



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 05:51 PM UTC

PDB ID : 3PGH / pdb_00003pgh
Title : CYCLOOXYGENASE-2 (PROSTAGLANDIN SYNTHASE-2) COM-
PLEXED WITH A NON-SELECTIVE INHIBITOR, FLURBIPROFEN
Authors : Kurumbail, R.; Stallings, W.
Deposited on : 1996-12-18
Resolution : 2.50 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

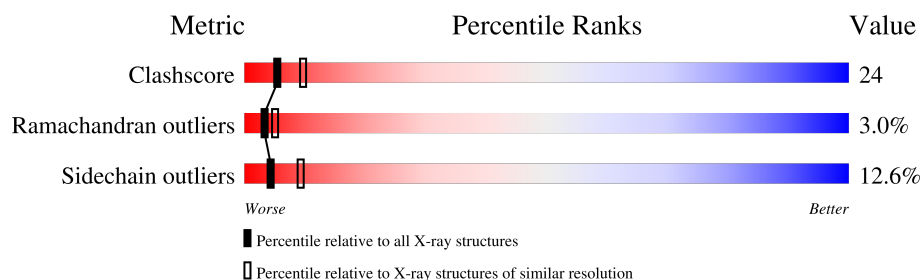
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	587	
1	B	587	
1	C	587	
1	D	587	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18304 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 CYCLOOXYGENASE-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4473	2886	748	814	25			
1	B	552	Total	C	N	O	S	0	0	0
			4473	2886	748	814	25			
1	C	552	Total	C	N	O	S	0	0	0
			4473	2886	748	814	25			
1	D	552	Total	C	N	O	S	0	0	0
			4473	2886	748	814	25			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	310	GLN	ASN	conflict	UNP Q05769
A	333	LYS	ARG	conflict	UNP Q05769
B	310	GLN	ASN	conflict	UNP Q05769
B	333	LYS	ARG	conflict	UNP Q05769
C	310	GLN	ASN	conflict	UNP Q05769
C	333	LYS	ARG	conflict	UNP Q05769
D	310	GLN	ASN	conflict	UNP Q05769
D	333	LYS	ARG	conflict	UNP Q05769

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



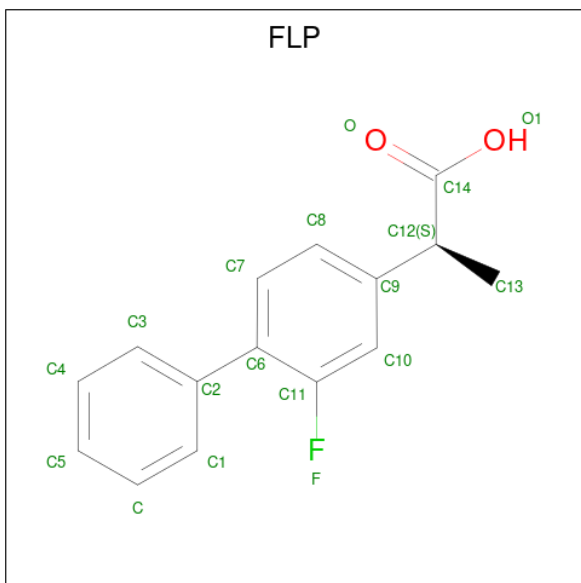
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 4 is FLURBIPROFEN (CCD ID: FLP) (formula: $C_{15}H_{13}FO_2$).



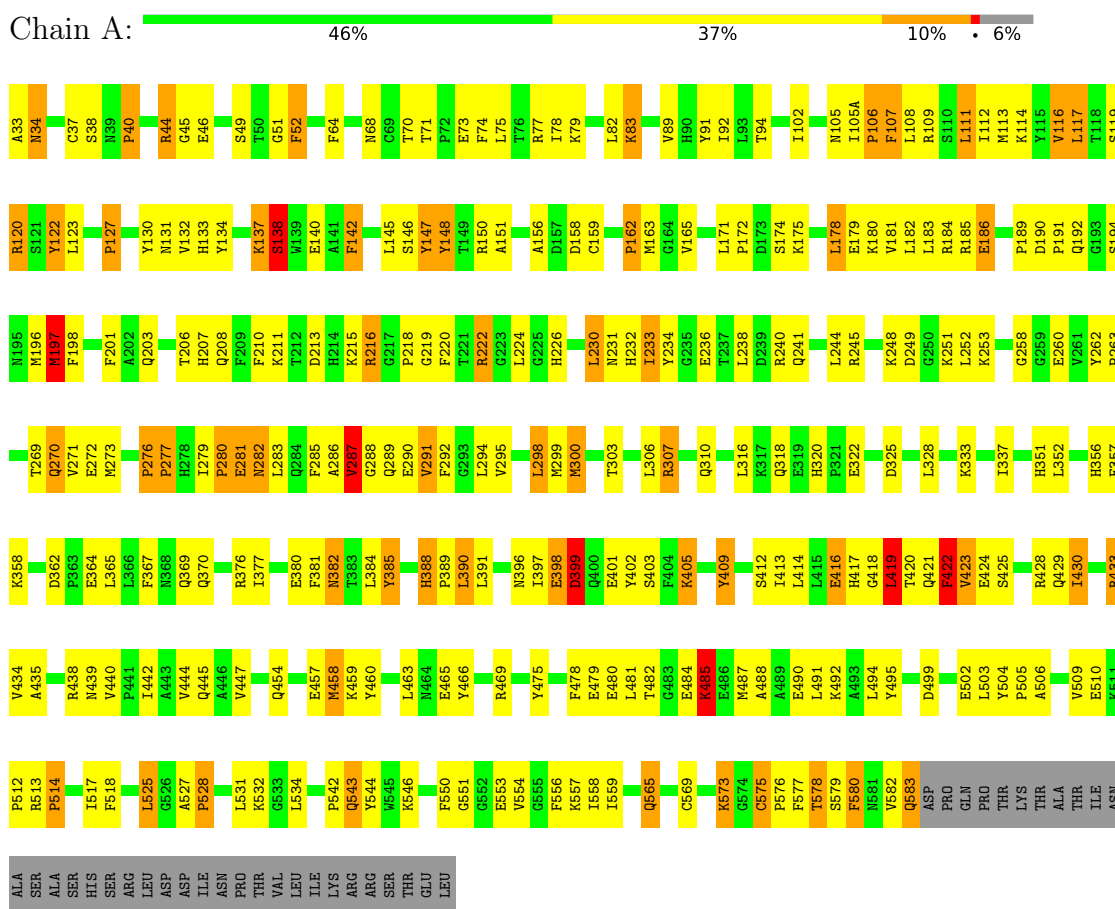
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 18	C 15	F 1	O 2	0	0
4	B	1	Total 18	C 15	F 1	O 2	0	0
4	C	1	Total 18	C 15	F 1	O 2	0	0
4	D	1	Total 18	C 15	F 1	O 2	0	0

3 Residue-property plots

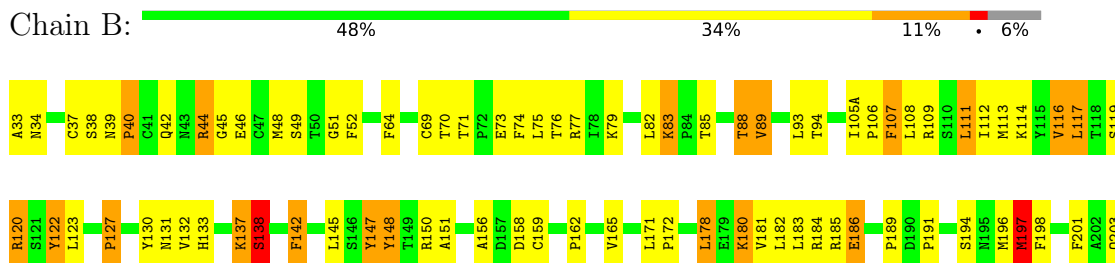
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: CYCLOOXYGENASE-2



• Molecule 1: CYCLOOXYGENASE-2





SER	P512	V434	Y355	E272	S194	V116	A33
HIS	R513	A435	H356	M273	N195	L117	N34
SER	P514	G436	F357	Y274	M196	T118	
ARG		G437	K358	Y275	S119	S119	C37
LEU	I517	R438	L359	P276	F198	S120	S38
ASP	F518	N439		P277	S121	R121	N39
ASP		V440	P363	H278	Q203	Y122	P40
ILE	L525	P441		I279	H204	L123	G41
ASN	G526	Y442	Q369	P280	F205		Q42
PRO	A527	Q445	Q370	E281	T206	P127	Q44
THR	P528	Q446	R376	N282	H207	R44	R44
VAL		V447	I377	L283	Q208	Y130	G45
LEU	L531	Q454		Q284	F209	N131	E46
ILE	K532		E380	F285	F210	N132	
LYS	G533	E457	F381	A286	K211	H133	S49
ARG	L534	E458	N382	V287	T212	Y134	T50
ARG		M458	T383	Q288	D213	G135	G51
SER	N537	K459	L384	Q289	H214	Y136	
THR		Y460	Y385	E290	K215	K137	F52
GLU	Q543			V291	R216	S138	
LEU	K546	L463		F292	G217	F64	
		N464	H388	G293	P218	F142	C69
	G551	E465	P389	L294	G219	T70	T70
	G552	Y466	L390	V295		T71	
	E553		L391	P296	R222	S146	P72
	V554	R469	P392	G297	L230	Y147	E73
	G555	Y475	N396	L298	M231	Y148	F74
	F556		E398	M299	H232	R150	L75
	K557	F478	S399	Q303	M300	A151	K79
	I558	E479	Q400	L306	E236	V155	L82
	I559	E480	E401	R307	T237	A156	K83
	C569	L481	Y402	Q310	L238	D157	P84
	K573	T482	S403		D239	D158	T85
	G574	G483	F404	L316	R240	C159	P86
	C575	E484	K405	K317	Q241	P162	N87
	P576	K485	Y409	Q318	H242	M163	T88
	F577	E486		E319	K243	G164	V89
	T578	M487	S412	L244	L245	V165	
	S579	A488	I413	H320	L246		L92
	F580	L491	L414	P321	F247	L171	L93
	N581	K492	L415	E322	K248	P172	T94
	V582	A493	E416				N95
	Q583	L494	H417	D325	K251	L178	F96
	ASP	Y495	G418		L252	E179	K97
PRO	PRO		L419	L328	K253	N104	
GLN	GLN	D499	T420	F329	Q258	N105	N104
PRO	PRO	V500	Q421		E260	T105A	T105A
THR	THR	M501	F422	K333	V261	F107	F107
LYS	LYS	E502	V423	I337	E186	L108	L108
THR	THR	L503	E424	V344	P189	R109	R109
ALA	ALA	Y504	S425		D190	S110	S110
ALA	P505	P505	R428	Q350	P191	L111	L111
THR	A506		Q429	H351	Q192	T112	T112
ILE	ILE		T430	L352	G193	K114	K114
ASN	ASN	V509					
ALA	ALA	E510					
SER	SER	K511					
ALA	ALA						

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	179.50Å 133.80Å 117.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	63.1 (8.00-2.50)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.236 , 0.316	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18304	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.82	2/4600 (0.0%)	1.26	56/6237 (0.9%)
1	B	0.81	0/4600	1.27	55/6237 (0.9%)
1	C	0.81	1/4600 (0.0%)	1.26	49/6237 (0.8%)
1	D	0.80	0/4600	1.26	54/6237 (0.9%)
All	All	0.81	3/18400 (0.0%)	1.26	214/24948 (0.9%)

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	1
1	B	0	1
1	C	0	2
1	D	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	458	MET	SD-CE	-7.93	1.59	1.79
1	C	458	MET	SD-CE	-5.82	1.65	1.79
1	A	224	LEU	C-O	-5.16	1.17	1.24

All (214) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	127	PRO	CA-C-N	10.12	130.20	119.78
1	C	127	PRO	C-N-CA	10.12	130.20	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	287	VAL	N-CA-C	9.59	129.30	109.34
1	B	485	LYS	N-CA-C	9.57	125.90	114.04
1	A	127	PRO	CA-C-N	9.18	129.75	119.92
1	A	127	PRO	C-N-CA	9.18	129.75	119.92
1	D	287	VAL	N-CA-C	9.14	128.35	109.34
1	A	287	VAL	N-CA-C	9.12	128.32	109.34
1	C	287	VAL	N-CA-C	9.02	128.09	109.34
1	D	127	PRO	CA-C-N	8.78	128.82	119.78
1	D	127	PRO	C-N-CA	8.78	128.82	119.78
1	D	485	LYS	N-CA-C	8.66	124.78	114.04
1	B	494	LEU	N-CA-C	8.52	120.19	111.07
1	C	423	VAL	N-CA-C	-8.52	102.12	110.72
1	D	494	LEU	N-CA-C	8.43	120.09	111.07
1	A	485	LYS	N-CA-C	8.32	124.36	114.04
1	B	423	VAL	N-CA-C	-8.32	102.32	110.72
1	B	513	ARG	N-CA-C	-8.22	98.36	110.20
1	A	148	TYR	N-CA-C	-8.16	98.40	110.48
1	D	423	VAL	N-CA-C	-8.14	102.50	110.72
1	C	485	LYS	N-CA-C	8.13	124.12	114.04
1	B	148	TYR	N-CA-C	-8.07	98.53	110.48
1	D	513	ARG	N-CA-C	-8.07	98.58	110.20
1	C	494	LEU	N-CA-C	7.91	119.68	111.14
1	A	494	LEU	N-CA-C	7.88	119.65	111.14
1	B	127	PRO	CA-C-N	7.86	127.87	119.78
1	B	127	PRO	C-N-CA	7.86	127.87	119.78
1	C	513	ARG	N-CA-C	-7.83	99.28	110.08
1	A	423	VAL	N-CA-C	-7.81	102.84	110.72
1	B	180	LYS	N-CA-C	7.76	119.74	111.28
1	C	251	LYS	N-CA-C	7.76	121.02	110.55
1	D	390	LEU	N-CA-C	-7.67	104.41	114.31
1	A	233	ILE	N-CA-C	-7.66	104.97	111.56
1	D	251	LYS	N-CA-C	7.41	121.45	110.48
1	A	390	LEU	N-CA-C	-7.38	104.79	114.31
1	A	513	ARG	N-CA-C	-7.37	99.59	110.20
1	B	251	LYS	N-CA-C	7.36	121.37	110.48
1	B	197	MET	N-CA-C	-7.34	102.25	112.45
1	D	197	MET	N-CA-C	-7.30	102.30	112.45
1	C	306	LEU	N-CA-C	-7.30	103.26	111.07
1	D	208	GLN	N-CA-C	-7.29	102.72	111.69
1	C	180	LYS	N-CA-C	7.28	118.86	111.07
1	C	208	GLN	N-CA-C	-7.24	102.38	112.45
1	D	148	TYR	N-CA-C	-7.23	98.78	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	388	HIS	CA-CB-CG	-7.16	106.64	113.80
1	B	388	HIS	CA-CB-CG	-7.09	106.71	113.80
1	B	233	ILE	N-CA-C	-7.08	105.47	111.56
1	B	390	LEU	N-CA-C	-7.03	105.25	114.31
1	A	251	LYS	N-CA-C	6.99	119.98	110.55
1	C	234	TYR	N-CA-C	6.97	121.79	113.28
1	A	40	PRO	N-CA-C	6.93	122.52	113.86
1	C	148	TYR	N-CA-C	-6.89	99.31	110.20
1	B	503	LEU	N-CA-C	6.86	118.41	111.07
1	D	306	LEU	N-CA-C	-6.82	103.77	111.07
1	A	73	GLU	N-CA-C	-6.77	101.41	110.55
1	C	218	PRO	N-CA-C	-6.77	100.61	111.38
1	D	283	LEU	N-CA-C	-6.69	103.71	114.09
1	B	500	VAL	N-CA-C	-6.69	106.78	113.20
1	D	180	LYS	N-CA-C	6.67	119.11	111.11
1	A	281	GLU	N-CA-C	-6.62	96.69	110.80
1	A	180	LYS	N-CA-C	6.60	118.47	111.28
1	A	306	LEU	N-CA-C	-6.56	104.05	111.07
1	D	218	PRO	N-CA-C	-6.55	101.58	111.41
1	D	233	ILE	N-CA-C	-6.51	105.96	111.56
1	C	233	ILE	N-CA-C	-6.49	105.98	111.56
1	C	40	PRO	N-CA-C	6.49	121.97	113.86
1	B	208	GLN	N-CA-C	-6.45	103.75	111.69
1	C	73	GLU	N-CA-C	-6.45	101.84	110.55
1	B	40	PRO	N-CA-C	6.43	121.90	113.86
1	C	390	LEU	N-CA-C	-6.43	105.98	113.88
1	D	281	GLU	N-CA-C	-6.42	97.12	110.80
1	A	503	LEU	N-CA-C	6.42	117.94	111.07
1	A	580	PHE	N-CA-C	-6.40	105.11	113.17
1	A	208	GLN	N-CA-C	-6.38	103.58	112.45
1	D	159	CYS	CA-C-N	6.38	125.61	118.97
1	D	159	CYS	C-N-CA	6.38	125.61	118.97
1	A	218	PRO	N-CA-C	-6.36	101.87	111.41
1	B	105(A)	ILE	CA-C-N	6.36	127.79	119.84
1	B	105(A)	ILE	C-N-CA	6.36	127.79	119.84
1	D	388	HIS	CA-CB-CG	-6.32	107.48	113.80
1	D	289	GLN	N-CA-C	-6.32	98.44	108.73
1	C	290	GLU	N-CA-C	6.29	120.41	112.87
1	C	281	GLU	N-CA-C	-6.25	97.48	110.80
1	A	388	HIS	CA-CB-CG	-6.25	107.55	113.80
1	B	580	PHE	N-CA-C	-6.23	105.31	113.17
1	C	197	MET	N-CA-C	-6.20	103.83	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	105(A)	ILE	CA-C-N	6.18	127.57	119.84
1	C	105(A)	ILE	C-N-CA	6.18	127.57	119.84
1	C	388	HIS	CG-CD2-NE2	-6.18	101.02	107.20
1	B	281	GLU	N-CA-C	-6.16	97.67	110.80
1	D	40	PRO	N-CA-C	6.16	121.56	113.86
1	D	328	LEU	N-CA-C	-6.16	103.89	111.40
1	C	276	PRO	CA-C-N	6.14	127.52	119.84
1	C	276	PRO	C-N-CA	6.14	127.52	119.84
1	A	34	ASN	CA-C-N	6.13	125.83	119.82
1	A	34	ASN	C-N-CA	6.13	125.83	119.82
1	D	233	ILE	CB-CA-C	-6.12	105.63	111.44
1	D	73	GLU	N-CA-C	-6.10	101.46	110.48
1	A	197	MET	N-CA-C	-6.08	104.00	112.45
1	C	503	LEU	N-CA-C	6.06	117.55	111.07
1	C	580	PHE	N-CA-C	-6.06	105.54	113.17
1	B	73	GLU	N-CA-C	-6.05	101.53	110.48
1	D	370	GLN	N-CA-C	-6.04	100.70	109.59
1	A	422	PHE	N-CA-C	-6.03	97.97	110.80
1	B	290	GLU	N-CA-C	6.01	120.09	112.87
1	B	258	GLY	N-CA-C	-6.01	98.94	113.18
1	A	388	HIS	ND1-CG-CD2	5.94	112.04	106.10
1	C	300	MET	N-CA-C	-5.93	104.74	111.14
1	D	388	HIS	ND1-CG-CD2	5.92	112.03	106.10
1	B	218	PRO	N-CA-C	-5.92	101.97	111.38
1	B	306	LEU	N-CA-C	-5.92	104.73	111.07
1	C	370	GLN	N-CA-C	-5.92	100.35	109.76
1	D	422	PHE	N-CA-C	-5.91	98.21	110.80
1	C	388	HIS	ND1-CG-CD2	5.90	112.00	106.10
1	C	201	PHE	N-CA-C	-5.90	104.77	111.14
1	B	422	PHE	N-CA-C	-5.90	98.24	110.80
1	B	88	THR	N-CA-C	-5.89	104.94	111.36
1	B	289	GLN	N-CA-C	-5.88	99.15	108.73
1	B	142	PHE	N-CA-C	5.88	117.36	111.07
1	A	370	GLN	N-CA-C	-5.83	100.50	109.76
1	B	328	LEU	N-CA-C	-5.82	104.86	111.14
1	C	480	GLU	N-CA-C	-5.81	105.03	111.36
1	D	258	GLY	N-CA-C	-5.81	99.41	113.18
1	A	388	HIS	CG-CD2-NE2	-5.79	101.41	107.20
1	A	105(A)	ILE	CA-C-N	5.75	127.03	119.84
1	A	105(A)	ILE	C-N-CA	5.75	127.03	119.84
1	D	105(A)	ILE	CA-C-N	5.74	127.02	119.84
1	D	105(A)	ILE	C-N-CA	5.74	127.02	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	88	THR	N-CA-C	-5.73	105.12	111.36
1	B	513	ARG	CA-C-N	5.72	126.98	119.84
1	B	513	ARG	C-N-CA	5.72	126.98	119.84
1	D	276	PRO	CA-C-N	5.71	126.97	119.84
1	D	276	PRO	C-N-CA	5.71	126.97	119.84
1	B	233	ILE	CB-CA-C	-5.70	106.02	111.44
1	C	388	HIS	CB-CG-CD2	-5.70	123.79	131.20
1	A	276	PRO	CA-C-N	5.68	126.94	119.84
1	A	276	PRO	C-N-CA	5.68	126.94	119.84
1	C	422	PHE	N-CA-C	-5.66	98.75	110.80
1	B	300	MET	N-CA-C	-5.65	105.03	111.14
1	A	258	GLY	N-CA-C	-5.65	99.86	110.77
1	A	234	TYR	N-CA-C	5.62	120.14	113.28
1	A	142	PHE	N-CA-C	5.62	117.08	111.07
1	B	560	ASN	N-CA-C	5.62	119.75	113.01
1	C	328	LEU	N-CA-C	-5.62	105.24	111.36
1	A	388	HIS	CB-CG-CD2	-5.60	123.92	131.20
1	A	325	ASP	N-CA-C	5.57	118.07	111.33
1	A	328	LEU	N-CA-C	-5.55	105.14	111.14
1	C	289	GLN	N-CA-C	-5.55	99.69	108.73
1	B	283	LEU	N-CA-C	-5.53	105.16	113.89
1	B	201	PHE	N-CA-C	-5.51	105.19	111.14
1	C	89	VAL	N-CA-C	-5.50	105.14	110.42
1	B	138	SER	N-CA-C	5.50	122.51	110.80
1	A	89	VAL	N-CA-C	-5.49	104.97	110.30
1	D	513	ARG	CA-C-N	5.49	126.70	119.84
1	D	513	ARG	C-N-CA	5.49	126.70	119.84
1	D	430	ILE	CB-CA-C	-5.48	104.17	111.13
1	A	222	ARG	N-CA-C	-5.46	106.54	114.12
1	D	388	HIS	CB-CG-CD2	-5.44	124.13	131.20
1	D	215	LYS	N-CA-C	-5.42	105.79	112.90
1	B	370	GLN	N-CA-C	-5.41	101.84	109.96
1	C	190	ASP	CA-C-N	5.41	125.23	119.28
1	C	190	ASP	C-N-CA	5.41	125.23	119.28
1	B	413	ILE	CB-CA-C	-5.40	104.77	112.22
1	B	573	LYS	N-CA-C	5.40	122.30	110.80
1	C	453	ASP	N-CA-C	5.40	116.84	111.07
1	A	201	PHE	N-CA-C	-5.36	105.35	111.14
1	A	362	ASP	CA-C-N	5.35	125.42	119.32
1	A	362	ASP	C-N-CA	5.35	125.42	119.32
1	D	537	ASN	N-CA-C	-5.35	102.07	110.14
1	A	413	ILE	N-CA-C	-5.33	105.34	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	573	LYS	N-CA-C	5.32	122.14	110.80
1	A	102	ILE	N-CA-C	-5.30	105.67	110.82
1	D	388	HIS	CG-CD2-NE2	-5.29	101.91	107.20
1	C	293	GLY	N-CA-C	-5.29	108.39	115.32
1	A	245	ARG	N-CA-C	5.29	118.69	110.17
1	D	290	GLU	N-CA-C	5.26	119.19	112.87
1	D	134	TYR	N-CA-C	5.26	116.98	108.41
1	C	41	CYS	N-CA-C	5.26	117.32	108.96
1	C	283	LEU	N-CA-C	-5.25	105.20	113.02
1	D	34	ASN	CA-C-N	5.24	126.39	119.84
1	D	34	ASN	C-N-CA	5.24	126.39	119.84
1	B	234	TYR	N-CA-C	5.23	119.72	113.23
1	D	413	ILE	CB-CA-C	-5.23	105.07	112.14
1	D	580	PHE	N-CA-C	-5.23	106.58	113.17
1	A	289	GLN	N-CA-C	-5.23	100.64	108.96
1	B	89	VAL	N-CA-C	-5.22	105.41	110.42
1	B	482	THR	N-CA-C	5.21	118.80	112.23
1	B	465	GLU	N-CA-C	-5.19	105.62	111.28
1	A	45	GLY	N-CA-C	-5.17	106.64	112.33
1	B	388	HIS	ND1-CG-CD2	5.15	111.25	106.10
1	C	573	LYS	N-CA-C	5.15	121.77	110.80
1	A	190	ASP	CA-C-N	5.14	124.94	119.28
1	A	190	ASP	C-N-CA	5.14	124.94	119.28
1	C	537	ASN	N-CA-C	-5.13	102.39	110.14
1	B	381	PHE	N-CA-C	-5.13	105.77	112.23
1	D	116	VAL	N-CA-C	-5.11	105.41	110.62
1	B	76	THR	N-CA-C	-5.11	105.61	111.07
1	C	430	ILE	CB-CA-C	-5.10	104.65	111.13
1	B	276	PRO	CA-C-N	5.09	126.21	119.84
1	B	276	PRO	C-N-CA	5.09	126.21	119.84
1	B	320	HIS	CA-C-N	5.09	124.89	119.28
1	B	320	HIS	C-N-CA	5.09	124.89	119.28
1	A	218	PRO	CA-C-N	-5.09	116.21	123.08
1	A	218	PRO	C-N-CA	-5.09	116.21	123.08
1	A	573	LYS	N-CA-C	5.08	121.61	110.80
1	D	137	LYS	N-CA-C	5.08	119.69	111.37
1	D	559	ILE	CB-CA-C	-5.07	105.38	112.02
1	D	45	GLY	N-CA-C	-5.07	106.76	112.33
1	A	134	TYR	N-CA-C	5.06	116.63	108.34
1	B	418	GLY	N-CA-C	5.04	125.13	113.18
1	A	290	GLU	N-CA-C	5.03	118.91	112.87
1	A	559	ILE	CB-CA-C	-5.03	105.53	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	503	LEU	N-CA-C	5.01	116.44	111.07
1	C	159	CYS	N-CA-C	-5.01	102.93	110.24

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	147	TYR	Sidechain
1	B	147	TYR	Sidechain
1	C	147	TYR	Sidechain
1	C	91	TYR	Sidechain
1	D	147	TYR	Sidechain

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	4473	0	4374	214	0
1	B	4473	0	4374	227	0
1	C	4473	0	4375	224	0
1	D	4473	0	4375	211	0
2	A	42	0	39	4	0
2	B	42	0	39	3	0
2	C	42	0	39	0	0
2	D	42	0	39	0	0
3	A	43	0	30	6	0
3	B	43	0	30	9	0
3	C	43	0	30	6	0
3	D	43	0	30	9	0
4	A	18	0	12	1	0
4	B	18	0	12	6	0
4	C	18	0	12	3	0
4	D	18	0	12	3	0
All	All	18304	0	17822	862	0

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 24.

All (862) 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:424:GLU:HA	1:C:428:ARG:HH21	1.27	0.97
1:C:458:MET:HE2	1:C:460:TYR:HE1	1.29	0.96
1:A:424:GLU:HA	1:A:428:ARG:HH21	1.31	0.96
1:D:424:GLU:HA	1:D:428:ARG:HH21	1.30	0.95
1:A:458:MET:HE2	1:A:460:TYR:HE1	1.27	0.95
1:B:479:GLU:HG2	1:B:485:LYS:NZ	1.82	0.95
1:C:230:LEU:HG	1:C:337:ILE:HG12	1.50	0.93
1:A:230:LEU:HG	1:A:337:ILE:HG12	1.52	0.92
1:D:230:LEU:HG	1:D:337:ILE:HG12	1.52	0.91
1:B:458:MET:HE2	1:B:460:TYR:HE1	1.32	0.91
1:A:479:GLU:HG2	1:A:485:LYS:NZ	1.85	0.91
1:A:430:ILE:HG23	1:A:582:VAL:HG11	1.53	0.90
1:C:253:LYS:HE3	1:C:269:THR:HG22	1.53	0.89
1:D:458:MET:HE2	1:D:460:TYR:HE1	1.38	0.89
1:B:230:LEU:HG	1:B:337:ILE:HG12	1.55	0.89
1:B:424:GLU:HA	1:B:428:ARG:HH21	1.38	0.88
1:A:291:VAL:HG22	1:A:294:LEU:HD12	1.57	0.87
1:B:430:ILE:HG23	1:B:582:VAL:HG11	1.57	0.86
1:D:156:ALA:HB3	1:D:159:CYS:SG	2.15	0.86
1:C:253:LYS:CE	1:C:269:THR:HG22	2.06	0.86
1:B:479:GLU:HG2	1:B:485:LYS:HZ2	1.41	0.85
1:D:405:LYS:H	1:D:405:LYS:HD2	1.42	0.85
1:B:156:ALA:HB3	1:B:159:CYS:SG	2.17	0.85
1:B:291:VAL:HG22	1:B:294:LEU:HD12	1.59	0.83
1:B:458:MET:HE2	1:B:460:TYR:CE1	2.13	0.82
1:C:479:GLU:HG2	1:C:485:LYS:NZ	1.95	0.81
1:A:458:MET:HE2	1:A:460:TYR:CE1	2.13	0.81
1:C:458:MET:HE2	1:C:460:TYR:CE1	2.15	0.80
1:D:430:ILE:HG23	1:D:582:VAL:HG11	1.61	0.80
1:C:291:VAL:HG22	1:C:294:LEU:HD12	1.64	0.80
1:A:253:LYS:HE3	1:A:269:THR:HG22	1.65	0.79
1:D:291:VAL:HG22	1:D:294:LEU:HD12	1.61	0.79
1:D:458:MET:HE2	1:D:460:TYR:CE1	2.18	0.78
1:C:430:ILE:HG23	1:C:582:VAL:HG11	1.63	0.78
1:A:420:THR:HG23	1:A:576:PRO:HG3	1.65	0.78
1:D:380:GLU:HG2	1:D:466:TYR:CE1	2.18	0.78
1:B:527:ALA:HB3	1:B:528:PRO:HD3	1.63	0.78
1:B:454:GLN:HA	1:B:457:GLU:HG2	1.65	0.78
1:C:156:ALA:HB3	1:C:159:CYS:SG	2.24	0.78
1:D:398:GLU:HG2	1:D:425:SER:OG	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ARG:HA	1:A:438:ARG:O	1.84	0.77
1:A:398:GLU:HG2	1:A:425:SER:OG	1.84	0.77
1:A:479:GLU:HG2	1:A:485:LYS:HZ2	1.48	0.77
1:B:184:ARG:HA	1:B:438:ARG:O	1.84	0.77
1:A:156:ALA:HB3	1:A:159:CYS:SG	2.25	0.76
1:D:447:VAL:HG13	3:D:682:HEM:HBA2	1.67	0.76
1:D:527:ALA:HB3	1:D:528:PRO:HD3	1.68	0.76
1:B:380:GLU:HG2	1:B:466:TYR:CE1	2.21	0.75
1:B:405:LYS:H	1:B:405:LYS:HD2	1.52	0.75
1:A:380:GLU:HG2	1:A:466:TYR:CE1	2.22	0.74
1:B:120:ARG:HG2	1:B:531:LEU:HD12	1.69	0.74
1:C:83:LYS:HB2	1:C:83:LYS:NZ	2.02	0.74
1:C:479:GLU:HG2	1:C:485:LYS:HZ2	1.53	0.74
1:B:420:THR:HG23	1:B:576:PRO:HG3	1.69	0.74
1:C:380:GLU:HG2	1:C:466:TYR:CE1	2.22	0.74
1:B:398:GLU:HG2	1:B:425:SER:OG	1.85	0.74
1:C:382:ASN:HD21	3:C:682:HEM:HAD2	1.52	0.73
1:C:184:ARG:HA	1:C:438:ARG:O	1.89	0.73
1:C:120:ARG:HG2	1:C:531:LEU:HD12	1.70	0.73
1:C:398:GLU:HG2	1:C:425:SER:OG	1.88	0.73
1:A:123:LEU:O	1:A:469:ARG:NH2	2.22	0.73
1:D:382:ASN:HD21	3:D:682:HEM:HAD2	1.54	0.73
1:C:197:MET:HA	1:C:197:MET:CE	2.18	0.72
1:B:333:LYS:O	1:B:337:ILE:HG13	1.90	0.72
1:C:123:LEU:O	1:C:469:ARG:NH2	2.22	0.72
1:D:280:PRO:CG	1:D:283:LEU:HD12	2.20	0.71
1:C:405:LYS:H	1:C:405:LYS:HD2	1.55	0.71
1:D:196:MET:HG2	1:D:429:GLN:HG2	1.73	0.71
1:D:420:THR:HG23	1:D:576:PRO:HG3	1.71	0.71
1:D:553:GLU:HG3	1:D:557:LYS:NZ	2.06	0.71
1:A:280:PRO:CG	1:A:283:LEU:HD12	2.20	0.70
1:C:420:THR:OG1	1:C:573:LYS:HB3	1.91	0.70
1:D:333:LYS:O	1:D:337:ILE:HG13	1.91	0.70
1:B:281:GLU:O	1:B:283:LEU:N	2.25	0.70
1:B:108:LEU:O	1:B:112:ILE:HG12	1.92	0.70
1:D:253:LYS:HE3	1:D:269:THR:HG22	1.72	0.70
1:A:120:ARG:HG2	1:A:531:LEU:HD12	1.72	0.70
1:A:295:VAL:CG1	1:A:298:LEU:HD22	2.22	0.69
1:A:333:LYS:O	1:A:337:ILE:HG13	1.91	0.69
1:A:382:ASN:HD21	3:A:682:HEM:HAD2	1.56	0.69
1:D:479:GLU:HG2	1:D:485:LYS:NZ	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:398:GLU:HG3	1:C:421:GLN:NE2	2.06	0.69
1:B:291:VAL:CG2	1:B:294:LEU:HD12	2.21	0.69
1:C:286:ALA:O	1:C:287:VAL:HG22	1.93	0.69
1:B:382:ASN:HD21	3:B:682:HEM:HAD2	1.56	0.68
1:C:197:MET:HA	1:C:197:MET:HE2	1.76	0.68
1:B:83:LYS:HB2	1:B:83:LYS:NZ	2.08	0.68
1:C:295:VAL:CG1	1:C:298:LEU:HD22	2.23	0.68
1:D:120:ARG:HG2	1:D:531:LEU:HD12	1.76	0.68
1:C:295:VAL:HG12	1:C:298:LEU:HD22	1.76	0.68
1:C:403:SER:HB2	1:C:405:LYS:HD2	1.76	0.68
1:A:253:LYS:CE	1:A:269:THR:HG22	2.24	0.67
1:B:287:VAL:HG11	1:B:299:MET:SD	2.34	0.67
1:D:295:VAL:CG1	1:D:298:LEU:HD22	2.25	0.67
1:C:454:GLN:HA	1:C:457:GLU:HG2	1.74	0.67
1:A:403:SER:HB2	1:A:405:LYS:HD2	1.76	0.67
1:D:291:VAL:CG2	1:D:294:LEU:HD12	2.23	0.67
1:D:454:GLN:HA	1:D:457:GLU:HG2	1.75	0.67
1:C:291:VAL:CG2	1:C:294:LEU:HD12	2.25	0.67
1:A:286:ALA:O	1:A:287:VAL:HG22	1.95	0.67
1:B:196:MET:HG2	1:B:429:GLN:HG2	1.77	0.67
1:C:420:THR:HG23	1:C:576:PRO:HG3	1.75	0.67
1:A:291:VAL:CG2	1:A:294:LEU:HD12	2.25	0.67
1:A:295:VAL:HG12	1:A:298:LEU:HD22	1.76	0.66
1:B:495:TYR:HE2	1:B:502:GLU:HG3	1.60	0.66
1:D:553:GLU:HG3	1:D:557:LYS:HZ1	1.60	0.66
1:A:213:ASP:OD1	1:A:215:LYS:HE2	1.96	0.66
1:A:194:SER:OG	1:A:351:HIS:HE1	1.78	0.66
1:D:108:LEU:O	1:D:112:ILE:HG12	1.95	0.66
1:D:458:MET:CE	1:D:460:TYR:HE1	2.08	0.66
1:A:191:PRO:HD2	1:A:433:ARG:HG3	1.75	0.66
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.77	0.66
1:D:123:LEU:O	1:D:469:ARG:NH2	2.29	0.66
1:A:83:LYS:NZ	1:A:83:LYS:HB2	2.11	0.66
1:D:276:PRO:HG2	1:D:409:TYR:CD2	2.29	0.66
1:B:280:PRO:CG	1:B:283:LEU:HD12	2.26	0.65
1:D:148:TYR:HD1	1:D:377:ILE:HG13	1.61	0.65
1:A:276:PRO:HG2	1:A:409:TYR:CD2	2.31	0.65
1:B:183:LEU:HD21	1:B:445:GLN:HB3	1.77	0.65
1:A:458:MET:CE	1:A:460:TYR:HE1	2.08	0.65
1:A:546:LYS:HD2	1:B:46:GLU:OE2	1.97	0.65
1:B:381:PHE:O	1:B:385:TYR:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:527:ALA:HB3	1:C:528:PRO:HD3	1.78	0.65
1:A:381:PHE:O	1:A:385:TYR:HB2	1.97	0.65
1:B:475:TYR:HA	1:B:480:GLU:OE2	1.97	0.65
1:D:280:PRO:HG3	1:D:283:LEU:HD12	1.79	0.64
1:D:83:LYS:HB2	1:D:83:LYS:NZ	2.12	0.64
1:D:295:VAL:HG12	1:D:298:LEU:HD22	1.79	0.64
1:C:132:VAL:HG21	1:C:219:GLY:HA3	1.80	0.64
1:D:184:ARG:HA	1:D:438:ARG:O	1.98	0.64
1:B:197:MET:HA	1:B:197:MET:CE	2.28	0.64
1:B:132:VAL:HG21	1:B:219:GLY:HA3	1.80	0.64
1:D:276:PRO:O	1:D:279:ILE:HG12	1.97	0.64
1:A:197:MET:HA	1:A:197:MET:CE	2.29	0.63
1:B:458:MET:CE	1:B:460:TYR:HE1	2.08	0.63
1:A:454:GLN:HA	1:A:457:GLU:HG2	1.80	0.63
1:B:215:LYS:NZ	1:B:222:ARG:HH21	1.96	0.63
1:C:46:GLU:OE2	1:D:546:LYS:HD2	1.99	0.63
1:D:120:ARG:HD3	4:D:701:FLP:O	1.99	0.63
1:D:420:THR:OG1	1:D:573:LYS:HB3	1.99	0.63
1:B:148:TYR:HD1	1:B:377:ILE:HG13	1.63	0.63
1:D:211:LYS:HZ1	1:D:236:GLU:HG2	1.64	0.63
1:C:196:MET:HG2	1:C:429:GLN:HG2	1.80	0.62
1:B:123:LEU:O	1:B:469:ARG:NH2	2.32	0.62
1:C:276:PRO:HG2	1:C:409:TYR:CD2	2.34	0.62
1:D:114:LYS:HD3	1:D:369:GLN:NE2	2.14	0.62
1:C:333:LYS:O	1:C:337:ILE:HG13	1.98	0.62
1:A:506:ALA:O	1:A:510:GLU:HB2	1.99	0.62
1:C:85:THR:O	1:C:89:VAL:HG23	2.00	0.62
1:B:398:GLU:HG3	1:B:421:GLN:NE2	2.15	0.62
1:C:504:TYR:HB3	1:C:505:PRO:HD3	1.80	0.62
1:C:506:ALA:O	1:C:510:GLU:HB2	1.99	0.62
1:A:38:SER:OG	1:A:40:PRO:HD3	1.99	0.62
1:C:131:ASN:HA	1:C:150:ARG:HG2	1.82	0.62
1:D:475:TYR:HA	1:D:480:GLU:OE2	1.99	0.62
1:C:191:PRO:HD2	1:C:433:ARG:HG3	1.80	0.62
1:D:506:ALA:O	1:D:510:GLU:HB2	1.99	0.62
1:C:491:LEU:HD11	1:C:509:VAL:HG11	1.82	0.62
1:A:287:VAL:HG11	1:A:299:MET:SD	2.40	0.61
1:B:253:LYS:HE3	1:B:269:THR:HG22	1.81	0.61
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.82	0.61
1:C:150:ARG:NH2	1:C:458:MET:O	2.33	0.61
1:C:108:LEU:O	1:C:112:ILE:HG12	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:GLU:HG3	1:A:421:GLN:NE2	2.16	0.61
1:A:475:TYR:HA	1:A:480:GLU:OE2	2.00	0.61
1:B:145:LEU:HD23	1:B:376:ARG:CZ	2.31	0.61
1:B:276:PRO:HG2	1:B:409:TYR:CD2	2.35	0.61
1:D:183:LEU:HD21	1:D:445:GLN:HB3	1.81	0.61
1:C:381:PHE:O	1:C:385:TYR:HB2	2.00	0.61
1:B:405:LYS:H	1:B:405:LYS:CD	2.14	0.61
1:A:116:VAL:O	1:A:120:ARG:HB2	2.00	0.60
1:A:491:LEU:HD11	1:A:509:VAL:HG11	1.82	0.60
1:D:145:LEU:HD23	1:D:376:ARG:CZ	2.31	0.60
1:D:281:GLU:O	1:D:283:LEU:N	2.34	0.60
1:D:381:PHE:O	1:D:385:TYR:HB2	2.00	0.60
1:A:46:GLU:OE2	1:B:546:LYS:HD2	2.01	0.60
1:A:575:CYS:N	1:A:576:PRO:HD3	2.17	0.60
1:D:197:MET:CE	1:D:197:MET:HA	2.31	0.60
1:A:132:VAL:HG21	1:A:219:GLY:HA3	1.82	0.60
1:A:281:GLU:O	1:A:283:LEU:N	2.34	0.60
1:A:147:TYR:OH	2:A:671:NAG:H62	2.01	0.60
1:B:211:LYS:NZ	1:B:236:GLU:CG	2.65	0.60
1:D:197:MET:HA	1:D:197:MET:HE2	1.84	0.60
1:C:148:TYR:HD1	1:C:377:ILE:HG13	1.64	0.60
1:C:183:LEU:HD21	1:C:445:GLN:HB3	1.83	0.60
1:D:215:LYS:NZ	1:D:222:ARG:HH21	2.00	0.60
1:A:148:TYR:HD1	1:A:377:ILE:HG13	1.66	0.59
1:B:475:TYR:CD1	1:B:480:GLU:HG2	2.37	0.59
1:D:132:VAL:HG21	1:D:219:GLY:HA3	1.83	0.59
1:D:211:LYS:NZ	1:D:236:GLU:CG	2.66	0.59
1:D:398:GLU:O	1:D:399:ASP:HB2	2.02	0.59
1:B:83:LYS:HB2	1:B:83:LYS:HZ3	1.66	0.59
1:B:420:THR:OG1	1:B:573:LYS:HB3	2.03	0.59
1:B:215:LYS:HD3	1:B:215:LYS:N	2.18	0.59
1:B:506:ALA:O	1:B:510:GLU:HB2	2.01	0.59
1:C:75:LEU:HG	1:C:79:LYS:HE2	1.83	0.59
1:C:133:HIS:CD2	1:C:147:TYR:HE2	2.21	0.59
1:C:281:GLU:O	1:C:283:LEU:N	2.35	0.59
1:D:479:GLU:HG2	1:D:485:LYS:HZ2	1.67	0.59
1:A:495:TYR:HE2	1:A:502:GLU:HG3	1.68	0.59
1:C:546:LYS:HD2	1:D:46:GLU:OE2	2.03	0.59
1:A:131:ASN:HA	1:A:150:ARG:HG2	1.85	0.59
1:A:412:SER:O	1:A:416:GLU:HB2	2.02	0.59
1:C:213:ASP:OD1	1:C:215:LYS:HE2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:GLU:HA	1:A:428:ARG:NH2	2.11	0.58
1:C:475:TYR:HA	1:C:480:GLU:OE2	2.03	0.58
1:D:287:VAL:HG11	1:D:299:MET:SD	2.44	0.58
1:D:504:TYR:HB3	1:D:505:PRO:HD3	1.85	0.58
1:B:447:VAL:HG13	3:B:682:HEM:HBA2	1.85	0.58
1:B:479:GLU:HG2	1:B:485:LYS:CE	2.31	0.58
1:D:83:LYS:HB2	1:D:83:LYS:HZ3	1.69	0.58
1:A:211:LYS:HZ1	1:A:236:GLU:HG2	1.67	0.58
1:B:180:LYS:O	1:B:438:ARG:NH2	2.36	0.58
1:C:83:LYS:HB2	1:C:83:LYS:HZ3	1.67	0.57
1:C:398:GLU:O	1:C:399:ASP:HB2	2.04	0.57
1:D:398:GLU:HG3	1:D:421:GLN:NE2	2.19	0.57
1:A:197:MET:HA	1:A:197:MET:HE2	1.85	0.57
1:A:553:GLU:O	1:A:557:LYS:HE3	2.05	0.57
1:D:211:LYS:NZ	1:D:236:GLU:HG2	2.18	0.57
1:D:253:LYS:CE	1:D:269:THR:HG22	2.34	0.57
1:A:108:LEU:O	1:A:112:ILE:HG12	2.04	0.57
1:A:150:ARG:NH2	1:A:458:MET:O	2.38	0.57
1:B:253:LYS:CE	1:B:269:THR:HG22	2.34	0.57
1:C:495:TYR:HE2	1:C:502:GLU:HG3	1.70	0.57
1:A:196:MET:HG2	1:A:429:GLN:HG2	1.86	0.57
1:C:525:LEU:O	1:C:528:PRO:HD2	2.04	0.57
1:D:575:CYS:N	1:D:576:PRO:HD3	2.20	0.57
1:A:276:PRO:O	1:A:279:ILE:HG12	2.05	0.57
1:A:398:GLU:O	1:A:399:ASP:HB2	2.05	0.57
1:B:89:VAL:O	1:B:93:LEU:HD23	2.04	0.57
1:B:211:LYS:HZ1	1:B:236:GLU:HG2	1.70	0.57
1:A:133:HIS:HD2	1:A:147:TYR:OH	1.87	0.56
1:A:475:TYR:CD1	1:A:480:GLU:HG2	2.40	0.56
1:C:116:VAL:O	1:C:120:ARG:HB2	2.05	0.56
1:C:287:VAL:HG11	1:C:299:MET:SD	2.44	0.56
1:A:420:THR:OG1	1:A:573:LYS:HB3	2.04	0.56
1:B:211:LYS:NZ	1:B:236:GLU:HG2	2.20	0.56
1:B:504:TYR:HB3	1:B:505:PRO:HD3	1.88	0.56
1:D:403:SER:HB2	1:D:405:LYS:HD2	1.87	0.56
1:C:107:PHE:CD1	1:C:107:PHE:N	2.72	0.56
1:C:475:TYR:CD1	1:C:480:GLU:HG2	2.41	0.56
1:D:402:TYR:OH	1:D:417:HIS:HE1	1.89	0.56
1:B:442:ILE:O	1:B:445:GLN:HG2	2.06	0.56
1:D:131:ASN:HA	1:D:150:ARG:HG2	1.87	0.56
1:D:215:LYS:HZ1	1:D:222:ARG:HH21	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:LEU:HG	1:B:79:LYS:HE2	1.87	0.55
1:B:281:GLU:C	1:B:283:LEU:H	2.15	0.55
1:D:405:LYS:H	1:D:405:LYS:CD	2.15	0.55
1:A:162:PRO:O	1:A:163:MET:HE2	2.07	0.55
1:B:295:VAL:CG1	1:B:298:LEU:HD22	2.37	0.55
1:D:286:ALA:O	1:D:287:VAL:HG22	2.07	0.55
1:C:458:MET:CE	1:C:460:TYR:HE1	2.12	0.55
1:A:203:GLN:HB3	1:A:298:LEU:HD11	1.89	0.55
1:C:405:LYS:H	1:C:405:LYS:CD	2.14	0.55
1:A:543:GLN:NE2	1:B:127:PRO:O	2.40	0.55
1:B:280:PRO:HG3	1:B:283:LEU:HD12	1.87	0.55
1:C:211:LYS:NZ	1:C:236:GLU:CG	2.70	0.55
1:D:133:HIS:CD2	1:D:147:TYR:HE2	2.25	0.55
1:D:495:TYR:HE2	1:D:502:GLU:HG3	1.72	0.55
1:A:183:LEU:HD21	1:A:445:GLN:HB3	1.89	0.54
1:A:525:LEU:O	1:A:528:PRO:HD2	2.07	0.54
1:C:276:PRO:O	1:C:279:ILE:HG12	2.07	0.54
1:A:211:LYS:NZ	1:A:236:GLU:CG	2.71	0.54
1:B:197:MET:HA	1:B:197:MET:HE2	1.88	0.54
1:B:419:LEU:HD23	1:B:419:LEU:H	1.72	0.54
1:C:553:GLU:HG3	1:C:557:LYS:HE3	1.90	0.54
1:D:211:LYS:HZ1	1:D:236:GLU:CG	2.19	0.54
1:B:181:VAL:HG12	1:B:487:MET:HG2	1.90	0.54
3:B:682:HEM:HBC2	3:B:682:HEM:HHD	1.90	0.54
1:C:215:LYS:HD3	1:C:215:LYS:N	2.22	0.54
1:D:203:GLN:HB3	1:D:298:LEU:HD11	1.89	0.54
1:C:318:GLN:NE2	1:C:318:GLN:HA	2.22	0.54
1:A:509:VAL:HG12	1:A:509:VAL:O	2.08	0.54
3:A:682:HEM:HBC2	3:A:682:HEM:HHD	1.89	0.54
1:C:575:CYS:N	1:C:576:PRO:HD3	2.23	0.54
1:A:107:PHE:CD1	1:A:107:PHE:N	2.73	0.54
1:B:107:PHE:CD1	1:B:107:PHE:N	2.74	0.54
1:C:478:PHE:CZ	1:C:495:TYR:HB2	2.43	0.54
1:B:116:VAL:O	1:B:120:ARG:HB2	2.08	0.54
1:B:478:PHE:CZ	1:B:495:TYR:HB2	2.43	0.54
1:C:253:LYS:HE2	1:C:269:THR:HG22	1.90	0.54
1:A:215:LYS:HD3	1:A:215:LYS:N	2.23	0.53
1:B:133:HIS:CD2	1:B:147:TYR:HE2	2.26	0.53
1:B:211:LYS:HZ1	1:B:236:GLU:CG	2.20	0.53
1:A:433:ARG:HD3	1:A:435:ALA:O	2.09	0.53
1:B:553:GLU:HG3	1:B:557:LYS:HE3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ALA:O	1:B:287:VAL:HG22	2.08	0.53
1:C:137:LYS:O	1:C:138:SER:O	2.27	0.53
1:C:145:LEU:HD23	1:C:376:ARG:CZ	2.39	0.53
1:C:215:LYS:NZ	1:C:222:ARG:HH21	2.06	0.53
1:D:181:VAL:HG12	1:D:487:MET:HG2	1.90	0.53
1:B:131:ASN:HA	1:B:150:ARG:HG2	1.90	0.53
1:C:114:LYS:HE2	1:C:365:LEU:O	2.08	0.53
1:D:238:LEU:HD22	1:D:242:HIS:CD2	2.44	0.53
1:A:215:LYS:NZ	1:A:222:ARG:HH21	2.07	0.53
1:B:64:PHE:HD2	1:B:70:THR:O	1.91	0.53
1:B:418:GLY:O	1:B:420:THR:N	2.41	0.53
1:C:320:HIS:HE1	1:C:551:GLY:O	1.92	0.53
1:A:183:LEU:HD22	1:A:442:ILE:HG12	1.90	0.53
1:B:206:THR:HB	1:B:210:PHE:CD2	2.44	0.53
1:B:355:TYR:HE2	4:B:701:FLP:O1	1.91	0.53
1:B:479:GLU:CG	1:B:485:LYS:HZ2	2.19	0.53
1:C:478:PHE:CE2	1:C:492:LYS:HA	2.43	0.53
1:D:418:GLY:O	1:D:420:THR:N	2.42	0.53
1:A:479:GLU:HG2	1:A:485:LYS:HZ1	1.70	0.53
1:B:398:GLU:O	1:B:399:ASP:HB2	2.09	0.53
1:D:206:THR:HB	1:D:210:PHE:CD2	2.44	0.53
1:B:402:TYR:OH	1:B:417:HIS:HE1	1.92	0.53
1:B:523:VAL:HA	4:B:701:FLP:H3	1.91	0.53
1:D:273:MET:SD	1:D:286:ALA:O	2.67	0.53
1:D:475:TYR:CD1	1:D:480:GLU:HG2	2.43	0.53
1:A:211:LYS:HZ1	1:A:236:GLU:CG	2.22	0.53
1:B:238:LEU:HD22	1:B:242:HIS:NE2	2.24	0.52
1:B:575:CYS:N	1:B:576:PRO:HD3	2.24	0.52
1:A:478:PHE:CZ	1:A:495:TYR:HB2	2.45	0.52
1:B:433:ARG:H	1:B:439:ASN:ND2	2.07	0.52
1:B:33:ALA:N	1:B:158:ASP:O	2.42	0.52
1:B:112:ILE:HB	1:B:357:PHE:CZ	2.45	0.52
1:C:423:VAL:HG13	1:C:578:THR:HG23	1.92	0.52
1:C:433:ARG:H	1:C:439:ASN:ND2	2.08	0.52
1:D:389:PRO:HG3	1:D:440:VAL:HG22	1.92	0.52
1:A:64:PHE:HD2	1:A:70:THR:O	1.93	0.52
1:A:127:PRO:O	1:B:543:GLN:NE2	2.43	0.52
1:A:280:PRO:HG2	1:A:283:LEU:HD12	1.92	0.52
1:A:418:GLY:O	1:A:420:THR:N	2.43	0.52
1:B:94:THR:O	1:B:356:HIS:CE1	2.63	0.52
1:C:203:GLN:HB3	1:C:298:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:TYR:OH	1:C:417:HIS:HE1	1.93	0.52
1:A:145:LEU:HD23	1:A:376:ARG:CZ	2.38	0.52
1:A:178:LEU:O	1:A:182:LEU:HB2	2.10	0.52
1:B:203:GLN:HG3	3:B:682:HEM:C2C	2.45	0.52
1:B:44:ARG:HD2	1:B:469:ARG:HD2	1.92	0.52
1:B:119:SER:O	1:B:122:TYR:HD1	1.93	0.52
1:D:419:LEU:HD23	1:D:419:LEU:H	1.75	0.52
1:A:402:TYR:OH	1:A:417:HIS:HE1	1.93	0.52
1:B:203:GLN:HB3	1:B:298:LEU:HD11	1.92	0.52
1:C:194:SER:OG	1:C:351:HIS:HE1	1.93	0.52
1:D:215:LYS:HD3	1:D:215:LYS:N	2.24	0.52
1:B:423:VAL:HG13	1:B:578:THR:HG23	1.90	0.51
1:C:509:VAL:HG12	1:C:509:VAL:O	2.10	0.51
1:D:382:ASN:ND2	3:D:682:HEM:HAD2	2.22	0.51
1:C:192:GLN:OE1	1:C:517:ILE:HG22	2.10	0.51
1:C:382:ASN:ND2	3:C:682:HEM:HAD2	2.24	0.51
1:C:553:GLU:O	1:C:557:LYS:HG2	2.10	0.51
1:D:150:ARG:NH2	1:D:458:MET:O	2.43	0.51
1:D:107:PHE:CD1	1:D:107:PHE:N	2.74	0.51
1:D:318:GLN:NE2	1:D:318:GLN:HA	2.25	0.51
1:B:38:SER:OG	1:B:40:PRO:HD3	2.09	0.51
1:B:238:LEU:HD22	1:B:242:HIS:CD2	2.45	0.51
1:B:403:SER:HB2	1:B:405:LYS:HD2	1.92	0.51
1:A:292:PHE:O	1:A:299:MET:HE2	2.11	0.51
1:C:206:THR:HB	1:C:210:PHE:CD2	2.45	0.51
1:D:276:PRO:HG2	1:D:409:TYR:CG	2.45	0.51
1:B:470:PHE:CG	1:B:525:LEU:HD22	2.46	0.51
3:C:682:HEM:HBC2	3:C:682:HEM:HHD	1.92	0.51
1:D:260:GLU:HB2	1:D:262:TYR:CE2	2.45	0.51
1:B:509:VAL:HG12	1:B:509:VAL:O	2.11	0.51
1:A:74:PHE:O	1:A:77:ARG:HB2	2.11	0.51
1:A:389:PRO:HG3	1:A:440:VAL:HG22	1.92	0.51
1:C:133:HIS:CD2	1:C:147:TYR:CE2	2.99	0.51
1:D:553:GLU:O	1:D:557:LYS:HG2	2.11	0.51
1:A:419:LEU:HD23	1:A:419:LEU:H	1.75	0.51
1:D:232:HIS:CD2	1:D:233:ILE:HG13	2.46	0.51
1:C:113:MET:HA	1:C:116:VAL:HG13	1.94	0.50
1:C:412:SER:O	1:C:416:GLU:HB2	2.11	0.50
1:D:42:GLN:O	1:D:69:CYS:HB2	2.10	0.50
1:A:211:LYS:NZ	1:A:236:GLU:HG2	2.26	0.50
1:B:525:LEU:O	1:B:528:PRO:HD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:447:VAL:HG13	3:D:682:HEM:CBA	2.39	0.50
1:C:119:SER:O	1:C:122:TYR:HD1	1.94	0.50
1:A:150:ARG:HD2	1:A:380:GLU:OE2	2.10	0.50
1:B:276:PRO:O	1:B:279:ILE:HG12	2.11	0.50
1:D:491:LEU:HD11	1:D:509:VAL:HG11	1.94	0.50
3:D:682:HEM:HBC2	3:D:682:HEM:HHD	1.94	0.50
1:C:424:GLU:HA	1:C:428:ARG:NH2	2.11	0.50
1:D:38:SER:OG	1:D:40:PRO:HD3	2.11	0.50
1:D:231:ASN:OD1	1:D:231:ASN:C	2.55	0.50
1:A:553:GLU:O	1:A:557:LYS:HG2	2.11	0.50
1:C:211:LYS:HZ1	1:C:236:GLU:CG	2.25	0.50
1:C:232:HIS:CD2	1:C:233:ILE:HG13	2.47	0.50
1:D:275:TYR:CD2	1:D:284:GLN:HG2	2.46	0.50
1:A:181:VAL:HG12	1:A:487:MET:HG2	1.92	0.50
1:A:414:LEU:HD11	1:A:419:LEU:CD2	2.42	0.50
1:C:198:PHE:HB2	1:C:580:PHE:HB3	1.94	0.50
1:D:75:LEU:HG	1:D:79:LYS:HE2	1.92	0.50
1:D:119:SER:O	1:D:122:TYR:HD1	1.95	0.50
1:C:211:LYS:NZ	1:C:236:GLU:HG2	2.26	0.50
1:A:433:ARG:H	1:A:439:ASN:ND2	2.09	0.50
1:B:260:GLU:HB2	1:B:262:TYR:CE2	2.47	0.50
1:B:478:PHE:CE2	1:B:492:LYS:HA	2.47	0.50
1:D:509:VAL:HG12	1:D:509:VAL:O	2.12	0.50
1:A:577:PHE:CE1	1:D:267:LYS:NZ	2.79	0.49
1:B:295:VAL:HG12	1:B:298:LEU:HD22	1.92	0.49
1:C:553:GLU:O	1:C:557:LYS:HE3	2.12	0.49
1:A:175:LYS:HD2	1:A:179:GLU:OE2	2.12	0.49
1:A:260:GLU:HB2	1:A:262:TYR:CE2	2.47	0.49
1:A:398:GLU:HG3	1:A:421:GLN:CD	2.37	0.49
1:B:389:PRO:HB2	1:B:434:VAL:HA	1.94	0.49
1:B:527:ALA:HA	4:B:701:FLP:C7	2.41	0.49
1:C:398:GLU:HG3	1:C:421:GLN:CD	2.37	0.49
1:C:414:LEU:HD11	1:C:419:LEU:CD2	2.41	0.49
1:C:269:THR:O	1:C:270:GLN:HB2	2.13	0.49
1:A:273:MET:SD	1:A:286:ALA:O	2.70	0.49
1:B:183:LEU:HD22	1:B:442:ILE:HG12	1.94	0.49
1:C:275:TYR:CD2	1:C:284:GLN:HG2	2.48	0.49
1:C:398:GLU:HG3	1:C:421:GLN:HE22	1.75	0.49
1:D:33:ALA:N	1:D:158:ASP:O	2.46	0.49
1:D:122:TYR:CD2	1:D:122:TYR:O	2.66	0.49
1:B:203:GLN:HG3	3:B:682:HEM:C1C	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:ILE:HB	1:C:357:PHE:CZ	2.47	0.49
1:D:33:ALA:HB3	1:D:158:ASP:OD2	2.12	0.49
1:B:382:ASN:ND2	3:B:682:HEM:HAD2	2.24	0.49
1:C:389:PRO:HG3	1:C:440:VAL:HG22	1.94	0.49
1:D:94:THR:O	1:D:356:HIS:CE1	2.65	0.49
1:A:206:THR:HB	1:A:210:PHE:CD2	2.47	0.49
1:B:303:THR:O	1:B:307:ARG:HD3	2.13	0.49
1:C:33:ALA:N	1:C:158:ASP:O	2.46	0.49
1:C:414:LEU:HD11	1:C:419:LEU:HD23	1.93	0.49
1:D:64:PHE:HD2	1:D:70:THR:O	1.95	0.49
1:D:423:VAL:HG13	1:D:578:THR:HG23	1.95	0.49
1:B:240:ARG:O	1:B:241:GLN:C	2.56	0.49
1:B:273:MET:SD	1:B:286:ALA:O	2.71	0.49
1:B:318:GLN:HA	1:B:318:GLN:NE2	2.27	0.49
1:B:423:VAL:CG1	1:B:578:THR:HG23	2.43	0.49
1:C:350:GLN:HE22	1:C:359:LEU:H	1.61	0.49
1:D:89:VAL:O	1:D:93:LEU:HD23	2.13	0.49
1:A:423:VAL:HG13	1:A:578:THR:HG23	1.95	0.48
1:C:133:HIS:HD2	1:C:147:TYR:OH	1.95	0.48
1:D:344:VAL:HG12	1:D:534:LEU:HD21	1.93	0.48
1:A:113:MET:HA	1:A:116:VAL:HG13	1.94	0.48
1:B:85:THR:O	1:B:89:VAL:HG23	2.14	0.48
1:C:74:PHE:O	1:C:77:ARG:HB2	2.13	0.48
1:D:133:HIS:HD2	1:D:147:TYR:OH	1.96	0.48
1:D:320:HIS:HE1	1:D:551:GLY:O	1.95	0.48
1:A:133:HIS:CD2	1:A:147:TYR:HE1	2.31	0.48
1:A:137:LYS:O	1:A:138:SER:O	2.30	0.48
1:A:551:GLY:HA2	1:B:48:MET:HE1	1.94	0.48
1:B:244:LEU:HD11	1:B:288:GLY:HA2	1.95	0.48
1:C:352:LEU:HD11	1:C:518:PHE:CZ	2.47	0.48
3:D:682:HEM:HHD	3:D:682:HEM:CBC	2.44	0.48
1:A:147:TYR:OH	2:A:671:NAG:C6	2.61	0.48
1:A:551:GLY:CA	1:B:48:MET:HE1	2.44	0.48
1:C:478:PHE:HZ	1:C:495:TYR:HB2	1.78	0.48
1:D:245:ARG:HD3	1:D:329:PHE:CD2	2.48	0.48
1:B:172:PRO:HG3	1:B:495:TYR:CE1	2.49	0.48
1:C:442:ILE:O	1:C:445:GLN:HG2	2.13	0.48
1:B:210:PHE:HB3	3:B:682:HEM:HBD1	1.95	0.48
1:D:172:PRO:HG3	1:D:495:TYR:CE1	2.48	0.48
1:C:350:GLN:HE22	1:C:359:LEU:N	2.11	0.48
1:C:280:PRO:CG	1:C:283:LEU:HD12	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:238:LEU:HD22	1:D:242:HIS:NE2	2.29	0.48
1:A:281:GLU:C	1:A:283:LEU:H	2.22	0.48
1:A:320:HIS:HE1	1:A:551:GLY:O	1.96	0.48
1:B:553:GLU:O	1:B:557:LYS:HE3	2.14	0.48
1:D:137:LYS:O	1:D:138:SER:O	2.32	0.48
1:A:33:ALA:HB3	1:A:158:ASP:OD2	2.14	0.47
1:A:75:LEU:HG	1:A:79:LYS:HE2	1.94	0.47
1:A:232:HIS:CD2	1:A:233:ILE:HG13	2.49	0.47
1:A:276:PRO:HG2	1:A:409:TYR:CG	2.49	0.47
1:D:244:LEU:HD11	1:D:288:GLY:HA2	1.96	0.47
1:A:140:GLU:OE2	2:A:671:NAG:O5	2.32	0.47
1:A:172:PRO:HG3	1:A:495:TYR:CE1	2.50	0.47
1:B:438:ARG:NH1	1:B:487:MET:HG3	2.29	0.47
1:C:64:PHE:HD2	1:C:70:THR:O	1.97	0.47
1:C:385:TYR:OH	4:C:701:FLP:H	2.15	0.47
1:D:85:THR:O	1:D:89:VAL:HG23	2.14	0.47
1:A:94:THR:O	1:A:356:HIS:CE1	2.68	0.47
1:B:42:GLN:O	1:B:69:CYS:HB2	2.14	0.47
1:B:414:LEU:HD11	1:B:419:LEU:CD2	2.44	0.47
1:C:260:GLU:HB2	1:C:262:TYR:CE2	2.49	0.47
1:A:108:LEU:O	1:A:111:LEU:HB3	2.14	0.47
1:B:119:SER:O	1:B:122:TYR:CD1	2.68	0.47
1:B:213:ASP:OD1	1:B:215:LYS:HE2	2.14	0.47
1:B:320:HIS:HE1	1:B:551:GLY:O	1.98	0.47
1:C:181:VAL:HG12	1:C:487:MET:HG2	1.96	0.47
1:D:527:ALA:HA	4:D:701:FLP:C7	2.44	0.47
1:B:215:LYS:HZ3	1:B:222:ARG:HH21	1.62	0.47
1:C:178:LEU:O	1:C:182:LEU:HB2	2.15	0.47
1:A:294:LEU:HD22	1:A:409:TYR:CE1	2.50	0.47
1:B:232:HIS:CD2	1:B:233:ILE:HG13	2.49	0.47
1:C:240:ARG:O	1:C:241:GLN:C	2.58	0.47
1:C:389:PRO:HB2	1:C:434:VAL:HA	1.96	0.47
1:C:543:GLN:NE2	1:D:127:PRO:O	2.48	0.47
1:D:104:ASN:ND2	1:D:358:LYS:HB2	2.30	0.47
1:D:116:VAL:O	1:D:120:ARG:HB2	2.14	0.47
1:B:150:ARG:NH2	1:B:458:MET:O	2.47	0.47
1:A:280:PRO:HG3	1:A:283:LEU:HD12	1.97	0.47
1:B:114:LYS:HD3	1:B:369:GLN:NE2	2.29	0.47
1:A:389:PRO:HB2	1:A:434:VAL:HA	1.97	0.47
1:B:113:MET:HA	1:B:116:VAL:HG13	1.97	0.47
1:B:352:LEU:HD11	1:B:518:PHE:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:GLU:HG3	1:B:421:GLN:CD	2.40	0.47
1:B:421:GLN:OE1	1:B:421:GLN:HA	2.15	0.47
3:B:682:HEM:HHD	3:B:682:HEM:CBC	2.44	0.47
1:C:249:ASP:CG	1:C:317:LYS:NZ	2.73	0.46
1:C:273:MET:SD	1:C:286:ALA:O	2.73	0.46
1:C:447:VAL:HG13	3:C:682:HEM:HBA2	1.97	0.46
1:D:119:SER:O	1:D:122:TYR:CD1	2.68	0.46
1:A:482:THR:HG22	1:A:509:VAL:HG12	1.98	0.46
1:B:388:HIS:C	1:B:390:LEU:H	2.24	0.46
1:B:420:THR:HA	1:B:576:PRO:HG2	1.98	0.46
1:D:155:VAL:HG12	1:D:459:LYS:NZ	2.31	0.46
1:A:33:ALA:N	1:A:158:ASP:O	2.48	0.46
1:B:230:LEU:HD13	1:B:233:ILE:HD12	1.96	0.46
1:C:108:LEU:O	1:C:111:LEU:HB3	2.16	0.46
1:C:183:LEU:HD22	1:C:442:ILE:HG12	1.97	0.46
1:C:419:LEU:HD23	1:C:419:LEU:H	1.78	0.46
1:D:230:LEU:N	1:D:230:LEU:HD23	2.30	0.46
1:D:269:THR:O	1:D:270:GLN:HB2	2.14	0.46
1:A:210:PHE:CE1	1:A:382:ASN:HA	2.50	0.46
1:A:244:LEU:HD11	1:A:288:GLY:HA2	1.96	0.46
1:B:387:TRP:HZ2	4:B:701:FLP:H5	1.81	0.46
1:B:319:GLU:HG3	1:B:554:VAL:HG11	1.96	0.46
1:C:89:VAL:O	1:C:93:LEU:HD23	2.14	0.46
1:C:203:GLN:O	1:C:207:HIS:ND1	2.48	0.46
1:C:482:THR:HG22	1:C:509:VAL:HG12	1.96	0.46
1:D:442:ILE:O	1:D:445:GLN:HG2	2.14	0.46
1:B:137:LYS:O	1:B:138:SER:O	2.33	0.46
1:B:478:PHE:HZ	1:B:495:TYR:HB2	1.80	0.46
1:C:34:ASN:HB3	1:C:37:CYS:SG	2.55	0.46
1:C:119:SER:O	1:C:122:TYR:CD1	2.68	0.46
1:C:249:ASP:CG	1:C:317:LYS:HZ2	2.23	0.46
1:C:385:TYR:CZ	4:C:701:FLP:H	2.50	0.46
1:C:553:GLU:HG3	1:C:557:LYS:CE	2.46	0.46
1:C:557:LYS:O	1:C:558:ILE:C	2.57	0.46
1:D:112:ILE:HB	1:D:357:PHE:CZ	2.50	0.46
1:C:109:ARG:HG3	1:C:357:PHE:CE1	2.50	0.46
1:C:122:TYR:O	1:C:122:TYR:CD2	2.69	0.46
1:D:198:PHE:HB2	1:D:580:PHE:HB3	1.98	0.46
1:A:114:LYS:HE2	1:A:365:LEU:O	2.16	0.46
1:D:178:LEU:O	1:D:182:LEU:HB2	2.16	0.46
1:A:388:HIS:C	1:A:390:LEU:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:TYR:OH	1:B:142:PHE:HB2	2.16	0.46
1:C:189:PRO:CB	1:C:430:ILE:HD12	2.46	0.46
1:C:204:HIS:ND1	1:C:292:PHE:CE2	2.84	0.46
1:C:388:HIS:C	1:C:390:LEU:H	2.24	0.46
1:C:388:HIS:CE1	1:C:447:VAL:HG11	2.51	0.46
1:D:113:MET:HA	1:D:116:VAL:HG13	1.97	0.46
1:D:355:TYR:HE2	4:D:701:FLP:O1	1.99	0.46
1:C:146:SER:O	1:C:220:PHE:HA	2.16	0.45
1:D:280:PRO:HG2	1:D:283:LEU:HD12	1.97	0.45
1:A:151:ALA:O	1:A:469:ARG:NH1	2.50	0.45
1:A:391:LEU:HD21	3:A:682:HEM:HHH	1.98	0.45
1:A:414:LEU:HD11	1:A:419:LEU:HD23	1.97	0.45
1:A:557:LYS:O	1:A:558:ILE:C	2.59	0.45
1:B:482:THR:HG22	1:B:509:VAL:HG12	1.97	0.45
3:C:682:HEM:HHH	3:C:682:HEM:CBH	2.45	0.45
1:B:276:PRO:HG2	1:B:409:TYR:CG	2.51	0.45
1:B:414:LEU:HD11	1:B:419:LEU:HD23	1.98	0.45
1:C:85:THR:OG1	1:C:88:THR:HG23	2.16	0.45
1:D:414:LEU:HD11	1:D:419:LEU:HD23	1.98	0.45
1:A:112:ILE:HB	1:A:357:PHE:CZ	2.52	0.45
1:A:240:ARG:O	1:A:241:GLN:C	2.60	0.45
1:A:269:THR:O	1:A:270:GLN:HB2	2.17	0.45
1:B:147:TYR:OH	2:B:671:NAG:C6	2.64	0.45
1:B:491:LEU:HD11	1:B:509:VAL:HG11	1.96	0.45
1:C:181:VAL:CG2	1:C:509:VAL:HG21	2.47	0.45
1:D:162:PRO:O	1:D:163:MET:HE2	2.15	0.45
1:A:183:LEU:HD23	1:A:183:LEU:HA	1.71	0.45
1:D:414:LEU:HD11	1:D:419:LEU:CD2	2.46	0.45
1:A:83:LYS:HB2	1:A:83:LYS:HZ3	1.82	0.45
1:D:412:SER:O	1:D:416:GLU:HB2	2.17	0.45
1:A:231:ASN:OD1	1:A:231:ASN:C	2.58	0.45
1:A:303:THR:O	1:A:307:ARG:HD3	2.17	0.45
1:B:553:GLU:O	1:B:557:LYS:HG2	2.17	0.45
1:C:196:MET:HE3	1:C:200:PHE:CE2	2.51	0.45
1:C:281:GLU:C	1:C:283:LEU:H	2.24	0.45
1:C:465:GLU:HA	1:C:465:GLU:OE1	2.17	0.45
1:C:510:GLU:O	1:C:512:PRO:HD3	2.17	0.45
1:D:34:ASN:HB3	1:D:37:CYS:SG	2.57	0.45
1:D:281:GLU:C	1:D:283:LEU:H	2.24	0.45
1:A:367:PHE:CD1	1:A:542:PRO:HG3	2.51	0.45
1:B:479:GLU:N	1:B:479:GLU:CD	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:LEU:HD22	1:C:242:HIS:NE2	2.32	0.45
1:C:583:GLN:H	1:C:583:GLN:CD	2.25	0.45
1:D:210:PHE:CE1	1:D:382:ASN:HA	2.52	0.45
1:A:294:LEU:HD22	1:A:409:TYR:CD1	2.52	0.45
1:B:384:LEU:HD12	1:B:384:LEU:C	2.42	0.45
1:C:418:GLY:O	1:C:420:THR:N	2.49	0.45
1:D:133:HIS:CD2	1:D:147:TYR:CE2	3.04	0.45
1:D:203:GLN:HG3	3:D:682:HEM:C1C	2.52	0.45
1:A:300:MET:HE3	1:A:300:MET:HB3	1.82	0.45
1:B:389:PRO:HG3	1:B:440:VAL:HG22	1.98	0.45
1:B:554:VAL:CG1	1:B:555:GLY:N	2.80	0.45
1:C:210:PHE:HB3	3:C:682:HEM:HBD1	1.99	0.45
1:C:500:VAL:HG12	1:C:500:VAL:O	2.17	0.45
1:D:44:ARG:HD2	1:D:469:ARG:HD2	1.98	0.45
1:D:465:GLU:OE1	1:D:465:GLU:HA	2.16	0.45
1:A:185:ARG:HB2	1:A:186:GLU:H	1.65	0.44
1:D:151:ALA:O	1:D:469:ARG:NH1	2.50	0.44
1:A:575:CYS:N	1:A:576:PRO:CD	2.80	0.44
1:C:216:ARG:HB3	1:C:220:PHE:CD2	2.53	0.44
1:D:83:LYS:HG3	1:D:83:LYS:O	2.17	0.44
1:D:388:HIS:C	1:D:390:LEU:H	2.25	0.44
1:A:105:ASN:O	1:A:106:PRO:HD3	2.18	0.44
1:A:482:THR:OG1	1:A:488:ALA:HB2	2.17	0.44
1:A:553:GLU:HG3	1:A:557:LYS:CE	2.47	0.44
1:B:33:ALA:HB3	1:B:158:ASP:OD2	2.18	0.44
1:C:244:LEU:HD11	1:C:288:GLY:HA2	2.00	0.44
1:D:155:VAL:HG12	1:D:459:LYS:HZ3	1.83	0.44
1:D:247:PHE:HA	1:D:325:ASP:CG	2.43	0.44
1:A:192:GLN:OE1	1:A:517:ILE:HG22	2.17	0.44
1:A:388:HIS:CE1	1:A:447:VAL:HG11	2.52	0.44
1:A:442:ILE:O	1:A:445:GLN:HG2	2.18	0.44
1:C:151:ALA:O	1:C:469:ARG:NH1	2.50	0.44
1:D:194:SER:OG	1:D:351:HIS:HE1	2.00	0.44
1:D:213:ASP:OD1	1:D:215:LYS:HE2	2.18	0.44
1:D:478:PHE:CZ	1:D:495:TYR:HB2	2.52	0.44
1:A:51:GLY:O	1:A:52:PHE:CB	2.66	0.44
1:A:138:SER:HB2	1:B:330:GLN:HB3	2.00	0.44
1:A:478:PHE:HZ	1:A:495:TYR:HB2	1.81	0.44
1:A:525:LEU:N	1:A:525:LEU:HD23	2.32	0.44
1:A:583:GLN:CD	1:A:583:GLN:H	2.24	0.44
1:D:316:LEU:HA	1:D:316:LEU:HD12	1.87	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:MET:O	1:B:117:LEU:HB2	2.17	0.44
1:B:122:TYR:CD2	1:B:122:TYR:O	2.71	0.44
1:B:344:VAL:HG12	1:B:534:LEU:HD21	1.99	0.44
1:C:183:LEU:HD23	1:C:183:LEU:HA	1.84	0.44
1:D:389:PRO:HB2	1:D:434:VAL:HA	1.98	0.44
1:A:120:ARG:HD3	4:A:701:FLP:O	2.18	0.44
1:A:382:ASN:ND2	3:A:682:HEM:HAD2	2.29	0.44
1:A:478:PHE:O	1:A:481:LEU:HB3	2.18	0.44
1:B:44:ARG:HD2	1:B:469:ARG:CD	2.48	0.44
1:B:142:PHE:CD2	1:B:142:PHE:C	2.95	0.44
1:C:33:ALA:HB3	1:C:158:ASP:OD2	2.17	0.44
1:C:276:PRO:HG2	1:C:409:TYR:CG	2.52	0.44
1:D:433:ARG:H	1:D:439:ASN:ND2	2.15	0.44
1:B:189:PRO:CB	1:B:430:ILE:HD12	2.48	0.44
1:B:350:GLN:HE22	1:B:359:LEU:N	2.16	0.44
1:D:482:THR:HG22	1:D:509:VAL:HG12	2.00	0.44
1:A:133:HIS:CD2	1:A:147:TYR:CE1	3.06	0.44
1:A:230:LEU:HD23	1:A:230:LEU:N	2.31	0.44
3:A:682:HEM:HHH	3:A:682:HEM:CBC	2.47	0.44
1:B:388:HIS:N	1:B:389:PRO:CD	2.81	0.44
1:C:197:MET:CE	1:C:197:MET:CA	2.93	0.44
1:D:96:PHE:O	1:D:97:LYS:C	2.61	0.44
1:D:109:ARG:HG3	1:D:357:PHE:CE1	2.53	0.44
1:D:500:VAL:HG12	1:D:500:VAL:O	2.17	0.44
1:D:557:LYS:O	1:D:558:ILE:C	2.60	0.44
1:A:352:LEU:HD11	1:A:518:PHE:CZ	2.52	0.43
1:A:565:GLN:HG3	1:D:268:ASP:OD1	2.18	0.43
1:C:231:ASN:OD1	1:C:231:ASN:C	2.61	0.43
1:D:482:THR:OG1	1:D:488:ALA:HB2	2.17	0.43
1:A:91:TYR:CD1	1:A:91:TYR:C	2.96	0.43
1:A:147:TYR:OH	2:A:671:NAG:C5	2.66	0.43
1:C:198:PHE:CD1	1:C:198:PHE:C	2.96	0.43
1:B:114:LYS:HB2	1:B:114:LYS:HE3	1.86	0.43
1:B:269:THR:O	1:B:270:GLN:HB2	2.17	0.43
1:C:352:LEU:HD11	1:C:518:PHE:HZ	1.81	0.43
1:A:92:ILE:HD12	1:A:92:ILE:H	1.83	0.43
1:A:114:LYS:HD3	1:A:369:GLN:NE2	2.32	0.43
1:A:119:SER:O	1:A:122:TYR:HD1	2.02	0.43
1:A:364:GLU:HA	1:A:367:PHE:CD2	2.53	0.43
1:B:133:HIS:CD2	1:B:147:TYR:CE2	3.07	0.43
1:B:172:PRO:HG3	1:B:495:TYR:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:LEU:O	1:B:182:LEU:HB2	2.18	0.43
1:C:48:MET:HE1	1:D:551:GLY:CA	2.49	0.43
1:C:122:TYR:CE1	1:C:123:LEU:CD2	3.01	0.43
1:C:210:PHE:CE1	1:C:382:ASN:HA	2.53	0.43
1:D:232:HIS:HD2	1:D:233:ILE:HG13	1.82	0.43
1:A:553:GLU:HG3	1:A:557:LYS:NZ	2.33	0.43
1:B:198:PHE:HB2	1:B:580:PHE:HB3	1.99	0.43
1:B:435:ALA:HB2	1:B:518:PHE:HA	2.00	0.43
1:D:39:ASN:N	1:D:40:PRO:CD	2.82	0.43
1:D:423:VAL:CG1	1:D:578:THR:HG23	2.48	0.43
1:A:203:GLN:O	1:A:207:HIS:ND1	2.51	0.43
1:A:318:GLN:NE2	1:A:318:GLN:HA	2.33	0.43
1:A:478:PHE:CE2	1:A:492:LYS:HA	2.53	0.43
1:B:232:HIS:HD2	1:B:233:ILE:HG13	1.84	0.43
1:C:230:LEU:N	1:C:230:LEU:HD23	2.33	0.43
1:C:396:ASN:HA	1:C:400:GLN:O	2.19	0.43
1:D:92:ILE:HD12	1:D:92:ILE:H	1.82	0.43
1:D:172:PRO:HG3	1:D:495:TYR:CD1	2.54	0.43
1:D:583:GLN:CD	1:D:583:GLN:H	2.26	0.43
1:B:557:LYS:O	1:B:558:ILE:C	2.62	0.43
1:C:544:TYR:O	1:C:546:LYS:N	2.51	0.43
1:D:189:PRO:CB	1:D:430:ILE:HD12	2.48	0.43
1:D:198:PHE:CZ	1:D:352:LEU:HD13	2.53	0.43
1:A:113:MET:O	1:A:117:LEU:HB2	2.18	0.43
1:B:34:ASN:HB3	1:B:37:CYS:SG	2.58	0.43
1:B:218:PRO:HB2	1:B:458:MET:SD	2.58	0.43
1:B:421:GLN:OE1	1:B:424:GLU:HB2	2.19	0.43
1:C:172:PRO:HG3	1:C:495:TYR:CE1	2.54	0.43
1:C:190:ASP:HA	1:C:191:PRO:HD2	1.84	0.43
1:B:459:LYS:HB3	1:B:459:LYS:HE2	1.75	0.43
1:C:117:LEU:HD12	1:C:117:LEU:HA	1.85	0.43
1:C:367:PHE:CD1	1:C:542:PRO:HG3	2.53	0.43
1:C:525:LEU:N	1:C:525:LEU:HD23	2.33	0.43
1:D:380:GLU:HG2	1:D:466:TYR:HE1	1.77	0.43
1:A:544:TYR:O	1:A:546:LYS:N	2.52	0.43
1:C:148:TYR:CE1	1:C:377:ILE:HD11	2.54	0.43
1:D:148:TYR:CD1	1:D:377:ILE:HG13	2.49	0.43
1:A:557:LYS:HA	1:A:557:LYS:HD3	1.81	0.42
1:B:350:GLN:HE22	1:B:359:LEU:H	1.66	0.42
1:B:478:PHE:CD1	1:B:491:LEU:HB3	2.54	0.42
1:C:554:VAL:CG1	1:C:555:GLY:N	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ASN:HB3	1:A:37:CYS:SG	2.59	0.42
1:A:405:LYS:HD2	1:A:405:LYS:H	1.84	0.42
1:B:39:ASN:N	1:B:40:PRO:CD	2.82	0.42
1:B:215:LYS:N	1:B:215:LYS:CD	2.81	0.42
1:B:352:LEU:HD11	1:B:518:PHE:HZ	1.83	0.42
1:C:349:VAL:CG1	4:C:701:FLP:H132	2.49	0.42
1:D:396:ASN:HA	1:D:400:GLN:O	2.19	0.42
1:D:525:LEU:O	1:D:528:PRO:HD2	2.19	0.42
1:B:183:LEU:HD23	1:B:183:LEU:HA	1.78	0.42
1:B:396:ASN:HA	1:B:401:GLU:HA	2.02	0.42
1:C:420:THR:HA	1:C:576:PRO:HG2	2.01	0.42
1:D:85:THR:OG1	1:D:88:THR:HG23	2.19	0.42
1:D:183:LEU:HD22	1:D:442:ILE:HG12	2.01	0.42
1:D:396:ASN:HA	1:D:401:GLU:HA	2.01	0.42
1:A:263:PRO:HB2	1:A:285:PHE:HB3	2.01	0.42
1:C:316:LEU:HD12	1:C:316:LEU:HA	1.89	0.42
1:C:424:GLU:O	1:C:428:ARG:NE	2.51	0.42
1:D:92:ILE:HD12	1:D:92:ILE:N	2.34	0.42
1:D:303:THR:O	1:D:307:ARG:HD3	2.20	0.42
1:A:44:ARG:HD2	1:A:469:ARG:HD2	2.01	0.42
1:B:45:GLY:HA3	1:B:69:CYS:SG	2.59	0.42
1:B:497:ASP:HB3	1:B:500:VAL:HG23	2.02	0.42
1:C:340:THR:O	1:C:344:VAL:HG23	2.20	0.42
1:C:578:THR:HG22	1:C:579:SER:H	1.84	0.42
1:D:230:LEU:HD13	1:D:233:ILE:HD12	2.01	0.42
1:A:109:ARG:HG3	1:A:357:PHE:CE1	2.54	0.42
1:A:198:PHE:CD1	1:A:198:PHE:C	2.97	0.42
1:A:216:ARG:HB3	1:A:220:PHE:CD2	2.54	0.42
1:B:565:GLN:HA	1:B:565:GLN:HE21	1.85	0.42
1:C:388:HIS:HB3	1:C:444:VAL:HG21	2.02	0.42
1:C:435:ALA:HB2	1:C:518:PHE:HA	2.01	0.42
1:D:403:SER:HB2	1:D:405:LYS:CD	2.49	0.42
1:D:478:PHE:CE2	1:D:492:LYS:HA	2.54	0.42
1:A:83:LYS:O	1:A:83:LYS:HG3	2.20	0.42
1:B:194:SER:OG	1:B:351:HIS:HE1	2.03	0.42
1:C:74:PHE:CZ	1:C:78:ILE:HD11	2.55	0.42
1:C:94:THR:O	1:C:356:HIS:CE1	2.73	0.42
1:D:240:ARG:O	1:D:241:GLN:C	2.61	0.42
1:A:510:GLU:O	1:A:512:PRO:HD3	2.20	0.42
1:B:208:GLN:HB3	1:B:232:HIS:ND1	2.35	0.42
1:B:245:ARG:HD3	1:B:329:PHE:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:TRP:HZ2	4:B:701:FLP:C5	2.33	0.42
1:B:498:ILE:C	1:B:500:VAL:H	2.28	0.42
1:B:583:GLN:CD	1:B:583:GLN:H	2.28	0.42
1:C:92:ILE:HD12	1:C:92:ILE:N	2.35	0.42
1:C:287:VAL:HG23	1:C:288:GLY:N	2.34	0.42
1:C:306:LEU:HD23	1:C:306:LEU:C	2.45	0.42
1:D:525:LEU:N	1:D:525:LEU:HD23	2.35	0.42
1:B:479:GLU:CD	1:B:479:GLU:H	2.28	0.42
1:C:162:PRO:O	1:C:163:MET:HE2	2.20	0.42
1:C:215:LYS:N	1:C:215:LYS:CD	2.82	0.42
1:C:330:GLN:HB3	1:D:138:SER:HB2	2.02	0.42
1:A:578:THR:HG22	1:A:579:SER:H	1.85	0.41
1:B:151:ALA:O	1:B:469:ARG:NH1	2.53	0.41
1:B:206:THR:HG21	1:B:385:TYR:CE1	2.55	0.41
1:B:210:PHE:CE1	1:B:382:ASN:HA	2.54	0.41
1:C:292:PHE:N	1:C:292:PHE:CD1	2.88	0.41
1:D:142:PHE:CD2	1:D:142:PHE:C	2.96	0.41
1:A:189:PRO:CB	1:A:430:ILE:HD12	2.50	0.41
1:A:405:LYS:H	1:A:405:LYS:CD	2.33	0.41
1:B:292:PHE:O	1:B:299:MET:HE2	2.20	0.41
1:B:479:GLU:HG3	1:B:488:ALA:HB1	2.02	0.41
1:D:352:LEU:HD11	1:D:518:PHE:CZ	2.55	0.41
1:D:478:PHE:CD1	1:D:491:LEU:HB3	2.56	0.41
1:D:510:GLU:O	1:D:512:PRO:HD3	2.19	0.41
1:A:191:PRO:HG3	1:A:433:ARG:NH2	2.35	0.41
1:B:185:ARG:HB2	1:B:186:GLU:H	1.68	0.41
1:C:44:ARG:HD2	1:C:469:ARG:HD2	2.03	0.41
1:C:96:PHE:O	1:C:97:LYS:C	2.63	0.41
1:D:108:LEU:O	1:D:111:LEU:HB3	2.20	0.41
1:D:210:PHE:HB3	3:D:682:HEM:HBD1	2.03	0.41
1:D:215:LYS:N	1:D:215:LYS:CD	2.83	0.41
1:D:554:VAL:CG1	1:D:555:GLY:N	2.81	0.41
1:A:396:ASN:HA	1:A:401:GLU:HA	2.03	0.41
1:A:465:GLU:HA	1:A:465:GLU:OE1	2.20	0.41
1:B:482:THR:OG1	1:B:488:ALA:HB2	2.20	0.41
1:C:238:LEU:HD22	1:C:242:HIS:CD2	2.54	0.41
1:D:150:ARG:HD2	1:D:380:GLU:OE2	2.20	0.41
1:A:40:PRO:O	1:A:68:ASN:HB3	2.20	0.41
1:A:92:ILE:HD12	1:A:92:ILE:N	2.36	0.41
1:B:191:PRO:HB2	1:B:515:ASP:HB3	2.00	0.41
1:B:340:THR:O	1:B:344:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:ILE:HD12	1:C:92:ILE:H	1.85	0.41
1:C:403:SER:HB2	1:C:405:LYS:CD	2.48	0.41
1:A:388:HIS:HB3	1:A:444:VAL:HG21	2.03	0.41
1:A:397:ILE:O	1:A:398:GLU:C	2.63	0.41
1:B:40:PRO:HB3	2:B:661:NAG:H62	2.03	0.41
1:C:232:HIS:HD2	1:C:233:ILE:HG13	1.85	0.41
1:C:298:LEU:HD12	1:C:298:LEU:HA	1.80	0.41
1:B:355:TYR:CE2	4:B:701:FLP:O1	2.71	0.41
1:B:465:GLU:OE1	1:B:465:GLU:HA	2.20	0.41
1:B:554:VAL:HG12	1:B:555:GLY:N	2.36	0.41
1:C:475:TYR:HD1	1:C:480:GLU:HG2	1.85	0.41
1:B:74:PHE:O	1:B:77:ARG:HB2	2.20	0.41
1:B:247:PHE:HA	1:B:325:ASP:CG	2.46	0.41
1:B:382:ASN:HD21	3:B:682:HEM:CAD	2.29	0.41
1:C:142:PHE:CD2	1:C:142:PHE:C	2.97	0.41
1:D:554:VAL:HG12	1:D:555:GLY:N	2.36	0.41
1:A:49:SER:O	1:B:320:HIS:CD2	2.74	0.41
1:A:198:PHE:HB2	1:A:580:PHE:HB3	2.02	0.41
1:A:210:PHE:HB3	3:A:682:HEM:HBD1	2.03	0.41
1:A:292:PHE:N	1:A:292:PHE:CD1	2.89	0.41
1:B:211:LYS:NZ	1:B:236:GLU:HG3	2.35	0.41
1:B:231:ASN:OD1	1:B:231:ASN:C	2.63	0.41
1:B:413:ILE:HG12	2:B:681:NAG:O6	2.21	0.41
1:B:510:GLU:O	1:B:512:PRO:HD3	2.21	0.41
1:C:42:GLN:O	1:C:69:CYS:HB2	2.20	0.41
1:C:320:HIS:HB3	1:C:323:TRP:CG	2.56	0.41
1:C:322:GLU:HG3	1:D:51:GLY:O	2.21	0.41
1:C:435:ALA:HB3	1:C:512:PRO:HG3	2.03	0.41
1:C:544:TYR:OH	1:D:142:PHE:HB2	2.20	0.41
1:D:204:HIS:ND1	1:D:292:PHE:CE2	2.88	0.41
1:D:398:GLU:HG3	1:D:421:GLN:HE22	1.86	0.41
1:A:146:SER:O	1:A:220:PHE:HA	2.21	0.41
1:A:381:PHE:HA	1:A:384:LEU:HG	2.03	0.41
1:A:565:GLN:HA	1:A:565:GLN:HE21	1.86	0.41
1:B:83:LYS:O	1:B:83:LYS:HG3	2.20	0.41
1:B:300:MET:HE3	1:B:300:MET:HB3	1.95	0.41
1:C:51:GLY:O	1:D:322:GLU:HG3	2.21	0.41
1:D:575:CYS:N	1:D:576:PRO:CD	2.84	0.41
1:D:578:THR:HG22	1:D:579:SER:H	1.85	0.41
1:A:74:PHE:CZ	1:A:78:ILE:HD11	2.56	0.40
1:A:215:LYS:N	1:A:215:LYS:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:PRO:O	1:B:281:GLU:CB	2.68	0.40
1:B:412:SER:O	1:B:416:GLU:HB2	2.21	0.40
1:D:350:GLN:HE22	1:D:359:LEU:H	1.70	0.40
1:D:436:GLY:O	1:D:487:MET:HE1	2.21	0.40
1:A:142:PHE:CD2	1:A:142:PHE:C	2.99	0.40
1:B:108:LEU:O	1:B:111:LEU:HB3	2.21	0.40
1:B:198:PHE:CZ	1:B:352:LEU:HD13	2.56	0.40
1:B:381:PHE:HA	1:B:384:LEU:HG	2.03	0.40
1:C:148:TYR:HE1	1:C:377:ILE:HD11	1.86	0.40
1:C:150:ARG:HD2	1:C:380:GLU:OE2	2.22	0.40
1:C:197:MET:HA	1:C:197:MET:HE3	2.00	0.40
1:C:276:PRO:HD2	1:C:279:ILE:HD11	2.02	0.40
1:C:320:HIS:CD2	1:D:49:SER:O	2.74	0.40
1:C:327:GLN:HG3	1:D:136:TYR:CE2	2.56	0.40
1:C:397:ILE:O	1:C:398:GLU:C	2.64	0.40
1:C:550:PHE:CD2	1:C:556:PHE:CD1	3.09	0.40
1:D:191:PRO:HD2	1:D:433:ARG:HG3	2.02	0.40
1:D:192:GLN:OE1	1:D:517:ILE:HG22	2.21	0.40
1:D:196:MET:SD	1:D:392:PRO:HD3	2.62	0.40
1:D:384:LEU:C	1:D:384:LEU:HD12	2.46	0.40
1:A:479:GLU:CD	1:A:479:GLU:H	2.30	0.40
1:A:550:PHE:CD2	1:A:556:PHE:CD1	3.09	0.40
1:B:85:THR:OG1	1:B:88:THR:HG23	2.21	0.40
1:B:181:VAL:CG2	1:B:509:VAL:HG21	2.51	0.40
1:C:211:LYS:HZ1	1:C:236:GLU:HG3	1.87	0.40
1:C:495:TYR:CE2	1:C:502:GLU:HG3	2.55	0.40
1:D:114:LYS:HE3	1:D:114:LYS:HB2	1.91	0.40
1:D:190:ASP:HA	1:D:191:PRO:HD2	1.87	0.40
1:A:276:PRO:HA	1:A:277:PRO:HD2	1.83	0.40
1:A:320:HIS:CD2	1:B:49:SER:O	2.74	0.40
1:A:388:HIS:N	1:A:389:PRO:CD	2.85	0.40
1:B:117:LEU:HD12	1:B:117:LEU:HA	1.85	0.40
1:C:384:LEU:HD12	1:C:384:LEU:C	2.46	0.40
1:C:569:CYS:HA	1:C:575:CYS:HA	2.03	0.40
1:D:203:GLN:HG3	3:D:682:HEM:C2C	2.56	0.40
1:A:122:TYR:CE1	1:A:123:LEU:CD2	3.05	0.40
1:A:424:GLU:CA	1:A:428:ARG:HH21	2.16	0.40
1:A:553:GLU:HG3	1:A:557:LYS:HE3	2.02	0.40
1:B:109:ARG:HG3	1:B:357:PHE:CE1	2.57	0.40
1:B:306:LEU:HD23	1:B:306:LEU:C	2.46	0.40
1:C:48:MET:O	1:C:56:LYS:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:LEU:HB2	1:C:441:PRO:HG2	2.03	0.40
1:D:294:LEU:HD22	1:D:409:TYR:CD1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	550/587 (94%)	473 (86%)	62 (11%)	15 (3%)	4	6
1	B	550/587 (94%)	484 (88%)	49 (9%)	17 (3%)	3	5
1	C	550/587 (94%)	479 (87%)	54 (10%)	17 (3%)	3	5
1	D	550/587 (94%)	477 (87%)	57 (10%)	16 (3%)	3	5
All	All	2200/2348 (94%)	1913 (87%)	222 (10%)	65 (3%)	3	5

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	PHE
1	A	82	LEU
1	A	130	TYR
1	A	138	SER
1	A	282	ASN
1	A	398	GLU
1	A	419	LEU
1	A	514	PRO
1	B	52	PHE
1	B	82	LEU
1	B	130	TYR
1	B	138	SER
1	B	282	ASN

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Mol	Chain	Res	Type
1	B	398	GLU
1	B	419	LEU
1	B	514	PRO
1	C	52	PHE
1	C	82	LEU
1	C	138	SER
1	C	282	ASN
1	C	398	GLU
1	C	419	LEU
1	C	514	PRO
1	D	52	PHE
1	D	82	LEU
1	D	130	TYR
1	D	138	SER
1	D	282	ASN
1	D	398	GLU
1	D	419	LEU
1	D	514	PRO
1	A	422	PHE
1	B	422	PHE
1	B	499	ASP
1	C	130	TYR
1	C	422	PHE
1	C	545	TRP
1	D	422	PHE
1	A	277	PRO
1	A	499	ASP
1	B	277	PRO
1	B	399	ASP
1	C	277	PRO
1	C	499	ASP
1	D	277	PRO
1	D	399	ASP
1	D	499	ASP
1	A	280	PRO
1	A	399	ASP
1	B	162	PRO
1	C	399	ASP
1	A	162	PRO
1	B	280	PRO
1	B	545	TRP
1	B	573	LYS

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Mol	Chain	Res	Type
1	C	162	PRO
1	C	280	PRO
1	C	573	LYS
1	D	162	PRO
1	D	280	PRO
1	D	573	LYS
1	A	226	HIS
1	C	226	HIS
1	B	51	GLY
1	D	51	GLY

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	493/525 (94%)	429 (87%)	64 (13%)	4	8
1	B	493/525 (94%)	433 (88%)	60 (12%)	5	10
1	C	493/525 (94%)	433 (88%)	60 (12%)	5	10
1	D	493/525 (94%)	428 (87%)	65 (13%)	4	8
All	All	1972/2100 (94%)	1723 (87%)	249 (13%)	4	9

All (249) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	71	THR
1	A	83	LYS
1	A	106	PRO
1	A	107	PHE
1	A	111	LEU
1	A	116	VAL
1	A	117	LEU
1	A	120	ARG
1	A	122	TYR
1	A	137	LYS

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Mol	Chain	Res	Type
1	A	138	SER
1	A	165	VAL
1	A	171	LEU
1	A	174	SER
1	A	178	LEU
1	A	186	GLU
1	A	197	MET
1	A	216	ARG
1	A	230	LEU
1	A	238	LEU
1	A	248	LYS
1	A	249	ASP
1	A	252	LEU
1	A	270	GLN
1	A	271	VAL
1	A	272	GLU
1	A	282	ASN
1	A	287	VAL
1	A	291	VAL
1	A	298	LEU
1	A	300	MET
1	A	307	ARG
1	A	310	GLN
1	A	316	LEU
1	A	322	GLU
1	A	358	LYS
1	A	382	ASN
1	A	385	TYR
1	A	399	ASP
1	A	405	LYS
1	A	409	TYR
1	A	416	GLU
1	A	419	LEU
1	A	422	PHE
1	A	430	ILE
1	A	433	ARG
1	A	459	LYS
1	A	463	LEU
1	A	484	GLU
1	A	485	LYS
1	A	490	GLU
1	A	514	PRO

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Mol	Chain	Res	Type
1	A	525	LEU
1	A	528	PRO
1	A	532	LYS
1	A	534	LEU
1	A	543	GLN
1	A	554	VAL
1	A	565	GLN
1	A	569	CYS
1	A	575	CYS
1	A	578	THR
1	A	583	GLN
1	B	44	ARG
1	B	71	THR
1	B	83	LYS
1	B	106	PRO
1	B	107	PHE
1	B	111	LEU
1	B	116	VAL
1	B	117	LEU
1	B	120	ARG
1	B	122	TYR
1	B	137	LYS
1	B	138	SER
1	B	165	VAL
1	B	171	LEU
1	B	178	LEU
1	B	186	GLU
1	B	197	MET
1	B	216	ARG
1	B	230	LEU
1	B	238	LEU
1	B	248	LYS
1	B	252	LEU
1	B	267	LYS
1	B	270	GLN
1	B	271	VAL
1	B	272	GLU
1	B	282	ASN
1	B	287	VAL
1	B	291	VAL
1	B	298	LEU
1	B	300	MET

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Mol	Chain	Res	Type
1	B	307	ARG
1	B	310	GLN
1	B	316	LEU
1	B	322	GLU
1	B	382	ASN
1	B	385	TYR
1	B	399	ASP
1	B	405	LYS
1	B	409	TYR
1	B	419	LEU
1	B	422	PHE
1	B	430	ILE
1	B	459	LYS
1	B	463	LEU
1	B	484	GLU
1	B	485	LYS
1	B	490	GLU
1	B	505	PRO
1	B	514	PRO
1	B	518	PHE
1	B	525	LEU
1	B	532	LYS
1	B	534	LEU
1	B	543	GLN
1	B	554	VAL
1	B	569	CYS
1	B	575	CYS
1	B	578	THR
1	B	583	GLN
1	C	44	ARG
1	C	71	THR
1	C	83	LYS
1	C	106	PRO
1	C	107	PHE
1	C	111	LEU
1	C	116	VAL
1	C	117	LEU
1	C	120	ARG
1	C	122	TYR
1	C	137	LYS
1	C	138	SER
1	C	165	VAL

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Mol	Chain	Res	Type
1	C	171	LEU
1	C	178	LEU
1	C	186	GLU
1	C	197	MET
1	C	216	ARG
1	C	230	LEU
1	C	238	LEU
1	C	245	ARG
1	C	248	LYS
1	C	252	LEU
1	C	270	GLN
1	C	271	VAL
1	C	272	GLU
1	C	282	ASN
1	C	287	VAL
1	C	291	VAL
1	C	298	LEU
1	C	300	MET
1	C	307	ARG
1	C	310	GLN
1	C	316	LEU
1	C	322	GLU
1	C	358	LYS
1	C	382	ASN
1	C	385	TYR
1	C	399	ASP
1	C	405	LYS
1	C	409	TYR
1	C	419	LEU
1	C	422	PHE
1	C	430	ILE
1	C	459	LYS
1	C	463	LEU
1	C	484	GLU
1	C	485	LYS
1	C	505	PRO
1	C	514	PRO
1	C	518	PHE
1	C	525	LEU
1	C	532	LYS
1	C	534	LEU
1	C	543	GLN

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Mol	Chain	Res	Type
1	C	554	VAL
1	C	569	CYS
1	C	575	CYS
1	C	578	THR
1	C	583	GLN
1	D	44	ARG
1	D	71	THR
1	D	83	LYS
1	D	86	PRO
1	D	106	PRO
1	D	107	PHE
1	D	111	LEU
1	D	116	VAL
1	D	117	LEU
1	D	120	ARG
1	D	122	TYR
1	D	137	LYS
1	D	138	SER
1	D	165	VAL
1	D	171	LEU
1	D	178	LEU
1	D	186	GLU
1	D	197	MET
1	D	216	ARG
1	D	230	LEU
1	D	238	LEU
1	D	248	LYS
1	D	252	LEU
1	D	267	LYS
1	D	270	GLN
1	D	271	VAL
1	D	272	GLU
1	D	282	ASN
1	D	287	VAL
1	D	291	VAL
1	D	296	PRO
1	D	298	LEU
1	D	300	MET
1	D	307	ARG
1	D	310	GLN
1	D	316	LEU
1	D	322	GLU

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Mol	Chain	Res	Type
1	D	358	LYS
1	D	363	PRO
1	D	382	ASN
1	D	385	TYR
1	D	399	ASP
1	D	409	TYR
1	D	416	GLU
1	D	419	LEU
1	D	422	PHE
1	D	430	ILE
1	D	459	LYS
1	D	463	LEU
1	D	484	GLU
1	D	485	LYS
1	D	505	PRO
1	D	514	PRO
1	D	518	PHE
1	D	525	LEU
1	D	528	PRO
1	D	532	LYS
1	D	534	LEU
1	D	543	GLN
1	D	554	VAL
1	D	569	CYS
1	D	575	CYS
1	D	578	THR
1	D	581	ASN
1	D	583	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	95	HIS
1	A	105	ASN
1	A	133	HIS
1	A	278	HIS
1	A	318	GLN
1	A	320	HIS
1	A	350	GLN
1	A	351	HIS
1	A	356	HIS

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Mol	Chain	Res	Type
1	A	368	ASN
1	A	369	GLN
1	A	382	ASN
1	A	396	ASN
1	A	417	HIS
1	A	454	GLN
1	A	464	ASN
1	A	543	GLN
1	B	42	GLN
1	B	90	HIS
1	B	133	HIS
1	B	214	HIS
1	B	278	HIS
1	B	318	GLN
1	B	320	HIS
1	B	350	GLN
1	B	351	HIS
1	B	356	HIS
1	B	369	GLN
1	B	382	ASN
1	B	396	ASN
1	B	417	HIS
1	B	454	GLN
1	B	464	ASN
1	C	42	GLN
1	C	90	HIS
1	C	95	HIS
1	C	101	ASN
1	C	105	ASN
1	C	133	HIS
1	C	278	HIS
1	C	318	GLN
1	C	320	HIS
1	C	350	GLN
1	C	351	HIS
1	C	356	HIS
1	C	368	ASN
1	C	369	GLN
1	C	382	ASN
1	C	396	ASN
1	C	417	HIS
1	C	454	GLN

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Mol	Chain	Res	Type
1	C	464	ASN
1	C	543	GLN
1	C	560	ASN
1	D	90	HIS
1	D	133	HIS
1	D	318	GLN
1	D	320	HIS
1	D	350	GLN
1	D	351	HIS
1	D	356	HIS
1	D	368	ASN
1	D	369	GLN
1	D	382	ASN
1	D	396	ASN
1	D	417	HIS
1	D	454	GLN
1	D	464	ASN
1	D	581	ASN

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](#)

20 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	HEM	A	682	1	50,50,50	1.29	6 (12%)	67,82,82	0.91	1 (1%)
2	NAG	B	661	1	14,14,15	0.54	0	17,19,21	1.01	1 (5%)
2	NAG	A	681	1	14,14,15	0.80	0	17,19,21	0.78	0
2	NAG	D	661	1	14,14,15	0.70	0	17,19,21	0.91	1 (5%)
3	HEM	C	682	1	50,50,50	1.22	5 (10%)	67,82,82	0.99	1 (1%)
2	NAG	C	681	1	14,14,15	0.62	0	17,19,21	0.82	0
2	NAG	A	671	1	14,14,15	0.74	0	17,19,21	1.60	5 (29%)
3	HEM	D	682	1	50,50,50	1.23	4 (8%)	67,82,82	0.99	1 (1%)
2	NAG	C	661	1	14,14,15	0.28	0	17,19,21	0.88	1 (5%)
4	FLP	C	701	-	19,19,19	1.08	1 (5%)	26,26,26	1.10	2 (7%)
2	NAG	B	681	1	14,14,15	0.75	0	17,19,21	0.93	1 (5%)
4	FLP	B	701	-	19,19,19	1.64	4 (21%)	26,26,26	1.12	1 (3%)
2	NAG	D	671	1	14,14,15	0.67	0	17,19,21	1.54	3 (17%)
2	NAG	A	661	1	14,14,15	0.61	0	17,19,21	0.89	1 (5%)
2	NAG	C	671	1	14,14,15	0.85	1 (7%)	17,19,21	1.64	4 (23%)
4	FLP	A	701	-	19,19,19	1.35	3 (15%)	26,26,26	1.08	2 (7%)
4	FLP	D	701	-	19,19,19	1.33	2 (10%)	26,26,26	0.99	1 (3%)
3	HEM	B	682	1	50,50,50	1.16	4 (8%)	67,82,82	1.04	1 (1%)
2	NAG	B	671	1	14,14,15	0.78	0	17,19,21	1.42	3 (17%)
2	NAG	D	681	1	14,14,15	0.80	0	17,19,21	0.88	0

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	HEM	A	682	1	-	3/14/54/54	-
2	NAG	B	661	1	-	0/6/23/26	0/1/1/1
2	NAG	A	681	1	-	2/6/23/26	0/1/1/1
2	NAG	D	661	1	-	0/6/23/26	0/1/1/1
3	HEM	C	682	1	-	5/14/54/54	-
2	NAG	C	681	1	-	2/6/23/26	0/1/1/1
2	NAG	A	671	1	-	2/6/23/26	0/1/1/1
3	HEM	D	682	1	-	3/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	661	1	-	0/6/23/26	0/1/1/1
4	FLP	C	701	-	-	0/12/12/12	0/2/2/2
2	NAG	B	681	1	-	2/6/23/26	0/1/1/1
4	FLP	B	701	-	-	0/12/12/12	0/2/2/2
2	NAG	D	671	1	-	2/6/23/26	0/1/1/1
2	NAG	A	661	1	-	0/6/23/26	0/1/1/1
2	NAG	C	671	1	-	2/6/23/26	0/1/1/1
4	FLP	A	701	-	-	0/12/12/12	0/2/2/2
4	FLP	D	701	-	-	0/12/12/12	0/2/2/2
3	HEM	B	682	1	-	3/14/54/54	-
2	NAG	B	671	1	-	2/6/23/26	0/1/1/1
2	NAG	D	681	1	-	2/6/23/26	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	682	HEM	CAC-C3C	-3.81	1.37	1.47
3	B	682	HEM	CAB-C3B	-3.62	1.37	1.47
4	B	701	FLP	C7-C6	3.58	1.45	1.40
3	A	682	HEM	CAC-C3C	-3.52	1.38	1.47
3	C	682	HEM	CAC-C3C	-3.45	1.38	1.47
3	D	682	HEM	CAB-C3B	-3.33	1.38	1.47
3	B	682	HEM	CAC-C3C	-3.28	1.38	1.47
3	A	682	HEM	CAB-C3B	-3.26	1.38	1.47
4	A	701	FLP	C8-C9	3.22	1.44	1.39
4	B	701	FLP	C8-C9	3.07	1.44	1.39
4	C	701	FLP	C8-C7	3.02	1.43	1.38
3	C	682	HEM	CAB-C3B	-3.01	1.39	1.47
3	A	682	HEM	CBC-CAC	2.86	1.44	1.30
3	D	682	HEM	CBB-CAB	2.84	1.44	1.30
3	C	682	HEM	CBC-CAC	2.82	1.43	1.30
4	D	701	FLP	C6-C11	2.82	1.43	1.39
3	C	682	HEM	CBB-CAB	2.80	1.43	1.30
4	A	701	FLP	C8-C7	2.77	1.43	1.38
3	D	682	HEM	CBC-CAC	2.76	1.43	1.30
3	A	682	HEM	CBB-CAB	2.72	1.43	1.30
3	B	682	HEM	CBC-CAC	2.63	1.43	1.30
3	B	682	HEM	CBB-CAB	2.53	1.42	1.30
2	C	671	NAG	C1-C2	2.30	1.55	1.52
3	C	682	HEM	C1B-NB	-2.23	1.36	1.40
3	A	682	HEM	O2D-CGD	-2.22	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	FLP	C6-C11	2.21	1.42	1.39
3	A	682	HEM	C1B-NB	-2.20	1.36	1.40
4	D	701	FLP	C8-C7	2.18	1.42	1.38
4	B	701	FLP	C9-C12	-2.12	1.49	1.52
4	B	701	FLP	C10-C11	2.04	1.41	1.37

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	682	HEM	C3B-C4B-NB	4.36	112.60	109.47
3	B	682	HEM	C3B-C4B-NB	4.07	112.39	109.47
2	D	671	NAG	C1-C2-N2	3.81	116.43	110.43
3	D	682	HEM	C3B-C4B-NB	3.79	112.19	109.47
2	A	671	NAG	C4-C3-C2	-3.31	106.17	111.02
2	C	671	NAG	C1-C2-N2	3.29	115.62	110.43
2	B	671	NAG	C4-C3-C2	-3.29	106.19	111.02
2	C	671	NAG	C1-O5-C5	3.11	116.35	112.19
2	D	671	NAG	C4-C3-C2	-3.05	106.55	111.02
3	A	682	HEM	C3B-C4B-NB	2.94	111.58	109.47
2	B	661	NAG	C3-C4-C5	-2.66	105.41	110.23
2	C	671	NAG	C2-N2-C7	-2.65	119.35	122.90
4	C	701	FLP	C2-C6-C11	-2.62	118.70	122.86
2	A	671	NAG	C1-C2-N2	2.59	114.51	110.43
2	A	671	NAG	O5-C1-C2	-2.52	107.39	111.29
2	B	671	NAG	C6-C5-C4	-2.51	106.85	113.02
2	D	661	NAG	C3-C4-C5	-2.44	105.81	110.23
2	A	661	NAG	C3-C4-C5	-2.39	105.90	110.23
2	C	671	NAG	C4-C3-C2	-2.31	107.63	111.02
4	B	701	FLP	C2-C6-C11	-2.29	119.23	122.86
4	A	701	FLP	O1-C14-O	-2.23	119.02	124.08
4	A	701	FLP	C2-C6-C11	-2.20	119.36	122.86
2	B	671	NAG	C1-O5-C5	2.19	115.12	112.19
2	B	681	NAG	C2-N2-C7	-2.09	120.10	122.90
2	A	671	NAG	C1-O5-C5	2.07	114.97	112.19
2	D	671	NAG	C1-O5-C5	2.06	114.95	112.19
2	C	661	NAG	C3-C4-C5	-2.05	106.52	110.23
2	A	671	NAG	C6-C5-C4	-2.03	108.03	113.02
4	C	701	FLP	C7-C6-C11	2.03	119.42	116.20
4	D	701	FLP	C2-C6-C11	-2.01	119.68	122.86

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	671	NAG	O5-C5-C6-O6
2	A	671	NAG	O5-C5-C6-O6
2	C	671	NAG	O5-C5-C6-O6
2	D	671	NAG	O5-C5-C6-O6
2	B	671	NAG	C4-C5-C6-O6
2	C	671	NAG	C4-C5-C6-O6
2	D	671	NAG	C4-C5-C6-O6
2	A	671	NAG	C4-C5-C6-O6
2	D	681	NAG	C4-C5-C6-O6
2	D	681	NAG	O5-C5-C6-O6
2	A	681	NAG	C4-C5-C6-O6
2	A	681	NAG	O5-C5-C6-O6
2	C	681	NAG	C4-C5-C6-O6
3	B	682	HEM	C2B-C3B-CAB-CBB
2	B	681	NAG	C4-C5-C6-O6
2	B	681	NAG	O5-C5-C6-O6
2	C	681	NAG	O5-C5-C6-O6
3	B	682	HEM	CAA-CBA-CGA-O2A
3	C	682	HEM	CAA-CBA-CGA-O2A
3	D	682	HEM	CAA-CBA-CGA-O2A
3	B	682	HEM	CAA-CBA-CGA-O1A
3	C	682	HEM	CAA-CBA-CGA-O1A
3	D	682	HEM	CAA-CBA-CGA-O1A
3	A	682	HEM	CAA-CBA-CGA-O1A
3	A	682	HEM	CAA-CBA-CGA-O2A
3	C	682	HEM	CAD-CBD-CGD-O2D
3	C	682	HEM	CAD-CBD-CGD-O1D
3	A	682	HEM	C2B-C3B-CAB-CBB
3	C	682	HEM	C2B-C3B-CAB-CBB
3	D	682	HEM	C2B-C3B-CAB-CBB

There are no ring outliers.

12 monomers are involved in 50 short contacts:

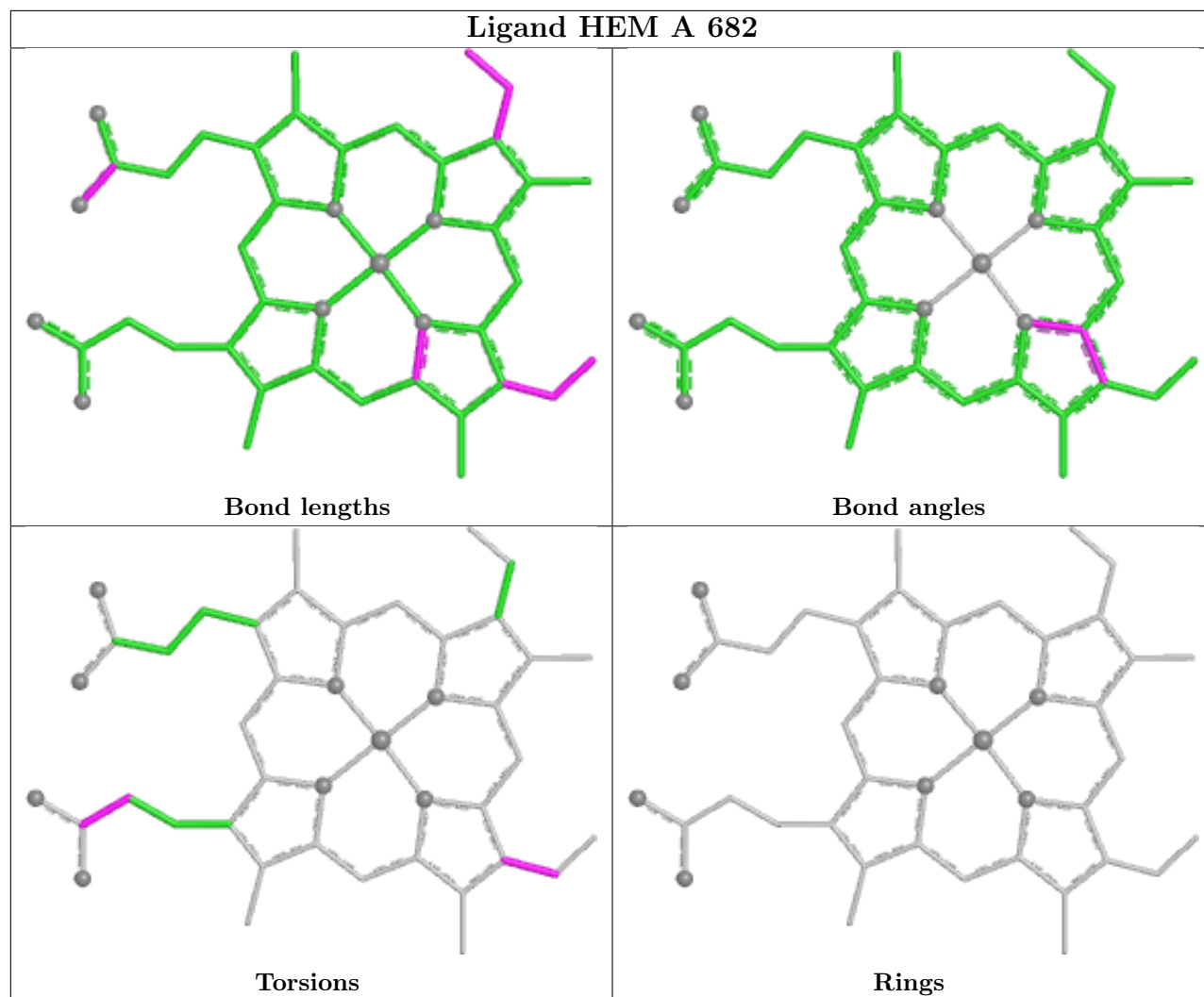
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	682	HEM	6	0
2	B	661	NAG	1	0
3	C	682	HEM	6	0
2	A	671	NAG	4	0
3	D	682	HEM	9	0
4	C	701	FLP	3	0
2	B	681	NAG	1	0
4	B	701	FLP	6	0

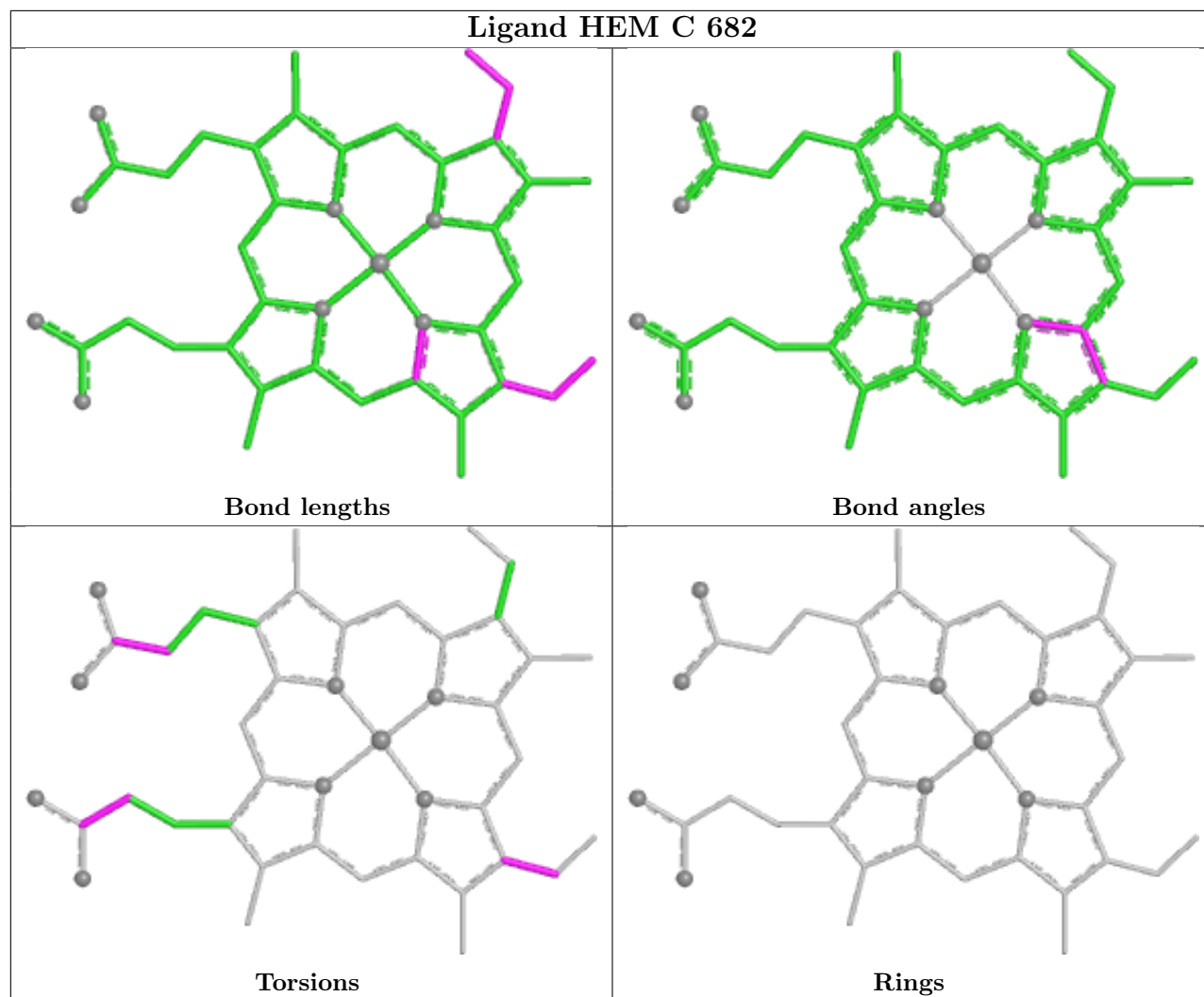
Continued on next page...

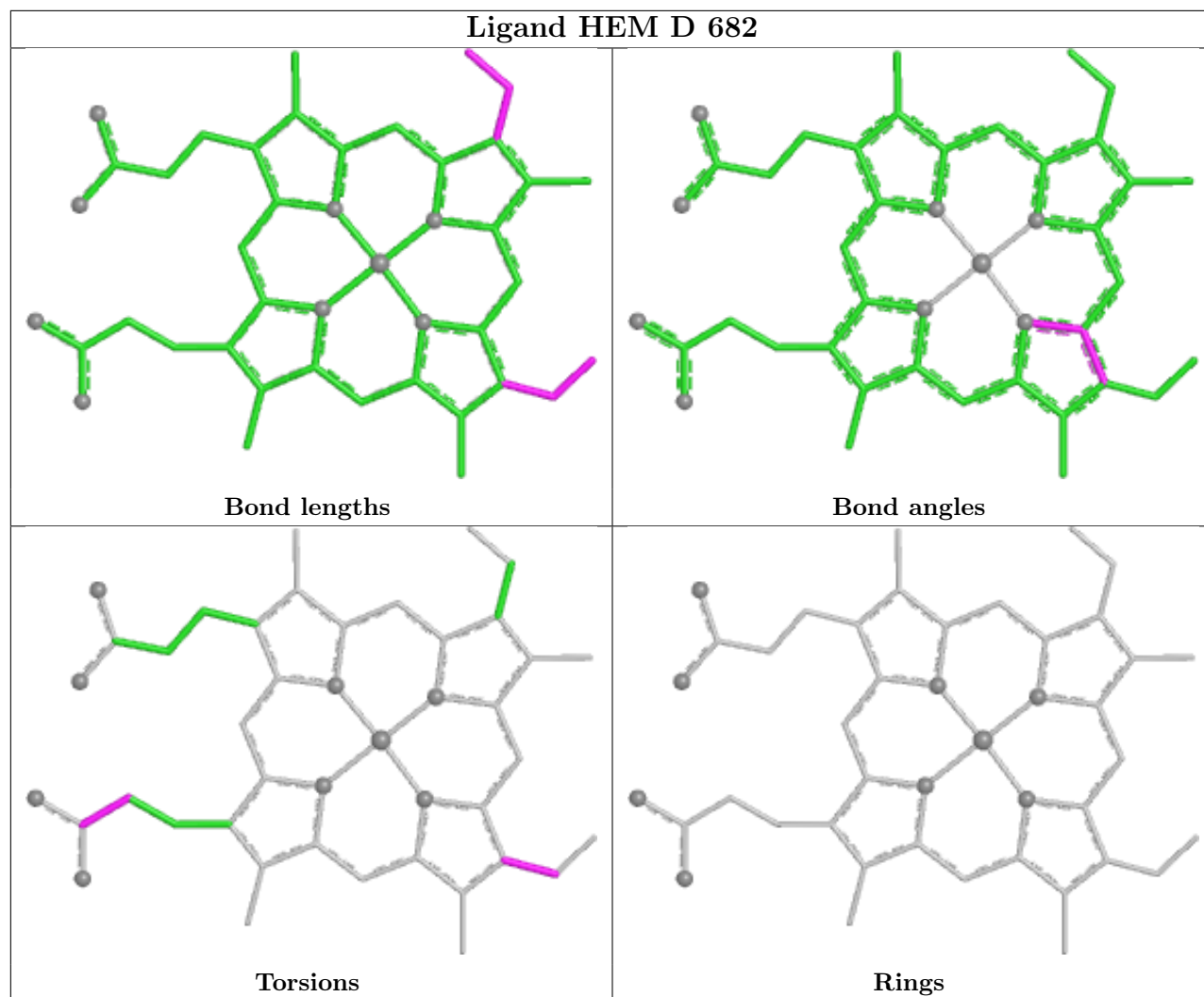
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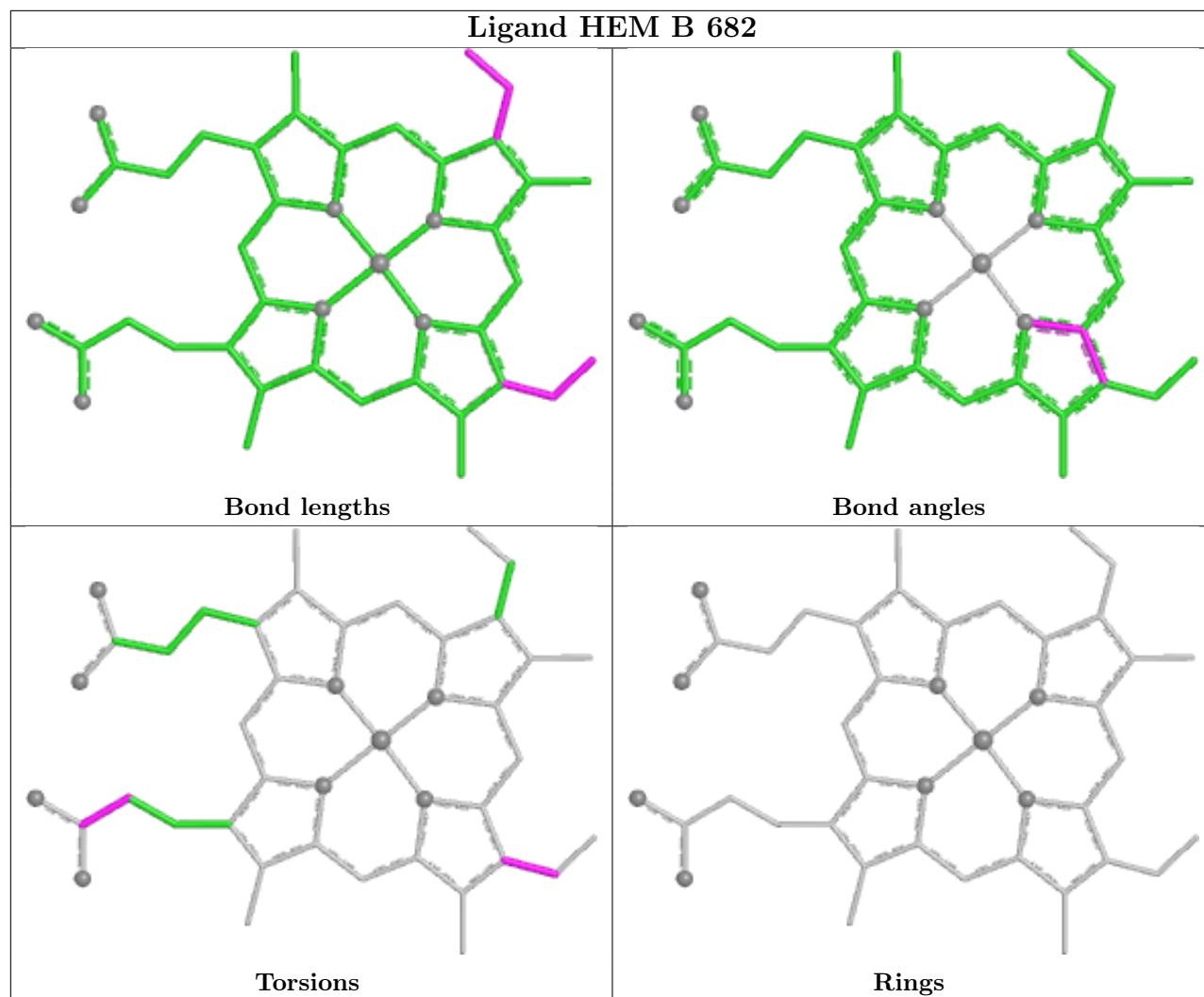
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	701	FLP	1	0
4	D	701	FLP	3	0
3	B	682	HEM	9	0
2	B	671	NAG	1	0

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.