C:313:TYR:C	1:C:315:GLY:N	2.72	0.44
1:A:74:ALA:O	1:A:75:LEU:C	2.61	0.44
1:A:118:MET:O	1:A:121:ASP:HB3	2.18	0.44
1:A:169:GLN:OE1	1:A:169:GLN:HA	2.18	0.44
1:A:381:ASN:HA	1:A:382:PRO:HD2	1.93	0.44
1:B:57:LEU:HD12	1:B:341:LEU:CD2	2.48	0.44
1:B:264:GLU:CG	2:B:472:HEM:CHD	2.96	0.44
1:C:70:ASN:HD21	1:C:352:GLU:HG2	1.81	0.44
1:A:102:ILE:HD12	1:A:249:LEU:CD2	2.48	0.44
1:A:320:GLU:HG3	1:A:376:PRO:HA	1.99	0.44
1:A:373:GLU:O	1:A:378:ARG:NH2	2.51	0.44
1:B:376:PRO:C	1:B:378:ARG:N	2.76	0.44
1:C:55:GLN:C	1:C:57:LEU:H	2.26	0.44
1:C:130:TRP:HZ3	1:C:417:MET:HG2	1.82	0.44
1:D:324:LEU:O	1:D:362:ARG:NH1	2.48	0.44
1:A:17:LEU:HD22	1:A:45:PRO:HD2	1.99	0.43
1:B:10:THR:O	1:B:11:PHE:CD1	2.69	0.43
1:B:111:ALA:O	1:B:114:GLY:N	2.51	0.43
1:C:69:LYS:HB2	1:C:398:ARG:HG3	1.99	0.43
1:C:296:ARG:HG2	1:C:297:VAL:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:MET:HE3	1:D:50:ARG:CD	2.48	0.43
1:D:283:ASN:HA	1:D:284:PRO:HD3	1.56	0.43
1:B:5:MET:HE1	1:B:39:ILE:CD1	2.43	0.43
1:B:27:GLN:O	1:B:28:ALA:C	2.58	0.43
1:B:242:ASP:O	1:B:243:PRO:C	2.61	0.43
1:B:251:ASP:O	1:B:252:GLU:C	2.60	0.43
1:B:301:PRO:CB	1:B:455:LEU:HA	2.48	0.43
1:B:433:ILE:HG21	1:B:433:ILE:HD13	1.79	0.43
1:C:91:THR:CG2	1:C:96:TRP:CE3	3.02	0.43
1:C:229:GLN:OE1	1:C:229:GLN:HA	2.17	0.43
1:C:427:THR:O	1:C:428:ASN:C	2.61	0.43
1:D:17:LEU:N	1:D:18:PRO:HD2	2.32	0.43
1:D:320:GLU:HG3	1:D:375:ARG:C	2.43	0.43
1:D:375:ARG:C	1:D:377:GLU:H	2.26	0.43
1:B:17:LEU:HB3	1:B:18:PRO:CD	2.47	0.43
1:B:118:MET:HE3	1:B:118:MET:HB2	1.91	0.43
1:D:64:GLU:OE2	1:D:397:GLN:HG3	2.18	0.43
1:D:318:LEU:HD11	1:D:414:LEU:HD12	1.99	0.43
1:A:104:LEU:HB3	1:A:105:PRO:HD3	2.01	0.43
1:A:292:GLU:O	1:A:293:GLU:C	2.62	0.43
1:A:390:PHE:O	1:A:392:PRO:HD2	2.18	0.43
1:A:407:LEU:HA	1:A:407:LEU:HD12	1.76	0.43
1:B:223:ARG:NH2	1:B:232:ASP:OD2	2.38	0.43
1:C:281:VAL:O	1:C:281:VAL:CG1	2.58	0.43
1:C:293:GLU:HG3	1:C:313:TYR:HB2	2.00	0.43
1:C:336:LYS:HD2	1:C:336:LYS:HA	1.41	0.43
1:D:20:LEU:HD12	1:D:20:LEU:HA	1.90	0.43
1:D:388:HIS:HA	1:D:391:LYS:HD2	2.00	0.43
1:B:30:MET:CE	1:B:325:TRP:CH2	2.88	0.43
1:C:122:ILE:O	1:C:123:ALA:C	2.61	0.43
1:C:329:PRO:HG3	1:C:439:LEU:HG	2.00	0.43
1:D:69:LYS:CB	1:D:398:ARG:HG3	2.48	0.43
1:D:115:TYR:HA	1:D:118:MET:HE2	1.99	0.43
1:D:274:SER:HB3	1:D:441:PRO:HG2	2.00	0.43
1:A:102:ILE:HD12	1:A:249:LEU:HD23	2.01	0.43
1:A:102:ILE:O	1:A:105:PRO:HD2	2.18	0.43
1:A:221:ALA:O	1:A:224:LYS:HB2	2.18	0.43
1:B:122:ILE:C	1:B:124:VAL:N	2.75	0.43
1:B:164:SER:C	1:B:166:TYR:N	2.76	0.43
1:C:118:MET:O	1:C:121:ASP:N	2.52	0.43
1:D:234:LEU:HA	1:D:237:MET:HE3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:355:VAL:O	1:D:357:ILE:N	2.52	0.43
1:A:84:ASP:HB2	1:A:89:SER:HB3	2.00	0.43
1:A:158:PHE:N	1:A:158:PHE:CD2	2.87	0.43
1:A:264:GLU:CG	2:A:472:HEM:C4C	3.01	0.43
1:A:407:LEU:N	1:A:407:LEU:HD13	2.33	0.43
1:B:164:SER:C	1:B:166:TYR:H	2.26	0.43
1:B:304:SER:OG	1:B:304:SER:O	2.36	0.43
1:B:359:GLN:O	1:B:360:LEU:C	2.60	0.43
1:C:79:ARG:O	1:C:81:PHE:N	2.52	0.43
1:C:164:SER:C	1:C:166:TYR:H	2.27	0.43
1:A:9:LYS:HD3	1:A:9:LYS:HA	1.67	0.43
1:A:245:THR:C	1:A:247:GLU:H	2.27	0.43
1:A:325:TRP:CE3	1:A:325:TRP:HA	2.54	0.43
1:B:100:HIS:ND1	1:B:100:HIS:C	2.77	0.43
1:B:262:LEU:O	1:B:266:HIS:CD2	2.70	0.43
1:B:364:LYS:O	1:B:368:GLY:N	2.50	0.43
1:C:260:THR:O	1:C:260:THR:CG2	2.64	0.43
1:C:393:PHE:HB3	1:C:400:CYS:HB3	2.01	0.43
1:D:79:ARG:O	1:D:83:GLY:N	2.44	0.43
1:A:16:ASN:HB2	1:A:43:GLU:O	2.19	0.43
1:A:134:ASN:N	1:A:134:ASN:HD22	2.00	0.43
1:B:15:LYS:HB3	1:B:43:GLU:HB3	2.00	0.43
1:B:20:LEU:HD22	1:B:42:PHE:CZ	2.54	0.43
1:B:149:THR:HG21	1:B:269:THR:HB	2.00	0.43
1:B:302:VAL:HA	1:B:303:PRO:HD3	1.77	0.43
1:C:111:ALA:O	1:C:112:MET:C	2.61	0.43
1:D:38:GLU:HB2	1:D:54:SER:OG	2.19	0.43
1:D:56:ARG:HG3	1:D:57:LEU:HD13	1.99	0.43
1:D:147:ARG:HD2	1:D:165:PHE:CD1	2.53	0.43
1:D:183:GLU:CD	1:D:190:ARG:HH22	2.25	0.43
1:D:400:CYS:HA	2:D:472:HEM:C4D	2.54	0.43
3:D:4465:PAM:H152	3:D:4465:PAM:H122	1.88	0.43
1:B:365:THR:C	1:B:366:ILE:HG12	2.44	0.43
1:C:147:ARG:HG3	1:C:164:SER:CB	2.41	0.43
1:C:196:PRO:CB	1:C:199:ASP:OD2	2.55	0.43
1:D:8:PRO:CD	1:D:36:LEU:CD1	2.93	0.43
1:A:371:VAL:CG2	1:A:372:GLU:N	2.82	0.42
1:B:27:GLN:HG3	1:B:27:GLN:H	1.36	0.42
1:B:280:LEU:HD21	1:B:317:VAL:HG13	2.01	0.42
1:B:323:ARG:CB	1:B:390:PHE:HE1	2.32	0.42
1:C:450:SER:C	1:C:452:LYS:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:MET:CB	1:A:155:LEU:HD23	2.25	0.42
1:A:158:PHE:CE1	1:A:258:ILE:HG12	2.54	0.42
1:A:387:GLN:OE1	1:A:388:HIS:HD2	2.00	0.42
1:B:58:ILE:HG21	1:B:360:LEU:CD2	2.49	0.42
1:B:210:LYS:O	1:B:211:VAL:C	2.60	0.42
1:B:427:THR:O	1:B:428:ASN:C	2.60	0.42
1:C:94:LYS:HE3	1:C:94:LYS:CA	2.37	0.42
1:C:108:SER:C	1:C:110:GLN:N	2.76	0.42
1:C:323:ARG:O	1:C:361:HIS:CB	2.68	0.42
1:D:56:ARG:NH2	1:D:342:GLY:O	2.52	0.42
1:A:57:LEU:O	1:A:58:ILE:C	2.62	0.42
1:C:24:LYS:HA	1:C:435:GLU:CG	2.49	0.42
1:C:68:ASP:O	1:C:333:LEU:HA	2.19	0.42
1:C:158:PHE:C	1:C:160:TYR:H	2.27	0.42
1:C:381:ASN:O	1:C:382:PRO:C	2.62	0.42
1:D:241:LYS:HG2	1:D:246:GLY:O	2.19	0.42
1:D:286:VAL:HG13	1:D:313:TYR:OH	2.19	0.42
1:B:262:LEU:HD23	1:B:262:LEU:HA	1.46	0.42
1:B:328:ALA:O	1:B:357:ILE:HD12	2.19	0.42
1:C:158:PHE:O	1:C:159:ASN:C	2.61	0.42
1:C:234:LEU:O	1:C:237:MET:HB2	2.19	0.42
1:D:77:PHE:CE2	1:D:187:LYS:HB3	2.54	0.42
1:D:118:MET:HE3	1:D:156:CYS:HA	2.01	0.42
1:A:336:LYS:HA	1:A:336:LYS:HD2	1.79	0.42
1:A:360:LEU:O	1:A:360:LEU:HG	2.16	0.42
1:A:387:GLN:NE2	1:A:387:GLN:HA	2.33	0.42
1:A:402:GLY:O	1:A:403:GLN:C	2.61	0.42
1:B:116:HIS:CD2	1:B:305:TYR:HA	2.55	0.42
1:B:332:SER:HB2	1:B:354:MET:HE2	2.00	0.42
1:B:362:ARG:O	1:B:363:ASP:C	2.62	0.42
1:C:17:LEU:N	1:C:18:PRO:CD	2.82	0.42
1:C:90:TRP:H	1:C:90:TRP:CD1	2.38	0.42
1:C:296:ARG:CG	1:C:297:VAL:N	2.82	0.42
1:C:327:THR:C	1:C:329:PRO:HD3	2.45	0.42
1:D:13:GLU:HG3	1:D:14:LEU:HD22	2.01	0.42
1:C:24:LYS:N	1:C:25:PRO:CD	2.82	0.42
1:C:118:MET:C	1:C:120:VAL:N	2.77	0.42
1:C:154:GLY:C	1:C:160:TYR:O	2.63	0.42
1:C:188:LEU:HD13	3:C:3465:PAM:O2	2.18	0.42
1:C:289:LYS:HE3	1:C:313:TYR:CZ	2.54	0.42
1:D:323:ARG:O	1:D:361:HIS:ND1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ARG:HG2	1:A:165:PHE:CD1	2.54	0.42
1:A:192:ASN:HA	1:A:193:PRO:HD2	1.84	0.42
1:A:195:ASP:OD1	1:A:196:PRO:HD2	2.20	0.42
1:A:320:GLU:C	1:A:323:ARG:H	2.26	0.42
1:A:401:ILE:HG12	1:A:401:ILE:H	1.45	0.42
1:D:86:LEU:CD1	1:D:99:ALA:CB	2.94	0.42
1:D:115:TYR:O	1:D:117:ALA:N	2.53	0.42
1:D:141:VAL:CB	1:D:142:PRO:CD	2.97	0.42
1:D:174:ILE:O	1:D:177:MET:N	2.50	0.42
1:D:314:VAL:HG21	1:D:411:THR:HG23	2.00	0.42
2:D:472:HEM:HBC2	2:D:472:HEM:HMC3	1.97	0.42
1:A:119:MET:O	1:A:120:VAL:C	2.61	0.42
1:B:2:ILE:HG12	1:B:346:PRO:HG3	2.00	0.42
1:B:3:LYS:HB3	1:B:3:LYS:HE3	1.59	0.42
1:B:153:ILE:HD12	1:B:153:ILE:HA	1.87	0.42
1:C:24:LYS:HA	1:C:435:GLU:CD	2.45	0.42
1:A:177:MET:CB	1:A:212:MET:CE	2.98	0.42
1:A:323:ARG:HG2	1:A:361:HIS:HB3	2.01	0.42
1:B:174:ILE:HD12	1:B:174:ILE:HG23	1.74	0.42
1:C:40:PHE:CZ	1:C:51:TYR:CB	3.03	0.42
1:C:129:LYS:O	1:C:132:ARG:N	2.46	0.42
1:C:188:LEU:CD1	3:C:3465:PAM:O2	2.68	0.42
1:D:97:LYS:O	1:D:98:LYS:C	2.62	0.42
1:D:232:ASP:C	1:D:234:LEU:N	2.75	0.42
1:D:301:PRO:HB3	1:D:455:LEU:HA	2.00	0.42
1:D:311:LEU:HD23	1:D:311:LEU:HA	1.72	0.42
1:D:316:MET:HB3	1:D:376:PRO:HB3	2.01	0.42
1:D:407:LEU:O	1:D:408:HIS:C	2.62	0.42
1:A:264:GLU:HG3	2:A:472:HEM:C4C	2.55	0.42
1:B:178:VAL:HG23	1:B:179:ARG:N	2.35	0.42
1:B:306:LYS:HB2	1:B:306:LYS:HE2	1.99	0.42
1:C:15:LYS:CB	1:C:43:GLU:O	2.68	0.42
1:C:322:LEU:HA	1:C:322:LEU:HD12	1.84	0.42
1:D:122:ILE:HG22	1:D:148:LEU:CD1	2.32	0.42
1:D:145:MET:C	1:D:147:ARG:N	2.76	0.42
1:D:322:LEU:HD12	1:D:322:LEU:HA	1.74	0.42
1:A:55:GLN:O	1:A:59:LYS:HG2	2.20	0.41
1:B:7:GLN:HB2	1:B:8:PRO:CD	2.45	0.41
1:B:320:GLU:O	1:B:321:ALA:C	2.62	0.41
1:C:273:LEU:HD23	1:C:273:LEU:HA	1.90	0.41
1:B:337:GLU:O	1:B:339:THR:HG22	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:LEU:HD11	1:C:261:PHE:CE2	2.56	0.41
1:D:73:GLN:HA	1:D:73:GLN:NE2	2.35	0.41
1:D:216:VAL:HG13	1:D:258:ILE:HD13	2.02	0.41
1:A:58:ILE:O	1:A:61:ALA:N	2.53	0.41
1:B:323:ARG:HA	1:B:361:HIS:HD1	1.85	0.41
1:B:390:PHE:C	1:B:392:PRO:HD2	2.45	0.41
1:C:1:THR:CG2	1:C:2:ILE:H	2.33	0.41
1:C:210:LYS:O	1:C:214:ASP:CG	2.63	0.41
1:C:223:ARG:HH21	1:C:234:LEU:CB	2.32	0.41
1:C:294:ALA:O	1:C:298:LEU:HD12	2.20	0.41
1:C:299:VAL:H	1:C:299:VAL:HG22	1.39	0.41
1:C:397:GLN:HG3	1:C:398:ARG:H	1.83	0.41
1:D:94:LYS:O	1:D:94:LYS:HG3	2.19	0.41
1:D:215:LEU:HD12	1:D:215:LEU:HA	1.84	0.41
1:A:62:CYS:SG	1:A:391:LYS:CD	3.09	0.41
1:A:279:PHE:O	1:A:283:ASN:ND2	2.50	0.41
1:A:318:LEU:HD13	1:A:414:LEU:HD12	2.01	0.41
1:C:18:PRO:C	1:C:20:LEU:N	2.78	0.41
1:C:150:LEU:HD21	1:C:162:PHE:CD1	2.55	0.41
1:D:29:LEU:O	1:D:30:MET:O	2.38	0.41
1:D:33:ALA:HB2	1:D:40:PHE:HE1	1.86	0.41
1:B:17:LEU:HD12	1:B:17:LEU:HA	1.90	0.41
1:B:354:MET:HE2	1:B:354:MET:HB2	1.88	0.41
1:C:147:ARG:HG2	1:C:165:PHE:CE1	2.55	0.41
1:D:26:VAL:HG12	1:D:27:GLN:N	2.35	0.41
1:D:30:MET:HE3	1:D:30:MET:HB3	1.89	0.41
1:D:33:ALA:HB3	1:D:359:GLN:HE21	1.85	0.41
1:D:47:ARG:C	1:D:48:VAL:HG12	2.45	0.41
1:D:345:TYR:HA	1:D:346:PRO:HD3	1.78	0.41
1:D:381:ASN:HD22	1:D:384:ALA:HB2	1.84	0.41
1:B:12:GLY:C	1:B:14:LEU:H	2.28	0.41
1:B:264:GLU:CG	2:B:472:HEM:C1D	3.04	0.41
1:B:319:ASN:O	1:B:379:PHE:CE1	2.74	0.41
1:B:401:ILE:HG12	1:B:401:ILE:H	1.79	0.41
1:C:29:LEU:HD23	1:C:29:LEU:HA	1.95	0.41
1:C:58:ILE:HD13	1:C:355:VAL:HG13	2.02	0.41
1:C:124:VAL:HG12	1:C:128:GLN:CG	2.40	0.41
1:C:278:TYR:CD2	1:C:278:TYR:C	2.99	0.41
2:C:472:HEM:HBC2	2:C:472:HEM:CMC	2.40	0.41
1:D:16:ASN:C	1:D:42:PHE:CZ	2.99	0.41
1:D:177:MET:HB2	1:D:212:MET:CE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:TYR:HA	1:A:118:MET:HE3	2.03	0.41
1:B:47:ARG:HH11	1:B:47:ARG:HD2	1.65	0.41
1:B:151:ASP:OD1	1:B:162:PHE:HB2	2.21	0.41
1:B:318:LEU:O	1:B:322:LEU:HB2	2.19	0.41
1:C:17:LEU:HD22	1:C:45:PRO:CD	2.50	0.41
1:D:152:THR:O	1:D:153:ILE:C	2.63	0.41
1:D:400:CYS:C	1:D:402:GLY:N	2.78	0.41
1:A:58:ILE:HD13	1:A:58:ILE:HA	1.82	0.41
1:A:401:ILE:CG1	2:A:472:HEM:HBD1	2.51	0.41
2:A:472:HEM:CMC	2:A:472:HEM:CBC	2.97	0.41
1:B:126:LEU:HD21	1:B:130:TRP:CE2	2.56	0.41
1:B:195:ASP:C	1:B:197:ALA:N	2.74	0.41
1:B:275:PHE:CZ	1:B:441:PRO:HD3	2.55	0.41
1:B:323:ARG:HD3	1:B:367:TRP:CZ3	2.56	0.41
1:C:313:TYR:O	1:C:314:VAL:C	2.64	0.41
1:C:418:LEU:HD23	1:C:418:LEU:HA	1.43	0.41
1:D:316:MET:HG2	1:D:379:PHE:O	2.21	0.41
1:D:422:ASP:OD1	1:D:451:LYS:HE2	2.20	0.41
1:B:12:GLY:C	1:B:14:LEU:N	2.78	0.41
1:B:115:TYR:HA	1:B:118:MET:HE2	2.00	0.41
1:B:122:ILE:C	1:B:124:VAL:H	2.28	0.41
1:B:128:GLN:O	1:B:132:ARG:HG2	2.20	0.41
1:B:223:ARG:O	1:B:224:LYS:C	2.64	0.41
1:B:253:ASN:O	1:B:254:ILE:C	2.61	0.41
1:B:272:LEU:N	1:B:327:THR:HG21	2.36	0.41
1:C:17:LEU:N	1:C:18:PRO:HD2	2.35	0.41
1:C:216:VAL:O	1:C:218:LYS:N	2.54	0.41
1:A:259:ILE:O	1:A:260:THR:C	2.63	0.41
1:B:421:PHE:HA	1:B:449:LYS:O	2.21	0.41
1:C:112:MET:HE2	1:C:115:TYR:CD2	2.56	0.41
1:D:71:LEU:C	1:D:72:SER:O	2.64	0.41
1:A:64:GLU:OE2	1:A:396:GLY:HA3	2.21	0.40
1:A:66:ARG:O	1:A:336:LYS:HB2	2.21	0.40
1:A:165:PHE:C	1:A:167:ARG:H	2.30	0.40
1:B:255:ARG:HD2	1:B:256:TYR:N	2.36	0.40
1:B:314:VAL:CG2	1:B:411:THR:HG23	2.51	0.40
1:B:402:GLY:O	1:B:405:PHE:HB3	2.21	0.40
1:C:47:ARG:NH1	1:C:49:THR:HG21	2.36	0.40
1:D:26:VAL:O	1:D:27:GLN:C	2.64	0.40
1:D:289:LYS:HE3	1:D:313:TYR:OH	2.21	0.40
1:A:55:GLN:OE1	1:A:56:ARG:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LEU:HD11	1:A:99:ALA:HB3	2.03	0.40
1:A:257:GLN:H	1:A:257:GLN:HG2	1.79	0.40
1:B:113:LYS:HA	1:B:305:TYR:CD2	2.57	0.40
1:C:147:ARG:CG	1:C:164:SER:HB3	2.42	0.40
1:D:281:VAL:CG1	1:D:425:ASP:HB2	2.51	0.40
1:A:171:HIS:O	1:A:172:PRO:C	2.62	0.40
1:A:218:LYS:HE2	1:A:218:LYS:N	2.35	0.40
1:B:174:ILE:O	1:B:175:THR:C	2.62	0.40
1:B:316:MET:HE3	1:B:316:MET:HB2	1.82	0.40
1:C:1:THR:CG2	1:C:2:ILE:N	2.84	0.40
1:D:193:PRO:O	1:D:198:TYR:HD2	2.03	0.40
1:D:242:ASP:N	1:D:247:GLU:O	2.53	0.40
1:D:256:TYR:O	1:D:257:GLN:C	2.59	0.40
1:A:418:LEU:HD22	1:A:418:LEU:HA	1.61	0.40
1:A:444:PHE:C	1:A:444:PHE:CD1	2.98	0.40
1:B:62:CYS:SG	1:B:391:LYS:NZ	2.92	0.40
1:C:130:TRP:O	1:C:131:GLU:C	2.60	0.40
1:C:348:GLU:O	1:C:349:LYS:C	2.64	0.40
1:A:10:THR:C	1:A:11:PHE:CD1	3.00	0.40
1:B:126:LEU:O	1:B:128:GLN:N	2.55	0.40
1:B:416:MET:HE1	1:B:455:LEU:HD12	2.03	0.40
1:C:21:ASN:HA	1:C:189:GLN:CD	2.40	0.40
1:C:158:PHE:O	1:C:160:TYR:N	2.53	0.40
1:C:212:MET:O	1:C:213:ASN:C	2.65	0.40
1:C:340:VAL:HG12	1:C:343:GLY:HA2	2.03	0.40
1:C:393:PHE:CE1	1:C:403:GLN:HA	2.57	0.40
1:D:2:ILE:HA	1:D:344:GLU:O	2.22	0.40
1:D:13:GLU:HG3	1:D:14:LEU:N	2.36	0.40
1:D:51:TYR:CD2	1:D:354:MET:HB3	2.57	0.40
1:D:245:THR:C	1:D:247:GLU:H	2.29	0.40
1:D:377:GLU:O	1:D:379:PHE:N	2.53	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ASP:OD2	1:C:23:ASP:OD2[2_664]	1.70	0.50
1:A:207:GLU:OE2	1:B:207:GLU:OE2[6_664]	2.04	0.16

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	453/471 (96%)	358 (79%)	66 (15%)	29 (6%)	1	1
1	B	453/471 (96%)	326 (72%)	89 (20%)	38 (8%)	0	0
1	C	453/471 (96%)	307 (68%)	102 (22%)	44 (10%)	0	0
1	D	452/471 (96%)	351 (78%)	72 (16%)	29 (6%)	1	1
All	All	1811/1884 (96%)	1342 (74%)	329 (18%)	140 (8%)	1	1

All (140) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	342	GLY
1	A	365	THR
1	A	377	GLU
1	A	425	ASP
1	A	452	LYS
1	B	13	GLU
1	B	62	CYS
1	B	141	VAL
1	B	240	GLY
1	B	264	GLU
1	B	317	VAL
1	B	322	LEU
1	B	391	LYS
1	B	425	ASP
1	C	19	LEU
1	C	116	HIS
1	C	126	LEU
1	C	127	VAL
1	C	165	PHE
1	C	338	ASP
1	C	377	GLU
1	C	452	LYS

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Mol	Chain	Res	Type
1	D	12	GLY
1	D	13	GLU
1	D	27	GLN
1	D	38	GLU
1	D	116	HIS
1	D	193	PRO
1	D	194	ASP
1	D	338	ASP
1	D	378	ARG
1	D	383	SER
1	D	403	GLN
1	D	437	LEU
1	A	58	ILE
1	A	83	GLY
1	A	93	GLU
1	A	254	ILE
1	A	293	GLU
1	A	311	LEU
1	A	378	ARG
1	A	396	GLY
1	B	85	GLY
1	B	126	LEU
1	B	127	VAL
1	B	251	ASP
1	B	305	TYR
1	B	321	ALA
1	B	327	THR
1	B	340	VAL
1	B	361	HIS
1	B	369	ASP
1	B	371	VAL
1	B	377	GLU
1	B	426	HIS
1	B	429	TYR
1	C	9	LYS
1	C	15	LYS
1	C	73	GLN
1	C	79	ARG
1	C	119	MET
1	C	154	GLY
1	C	217	ASP
1	C	256	TYR

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Mol	Chain	Res	Type
1	C	263	ILE
1	C	264	GLU
1	D	8	PRO
1	D	26	VAL
1	D	64	GLU
1	D	74	ALA
1	A	34	ASP
1	A	100	HIS
1	A	366	ILE
1	A	403	GLN
1	B	47	ARG
1	B	155	LEU
1	B	193	PRO
1	B	263	ILE
1	C	80	ASP
1	C	109	GLN
1	C	155	LEU
1	C	159	ASN
1	C	287	LEU
1	C	372	GLU
1	C	451	LYS
1	D	158	PHE
1	D	356	LEU
1	D	382	PRO
1	A	227	GLY
1	A	237	MET
1	A	238	LEU
1	A	412	LEU
1	A	437	LEU
1	B	96	TRP
1	B	123	ALA
1	B	409	GLU
1	C	77	PHE
1	C	136	ASP
1	C	188	LEU
1	C	339	THR
1	C	369	ASP
1	D	96	TRP
1	D	410	ALA
1	D	438	THR
1	A	62	CYS
1	A	105	PRO

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Mol	Chain	Res	Type
1	A	123	ALA
1	B	403	GLN
1	B	408	HIS
1	B	437	LEU
1	C	146	THR
1	C	156	CYS
1	C	191	ALA
1	C	196	PRO
1	C	224	LYS
1	C	259	ILE
1	C	281	VAL
1	C	288	GLN
1	C	425	ASP
1	D	289	LYS
1	D	293	GLU
1	A	248	PRO
1	A	305	TYR
1	A	418	LEU
1	B	119	MET
1	B	252	GLU
1	C	151	ASP
1	C	365	THR
1	C	391	LYS
1	D	228	GLU
1	D	248	PRO
1	B	243	PRO
1	B	326	PRO
1	C	12	GLY
1	C	317	VAL
1	B	48	VAL
1	D	216	VAL
1	A	8	PRO
1	D	153	ILE
1	D	196	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	397/413 (96%)	318 (80%)	79 (20%)	1	2
1	B	399/413 (97%)	304 (76%)	95 (24%)	1	1
1	C	399/413 (97%)	312 (78%)	87 (22%)	1	1
1	D	399/413 (97%)	310 (78%)	89 (22%)	1	1
All	All	1594/1652 (96%)	1244 (78%)	350 (22%)	1	1

All (350) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	5	MET
1	A	7	GLN
1	A	9	LYS
1	A	11	PHE
1	A	13	GLU
1	A	14	LEU
1	A	21	ASN
1	A	38	GLU
1	A	39	ILE
1	A	48	VAL
1	A	49	THR
1	A	53	SER
1	A	57	LEU
1	A	69	LYS
1	A	70	ASN
1	A	71	LEU
1	A	86	LEU
1	A	97	LYS
1	A	103	LEU
1	A	106	SER
1	A	112	MET
1	A	126	LEU
1	A	128	GLN
1	A	133	LEU
1	A	134	ASN
1	A	136	ASP
1	A	139	ILE
1	A	143	GLU
1	A	145	MET
1	A	148	LEU
1	A	149	THR
1	A	172	PRO

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Mol	Chain	Res	Type
1	A	200	GLU
1	A	201	ASN
1	A	209	ILE
1	A	215	LEU
1	A	218	LYS
1	A	222	ASP
1	A	224	LYS
1	A	226	SER
1	A	230	SER
1	A	247	GLU
1	A	248	PRO
1	A	254	ILE
1	A	255	ARG
1	A	260	THR
1	A	266	HIS
1	A	281	VAL
1	A	282	LYS
1	A	283	ASN
1	A	287	LEU
1	A	293	GLU
1	A	296	ARG
1	A	312	LYS
1	A	314	VAL
1	A	318	LEU
1	A	320	GLU
1	A	322	LEU
1	A	324	LEU
1	A	336	LYS
1	A	338	ASP
1	A	340	VAL
1	A	364	LYS
1	A	365	THR
1	A	366	ILE
1	A	378	ARG
1	A	385	ILE
1	A	387	GLN
1	A	391	LYS
1	A	401	ILE
1	A	407	LEU
1	A	414	LEU
1	A	416	MET
1	A	418	LEU

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Mol	Chain	Res	Type
1	A	419	LYS
1	A	445	VAL
1	A	447	LYS
1	A	455	LEU
1	B	1	THR
1	B	4	GLU
1	B	9	LYS
1	B	11	PHE
1	B	13	GLU
1	B	14	LEU
1	B	22	THR
1	B	32	ILE
1	B	35	GLU
1	B	38	GLU
1	B	39	ILE
1	B	41	LYS
1	B	48	VAL
1	B	52	LEU
1	B	53	SER
1	B	56	ARG
1	B	57	LEU
1	B	62	CYS
1	B	64	GLU
1	B	76	LYS
1	B	78	VAL
1	B	79	ARG
1	B	86	LEU
1	B	88	THR
1	B	97	LYS
1	B	102	ILE
1	B	103	LEU
1	B	106	SER
1	B	109	GLN
1	B	112	MET
1	B	121	ASP
1	B	126	LEU
1	B	128	GLN
1	B	129	LYS
1	B	133	LEU
1	B	134	ASN
1	B	136	ASP
1	B	139	ILE

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Mol	Chain	Res	Type
1	B	148	LEU
1	B	153	ILE
1	B	155	LEU
1	B	189	GLN
1	B	200	GLU
1	B	201	ASN
1	B	210	LYS
1	B	218	LYS
1	B	224	LYS
1	B	230	SER
1	B	233	LEU
1	B	235	THR
1	B	244	GLU
1	B	250	ASP
1	B	254	ILE
1	B	255	ARG
1	B	258	ILE
1	B	259	ILE
1	B	260	THR
1	B	268	THR
1	B	274	SER
1	B	278	TYR
1	B	280	LEU
1	B	282	LYS
1	B	283	ASN
1	B	287	LEU
1	B	293	GLU
1	B	299	VAL
1	B	302	VAL
1	B	306	LYS
1	B	309	LYS
1	B	312	LYS
1	B	314	VAL
1	B	318	LEU
1	B	320	GLU
1	B	322	LEU
1	B	323	ARG
1	B	324	LEU
1	B	339	THR
1	B	352	GLU
1	B	355	VAL
1	B	356	LEU

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Mol	Chain	Res	Type
1	B	364	LYS
1	B	366	ILE
1	B	371	VAL
1	B	383	SER
1	B	391	LYS
1	B	401	ILE
1	B	403	GLN
1	B	404	GLN
1	B	407	LEU
1	B	412	LEU
1	B	414	LEU
1	B	416	MET
1	B	422	ASP
1	B	447	LYS
1	B	450	SER
1	C	2	ILE
1	C	13	GLU
1	C	14	LEU
1	C	32	ILE
1	C	38	GLU
1	C	39	ILE
1	C	43	GLU
1	C	56	ARG
1	C	57	LEU
1	C	58	ILE
1	C	64	GLU
1	C	65	SER
1	C	71	LEU
1	C	78	VAL
1	C	79	ARG
1	C	86	LEU
1	C	88	THR
1	C	89	SER
1	C	94	LYS
1	C	97	LYS
1	C	100	HIS
1	C	103	LEU
1	C	125	GLN
1	C	126	LEU
1	C	133	LEU
1	C	134	ASN
1	C	139	ILE

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Mol	Chain	Res	Type
1	C	145	MET
1	C	147	ARG
1	C	148	LEU
1	C	167	ARG
1	C	172	PRO
1	C	176	SER
1	C	177	MET
1	C	181	LEU
1	C	192	ASN
1	C	194	ASP
1	C	201	ASN
1	C	218	LYS
1	C	219	ILE
1	C	224	LYS
1	C	230	SER
1	C	231	ASP
1	C	235	THR
1	C	238	LEU
1	C	252	GLU
1	C	259	ILE
1	C	260	THR
1	C	266	HIS
1	C	268	THR
1	C	283	ASN
1	C	287	LEU
1	C	289	LYS
1	C	293	GLU
1	C	296	ARG
1	C	298	LEU
1	C	299	VAL
1	C	306	LYS
1	C	310	GLN
1	C	312	LYS
1	C	316	MET
1	C	317	VAL
1	C	318	LEU
1	C	320	GLU
1	C	324	LEU
1	C	333	LEU
1	C	336	LYS
1	C	337	GLU
1	C	344	GLU

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Mol	Chain	Res	Type
1	C	349	LYS
1	C	364	LYS
1	C	365	THR
1	C	366	ILE
1	C	371	VAL
1	C	378	ARG
1	C	387	GLN
1	C	391	LYS
1	C	398	ARG
1	C	403	GLN
1	C	407	LEU
1	C	413	VAL
1	C	414	LEU
1	C	430	GLU
1	C	433	ILE
1	C	438	THR
1	C	447	LYS
1	C	455	LEU
1	D	3	LYS
1	D	7	GLN
1	D	14	LEU
1	D	17	LEU
1	D	30	MET
1	D	31	LYS
1	D	39	ILE
1	D	48	VAL
1	D	56	ARG
1	D	57	LEU
1	D	64	GLU
1	D	65	SER
1	D	71	LEU
1	D	72	SER
1	D	73	GLN
1	D	88	THR
1	D	94	LYS
1	D	97	LYS
1	D	103	LEU
1	D	121	ASP
1	D	122	ILE
1	D	124	VAL
1	D	126	LEU
1	D	127	VAL

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Mol	Chain	Res	Type
1	D	128	GLN
1	D	133	LEU
1	D	134	ASN
1	D	136	ASP
1	D	137	GLU
1	D	139	ILE
1	D	141	VAL
1	D	153	ILE
1	D	178	VAL
1	D	179	ARG
1	D	195	ASP
1	D	196	PRO
1	D	200	GLU
1	D	201	ASN
1	D	209	ILE
1	D	210	LYS
1	D	218	LYS
1	D	226	SER
1	D	228	GLU
1	D	230	SER
1	D	233	LEU
1	D	235	THR
1	D	255	ARG
1	D	260	THR
1	D	266	HIS
1	D	281	VAL
1	D	286	VAL
1	D	287	LEU
1	D	293	GLU
1	D	299	VAL
1	D	310	GLN
1	D	314	VAL
1	D	317	VAL
1	D	318	LEU
1	D	320	GLU
1	D	322	LEU
1	D	324	LEU
1	D	332	SER
1	D	333	LEU
1	D	336	LYS
1	D	344	GLU
1	D	349	LYS

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Mol	Chain	Res	Type
1	D	352	GLU
1	D	360	LEU
1	D	364	LYS
1	D	365	THR
1	D	370	ASP
1	D	371	VAL
1	D	383	SER
1	D	385	ILE
1	D	391	LYS
1	D	392	PRO
1	D	397	GLN
1	D	398	ARG
1	D	403	GLN
1	D	407	LEU
1	D	413	VAL
1	D	414	LEU
1	D	419	LYS
1	D	420	HIS
1	D	427	THR
1	D	430	GLU
1	D	438	THR
1	D	440	LYS
1	D	452	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	27	GLN
1	A	73	GLN
1	A	95	ASN
1	A	100	HIS
1	A	101	ASN
1	A	116	HIS
1	A	134	ASN
1	A	138	HIS
1	A	171	HIS
1	A	189	GLN
1	A	201	ASN
1	A	236	HIS
1	A	239	ASN
1	A	307	GLN

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Mol	Chain	Res	Type
1	A	359	GLN
1	A	387	GLN
1	A	388	HIS
1	A	403	GLN
1	A	404	GLN
1	A	426	HIS
1	B	7	GLN
1	B	70	ASN
1	B	92	HIS
1	B	116	HIS
1	B	159	ASN
1	B	171	HIS
1	B	192	ASN
1	B	201	ASN
1	B	239	ASN
1	B	266	HIS
1	B	283	ASN
1	B	310	GLN
1	B	388	HIS
1	B	395	ASN
1	B	403	GLN
1	B	420	HIS
1	B	426	HIS
1	B	428	ASN
1	C	7	GLN
1	C	21	ASN
1	C	100	HIS
1	C	116	HIS
1	C	128	GLN
1	C	134	ASN
1	C	171	HIS
1	C	201	ASN
1	C	204	GLN
1	C	236	HIS
1	C	239	ASN
1	C	388	HIS
1	C	403	GLN
1	D	73	GLN
1	D	100	HIS
1	D	110	GLN
1	D	116	HIS
1	D	138	HIS

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Mol	Chain	Res	Type
1	D	169	GLN
1	D	171	HIS
1	D	201	ASN
1	D	204	GLN
1	D	239	ASN
1	D	307	GLN
1	D	388	HIS
1	D	397	GLN
1	D	403	GLN
1	D	404	GLN
1	D	420	HIS
1	D	426	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PAM	C	3465	-	17,17,17	1.32	1 (5%)	17,17,17	1.34	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	A	472	1	50,50,50	1.88	14 (28%)	67,82,82	2.22	25 (37%)
2	HEM	C	472	1	50,50,50	2.06	18 (36%)	67,82,82	2.79	30 (44%)
2	HEM	D	472	1	50,50,50	2.10	15 (30%)	67,82,82	2.04	23 (34%)
3	PAM	A	1465	-	17,17,17	1.23	2 (11%)	17,17,17	1.23	1 (5%)
2	HEM	B	472	1	50,50,50	2.41	21 (42%)	67,82,82	2.09	21 (31%)
3	PAM	B	2465	-	17,17,17	1.29	2 (11%)	17,17,17	1.38	2 (11%)
3	PAM	D	4465	-	17,17,17	1.22	1 (5%)	17,17,17	1.36	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PAM	C	3465	-	-	6/15/15/15	-
2	HEM	A	472	1	-	3/14/54/54	-
2	HEM	C	472	1	-	4/14/54/54	-
2	HEM	D	472	1	-	4/14/54/54	-
3	PAM	A	1465	-	-	5/15/15/15	-
2	HEM	B	472	1	-	3/14/54/54	-
3	PAM	B	2465	-	-	12/15/15/15	-
3	PAM	D	4465	-	-	10/15/15/15	-

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	472	HEM	FE-ND	6.54	2.15	1.94
2	C	472	HEM	C3D-C2D	6.41	1.50	1.36
2	B	472	HEM	CHA-C1A	-5.84	1.26	1.39
2	D	472	HEM	C3D-C2D	5.76	1.49	1.36
2	C	472	HEM	FE-NB	5.59	2.12	1.94
2	D	472	HEM	FE-ND	5.36	2.11	1.94
2	B	472	HEM	C4D-ND	-5.36	1.31	1.40
2	A	472	HEM	C3D-C2D	4.65	1.46	1.36
2	D	472	HEM	FE-NA	4.64	2.10	1.95
2	A	472	HEM	FE-NA	-4.38	1.80	1.95
2	D	472	HEM	FE-NC	4.31	2.09	1.95
2	B	472	HEM	CHA-C4D	-4.28	1.29	1.38
2	B	472	HEM	C3D-C2D	4.26	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3465	PAM	C10-C9	4.21	1.55	1.31
3	D	4465	PAM	C10-C9	4.15	1.55	1.31
2	C	472	HEM	CMB-C2B	4.12	1.59	1.50
2	B	472	HEM	FE-NC	-4.09	1.81	1.95
2	D	472	HEM	FE-NB	-4.09	1.82	1.94
2	B	472	HEM	C3B-C2B	-4.05	1.28	1.37
3	B	2465	PAM	C10-C9	3.97	1.54	1.31
2	B	472	HEM	C1C-NC	-3.94	1.32	1.39
3	A	1465	PAM	C10-C9	3.86	1.53	1.31
2	B	472	HEM	CMA-C3A	3.81	1.58	1.50
2	B	472	HEM	CHB-C1B	-3.72	1.31	1.38
2	D	472	HEM	CMB-C2B	3.48	1.57	1.50
2	D	472	HEM	CHD-C4C	-3.48	1.31	1.38
2	B	472	HEM	CHB-C4A	-3.44	1.31	1.39
2	C	472	HEM	FE-NA	-3.43	1.83	1.95
2	D	472	HEM	CAA-C2A	3.38	1.60	1.51
2	A	472	HEM	C1D-ND	-3.28	1.32	1.38
2	B	472	HEM	C3B-C4B	3.20	1.51	1.44
2	B	472	HEM	FE-ND	3.13	2.04	1.94
2	B	472	HEM	C1A-NA	-2.94	1.34	1.39
2	D	472	HEM	C4C-NC	-2.88	1.34	1.39
2	A	472	HEM	CHD-C4C	-2.78	1.32	1.38
2	C	472	HEM	CHB-C1B	-2.76	1.33	1.38
2	C	472	HEM	CAC-C3C	2.71	1.54	1.47
2	C	472	HEM	CAB-C3B	2.68	1.54	1.47
2	C	472	HEM	CMA-C3A	2.65	1.56	1.50
2	C	472	HEM	C4A-C3A	2.64	1.49	1.43
2	A	472	HEM	CAB-C3B	2.53	1.54	1.47
2	D	472	HEM	CMA-C3A	2.51	1.55	1.50
2	C	472	HEM	C1B-NB	-2.50	1.35	1.40
2	B	472	HEM	O1D-CGD	2.48	1.30	1.22
2	A	472	HEM	CMA-C3A	2.46	1.55	1.50
2	B	472	HEM	C1B-C2B	2.37	1.49	1.44
2	C	472	HEM	C1C-C2C	-2.37	1.40	1.45
2	B	472	HEM	CAC-C3C	2.36	1.53	1.47
2	C	472	HEM	C3C-C4C	-2.36	1.41	1.46
2	B	472	HEM	C4A-C3A	2.35	1.48	1.43
3	B	2465	PAM	O2-C1	2.34	1.29	1.22
2	D	472	HEM	C3C-C4C	-2.33	1.41	1.46
2	A	472	HEM	C4D-ND	-2.33	1.36	1.40
2	B	472	HEM	C3C-C2C	-2.33	1.32	1.37
2	C	472	HEM	FE-ND	-2.31	1.87	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	472	HEM	FE-NB	-2.31	1.87	1.94
2	C	472	HEM	FE-NC	-2.30	1.87	1.95
2	C	472	HEM	C4A-NA	-2.30	1.35	1.39
2	A	472	HEM	CHC-C1C	-2.24	1.33	1.38
2	C	472	HEM	CHB-C4A	-2.24	1.34	1.39
2	D	472	HEM	CAD-C3D	2.22	1.57	1.51
2	D	472	HEM	C1A-NA	-2.21	1.35	1.39
3	A	1465	PAM	O2-C1	2.17	1.29	1.22
2	D	472	HEM	C3C-C2C	-2.17	1.32	1.37
2	C	472	HEM	O1D-CGD	2.14	1.29	1.22
2	D	472	HEM	O1D-CGD	2.10	1.29	1.22
2	A	472	HEM	CMB-C2B	2.09	1.55	1.50
2	C	472	HEM	CHC-C1C	-2.08	1.34	1.38
2	A	472	HEM	FE-NB	2.07	2.01	1.94
2	A	472	HEM	CMD-C2D	2.07	1.55	1.50
2	B	472	HEM	CMB-C2B	2.05	1.55	1.50
2	A	472	HEM	C4A-C3A	2.05	1.47	1.43
2	A	472	HEM	CAC-C3C	2.05	1.52	1.47
2	B	472	HEM	C1C-C2C	2.01	1.49	1.45

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	472	HEM	CHD-C4C-NC	8.24	133.43	124.45
2	C	472	HEM	CHC-C1C-NC	7.49	132.60	124.45
2	A	472	HEM	CMD-C2D-C1D	6.40	135.03	125.03
2	D	472	HEM	C3B-C4B-NB	-6.08	105.10	109.47
2	C	472	HEM	C1C-CHC-C4B	-5.97	113.32	126.02
2	C	472	HEM	CHD-C4C-C3C	-5.72	115.57	125.21
2	B	472	HEM	C2A-C1A-NA	5.58	116.34	110.15
2	C	472	HEM	CAD-CBD-CGD	-5.13	100.06	113.67
2	D	472	HEM	C4B-C3B-C2B	5.12	111.99	107.28
2	C	472	HEM	C4D-ND-C1D	4.96	111.09	105.21
2	A	472	HEM	CAA-CBA-CGA	-4.76	101.05	113.67
2	C	472	HEM	CAA-CBA-CGA	-4.68	101.26	113.67
2	B	472	HEM	C3D-C4D-ND	4.64	115.26	110.17
2	B	472	HEM	CMD-C2D-C1D	4.51	132.08	125.03
2	A	472	HEM	CHD-C1D-ND	-4.50	119.58	124.42
2	C	472	HEM	CBD-CAD-C3D	-4.49	100.13	112.53
2	A	472	HEM	CAD-CBD-CGD	-4.33	102.17	113.67
2	C	472	HEM	CHC-C1C-C2C	-4.18	116.79	125.49
2	B	472	HEM	C4C-CHD-C1D	-4.03	117.45	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	472	HEM	CBB-CAB-C3B	-3.98	107.65	127.53
2	A	472	HEM	O1D-CGD-CBD	-3.96	110.52	123.09
2	A	472	HEM	CAD-C3D-C4D	3.94	131.56	124.70
2	C	472	HEM	CBB-CAB-C3B	-3.91	108.00	127.53
2	D	472	HEM	C3B-C2B-C1B	-3.89	103.49	106.41
2	B	472	HEM	CBA-CAA-C2A	-3.89	101.79	112.53
2	C	472	HEM	O2A-CGA-CBA	3.86	126.18	114.00
2	A	472	HEM	CMB-C2B-C1B	-3.82	119.06	125.03
2	B	472	HEM	CHA-C4D-C3D	-3.77	118.28	125.23
2	D	472	HEM	C4D-ND-C1D	3.71	109.61	105.21
2	C	472	HEM	CHA-C4D-ND	3.71	128.96	124.37
2	C	472	HEM	C2A-C1A-NA	3.65	114.21	110.15
2	A	472	HEM	O1A-CGA-CBA	-3.60	111.67	123.09
2	A	472	HEM	O2A-CGA-CBA	3.53	125.16	114.00
2	D	472	HEM	CMD-C2D-C1D	3.53	130.55	125.03
2	D	472	HEM	CHC-C4B-NB	3.51	128.20	124.42
2	B	472	HEM	CHB-C4A-C3A	-3.44	117.44	127.43
2	C	472	HEM	CMA-C3A-C4A	-3.37	120.29	125.42
2	D	472	HEM	CHA-C4D-ND	3.34	128.50	124.37
2	C	472	HEM	C4C-CHD-C1D	-3.32	118.96	126.02
2	A	472	HEM	C1D-C2D-C3D	-3.31	103.50	106.98
2	B	472	HEM	CHB-C4A-NA	3.28	129.81	123.86
2	B	472	HEM	C4A-NA-C1A	-3.27	100.49	105.82
2	C	472	HEM	CMB-C2B-C1B	-3.24	119.97	125.03
2	B	472	HEM	C4A-CHB-C1B	-3.24	118.64	126.25
2	C	472	HEM	CHB-C4A-NA	3.23	129.72	123.86
2	D	472	HEM	C1B-NB-C4B	3.23	109.03	105.21
2	B	472	HEM	CHD-C4C-NC	3.18	127.91	124.45
2	B	472	HEM	CHA-C1A-C2A	-3.13	118.44	125.30
2	D	472	HEM	CHD-C4C-NC	3.08	127.80	124.45
2	B	472	HEM	C4D-C3D-C2D	-3.06	102.43	106.89
2	A	472	HEM	C4D-ND-C1D	3.05	108.82	105.21
2	C	472	HEM	CHB-C1B-NB	3.03	128.12	124.37
2	A	472	HEM	CHD-C4C-NC	3.01	127.73	124.45
2	B	472	HEM	C2B-C1B-NB	3.01	113.30	109.84
2	D	472	HEM	CAD-C3D-C4D	2.98	129.90	124.70
2	B	472	HEM	CHC-C4B-NB	-2.96	121.23	124.42
2	A	472	HEM	CHA-C1A-NA	2.94	129.20	123.86
2	C	472	HEM	O1A-CGA-CBA	-2.93	113.81	123.09
2	D	472	HEM	CHB-C1B-NB	2.89	127.95	124.37
2	B	472	HEM	CAD-C3D-C4D	2.85	129.67	124.70
2	C	472	HEM	CBA-CAA-C2A	2.75	120.13	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	472	HEM	CMA-C3A-C4A	-2.71	121.29	125.42
2	B	472	HEM	CBD-CAD-C3D	-2.69	105.09	112.53
2	D	472	HEM	CAD-CBD-CGD	-2.66	106.61	113.67
2	D	472	HEM	C3C-C2C-C1C	-2.64	104.55	107.05
3	B	2465	PAM	O1-C1-C2	2.61	122.24	114.00
2	C	472	HEM	C1A-C2A-C3A	-2.61	102.83	106.87
2	D	472	HEM	CMA-C3A-C2A	2.61	131.15	125.62
2	A	472	HEM	CMB-C2B-C3B	2.58	134.68	128.43
2	B	472	HEM	CMA-C3A-C2A	2.58	131.09	125.62
2	A	472	HEM	C4C-CHD-C1D	2.56	131.46	126.02
2	C	472	HEM	O1D-CGD-CBD	-2.55	114.99	123.09
2	D	472	HEM	C4C-C3C-C2C	2.52	109.00	106.81
2	A	472	HEM	CHA-C1A-C2A	-2.52	119.78	125.30
3	D	4465	PAM	C3-C2-C1	-2.52	107.93	114.51
3	C	3465	PAM	O1-C1-O2	-2.52	116.86	123.33
2	C	472	HEM	O2D-CGD-O1D	2.49	129.75	123.33
3	C	3465	PAM	C11-C10-C9	-2.49	106.15	124.83
2	A	472	HEM	O2D-CGD-CBD	2.47	121.79	114.00
2	A	472	HEM	CHB-C4A-C3A	-2.46	120.28	127.43
3	C	3465	PAM	C7-C6-C5	-2.42	102.11	114.37
2	A	472	HEM	CAD-C3D-C2D	-2.40	123.37	127.87
2	D	472	HEM	CBB-CAB-C3B	-2.40	115.53	127.53
2	C	472	HEM	CHB-C4A-C3A	-2.40	120.46	127.43
2	A	472	HEM	CHB-C4A-NA	2.40	128.21	123.86
2	B	472	HEM	CBC-CAC-C3C	-2.39	115.56	127.53
2	A	472	HEM	C2D-C1D-ND	2.35	112.62	109.90
3	B	2465	PAM	O1-C1-O2	-2.33	117.33	123.33
2	C	472	HEM	C3D-C4D-ND	-2.32	107.63	110.17
2	D	472	HEM	C2A-C1A-NA	2.32	112.72	110.15
2	C	472	HEM	C4A-C3A-C2A	2.28	109.43	106.82
2	C	472	HEM	CAA-C2A-C1A	2.26	129.35	124.94
2	D	472	HEM	O2A-CGA-CBA	2.21	120.99	114.00
2	A	472	HEM	C4A-CHB-C1B	-2.19	121.10	126.25
2	D	472	HEM	O1A-CGA-CBA	-2.18	116.18	123.09
2	D	472	HEM	CHD-C1D-ND	2.16	126.74	124.42
2	C	472	HEM	C4A-CHB-C1B	-2.15	121.19	126.25
2	C	472	HEM	C1D-C2D-C3D	-2.13	104.74	106.98
3	D	4465	PAM	O1-C1-C2	2.12	120.71	114.00
2	A	472	HEM	CHD-C4C-C3C	-2.11	121.64	125.21
2	D	472	HEM	CHC-C1C-NC	-2.10	122.17	124.45
2	A	472	HEM	CMC-C2C-C3C	-2.09	123.38	128.43
2	C	472	HEM	CMA-C3A-C2A	2.07	130.01	125.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1465	PAM	O1-C1-C2	2.05	120.46	114.00
2	B	472	HEM	C1B-NB-C4B	-2.02	102.81	105.21
2	D	472	HEM	O1D-CGD-CBD	-2.02	116.69	123.09
2	B	472	HEM	CHB-C1B-NB	-2.01	121.88	124.37

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	4465	PAM	C10-C11-C12-C13
3	A	1465	PAM	C1-C2-C3-C4
3	D	4465	PAM	C12-C13-C14-C15
3	D	4465	PAM	C1-C2-C3-C4
3	B	2465	PAM	C11-C10-C9-C8
3	B	2465	PAM	C2-C3-C4-C5
3	D	4465	PAM	C2-C3-C4-C5
3	B	2465	PAM	C1-C2-C3-C4
3	A	1465	PAM	C12-C13-C14-C15
3	D	4465	PAM	C4-C5-C6-C7
3	C	3465	PAM	C2-C3-C4-C5
2	D	472	HEM	C4D-C3D-CAD-CBD
3	D	4465	PAM	C6-C7-C8-C9
2	D	472	HEM	C2D-C3D-CAD-CBD
3	B	2465	PAM	C3-C4-C5-C6
3	B	2465	PAM	C5-C6-C7-C8
3	B	2465	PAM	C11-C12-C13-C14
3	B	2465	PAM	C10-C11-C12-C13
3	C	3465	PAM	C12-C13-C14-C15
3	A	1465	PAM	C3-C4-C5-C6
3	C	3465	PAM	C10-C11-C12-C13
3	D	4465	PAM	C11-C10-C9-C8
3	A	1465	PAM	C13-C14-C15-C16
3	C	3465	PAM	C11-C12-C13-C14
3	C	3465	PAM	C4-C5-C6-C7
2	C	472	HEM	C1A-C2A-CAA-CBA
3	D	4465	PAM	C3-C4-C5-C6
3	B	2465	PAM	C6-C7-C8-C9
3	B	2465	PAM	C12-C13-C14-C15
3	B	2465	PAM	C4-C5-C6-C7
3	B	2465	PAM	C13-C14-C15-C16
3	C	3465	PAM	C9-C10-C11-C12
2	A	472	HEM	CAD-CBD-CGD-O1D

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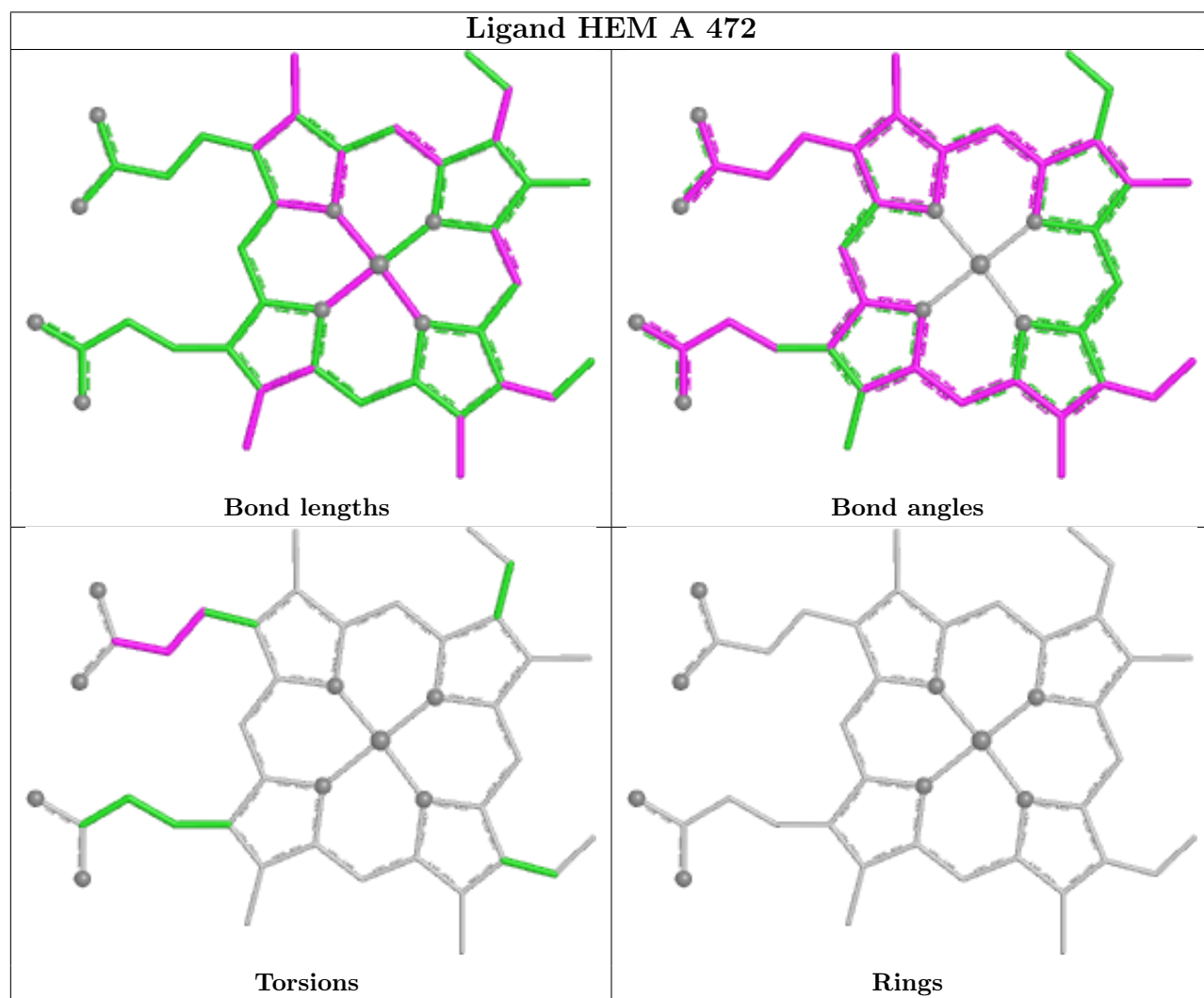
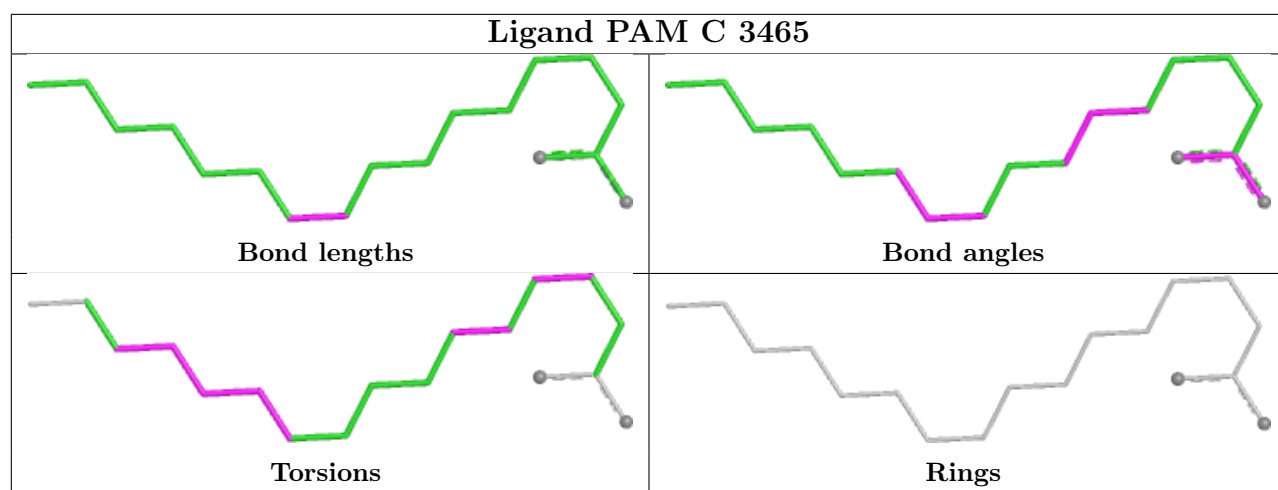
Mol	Chain	Res	Type	Atoms
2	B	472	HEM	CAD-CBD-CGD-O2D
2	C	472	HEM	CAD-CBD-CGD-O1D
2	A	472	HEM	C3D-CAD-CBD-CGD
2	B	472	HEM	CAD-CBD-CGD-O1D
2	C	472	HEM	CAD-CBD-CGD-O2D
3	D	4465	PAM	C7-C8-C9-C10
2	D	472	HEM	CAD-CBD-CGD-O1D
2	C	472	HEM	C3A-C2A-CAA-CBA
2	A	472	HEM	CAD-CBD-CGD-O2D
3	D	4465	PAM	C9-C10-C11-C12
2	D	472	HEM	CAD-CBD-CGD-O2D
3	A	1465	PAM	C9-C10-C11-C12
2	B	472	HEM	CAA-CBA-CGA-O1A
3	B	2465	PAM	C7-C8-C9-C10

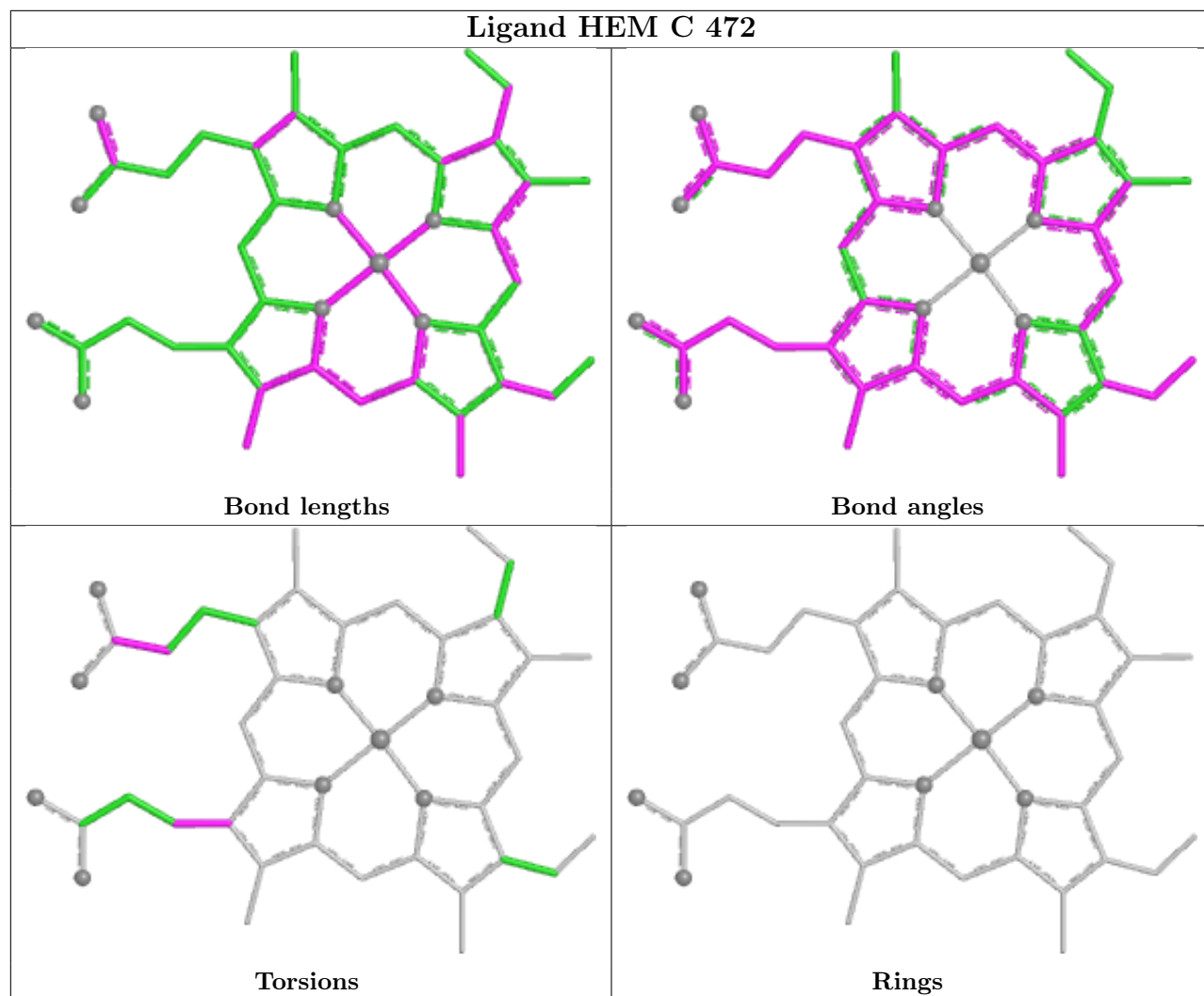
There are no ring outliers.

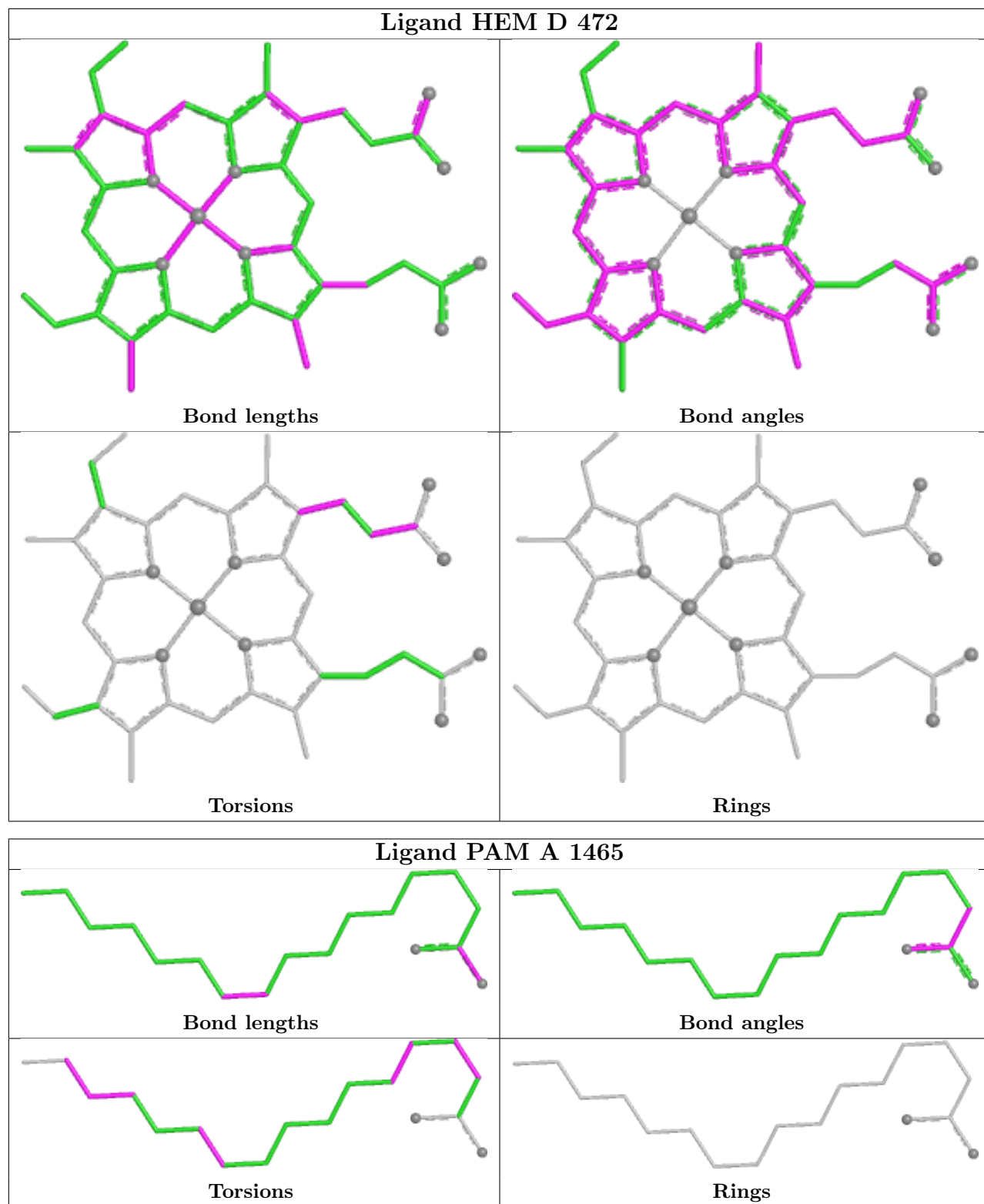
7 monomers are involved in 57 short contacts:

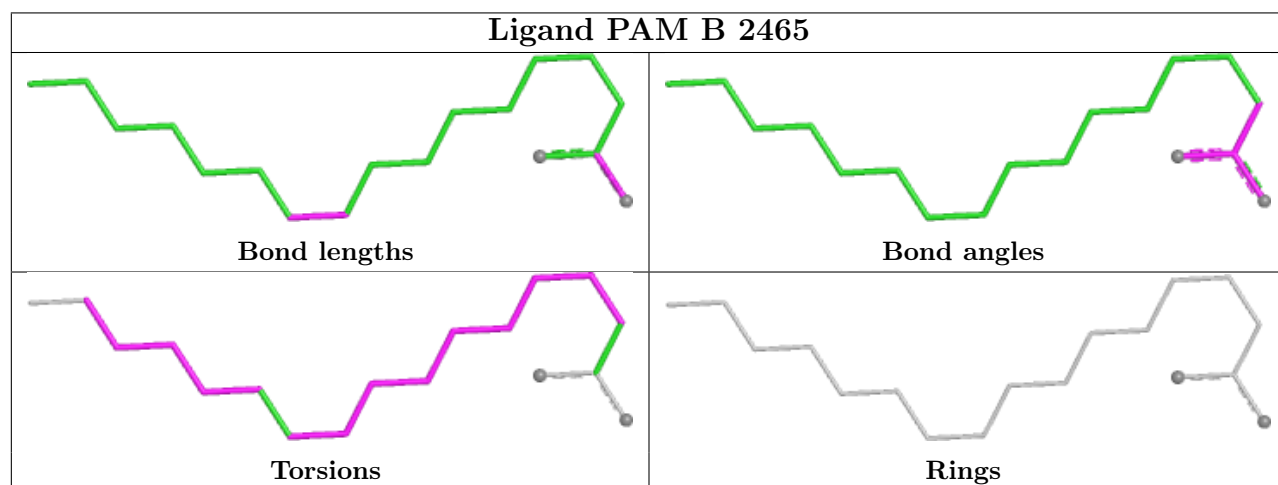
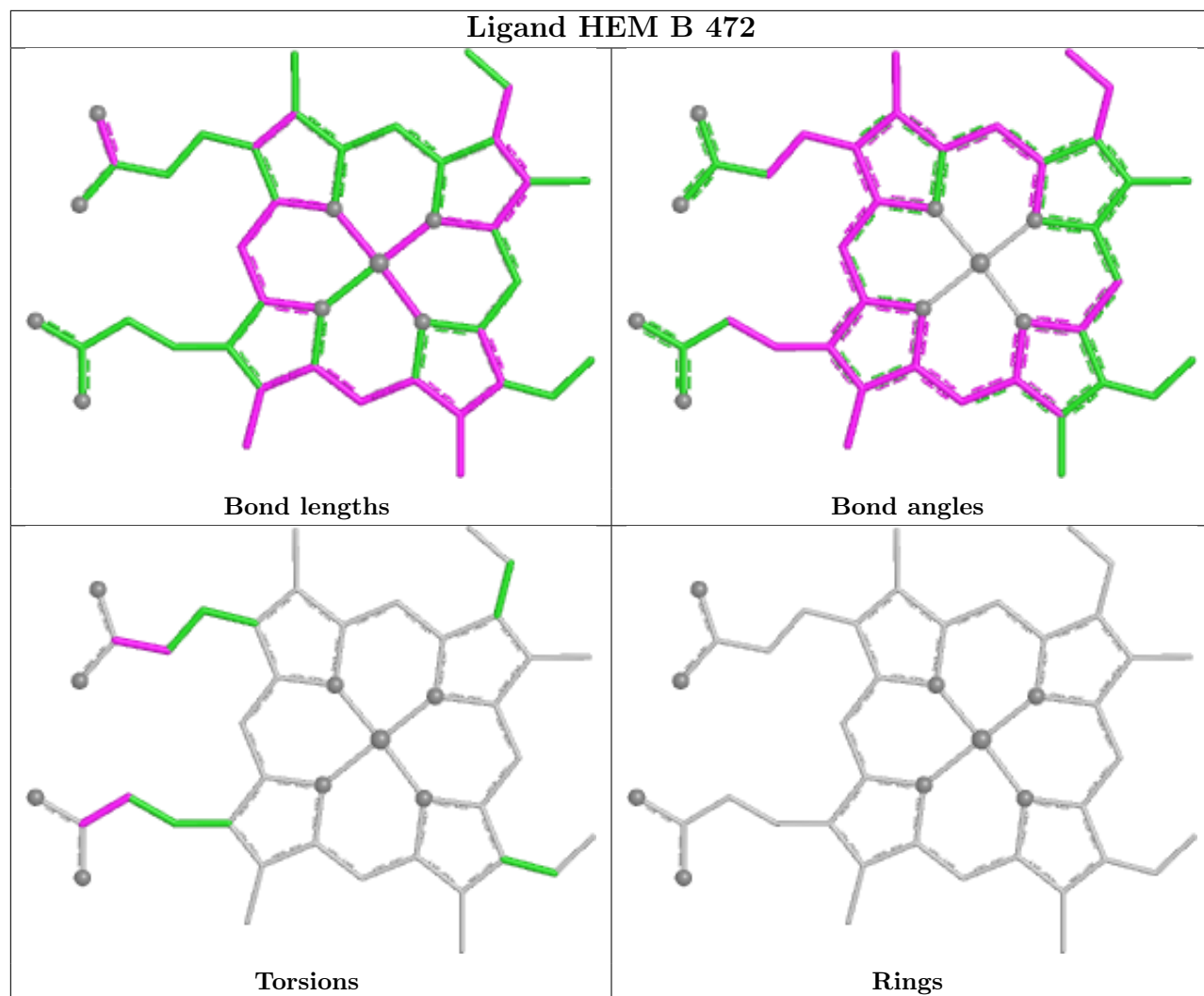
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3465	PAM	6	0
2	A	472	HEM	14	0
2	C	472	HEM	4	0
2	D	472	HEM	13	0
3	A	1465	PAM	3	0
2	B	472	HEM	15	0
3	D	4465	PAM	2	0

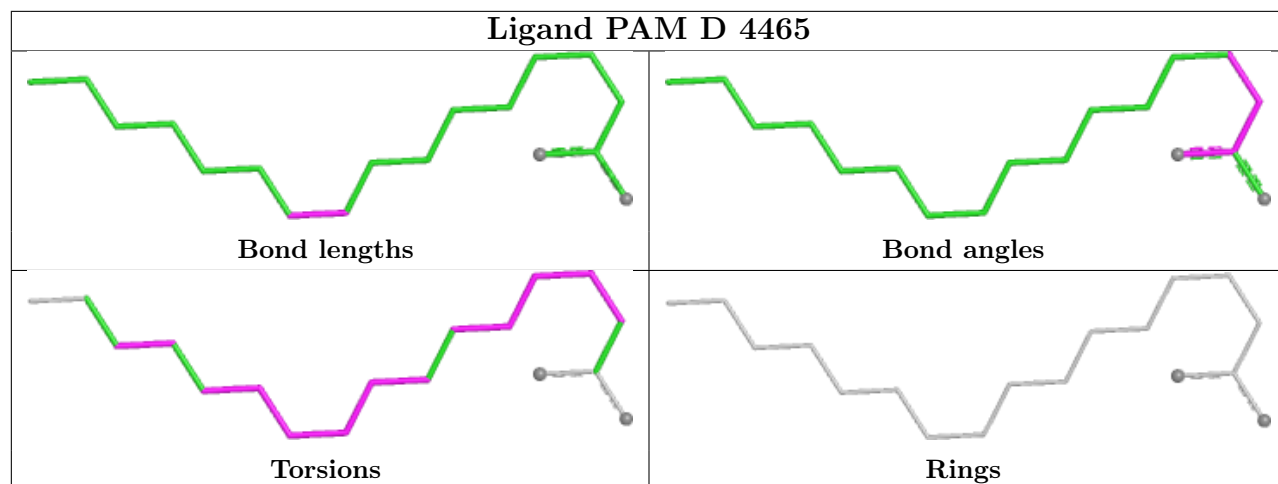
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	455/471 (96%)	-0.48	0 100 100	24, 46, 66, 87	0
1	B	455/471 (96%)	-0.17	4 (0%) 81 81	31, 58, 83, 96	0
1	C	455/471 (96%)	-0.09	1 (0%) 91 92	32, 58, 80, 90	0
1	D	454/471 (96%)	-0.09	5 (1%) 78 77	38, 62, 80, 92	0
All	All	1819/1884 (96%)	-0.21	10 (0%) 87 87	24, 56, 80, 96	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	196	PRO	2.7
1	B	242	ASP	2.5
1	B	245	THR	2.4
1	D	335	ALA	2.4
1	C	6	PRO	2.3
1	B	1	THR	2.2
1	B	292	GLU	2.2
1	D	243	PRO	2.2
1	D	197	ALA	2.1
1	D	222	ASP	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

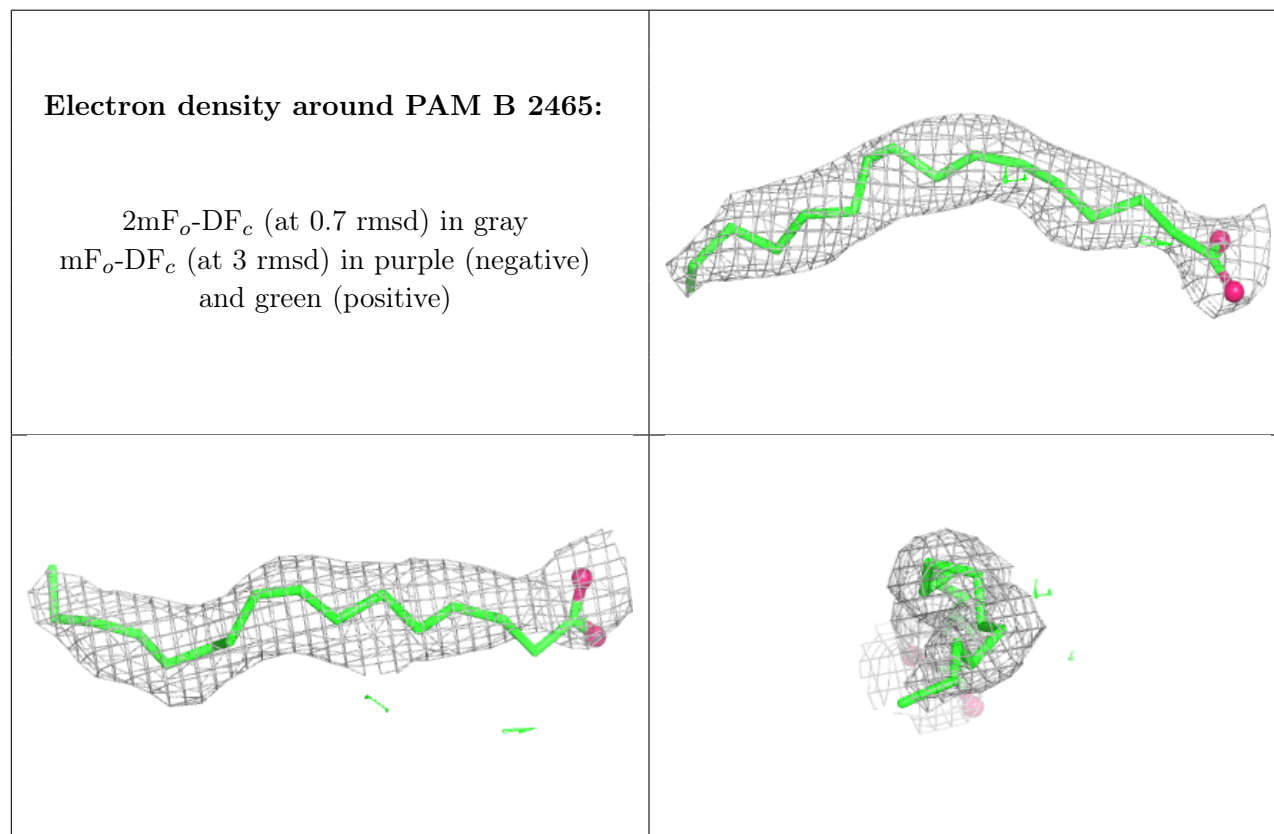
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

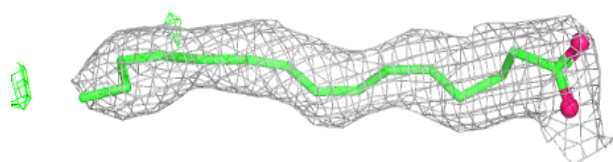
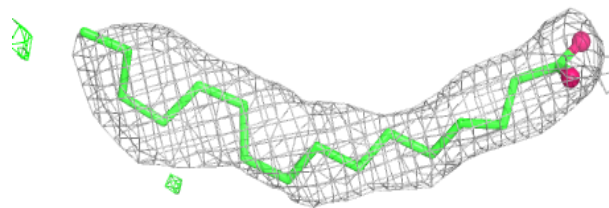
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PAM	B	2465	18/18	0.83	0.10	57,68,74,76	0
3	PAM	D	4465	18/18	0.85	0.10	45,59,78,79	0
3	PAM	C	3465	18/18	0.88	0.09	43,50,71,73	0
3	PAM	A	1465	18/18	0.90	0.07	30,45,62,64	0
2	HEM	C	472	43/43	0.96	0.07	23,30,48,54	0
2	HEM	D	472	43/43	0.96	0.07	29,40,55,60	0
2	HEM	B	472	43/43	0.96	0.07	27,35,59,68	0
2	HEM	A	472	43/43	0.98	0.06	18,27,38,43	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

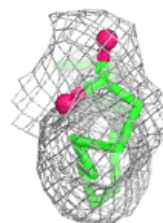
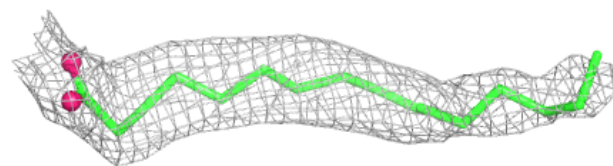
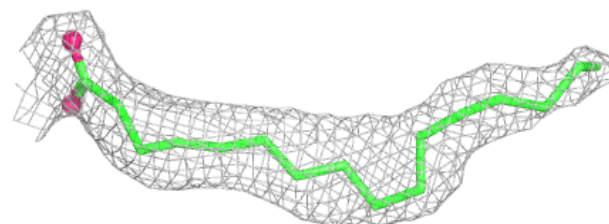


Electron density around PAM D 4465:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

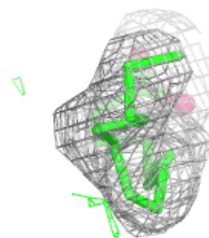
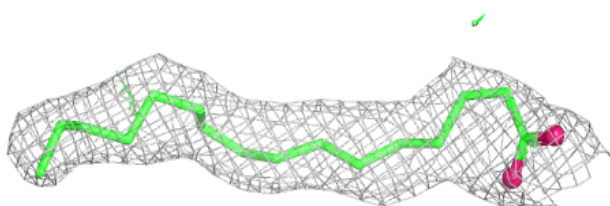
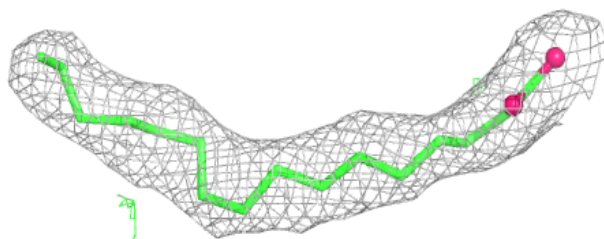
**Electron density around PAM C 3465:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

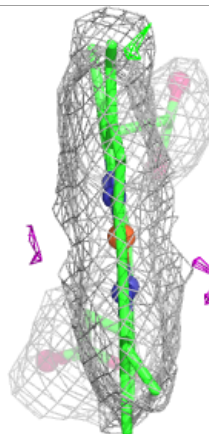
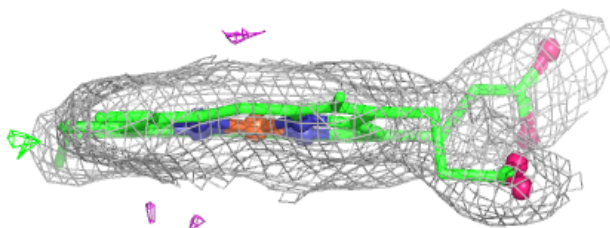
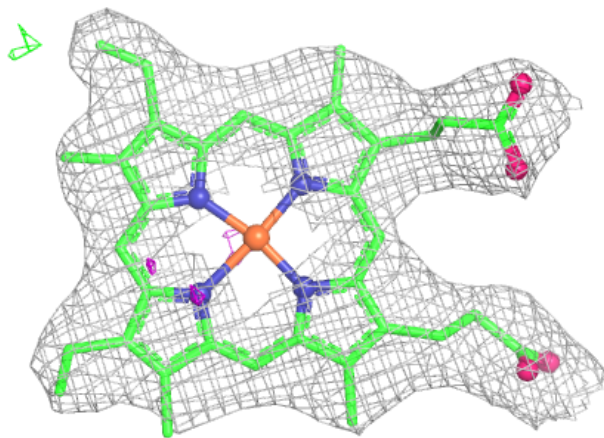


Electron density around PAM A 1465:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

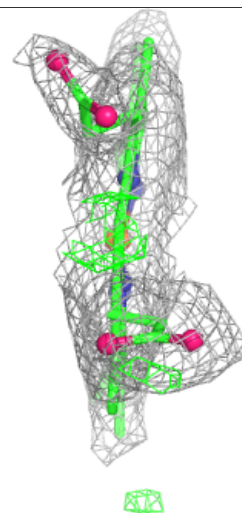
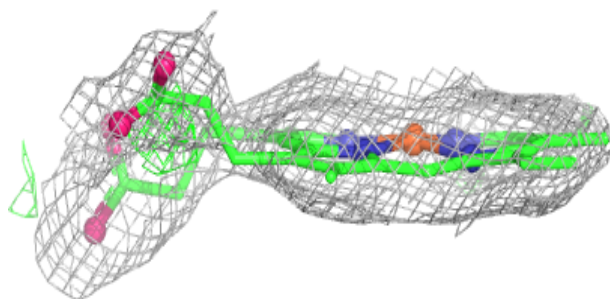
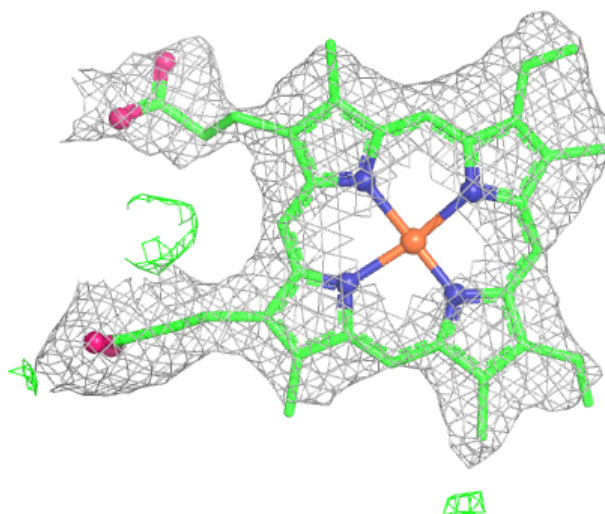
**Electron density around HEM C 472:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



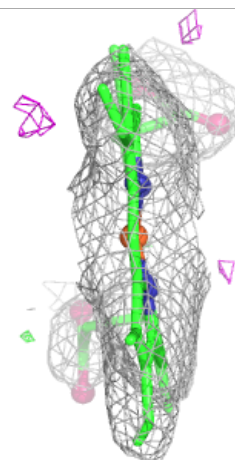
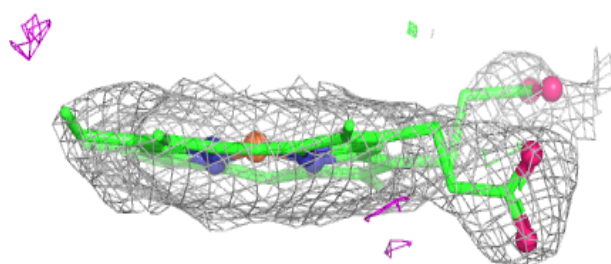
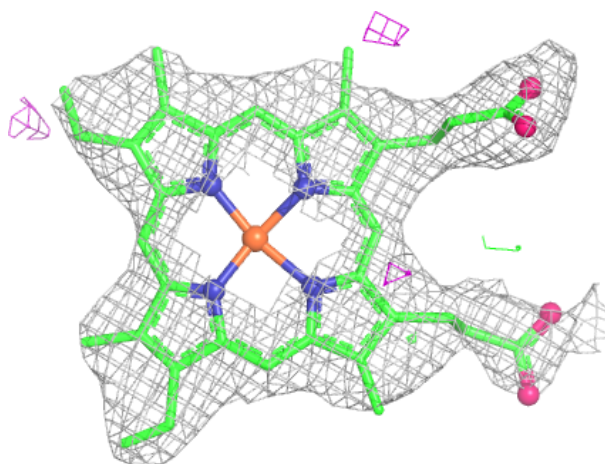
Electron density around HEM D 472:

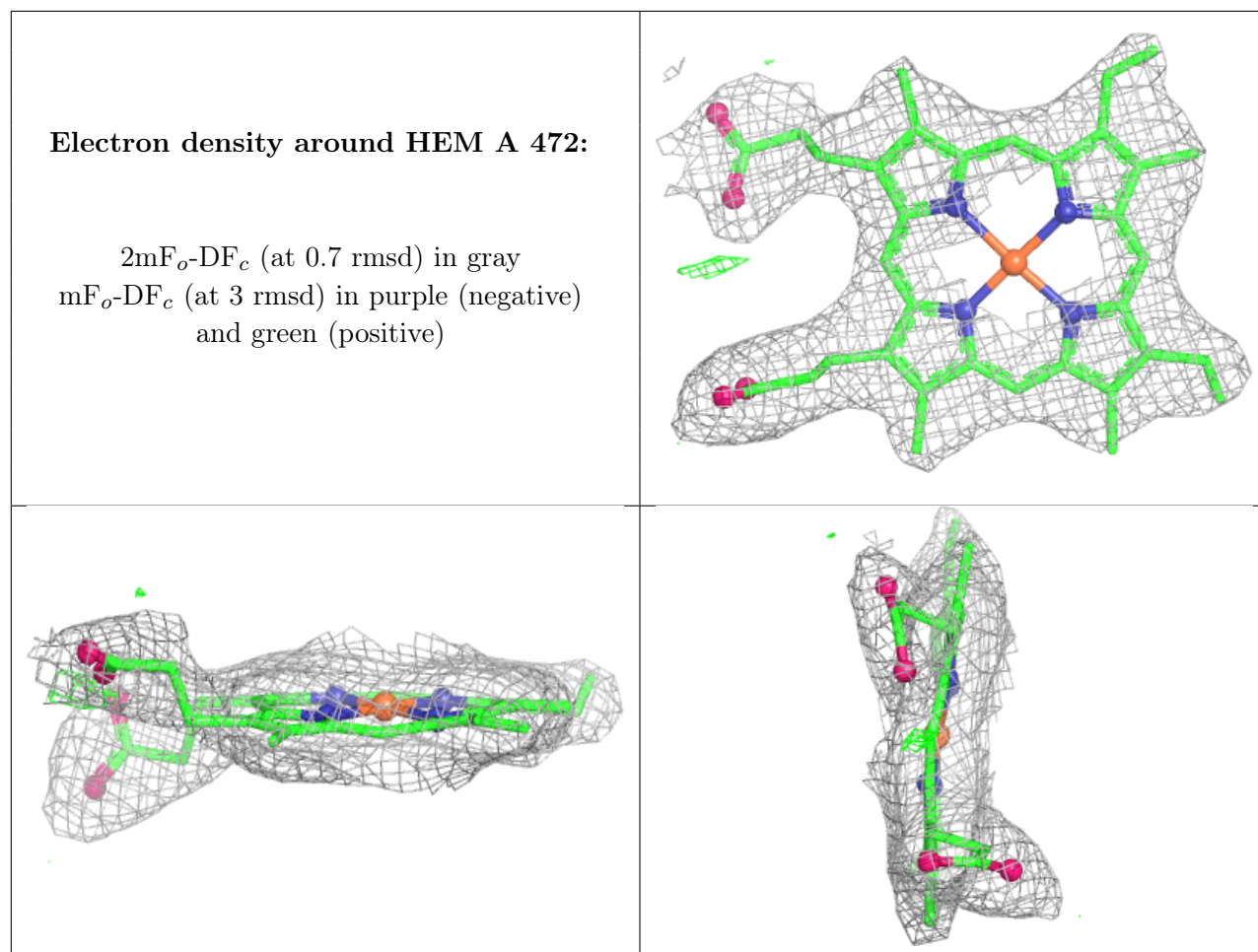
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 472:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.