



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 12:13 PM EDT

PDB ID : 1GGF / pdb_00001ggf
Title : CRYSTAL STRUCTURE OF CATALASE HP11 FROM ESCHERICHIA COLI, VARIANT HIS128ASN, COMPLEX WITH HYDROGEN PEROXIDE.
Authors : Melik-Adamyany, W.R.; Bravo, J.; Carpena, X.; Switala, J.; Mate, M.J.; Fita, I.; Loewen, P.C.
Deposited on : 2000-08-21
Resolution : 2.28 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](#) ①) were used in the production of this report:

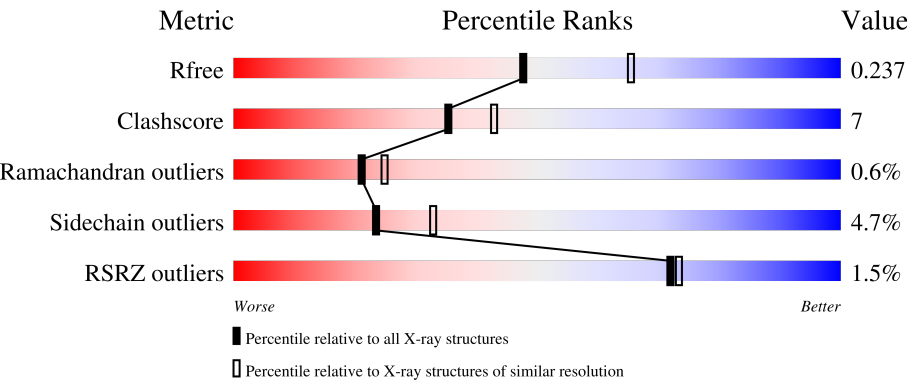
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	753	2% 74% 19% . .
1	B	753	2% 68% 23% 5% . . .
1	C	753	% 74% 19% . .
1	D	753	% 72% 21% . . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PEO	A	3002	-	-	X	-
3	PEO	A	3003	-	-	X	-
3	PEO	D	6002	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25199 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.

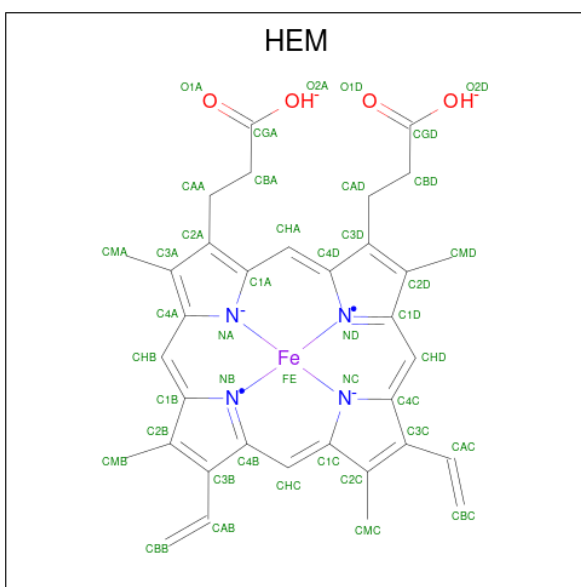
- Molecule 1 is a protein called CATALASE HPIL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5744	3645	1004	1083	12			
1	B	727	Total	C	N	O	S	0	0	0
			5744	3645	1004	1083	12			
1	C	727	Total	C	N	O	S	0	0	0
			5744	3645	1004	1083	12			
1	D	727	Total	C	N	O	S	0	0	0
			5744	3645	1004	1083	12			

There are 4 discrepancies between the modelled and reference sequences:

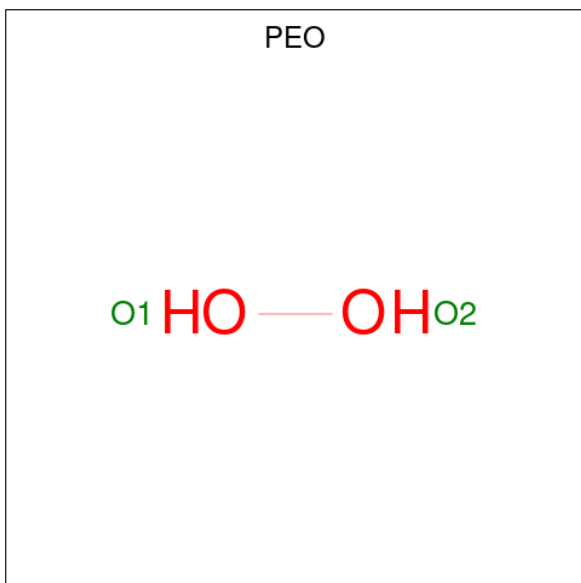
Chain	Residue	Modelled	Actual	Comment	Reference
A	128	ASN	HIS	engineered mutation	UNP P21179
B	128	ASN	HIS	engineered mutation	UNP P21179
C	128	ASN	HIS	engineered mutation	UNP P21179
D	128	ASN	HIS	engineered mutation	UNP P21179

- 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 HYDROGEN PEROXIDE (CCD ID: PEO) (formula: H_2O_2).



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

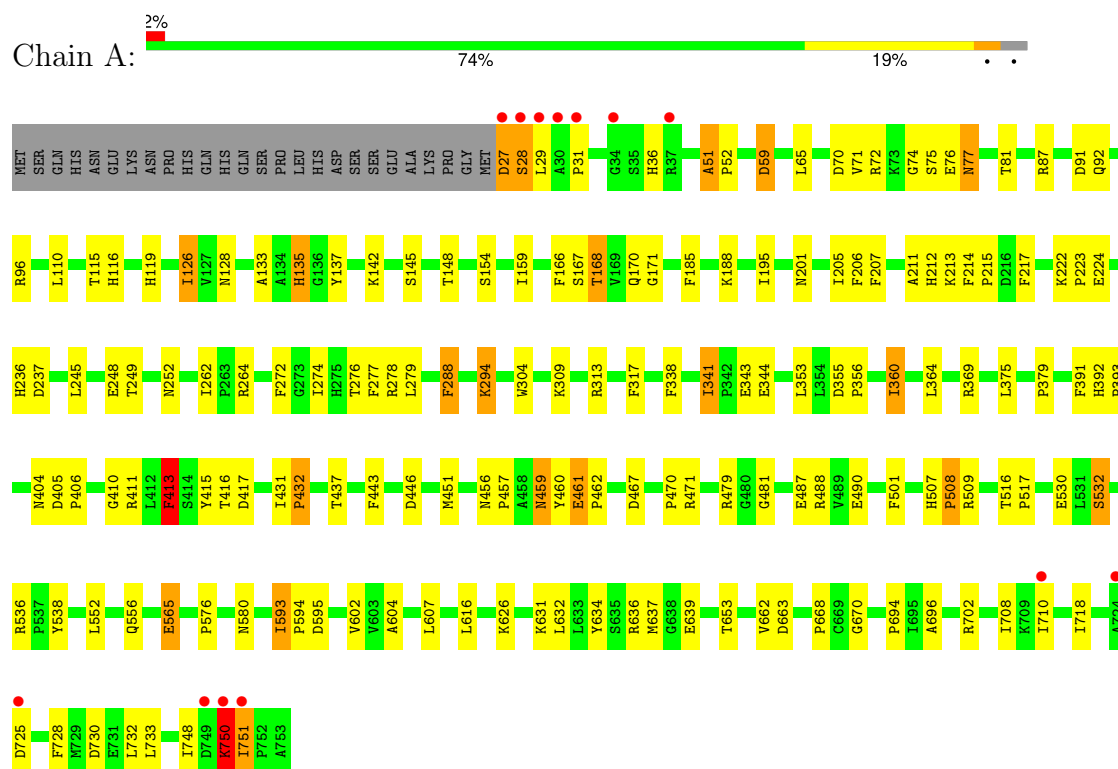
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	581	Total O 581 581	0	0
4	B	440	Total O 440 440	0	0
4	C	474	Total O 474 474	0	0
4	D	530	Total O 530 530	0	0

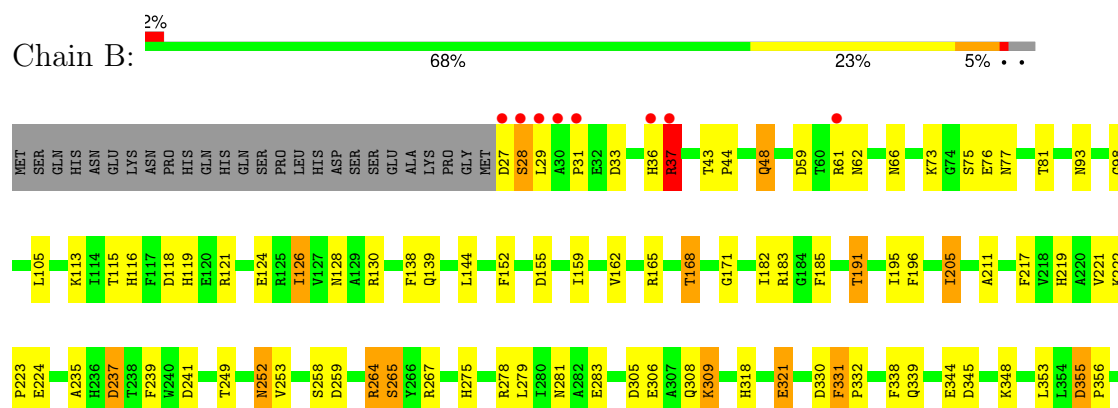
3 Residue-property plots [i](#)

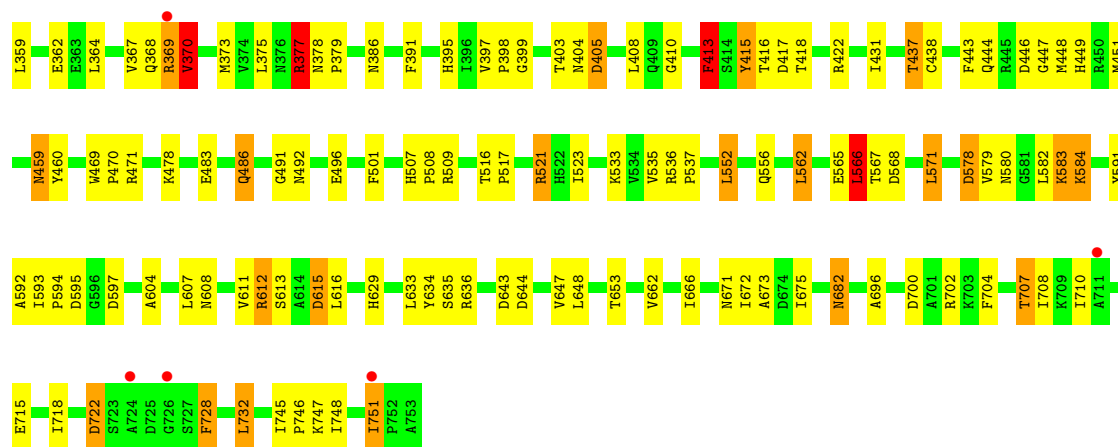
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

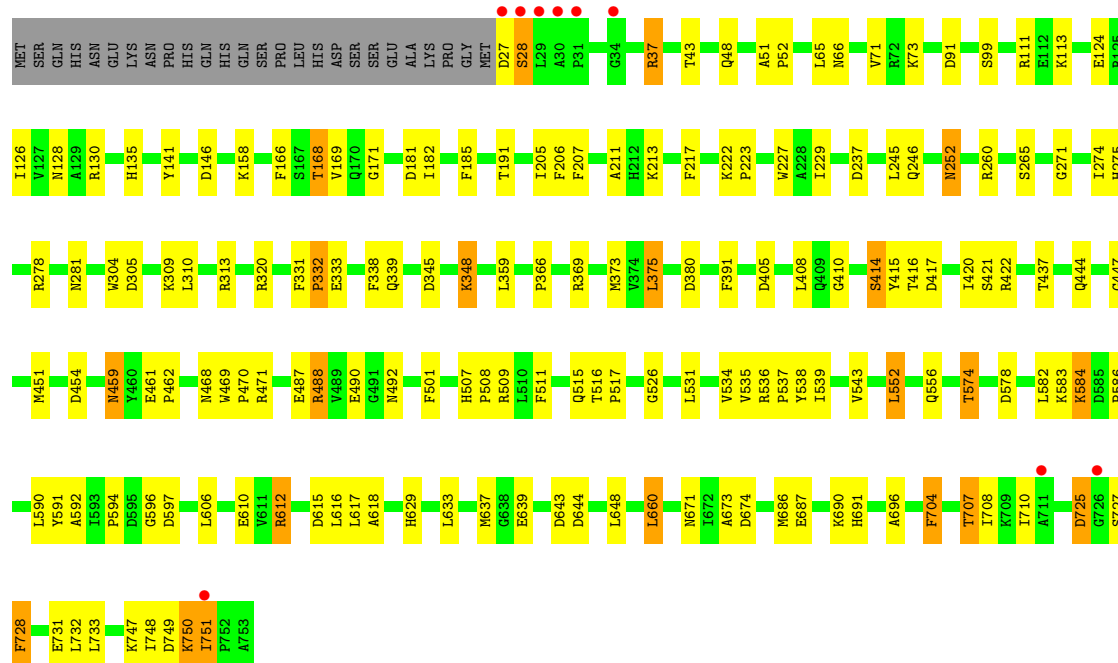
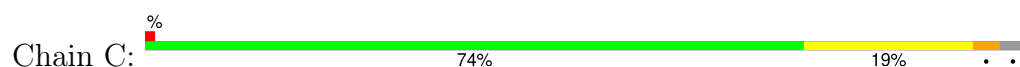


• Molecule 1: CATALASE HPII

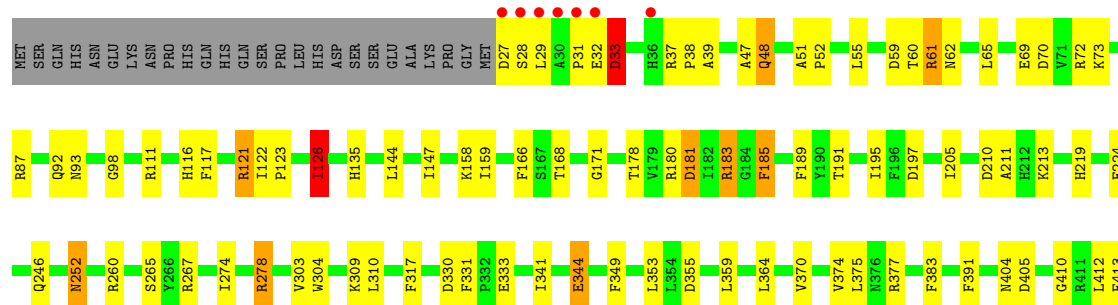
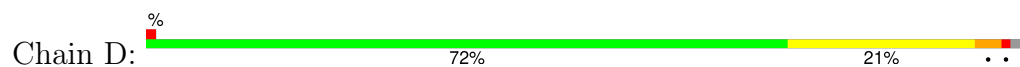


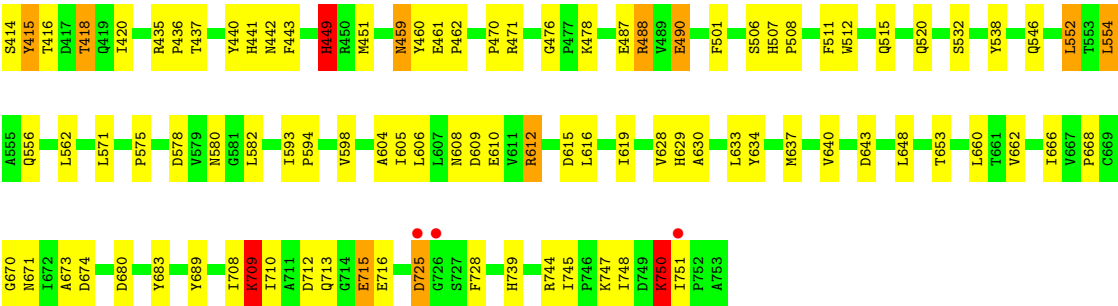


• Molecule 1: CATALASE HPII



• Molecule 1: CATALASE HPII





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.37Å 133.41Å 121.92Å 90.00° 109.63° 90.00°	Depositor
Resolution (Å)	87.95 – 2.28 87.95 – 2.28	Depositor EDS
% Data completeness (in resolution range)	98.3 (87.95-2.28) 98.3 (87.95-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.28Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.174 , 0.254 0.171 , 0.237	Depositor DCC
R_{free} test set	6348 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25199	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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, PEO

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	0.67	0/5899	1.66	80/8020 (1.0%)
1	B	0.64	0/5899	1.68	86/8020 (1.1%)
1	C	0.64	0/5899	1.62	61/8020 (0.8%)
1	D	0.66	0/5899	1.67	76/8020 (0.9%)
All	All	0.65	0/23596	1.66	303/32080 (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	C	0	1

There are no bond length outliers.

All (303) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	449	HIS	CA-CB-CG	16.40	130.20	113.80
1	D	488	ARG	CD-NE-CZ	13.96	143.95	124.40
1	B	37	ARG	CD-NE-CZ	11.18	140.05	124.40
1	B	722	ASP	CA-CB-CG	-10.41	102.19	112.60
1	D	33	ASP	CA-CB-CG	10.27	122.87	112.60
1	D	27	ASP	CA-CB-CG	9.90	122.50	112.60
1	B	413	PHE	CA-CB-CG	9.75	123.55	113.80
1	B	615	ASP	CA-CB-CG	9.40	122.00	112.60
1	D	185	PHE	CA-CB-CG	9.03	122.83	113.80
1	A	185	PHE	CA-CB-CG	8.91	122.71	113.80
1	C	338	PHE	CA-CB-CG	8.83	122.63	113.80
1	D	278	ARG	CD-NE-CZ	8.69	136.57	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	PHE	CA-CB-CG	8.65	122.45	113.80
1	B	33	ASP	CA-CB-CG	8.64	121.24	112.60
1	C	271	GLY	O-C-N	-8.60	116.26	123.23
1	C	728	PHE	CA-CB-CG	8.35	122.15	113.80
1	C	171	GLY	N-CA-C	8.30	121.46	112.33
1	B	521	ARG	CD-NE-CZ	8.29	136.01	124.40
1	B	567	THR	CA-C-N	8.23	131.66	120.54
1	B	567	THR	C-N-CA	8.23	131.66	120.54
1	B	165	ARG	NE-CZ-NH2	8.11	126.50	119.20
1	D	739	HIS	CA-CB-CG	7.94	121.74	113.80
1	B	338	PHE	CA-CB-CG	7.92	121.72	113.80
1	D	55	LEU	N-CA-C	-7.87	103.81	113.41
1	B	682	ASN	CA-CB-CG	-7.82	104.78	112.60
1	C	181	ASP	CA-CB-CG	7.78	120.38	112.60
1	D	59	ASP	CA-CB-CG	-7.77	104.83	112.60
1	A	170	GLN	CA-C-N	7.74	128.87	120.44
1	A	170	GLN	C-N-CA	7.74	128.87	120.44
1	A	70	ASP	CA-CB-CG	7.63	120.23	112.60
1	B	121	ARG	NE-CZ-NH2	-7.62	112.34	119.20
1	A	416	THR	CA-C-O	7.51	128.94	120.90
1	A	116	HIS	CA-CB-CG	-7.48	106.32	113.80
1	B	182	ILE	N-CA-C	-7.39	101.99	110.05
1	C	674	ASP	CA-CB-CG	7.37	119.97	112.60
1	C	237	ASP	CA-C-O	-7.35	113.03	120.90
1	A	536	ARG	O-C-N	7.35	127.18	121.23
1	C	217	PHE	CA-CB-CG	-7.32	106.48	113.80
1	B	331	PHE	CA-C-O	7.31	125.85	119.71
1	D	442	ASN	CA-C-O	-7.30	113.38	121.05
1	B	391	PHE	CA-CB-CG	7.19	120.99	113.80
1	B	185	PHE	CA-CB-CG	7.16	120.96	113.80
1	A	355	ASP	CA-C-O	7.15	124.61	119.32
1	A	277	PHE	CA-CB-CG	7.14	120.94	113.80
1	D	126	ILE	N-CA-CB	7.12	118.88	110.55
1	A	417	ASP	N-CA-CB	-7.11	98.48	110.49
1	D	166	PHE	CA-C-O	-7.10	112.90	121.28
1	A	135	HIS	CA-CB-CG	7.05	120.85	113.80
1	B	597	ASP	CA-CB-CG	7.03	119.63	112.60
1	D	126	ILE	CB-CG1-CD1	-7.02	99.06	113.80
1	B	152	PHE	CA-CB-CG	7.01	120.81	113.80
1	B	237	ASP	N-CA-C	7.00	118.56	111.07
1	A	479	ARG	CD-NE-CZ	6.99	134.18	124.40
1	B	702	ARG	CA-C-N	6.98	130.20	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	702	ARG	C-N-CA	6.98	130.20	120.29
1	C	66	ASN	CA-CB-CG	6.97	119.57	112.60
1	C	447	GLY	CA-C-O	-6.96	117.43	122.23
1	D	725	ASP	CA-CB-CG	-6.91	105.69	112.60
1	D	197	ASP	CA-CB-CG	6.91	119.51	112.60
1	B	416	THR	CA-C-N	6.85	132.09	121.19
1	B	416	THR	C-N-CA	6.85	132.09	121.19
1	D	377	ARG	NE-CZ-NH1	-6.84	114.66	121.50
1	D	126	ILE	CB-CA-C	-6.84	103.22	111.97
1	D	728	PHE	CA-CB-CG	6.83	120.63	113.80
1	B	636	ARG	CA-C-O	-6.82	114.15	121.45
1	C	597	ASP	CA-CB-CG	6.78	119.38	112.60
1	A	413	PHE	N-CA-C	-6.78	104.76	113.16
1	D	709	LYS	CA-CB-CG	6.77	127.64	114.10
1	A	87	ARG	CA-C-O	6.77	128.63	121.19
1	B	264	ARG	CA-C-O	6.72	127.70	119.97
1	A	431	ILE	N-CA-C	-6.71	102.37	108.95
1	B	155	ASP	CA-CB-CG	6.66	119.26	112.60
1	B	62	ASN	CA-CB-CG	6.66	119.26	112.60
1	B	447	GLY	CA-C-O	-6.65	117.64	122.23
1	D	61	ARG	NE-CZ-NH1	-6.60	114.90	121.50
1	B	405	ASP	CA-CB-CG	6.58	119.18	112.60
1	A	170	GLN	N-CA-C	6.56	118.31	111.03
1	A	59	ASP	CA-CB-CG	6.56	119.16	112.60
1	D	383	PHE	CA-CB-CG	-6.55	107.25	113.80
1	A	236	HIS	CA-CB-CG	6.55	120.35	113.80
1	B	501	PHE	CA-CB-CG	6.53	120.33	113.80
1	D	260	ARG	NH1-CZ-NH2	6.53	127.78	119.30
1	D	501	PHE	CA-CB-CG	6.46	120.26	113.80
1	A	730	ASP	CA-CB-CG	6.43	119.03	112.60
1	A	133	ALA	N-CA-C	6.42	119.47	109.52
1	C	391	PHE	CA-CB-CG	6.42	120.22	113.80
1	A	631	LYS	CA-CB-CG	6.40	126.90	114.10
1	C	320	ARG	NE-CZ-NH2	-6.39	113.44	119.20
1	B	128	ASN	CA-CB-CG	6.38	118.98	112.60
1	D	355	ASP	CA-C-O	6.37	123.43	119.29
1	D	181	ASP	CA-CB-CG	6.33	118.93	112.60
1	A	248	GLU	CB-CG-CD	6.32	123.34	112.60
1	D	116	HIS	CA-CB-CG	-6.31	107.49	113.80
1	A	77	ASN	CA-CB-CG	-6.29	106.31	112.60
1	D	441	HIS	CA-CB-CG	-6.29	107.51	113.80
1	D	712	ASP	CA-C-N	6.28	129.02	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	712	ASP	C-N-CA	6.28	129.02	120.54
1	B	379	PRO	CB-CA-C	-6.26	101.77	111.22
1	B	578	ASP	CA-CB-CG	6.26	118.86	112.60
1	C	237	ASP	N-CA-C	6.26	118.62	111.11
1	B	165	ARG	NE-CZ-NH1	-6.24	115.26	121.50
1	C	596	GLY	N-CA-C	6.23	120.01	111.54
1	B	437	THR	CB-CA-C	6.22	120.64	110.88
1	D	391	PHE	CA-CB-CG	6.20	120.00	113.80
1	B	116	HIS	CA-CB-CG	-6.20	107.60	113.80
1	D	546	GLN	OE1-CD-NE2	-6.19	116.41	122.60
1	A	461	GLU	O-C-N	6.18	126.18	121.85
1	C	629	HIS	CA-CB-CG	-6.18	107.62	113.80
1	D	488	ARG	NE-CZ-NH1	6.18	127.68	121.50
1	D	578	ASP	CA-CB-CG	6.17	118.77	112.60
1	D	61	ARG	NE-CZ-NH2	6.17	124.75	119.20
1	A	288	PHE	CA-CB-CG	6.15	119.95	113.80
1	D	575	PRO	N-CA-CB	6.13	106.62	103.19
1	C	501	PHE	CA-CB-CG	6.13	119.93	113.80
1	A	565	GLU	CA-C-O	-6.06	113.65	120.32
1	A	417	ASP	CA-CB-CG	-6.06	106.54	112.60
1	C	135	HIS	CA-C-O	-6.05	114.58	121.72
1	C	615	ASP	CA-CB-CG	6.03	118.63	112.60
1	A	595	ASP	CA-CB-CG	5.99	118.59	112.60
1	C	691	HIS	CA-C-O	5.99	126.67	119.43
1	D	210	ASP	CA-CB-CG	5.97	118.57	112.60
1	A	237	ASP	N-CA-C	5.97	117.45	111.07
1	B	138	PHE	CA-C-O	-5.97	114.37	121.11
1	B	700	ASP	CA-CB-CG	-5.95	106.65	112.60
1	B	417	ASP	CA-C-O	5.93	127.96	121.02
1	B	171	GLY	N-CA-C	5.93	120.14	112.54
1	C	405	ASP	CA-CB-CG	5.92	118.52	112.60
1	A	72	ARG	CB-CA-C	-5.92	100.42	109.89
1	B	492	ASN	CA-CB-CG	-5.91	106.69	112.60
1	C	454	ASP	CA-CB-CG	-5.89	106.71	112.60
1	A	87	ARG	O-C-N	-5.88	115.64	122.87
1	B	195	ILE	CB-CA-C	-5.86	103.02	111.34
1	D	750	LYS	N-CA-C	5.86	118.89	111.69
1	A	490	GLU	CB-CG-CD	5.84	122.53	112.60
1	A	456	ASN	O-C-N	-5.82	116.24	121.31
1	A	272	PHE	CA-C-O	-5.82	114.47	120.99
1	B	331	PHE	N-CA-C	5.82	116.72	109.57
1	D	61	ARG	CD-NE-CZ	5.81	132.54	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	417	ASP	N-CA-CB	-5.81	99.84	109.72
1	B	422	ARG	CA-CB-CG	5.80	125.71	114.10
1	B	377	ARG	NE-CZ-NH2	-5.79	113.99	119.20
1	B	483	GLU	CA-C-O	-5.79	113.90	120.32
1	B	224	GLU	CA-C-N	5.78	125.64	119.28
1	B	224	GLU	C-N-CA	5.78	125.64	119.28
1	C	414	SER	O-C-N	-5.78	114.91	122.59
1	C	405	ASP	CA-C-O	5.77	124.61	119.59
1	B	217	PHE	CA-CB-CG	-5.76	108.03	113.80
1	A	456	ASN	CA-C-O	5.76	125.16	119.51
1	D	374	VAL	CA-C-O	-5.76	114.34	120.39
1	D	73	LYS	CA-CB-CG	5.76	125.61	114.10
1	B	121	ARG	CD-NE-CZ	5.75	132.45	124.40
1	D	304	TRP	N-CA-C	5.74	117.99	111.11
1	B	566	LEU	N-CA-CB	5.73	118.46	110.04
1	A	750	LYS	N-CA-C	-5.72	105.97	113.12
1	B	595	ASP	CA-CB-CG	5.71	118.31	112.60
1	C	339	GLN	CA-C-O	-5.70	114.27	120.36
1	D	712	ASP	CA-C-O	5.70	126.59	120.55
1	C	366	PRO	CA-C-O	5.69	128.16	121.56
1	B	265	SER	N-CA-CB	-5.66	102.95	111.56
1	B	438	CYS	CA-C-N	5.66	125.66	119.89
1	B	438	CYS	C-N-CA	5.66	125.66	119.89
1	C	691	HIS	CA-C-N	5.65	130.60	122.35
1	C	691	HIS	C-N-CA	5.65	130.60	122.35
1	D	171	GLY	N-CA-C	5.63	119.74	112.54
1	D	98	GLY	N-CA-C	-5.62	104.65	112.18
1	D	412	LEU	CA-C-O	-5.62	113.75	120.10
1	D	471	ARG	N-CA-C	5.60	118.86	109.95
1	C	237	ASP	O-C-N	5.60	127.91	122.09
1	C	373	MET	CA-C-N	-5.60	115.81	123.14
1	C	373	MET	C-N-CA	-5.60	115.81	123.14
1	C	206	PHE	CA-CB-CG	-5.59	108.20	113.80
1	A	313	ARG	NE-CZ-NH2	5.59	124.23	119.20
1	A	74	GLY	CA-C-O	-5.57	116.07	121.92
1	B	93	ASN	N-CA-C	5.57	118.54	109.24
1	A	51	ALA	O-C-N	5.57	127.07	121.56
1	C	509	ARG	NE-CZ-NH2	5.57	124.21	119.20
1	A	416	THR	CA-C-N	5.56	132.16	121.54
1	A	416	THR	C-N-CA	5.56	132.16	121.54
1	B	471	ARG	N-CA-C	5.56	118.76	110.14
1	A	72	ARG	CA-C-O	-5.55	114.43	120.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	435	ARG	CB-CA-C	-5.54	100.71	109.42
1	C	168	THR	N-CA-C	-5.52	101.84	110.17
1	A	217	PHE	CA-CB-CG	-5.51	108.29	113.80
1	D	70	ASP	CA-CB-CG	5.51	118.11	112.60
1	D	62	ASN	CA-CB-CG	5.50	118.10	112.60
1	D	317	PHE	CA-C-O	-5.50	115.05	120.82
1	D	414	SER	O-C-N	-5.50	115.28	122.59
1	C	65	LEU	CA-C-O	-5.49	114.73	120.55
1	D	554	LEU	CB-CA-C	-5.49	102.26	110.88
1	B	369	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	A	304	TRP	N-CA-C	5.49	117.69	111.11
1	A	212	HIS	CA-CB-CG	-5.48	108.32	113.80
1	D	615	ASP	CA-CB-CG	5.48	118.08	112.60
1	A	168	THR	CA-C-N	-5.47	117.56	123.08
1	A	168	THR	C-N-CA	-5.47	117.56	123.08
1	C	130	ARG	NE-CZ-NH2	-5.47	114.28	119.20
1	D	93	ASN	OD1-CG-ND2	-5.47	117.13	122.60
1	B	355	ASP	CA-C-O	5.46	123.94	119.36
1	A	616	LEU	CA-C-N	5.46	127.53	120.44
1	A	616	LEU	C-N-CA	5.46	127.53	120.44
1	A	166	PHE	CA-C-O	-5.45	114.82	121.36
1	A	279	LEU	CA-C-O	-5.45	114.94	120.71
1	A	446	ASP	CA-CB-CG	5.45	118.05	112.60
1	B	431	ILE	N-CA-C	-5.44	103.61	108.95
1	C	526	GLY	N-CA-C	-5.44	106.19	112.50
1	B	509	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	B	278	ARG	CD-NE-CZ	5.41	131.97	124.40
1	B	403	THR	N-CA-CB	5.41	120.34	111.31
1	D	98	GLY	CA-C-O	-5.40	117.67	121.88
1	A	668	PRO	CA-C-O	-5.38	115.44	122.12
1	C	304	TRP	N-CA-C	5.38	117.58	111.02
1	C	492	ASN	CB-CG-ND2	-5.38	108.33	116.40
1	A	481	GLY	CA-C-O	-5.38	115.10	122.31
1	D	168	THR	CA-C-O	-5.38	115.31	121.82
1	D	416	THR	CA-C-N	5.38	128.26	120.79
1	D	416	THR	C-N-CA	5.38	128.26	120.79
1	B	648	LEU	N-CA-C	5.37	117.21	109.04
1	C	574	THR	CB-CA-C	-5.37	100.80	109.67
1	B	306	GLU	CA-C-N	5.37	127.42	120.44
1	B	306	GLU	C-N-CA	5.37	127.42	120.44
1	B	422	ARG	N-CA-CB	-5.36	102.20	110.13
1	B	478	LYS	N-CA-CB	-5.36	101.50	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	281	ASN	CA-CB-CG	5.34	117.94	112.60
1	A	317	PHE	CA-C-O	-5.33	114.90	120.55
1	D	178	THR	N-CA-C	5.32	118.61	112.97
1	B	279	LEU	CA-C-O	-5.31	115.08	120.71
1	A	670	GLY	N-CA-C	-5.30	103.42	110.58
1	D	189	PHE	CA-CB-CG	5.30	119.11	113.80
1	D	183	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	B	486	GLN	OE1-CD-NE2	-5.29	117.31	122.60
1	D	246	GLN	CA-C-N	5.29	124.96	119.56
1	D	246	GLN	C-N-CA	5.29	124.96	119.56
1	D	640	VAL	N-CA-CB	5.29	121.72	111.93
1	A	279	LEU	N-CA-C	-5.29	101.08	109.59
1	A	467	ASP	CA-CB-CG	5.28	117.88	112.60
1	D	47	ALA	N-CA-C	5.28	117.11	111.36
1	B	81	THR	CA-CB-CG2	5.28	119.47	110.50
1	D	147	ILE	N-CA-C	5.27	119.58	113.42
1	C	421	SER	CA-C-O	5.26	126.35	120.82
1	A	171	GLY	N-CA-C	5.26	118.12	112.33
1	A	360	ILE	N-CA-CB	5.26	118.40	111.40
1	B	259	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	471	ARG	N-CA-C	5.24	118.29	109.95
1	C	185	PHE	CA-CB-CG	5.24	119.04	113.80
1	A	168	THR	N-CA-C	-5.24	101.75	109.86
1	D	506	SER	CB-CA-C	5.23	120.72	110.67
1	B	444	GLN	OE1-CD-NE2	-5.23	117.37	122.60
1	A	195	ILE	CB-CA-C	-5.22	104.36	111.15
1	B	318	HIS	N-CA-C	5.22	117.05	111.36
1	B	128	ASN	OD1-CG-ND2	-5.20	117.40	122.60
1	C	618	ALA	O-C-N	5.20	127.43	122.07
1	A	206	PHE	CA-CB-CG	-5.20	108.61	113.80
1	A	694	PRO	O-C-N	-5.19	117.04	123.01
1	D	715	GLU	CA-CB-CG	5.19	124.48	114.10
1	A	167	SER	O-C-N	5.19	128.71	123.26
1	B	241	ASP	CA-CB-CG	5.19	117.79	112.60
1	B	370	VAL	N-CA-CB	-5.19	105.12	112.12
1	B	399	GLY	N-CA-C	-5.18	107.84	114.37
1	D	680	ASP	CA-CB-CG	5.18	117.78	112.60
1	D	303	VAL	CA-C-O	-5.18	114.49	121.32
1	B	168	THR	CA-C-N	-5.17	117.67	123.16
1	B	168	THR	C-N-CA	-5.17	117.67	123.16
1	D	121	ARG	NE-CZ-NH1	5.17	126.67	121.50
1	D	260	ARG	NE-CZ-NH2	-5.17	114.55	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	725	ASP	CA-C-N	5.17	125.68	120.00
1	C	725	ASP	C-N-CA	5.17	125.68	120.00
1	A	309	LYS	CA-C-N	5.16	128.16	120.31
1	A	309	LYS	C-N-CA	5.16	128.16	120.31
1	C	536	ARG	CA-C-O	5.16	122.65	119.29
1	A	224	GLU	CA-C-O	5.15	124.95	119.80
1	D	344	GLU	CB-CA-C	-5.15	99.55	110.31
1	B	446	ASP	CB-CA-C	-5.14	109.10	115.89
1	D	267	ARG	NE-CZ-NH1	-5.14	116.36	121.50
1	C	444	GLN	CA-C-O	-5.14	115.40	121.16
1	A	154	SER	CA-C-O	-5.14	113.07	119.18
1	B	707	THR	N-CA-CB	5.14	117.67	110.12
1	C	169	VAL	CB-CA-C	-5.13	106.57	111.44
1	A	702	ARG	CA-C-N	5.13	128.80	120.60
1	A	702	ARG	C-N-CA	5.13	128.80	120.60
1	A	379	PRO	CB-CA-C	-5.10	103.52	111.22
1	A	501	PHE	CA-CB-CG	5.10	118.90	113.80
1	C	509	ARG	NE-CZ-NH1	-5.10	116.40	121.50
1	A	355	ASP	CA-CB-CG	5.09	117.69	112.60
1	B	48	GLN	O-C-N	5.09	125.52	121.55
1	A	81	THR	CA-CB-CG2	5.09	119.16	110.50
1	C	146	ASP	CA-CB-CG	-5.09	107.51	112.60
1	C	543	VAL	N-CA-C	-5.09	105.58	110.72
1	D	224	GLU	CB-CA-C	5.09	117.56	109.52
1	C	182	ILE	CA-C-O	-5.08	115.84	121.98
1	D	87	ARG	NE-CZ-NH1	5.07	126.57	121.50
1	B	98	GLY	N-CA-C	-5.07	106.34	112.48
1	A	593	ILE	CA-C-O	5.07	122.90	119.20
1	C	71	VAL	CA-C-O	-5.07	113.83	119.20
1	A	110	LEU	CA-C-O	-5.04	115.53	120.82
1	B	496	GLU	N-CA-CB	-5.04	102.00	111.13
1	C	166	PHE	CA-C-O	-5.04	115.33	121.28
1	C	416	THR	CA-C-N	5.03	127.78	120.79
1	C	416	THR	C-N-CA	5.03	127.78	120.79
1	A	636	ARG	CA-C-O	-5.02	116.08	121.45
1	C	246	GLN	CA-C-N	5.02	124.68	119.56
1	C	246	GLN	C-N-CA	5.02	124.68	119.56
1	C	704	PHE	CA-CB-CG	-5.02	108.78	113.80
1	C	422	ARG	N-CA-C	5.02	116.56	111.14

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	207	PHE	Mainchain

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	5744	0	5577	77	1
1	B	5744	0	5577	111	1
1	C	5744	0	5577	80	0
1	D	5744	0	5577	94	0
2	A	43	0	30	2	0
2	B	43	0	30	3	0
2	C	43	0	30	3	0
2	D	43	0	30	4	0
3	A	6	0	0	5	0
3	B	6	0	0	3	0
3	C	6	0	0	2	0
3	D	8	0	0	4	0
4	A	581	0	0	5	0
4	B	440	0	0	12	0
4	C	474	0	0	8	0
4	D	530	0	0	7	0
All	All	25199	0	22428	335	1

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 7.

All (335) 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)
3:C:5003:PEO:O2	3:C:5003:PEO:O1	1.53	1.27
3:A:3002:PEO:O2	3:A:3002:PEO:O1	1.53	1.26
3:C:5001:PEO:O2	3:C:5001:PEO:O1	1.52	1.26
3:A:3003:PEO:O2	3:A:3003:PEO:O1	1.53	1.25
3:D:6002:PEO:O1	3:D:6002:PEO:O2	1.52	1.25
3:D:3004:PEO:O1	3:D:3004:PEO:O2	1.54	1.25
3:D:6003:PEO:O2	3:D:6003:PEO:O1	1.54	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:4003:PEO:O2	3:B:4003:PEO:O1	1.54	1.24
3:B:4002:PEO:O2	3:B:4002:PEO:O1	1.54	1.22
3:B:4001:PEO:O2	3:B:4001:PEO:O1	1.54	1.20
1:A:451:MET:HE2	1:C:451:MET:HE2	1.41	1.01
1:D:709:LYS:HG2	1:D:751:ILE:HD11	1.52	0.91
1:C:126:ILE:HD12	2:C:760:HEM:HMD1	1.51	0.90
1:D:39:ALA:H	1:D:48:GLN:HE21	1.20	0.89
1:D:39:ALA:H	1:D:48:GLN:NE2	1.74	0.85
1:B:451:MET:HE2	1:D:451:MET:HE2	1.58	0.83
1:A:710:ILE:HD13	1:A:718:ILE:HG13	1.63	0.80
2:C:760:HEM:HMC2	2:C:760:HEM:HBC2	1.62	0.80
1:D:126:ILE:HD11	2:D:760:HEM:HMD1	1.63	0.80
1:C:345:ASP:HA	1:C:348:LYS:HD3	1.64	0.78
1:B:710:ILE:HD13	1:B:718:ILE:HG13	1.66	0.77
1:B:345:ASP:HA	1:B:348:LYS:HD2	1.67	0.76
1:D:126:ILE:CD1	2:D:760:HEM:HMD1	2.17	0.75
1:C:584:LYS:HE3	1:C:586:PRO:HG3	1.68	0.75
1:A:457:PRO:HG2	1:C:37:ARG:NH2	2.01	0.74
2:B:760:HEM:HBC2	2:B:760:HEM:HMC2	1.66	0.74
1:D:126:ILE:H	1:D:126:ILE:HD12	1.54	0.73
1:B:29:LEU:HD13	1:C:245:LEU:HD13	1.73	0.71
1:C:490:GLU:HG3	1:D:490:GLU:HG3	1.71	0.70
1:B:583:LYS:O	1:B:584:LYS:HB3	1.92	0.69
1:D:144:LEU:HD11	1:D:370:VAL:HG13	1.73	0.69
1:D:710:ILE:HG23	1:D:715:GLU:HG2	1.74	0.69
1:A:639:GLU:HG3	4:A:3553:HOH:O	1.93	0.69
1:B:666:ILE:HG12	1:B:696:ALA:HB3	1.75	0.68
1:D:671:ASN:HD21	1:D:673:ALA:HB3	1.58	0.67
1:C:552:LEU:HD22	1:C:556:GLN:HG3	1.75	0.67
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.09	0.67
1:A:532:SER:HB2	1:D:637:MET:HG3	1.75	0.66
4:A:3560:HOH:O	1:C:28:SER:HA	1.94	0.66
1:A:96:ARG:HD3	4:A:3378:HOH:O	1.97	0.64
1:B:183:ARG:HG2	4:B:4287:HOH:O	1.97	0.64
1:D:552:LEU:HD11	1:D:571:LEU:HD23	1.80	0.64
1:B:222:LYS:HB3	1:B:223:PRO:HD2	1.80	0.64
1:D:32:GLU:O	1:D:33:ASP:HB3	1.98	0.63
1:B:281:ASN:OD1	1:B:283:GLU:HG2	1.98	0.62
1:B:413:PHE:CZ	1:C:111:ARG:HB2	2.34	0.62
1:B:583:LYS:HE2	1:B:583:LYS:H	1.63	0.62
1:D:180:ARG:O	1:D:181:ASP:HB2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.83	0.61
1:B:139:GLN:HG3	1:B:159:ILE:HG12	1.83	0.61
1:B:556:GLN:HG2	1:B:566:LEU:CD2	2.31	0.61
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.85	0.60
1:D:126:ILE:HD12	1:D:126:ILE:N	2.14	0.60
1:D:689:TYR:HA	1:D:744:ARG:NH1	2.16	0.59
1:A:92:GLN:HA	1:D:213:LYS:HD3	1.83	0.59
1:C:696:ALA:HB1	1:C:728:PHE:CZ	2.39	0.57
1:B:275:HIS:CD2	1:B:408:LEU:HB2	2.39	0.57
1:B:604:ALA:HB2	1:B:662:VAL:HG11	1.85	0.57
1:B:36:HIS:NE2	1:B:37:ARG:NE	2.52	0.56
1:C:610:GLU:OE1	1:C:643:ASP:HA	2.05	0.56
1:B:144:LEU:HD11	1:B:370:VAL:HG13	1.87	0.56
1:D:612:ARG:HA	1:D:643:ASP:OD2	2.05	0.56
1:A:341:ILE:HD11	1:A:360:ILE:HD13	1.86	0.56
1:C:43:THR:HG21	1:C:48:GLN:HG3	1.87	0.56
1:B:696:ALA:HB1	1:B:728:PHE:CZ	2.41	0.56
1:A:274:ILE:HD12	2:A:760:HEM:HMB1	1.88	0.56
1:B:415:TYR:O	1:B:418:THR:HG22	2.06	0.56
1:D:51:ALA:HB1	1:D:52:PRO:HD2	1.88	0.56
1:B:634:TYR:O	1:B:653:THR:HA	2.06	0.55
1:A:637:MET:HG3	1:D:532:SER:HB2	1.89	0.55
1:B:449:HIS:ND1	4:B:4438:HOH:O	2.33	0.55
1:A:748:ILE:O	1:A:751:ILE:HG13	2.07	0.55
1:A:214:PHE:HB3	1:A:215:PRO:HD3	1.89	0.55
1:D:183:ARG:HG2	4:D:6381:HOH:O	2.06	0.55
1:D:278:ARG:HH12	1:D:487:GLU:CD	2.14	0.55
1:D:629:HIS:HD2	4:D:6324:HOH:O	1.90	0.54
1:D:745:ILE:O	1:D:748:ILE:HG12	2.07	0.54
1:A:294:LYS:NZ	4:A:3246:HOH:O	2.40	0.54
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.89	0.54
1:C:211:ALA:CB	1:C:410:GLY:HA3	2.38	0.54
1:D:341:ILE:HD13	1:D:349:PHE:CZ	2.43	0.53
2:B:760:HEM:HMB2	2:B:760:HEM:HBB2	1.90	0.53
1:D:359:LEU:H	1:D:507:HIS:HD2	1.57	0.53
1:C:37:ARG:NH1	4:C:5406:HOH:O	2.41	0.52
1:D:488:ARG:NH2	4:D:6503:HOH:O	2.36	0.52
1:B:196:PHE:HA	1:B:395:HIS:O	2.09	0.52
1:C:124:GLU:HG2	4:C:5100:HOH:O	2.09	0.52
1:C:552:LEU:HD13	1:C:556:GLN:NE2	2.25	0.52
1:D:443:PHE:CZ	1:D:470:PRO:HD2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:LEU:HD13	1:D:29:LEU:HD13	1.91	0.52
1:D:608:ASN:HD21	1:D:670:GLY:HA3	1.75	0.52
1:C:552:LEU:HD22	1:C:552:LEU:O	2.10	0.51
1:B:344:GLU:CD	1:B:344:GLU:H	2.18	0.51
1:C:141:TYR:CD1	1:C:369:ARG:HG3	2.45	0.51
1:C:113:LYS:HD2	4:C:5215:HOH:O	2.10	0.51
1:C:222:LYS:HB3	1:C:223:PRO:CD	2.41	0.51
1:D:158:LYS:NZ	4:D:6515:HOH:O	2.38	0.51
1:D:619:ILE:HD13	1:D:666:ILE:HG21	1.92	0.51
1:C:274:ILE:HD12	2:C:760:HEM:HMB1	1.91	0.51
1:D:61:ARG:HH12	1:D:72:ARG:HH12	1.57	0.51
1:B:359:LEU:H	1:B:507:HIS:HD2	1.58	0.51
1:C:591:TYR:O	1:C:592:ALA:C	2.54	0.51
1:A:457:PRO:HG2	1:C:37:ARG:HH21	1.72	0.50
1:A:51:ALA:HB1	1:A:52:PRO:HD2	1.93	0.50
1:C:310:LEU:HD13	1:C:660:LEU:HB3	1.93	0.50
1:C:345:ASP:O	1:C:348:LYS:HB2	2.11	0.50
1:D:69:GLU:OE2	1:D:72:ARG:NH1	2.43	0.50
1:C:671:ASN:HD21	1:C:673:ALA:HB3	1.75	0.50
1:A:65:LEU:HD21	1:A:135:HIS:CG	2.47	0.50
1:D:274:ILE:HD12	2:D:760:HEM:HMB1	1.91	0.50
1:D:605:ILE:HD12	1:D:630:ALA:HB1	1.94	0.50
1:C:158:LYS:HD2	4:C:5466:HOH:O	2.12	0.49
1:A:696:ALA:HB1	1:A:728:PHE:CZ	2.47	0.49
1:D:476:GLY:HA3	4:D:6087:HOH:O	2.12	0.49
1:B:552:LEU:O	1:B:556:GLN:HG3	2.12	0.49
1:C:222:LYS:HB3	1:C:223:PRO:HD2	1.94	0.49
1:D:604:ALA:HB2	1:D:662:VAL:HG11	1.93	0.49
1:A:725:ASP:H	1:A:728:PHE:HB3	1.77	0.49
1:B:562:LEU:HA	1:C:637:MET:HB2	1.95	0.49
1:C:211:ALA:HB3	1:C:410:GLY:HA3	1.94	0.49
1:B:615:ASP:O	1:B:616:LEU:C	2.56	0.49
1:A:532:SER:HB2	1:D:637:MET:CG	2.43	0.49
1:B:222:LYS:HB3	1:B:223:PRO:CD	2.42	0.48
1:C:690:LYS:HE2	4:C:5271:HOH:O	2.12	0.48
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.21	0.48
1:B:73:LYS:HE3	1:D:440:TYR:O	2.13	0.48
1:B:682:ASN:HB3	1:B:707:THR:HG21	1.94	0.48
1:D:364:LEU:HD11	1:D:580:ASN:HB2	1.93	0.48
1:B:469:TRP:HA	1:B:470:PRO:C	2.38	0.48
1:D:404:ASN:O	1:D:405:ASP:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:ASN:O	1:A:405:ASP:C	2.55	0.48
1:B:59:ASP:HA	1:B:61:ARG:CZ	2.44	0.48
1:B:718:ILE:HG12	4:B:4021:HOH:O	2.13	0.48
1:D:126:ILE:CD1	1:D:126:ILE:H	2.21	0.48
4:A:3295:HOH:O	1:D:126:ILE:HG13	2.12	0.48
1:B:666:ILE:HD11	1:B:732:LEU:CD1	2.44	0.48
4:B:4182:HOH:O	1:D:52:PRO:HG3	2.13	0.48
1:D:252:ASN:HD22	1:D:252:ASN:HA	1.61	0.48
1:C:158:LYS:HB3	4:C:5466:HOH:O	2.13	0.48
1:A:459:ASN:CG	1:B:219:HIS:HB3	2.39	0.48
1:B:275:HIS:CG	1:B:408:LEU:HB2	2.49	0.48
1:B:43:THR:HG21	1:B:48:GLN:HG3	1.96	0.47
1:A:509:ARG:HD2	1:A:576:PRO:HD2	1.96	0.47
1:C:749:ASP:HB3	1:C:750:LYS:HE2	1.96	0.47
1:D:750:LYS:HD2	1:D:751:ILE:HG13	1.96	0.47
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.28	0.47
1:A:604:ALA:HB2	1:A:662:VAL:HG11	1.96	0.47
1:B:76:GLU:O	1:B:77:ASN:HB2	2.14	0.47
1:B:267:ARG:HG2	1:B:332:PRO:HB3	1.96	0.47
1:D:511:PHE:O	1:D:515:GLN:HG2	2.15	0.47
3:A:3001:PEO:O2	3:A:3002:PEO:O2	2.31	0.47
1:C:612:ARG:HB2	1:C:612:ARG:CZ	2.45	0.47
1:D:122:ILE:HB	1:D:123:PRO:HD2	1.97	0.47
1:A:516:THR:HB	1:A:517:PRO:HD2	1.97	0.47
1:B:535:VAL:O	1:B:537:PRO:HD3	2.15	0.47
1:D:598:VAL:HG22	1:D:628:VAL:HG22	1.97	0.47
1:B:211:ALA:HB3	1:B:410:GLY:HA3	1.96	0.47
1:D:60:THR:O	1:D:61:ARG:HD2	2.15	0.47
1:A:607:LEU:HD11	1:A:632:LEU:HB3	1.96	0.47
1:B:249:THR:O	1:B:253:VAL:HG23	2.15	0.47
1:B:305:ASP:O	1:B:309:LYS:HB2	2.15	0.47
1:B:748:ILE:O	1:B:751:ILE:HG22	2.15	0.47
1:C:260:ARG:HD3	1:C:590:LEU:HD21	1.95	0.47
1:C:275:HIS:CD2	1:C:408:LEU:HD13	2.49	0.47
1:A:36:HIS:CD2	1:A:36:HIS:H	2.33	0.46
1:B:449:HIS:CD2	1:D:449:HIS:CD2	3.03	0.46
1:D:359:LEU:H	1:D:507:HIS:CD2	2.33	0.46
1:C:727:SER:O	1:C:731:GLU:HG3	2.14	0.46
1:B:191:THR:HB	4:B:4063:HOH:O	2.15	0.46
1:B:258:SER:HA	1:B:523:ILE:HG12	1.97	0.46
1:A:626:LYS:HG3	1:A:733:LEU:HD13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:ASN:HD22	1:B:460:TYR:HD2	1.63	0.46
1:B:162:VAL:HG21	1:B:373:MET:SD	2.55	0.46
1:C:52:PRO:HB3	1:C:380:ASP:HA	1.97	0.46
1:B:309:LYS:HE2	4:B:4213:HOH:O	2.15	0.46
1:C:535:VAL:O	1:C:537:PRO:HD3	2.16	0.46
1:C:583:LYS:O	1:C:584:LYS:HB3	2.15	0.46
1:B:205:ILE:HB	1:B:356:PRO:O	2.16	0.46
1:A:119:HIS:CE1	1:C:420:ILE:HG21	2.52	0.46
1:B:44:PRO:HB3	1:B:629:HIS:CD2	2.51	0.46
1:B:118:ASP:OD1	1:C:417:ASP:OD2	2.34	0.45
1:C:332:PRO:HB2	1:C:375:LEU:HB2	1.97	0.45
1:C:469:TRP:HA	1:C:470:PRO:C	2.40	0.45
1:B:364:LEU:HD11	1:B:580:ASN:HB2	1.98	0.45
1:D:65:LEU:HD21	1:D:135:HIS:CG	2.51	0.45
1:A:459:ASN:HD22	1:A:460:TYR:HD2	1.65	0.45
1:C:331:PHE:O	1:C:333:GLU:HG3	2.16	0.45
1:C:488:ARG:HE	1:C:488:ARG:HB2	1.54	0.45
1:B:264:ARG:HH12	1:B:321:GLU:CD	2.24	0.45
1:C:643:ASP:OD1	1:C:644:ASP:N	2.50	0.45
1:B:448:MET:HG3	1:D:122:ILE:HG22	1.98	0.45
1:A:413:PHE:CZ	1:D:111:ARG:HB2	2.52	0.45
1:B:591:TYR:O	1:B:592:ALA:C	2.59	0.45
1:A:211:ALA:CB	1:A:410:GLY:HA3	2.47	0.45
1:D:331:PHE:O	1:D:333:GLU:HG3	2.17	0.45
1:C:617:LEU:HD12	4:C:5419:HOH:O	2.16	0.45
1:D:606:LEU:O	1:D:668:PRO:HD2	2.17	0.45
1:C:748:ILE:O	1:C:751:ILE:HG23	2.17	0.45
1:D:126:ILE:HD13	2:D:760:HEM:HMD1	1.98	0.44
1:B:486:GLN:OE1	4:B:4416:HOH:O	2.21	0.44
1:B:583:LYS:H	1:B:583:LYS:CE	2.30	0.44
1:B:355:ASP:HA	1:B:356:PRO:HD2	1.92	0.44
1:B:309:LYS:HD2	1:C:313:ARG:NH2	2.32	0.44
1:B:331:PHE:HA	1:B:332:PRO:HD3	1.85	0.44
1:D:415:TYR:O	1:D:418:THR:HG22	2.16	0.44
1:A:530:GLU:OE2	3:A:3003:PEO:O1	2.36	0.44
1:B:339:GLN:HG3	1:B:367:VAL:HG22	1.99	0.44
1:B:362:GLU:HG2	1:B:367:VAL:HG23	1.98	0.44
1:B:449:HIS:HB2	1:D:449:HIS:CE1	2.53	0.44
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.47	0.44
1:A:27:ASP:HA	1:C:471:ARG:CZ	2.48	0.44
1:A:29:LEU:HD12	1:C:468:ASN:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:634:TYR:O	1:D:653:THR:HA	2.17	0.44
1:A:364:LEU:HD11	1:A:580:ASN:HB2	1.98	0.44
1:D:309:LYS:NZ	1:D:683:TYR:OH	2.50	0.44
1:D:512:TRP:CH2	1:D:520:GLN:HB3	2.53	0.44
1:B:629:HIS:HD2	4:B:4242:HOH:O	2.00	0.43
1:C:490:GLU:HG3	1:D:490:GLU:CG	2.45	0.43
1:D:195:ILE:HD11	1:D:436:PRO:HA	2.01	0.43
1:D:310:LEU:HD13	1:D:660:LEU:HB3	1.98	0.43
1:A:207:PHE:O	1:A:249:THR:HA	2.19	0.43
1:A:276:THR:CG2	1:A:288:PHE:HB3	2.49	0.43
1:B:115:THR:O	1:B:119:HIS:HD2	2.01	0.43
1:B:404:ASN:O	1:B:405:ASP:C	2.61	0.43
1:C:578:ASP:HB2	1:C:582:LEU:O	2.18	0.43
1:A:392:HIS:ND1	1:A:393:PRO:HD2	2.33	0.43
1:B:579:VAL:O	1:B:580:ASN:C	2.62	0.43
1:B:397:VAL:HB	1:B:398:PRO:HD2	2.01	0.43
1:B:507:HIS:N	1:B:508:PRO:CD	2.81	0.43
1:D:158:LYS:HB2	1:D:158:LYS:HE3	1.92	0.43
1:A:71:VAL:HG21	1:A:432:PRO:HG2	2.01	0.43
1:C:305:ASP:O	1:C:309:LYS:HG3	2.18	0.43
1:C:732:LEU:HD13	1:C:732:LEU:C	2.44	0.43
1:A:115:THR:O	1:A:119:HIS:HD2	2.01	0.43
1:A:211:ALA:HB3	1:A:410:GLY:HA3	2.00	0.43
1:A:213:LYS:HD3	1:D:92:GLN:HA	2.00	0.43
1:B:593:ILE:HA	1:B:594:PRO:HD2	1.76	0.43
1:A:76:GLU:O	1:A:77:ASN:HB2	2.19	0.43
1:B:443:PHE:CZ	1:B:470:PRO:HD2	2.54	0.43
1:C:359:LEU:H	1:C:507:HIS:HD2	1.66	0.43
1:A:145:SER:HA	1:A:148:THR:O	2.19	0.43
1:B:31:PRO:HG3	1:C:538:TYR:CE2	2.53	0.43
1:B:126:ILE:CG2	2:B:760:HEM:HMD1	2.49	0.43
1:B:451:MET:SD	4:B:4438:HOH:O	2.62	0.43
1:C:227:TRP:CE3	1:C:229:ILE:HD12	2.54	0.43
1:C:686:MET:O	1:C:751:ILE:HD11	2.19	0.43
1:D:478:LYS:HE2	4:D:6481:HOH:O	2.19	0.43
1:A:126:ILE:HG12	1:D:117:PHE:CZ	2.54	0.42
3:D:6001:PEO:O2	3:D:6002:PEO:O2	2.37	0.42
1:C:461:GLU:HA	1:C:462:PRO:C	2.45	0.42
1:A:356:PRO:HG3	1:A:405:ASP:OD1	2.19	0.42
1:B:578:ASP:HB3	1:B:582:LEU:O	2.20	0.42
1:A:27:ASP:O	1:A:28:SER:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:ILE:HA	1:A:594:PRO:HD2	1.88	0.42
1:B:521:ARG:HE	1:B:745:ILE:HG21	1.84	0.42
1:D:671:ASN:ND2	1:D:673:ALA:HB3	2.29	0.42
1:A:31:PRO:HD2	1:A:36:HIS:CD2	2.55	0.42
1:A:288:PHE:CE2	1:A:343:GLU:HA	2.54	0.42
1:A:538:TYR:CE2	1:D:31:PRO:HG3	2.54	0.42
1:C:704:PHE:O	1:C:707:THR:HG22	2.20	0.42
1:D:211:ALA:HB3	1:D:410:GLY:HA3	2.01	0.42
1:D:593:ILE:HA	1:D:594:PRO:HD2	1.86	0.42
1:B:61:ARG:HG2	1:B:66:ASN:OD1	2.20	0.42
1:B:377:ARG:HD2	1:B:378:ASN:O	2.20	0.42
1:D:459:ASN:HD22	1:D:460:TYR:HD2	1.67	0.42
1:B:119:HIS:CE1	1:D:420:ILE:HG21	2.54	0.42
1:B:130:ARG:HB3	1:B:168:THR:OG1	2.20	0.42
1:A:31:PRO:HG3	1:D:538:TYR:CE2	2.55	0.42
1:B:118:ASP:HA	1:C:126:ILE:CD1	2.49	0.42
1:B:607:LEU:HD22	1:B:611:VAL:HG21	2.01	0.42
1:B:612:ARG:HD2	1:B:643:ASP:OD2	2.20	0.42
1:B:643:ASP:OD1	1:B:644:ASP:N	2.53	0.42
1:C:51:ALA:HB1	1:C:52:PRO:CD	2.49	0.42
1:D:609:ASP:N	1:D:674:ASP:OD1	2.53	0.42
1:A:634:TYR:O	1:A:653:THR:HA	2.20	0.42
1:B:708:ILE:HG13	1:B:710:ILE:HD12	2.02	0.42
1:D:552:LEU:HD13	1:D:556:GLN:HG3	2.02	0.42
1:D:708:ILE:HD12	1:D:710:ILE:HD11	2.01	0.42
1:A:91:ASP:HB3	1:C:461:GLU:OE1	2.20	0.42
1:B:235:ALA:HB1	1:B:533:LYS:HD3	2.01	0.42
1:B:604:ALA:HB1	1:B:633:LEU:HD22	2.00	0.42
1:B:675:ILE:HG13	1:B:704:PHE:HZ	1.84	0.42
1:A:137:TYR:HB2	1:A:159:ILE:HG23	2.01	0.41
1:A:708:ILE:HG13	1:A:710:ILE:HD12	2.02	0.41
1:B:330:ASP:OD1	1:B:629:HIS:HE1	2.02	0.41
1:B:368:GLN:HB2	4:B:4375:HOH:O	2.19	0.41
1:A:201:ASN:OD1	3:A:3002:PEO:O1	2.38	0.41
1:B:221:VAL:HG23	1:B:239:PHE:CD1	2.55	0.41
1:C:252:ASN:HD22	1:C:252:ASN:HA	1.62	0.41
1:D:37:ARG:HA	1:D:38:PRO:HD2	1.92	0.41
1:A:443:PHE:CZ	1:A:470:PRO:HD2	2.55	0.41
1:A:126:ILE:HD12	1:D:121:ARG:CZ	2.51	0.41
1:B:386:ASN:OD1	1:B:386:ASN:C	2.63	0.41
1:C:511:PHE:O	1:C:515:GLN:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:592:ALA:O	1:C:594:PRO:HD3	2.20	0.41
1:A:461:GLU:HA	1:A:462:PRO:C	2.46	0.41
1:B:124:GLU:HG2	4:C:5045:HOH:O	2.20	0.41
1:B:745:ILE:HB	1:B:746:PRO:HD3	2.01	0.41
1:C:278:ARG:HH12	1:C:487:GLU:CD	2.29	0.41
1:A:262:ILE:O	1:A:262:ILE:HG13	2.21	0.41
1:A:516:THR:HB	1:A:517:PRO:CD	2.51	0.41
1:B:237:ASP:OD2	1:B:536:ARG:HG3	2.20	0.41
1:B:516:THR:HB	1:B:517:PRO:CD	2.51	0.41
1:C:51:ALA:HB1	1:C:52:PRO:HD2	2.01	0.41
1:B:113:LYS:HD2	4:B:4183:HOH:O	2.19	0.41
1:B:451:MET:HG3	1:D:451:MET:HE2	2.02	0.41
1:C:660:LEU:HD13	1:C:687:GLU:CD	2.46	0.41
1:A:222:LYS:HB3	1:A:223:PRO:HD2	2.03	0.41
1:A:488:ARG:NH1	1:B:491:GLY:HA2	2.36	0.41
1:A:602:VAL:HG13	1:A:662:VAL:HA	2.03	0.41
1:A:637:MET:HB2	1:D:562:LEU:HA	2.03	0.41
1:B:252:ASN:HD22	1:B:252:ASN:HA	1.75	0.41
1:B:616:LEU:HD23	1:B:616:LEU:HA	1.81	0.41
1:C:128:ASN:HA	1:C:168:THR:O	2.20	0.41
1:D:488:ARG:NH1	1:D:490:GLU:OE1	2.49	0.41
1:A:128:ASN:HA	1:A:168:THR:O	2.22	0.41
1:A:264:ARG:HH21	1:A:663:ASP:CG	2.28	0.41
1:A:461:GLU:OE1	1:C:91:ASP:HB3	2.20	0.41
1:C:507:HIS:N	1:C:508:PRO:HD2	2.35	0.41
1:D:461:GLU:HB2	1:D:462:PRO:HA	2.02	0.41
1:A:405:ASP:HA	1:A:406:PRO:HD2	1.97	0.40
1:B:535:VAL:HG22	4:B:4320:HOH:O	2.21	0.40
1:B:671:ASN:OD1	1:B:673:ALA:HB3	2.21	0.40
1:B:715:GLU:CG	1:B:747:LYS:HE2	2.51	0.40
1:A:507:HIS:N	1:A:508:PRO:CD	2.84	0.40
1:B:105:LEU:HD11	1:D:413:PHE:HB2	2.03	0.40
1:C:516:THR:HB	1:C:517:PRO:CD	2.51	0.40
1:C:534:VAL:HG11	1:C:539:ILE:HB	2.04	0.40
1:D:507:HIS:N	1:D:508:PRO:CD	2.84	0.40
1:B:608:ASN:HD22	1:B:672:ILE:HD13	1.86	0.40
1:D:158:LYS:HD2	4:D:6525:HOH:O	2.20	0.40
1:A:188:LYS:HB2	1:A:391:PHE:CE1	2.57	0.40
1:A:411:ARG:HG2	2:A:760:HEM:C2C	2.57	0.40
1:A:750:LYS:HE3	1:A:750:LYS:C	2.46	0.40
1:B:308:GLN:OE1	1:C:313:ARG:NH1	2.51	0.40

All (1) 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:59:ASP:OD1	1:B:369:ARG:NH2[2_545]	2.17	0.03

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	725/753 (96%)	701 (97%)	21 (3%)	3 (0%)	30	36
1	B	725/753 (96%)	686 (95%)	34 (5%)	5 (1%)	18	21
1	C	725/753 (96%)	698 (96%)	23 (3%)	4 (1%)	21	25
1	D	725/753 (96%)	699 (96%)	22 (3%)	4 (1%)	21	25
All	All	2900/3012 (96%)	2784 (96%)	100 (3%)	16 (1%)	21	25

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	B	28	SER
1	C	28	SER
1	C	725	ASP
1	D	33	ASP
1	B	584	LYS
1	D	725	ASP
1	A	75	SER
1	A	415	TYR
1	B	75	SER
1	B	613	SER
1	C	414	SER
1	D	28	SER
1	D	415	TYR
1	B	415	TYR

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Mol	Chain	Res	Type
1	C	415	TYR

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	612/636 (96%)	589 (96%)	23 (4%)	29	42
1	B	612/636 (96%)	581 (95%)	31 (5%)	21	29
1	C	612/636 (96%)	581 (95%)	31 (5%)	21	29
1	D	612/636 (96%)	583 (95%)	29 (5%)	23	33
All	All	2448/2544 (96%)	2334 (95%)	114 (5%)	23	33

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASP
1	A	126	ILE
1	A	142	LYS
1	A	205	ILE
1	A	252	ASN
1	A	294	LYS
1	A	341	ILE
1	A	344	GLU
1	A	353	LEU
1	A	369	ARG
1	A	375	LEU
1	A	413	PHE
1	A	432	PRO
1	A	437	THR
1	A	459	ASN
1	A	508	PRO
1	A	532	SER
1	A	552	LEU
1	A	556	GLN
1	A	565	GLU

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Mol	Chain	Res	Type
1	A	732	LEU
1	A	750	LYS
1	A	751	ILE
1	B	27	ASP
1	B	28	SER
1	B	37	ARG
1	B	126	ILE
1	B	191	THR
1	B	205	ILE
1	B	252	ASN
1	B	265	SER
1	B	309	LYS
1	B	321	GLU
1	B	353	LEU
1	B	370	VAL
1	B	375	LEU
1	B	377	ARG
1	B	413	PHE
1	B	437	THR
1	B	459	ASN
1	B	552	LEU
1	B	562	LEU
1	B	565	GLU
1	B	566	LEU
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	612	ARG
1	B	635	SER
1	B	647	VAL
1	B	722	ASP
1	B	728	PHE
1	B	732	LEU
1	B	751	ILE
1	C	27	ASP
1	C	37	ARG
1	C	73	LYS
1	C	99	SER
1	C	191	THR
1	C	205	ILE
1	C	213	LYS
1	C	252	ASN

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Mol	Chain	Res	Type
1	C	265	SER
1	C	332	PRO
1	C	348	LYS
1	C	375	LEU
1	C	437	THR
1	C	459	ASN
1	C	488	ARG
1	C	531	LEU
1	C	552	LEU
1	C	574	THR
1	C	584	LYS
1	C	606	LEU
1	C	612	ARG
1	C	616	LEU
1	C	633	LEU
1	C	639	GLU
1	C	648	LEU
1	C	660	LEU
1	C	707	THR
1	C	733	LEU
1	C	747	LYS
1	C	750	LYS
1	C	751	ILE
1	D	48	GLN
1	D	126	ILE
1	D	159	ILE
1	D	185	PHE
1	D	191	THR
1	D	205	ILE
1	D	252	ASN
1	D	265	SER
1	D	344	GLU
1	D	353	LEU
1	D	375	LEU
1	D	418	THR
1	D	437	THR
1	D	449	HIS
1	D	459	ASN
1	D	490	GLU
1	D	552	LEU
1	D	554	LEU
1	D	582	LEU

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Mol	Chain	Res	Type
1	D	610	GLU
1	D	612	ARG
1	D	616	LEU
1	D	633	LEU
1	D	648	LEU
1	D	709	LYS
1	D	713	GLN
1	D	716	GLU
1	D	747	LYS
1	D	750	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	119	HIS
1	A	212	HIS
1	A	252	ASN
1	A	449	HIS
1	A	459	ASN
1	A	486	GLN
1	A	515	GLN
1	A	556	GLN
1	A	713	GLN
1	B	84	GLN
1	B	119	HIS
1	B	139	GLN
1	B	157	ASN
1	B	212	HIS
1	B	252	ASN
1	B	449	HIS
1	B	459	ASN
1	B	486	GLN
1	B	507	HIS
1	B	629	HIS
1	C	84	GLN
1	C	246	GLN
1	C	252	ASN
1	C	441	HIS
1	C	459	ASN
1	C	507	HIS
1	C	546	GLN

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Mol	Chain	Res	Type
1	C	556	GLN
1	C	629	HIS
1	C	671	ASN
1	D	48	GLN
1	D	252	ASN
1	D	449	HIS
1	D	459	ASN
1	D	507	HIS
1	D	629	HIS
1	D	671	ASN
1	D	713	GLN

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](#)

17 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	PEO	D	6003	-	1,1,1	0.83	0	-		
3	PEO	B	4002	2	1,1,1	0.81	0	-		
3	PEO	A	3001	-	1,1,1	0.60	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	C	760	1	50,50,50	1.41	9 (18%)	67,82,82	1.12	6 (8%)
3	PEO	A	3002	-	1,1,1	0.74	0	-		
3	PEO	D	3004	-	1,1,1	0.86	0	-		
3	PEO	D	6002	-	1,1,1	0.72	0	-		
3	PEO	B	4003	-	1,1,1	0.79	0	-		
3	PEO	D	6001	-	1,1,1	0.67	0	-		
3	PEO	C	5001	-	1,1,1	0.69	0	-		
2	HEM	A	760	1	50,50,50	1.46	9 (18%)	67,82,82	1.05	5 (7%)
3	PEO	A	3003	-	1,1,1	0.77	0	-		
3	PEO	B	4001	-	1,1,1	0.80	0	-		
3	PEO	C	5002	-	1,1,1	0.67	0	-		
2	HEM	D	760	1	50,50,50	1.38	9 (18%)	67,82,82	0.86	3 (4%)
3	PEO	C	5003	-	1,1,1	0.72	0	-		
2	HEM	B	760	3,1	50,50,50	1.37	10 (20%)	67,82,82	1.05	6 (8%)

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
2	HEM	B	760	3,1	-	2/14/54/54	-
2	HEM	D	760	1	-	4/14/54/54	-
2	HEM	C	760	1	-	2/14/54/54	-
2	HEM	A	760	1	-	2/14/54/54	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	760	HEM	CAC-C3C	3.42	1.56	1.47
2	A	760	HEM	FE-NB	3.32	2.05	1.94
2	C	760	HEM	CAC-C3C	3.30	1.56	1.47
2	D	760	HEM	CAB-C3B	2.98	1.55	1.47
2	C	760	HEM	FE-NB	2.88	2.03	1.94
2	B	760	HEM	CAB-C3B	2.88	1.55	1.47
2	B	760	HEM	CAC-C3C	2.85	1.55	1.47
2	B	760	HEM	FE-ND	2.82	2.03	1.94
2	C	760	HEM	CAB-C3B	2.81	1.54	1.47
2	A	760	HEM	CMD-C2D	2.78	1.56	1.50
2	C	760	HEM	FE-ND	2.78	2.03	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	760	HEM	FE-NB	2.78	2.03	1.94
2	D	760	HEM	FE-NC	2.73	2.04	1.95
2	D	760	HEM	FE-NA	2.60	2.03	1.95
2	D	760	HEM	FE-ND	2.59	2.02	1.94
2	C	760	HEM	FE-NC	2.49	2.03	1.95
2	D	760	HEM	CAC-C3C	2.49	1.54	1.47
2	D	760	HEM	CMB-C2B	2.42	1.55	1.50
2	A	760	HEM	CMB-C2B	2.41	1.55	1.50
2	C	760	HEM	CMB-C2B	2.37	1.55	1.50
2	A	760	HEM	CAB-C3B	2.35	1.53	1.47
2	C	760	HEM	CMD-C2D	2.34	1.55	1.50
2	D	760	HEM	CMD-C2D	2.32	1.55	1.50
2	D	760	HEM	CMC-C2C	2.29	1.55	1.50
2	C	760	HEM	CMC-C2C	2.27	1.55	1.50
2	B	760	HEM	CMD-C2D	2.23	1.55	1.50
2	B	760	HEM	FE-NC	2.22	2.02	1.95
2	B	760	HEM	C3B-C2B	-2.22	1.32	1.37
2	B	760	HEM	CMB-C2B	2.19	1.55	1.50
2	A	760	HEM	CMC-C2C	2.15	1.55	1.50
2	B	760	HEM	FE-NB	2.13	2.01	1.94
2	C	760	HEM	C3D-C2D	-2.13	1.32	1.36
2	B	760	HEM	CMC-C2C	2.11	1.55	1.50
2	B	760	HEM	CAD-C3D	2.09	1.56	1.51
2	A	760	HEM	FE-NA	2.09	2.02	1.95
2	A	760	HEM	FE-ND	2.04	2.01	1.94
2	A	760	HEM	C3C-C2C	-2.01	1.33	1.37

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	760	HEM	CHC-C1C-NC	3.29	128.04	124.45
2	C	760	HEM	O1A-CGA-CBA	-3.27	112.72	123.09
2	B	760	HEM	CMA-C3A-C4A	-3.01	120.83	125.42
2	B	760	HEM	CBA-CAA-C2A	2.79	120.24	112.53
2	A	760	HEM	CHC-C4B-NB	2.70	127.33	124.42
2	B	760	HEM	CMA-C3A-C2A	2.65	131.24	125.62
2	A	760	HEM	O1A-CGA-CBA	-2.59	114.87	123.09
2	A	760	HEM	CBC-CAC-C3C	-2.56	114.73	127.53
2	A	760	HEM	C1C-CHC-C4B	-2.56	120.58	126.02
2	D	760	HEM	O1A-CGA-CBA	-2.55	115.00	123.09
2	C	760	HEM	CAD-CBD-CGD	2.49	120.27	113.67
2	B	760	HEM	O1D-CGD-CBD	-2.44	115.36	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	760	HEM	O2A-CGA-O1A	2.21	129.03	123.33
2	C	760	HEM	CMD-C2D-C1D	-2.20	121.59	125.03
2	D	760	HEM	CHD-C1D-ND	2.17	126.76	124.42
2	C	760	HEM	CHA-C1A-NA	2.15	127.75	123.86
2	B	760	HEM	O2D-CGD-CBD	2.14	120.77	114.00
2	D	760	HEM	CMD-C2D-C1D	-2.05	121.82	125.03
2	B	760	HEM	CBC-CAC-C3C	-2.02	117.45	127.53
2	C	760	HEM	CMA-C3A-C2A	2.01	129.88	125.62

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	760	HEM	C2C-C3C-CAC-CBC
2	C	760	HEM	CAA-CBA-CGA-O2A
2	B	760	HEM	CAA-CBA-CGA-O1A
2	D	760	HEM	CAA-CBA-CGA-O2A
2	B	760	HEM	CAA-CBA-CGA-O2A
2	D	760	HEM	CAA-CBA-CGA-O1A
2	A	760	HEM	CAA-CBA-CGA-O1A
2	C	760	HEM	CAA-CBA-CGA-O1A
2	A	760	HEM	CAA-CBA-CGA-O2A
2	D	760	HEM	C4C-C3C-CAC-CBC

There are no ring outliers.

16 monomers are involved in 26 short contacts:

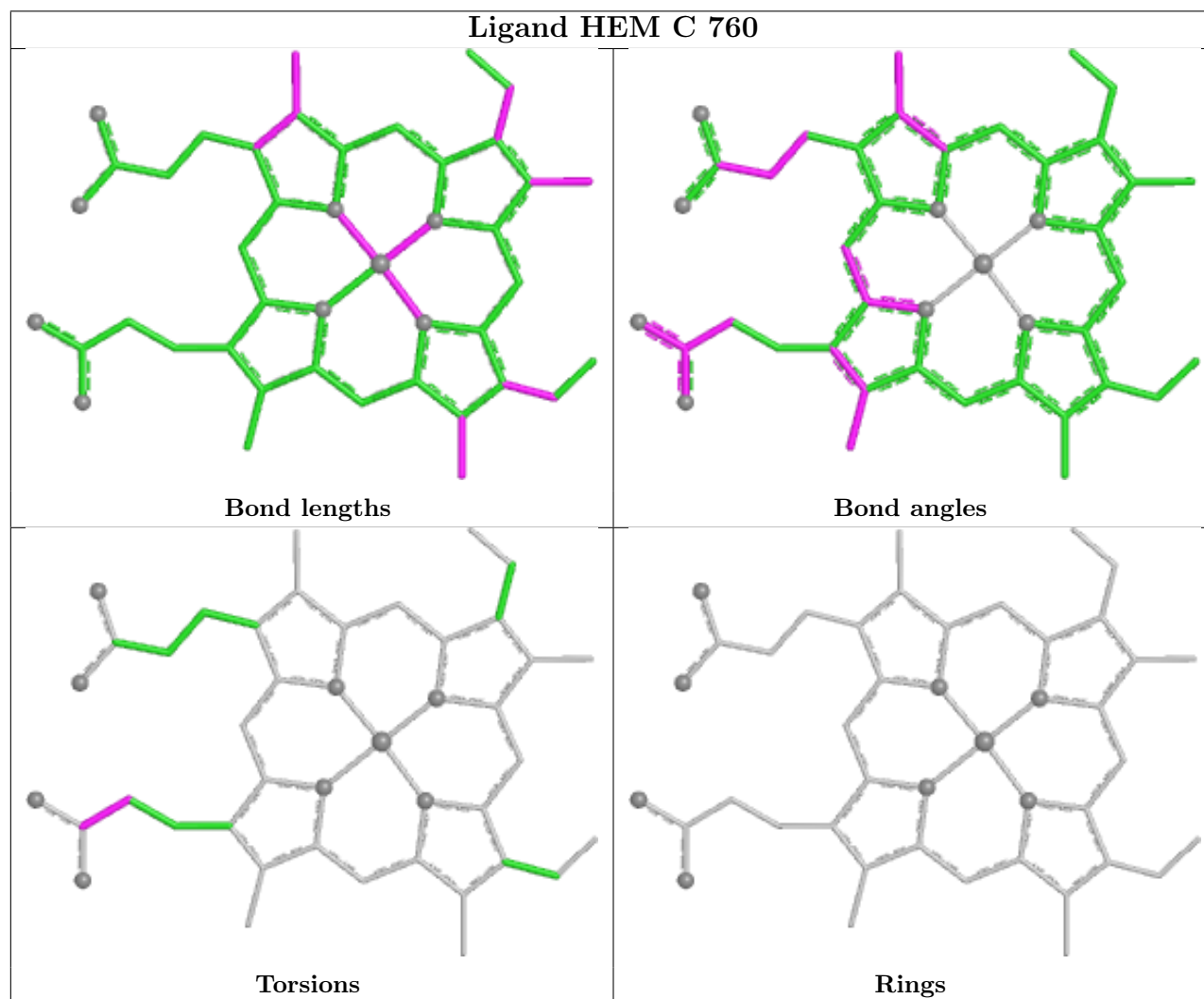
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	6003	PEO	1	0
3	B	4002	PEO	1	0
3	A	3001	PEO	1	0
2	C	760	HEM	3	0
3	A	3002	PEO	3	0
3	D	3004	PEO	1	0
3	D	6002	PEO	2	0
3	B	4003	PEO	1	0
3	D	6001	PEO	1	0
3	C	5001	PEO	1	0
2	A	760	HEM	2	0
3	A	3003	PEO	2	0
3	B	4001	PEO	1	0

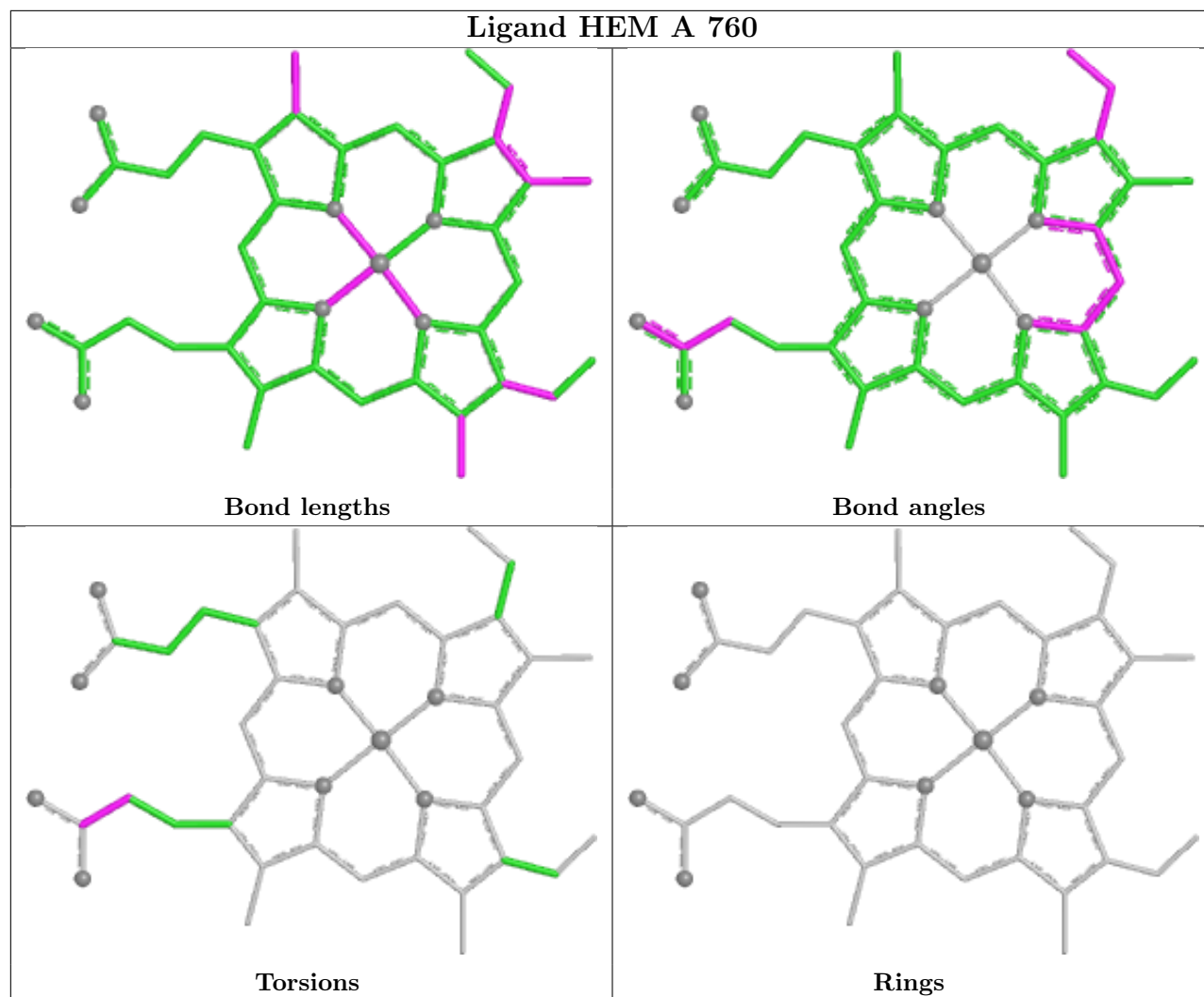
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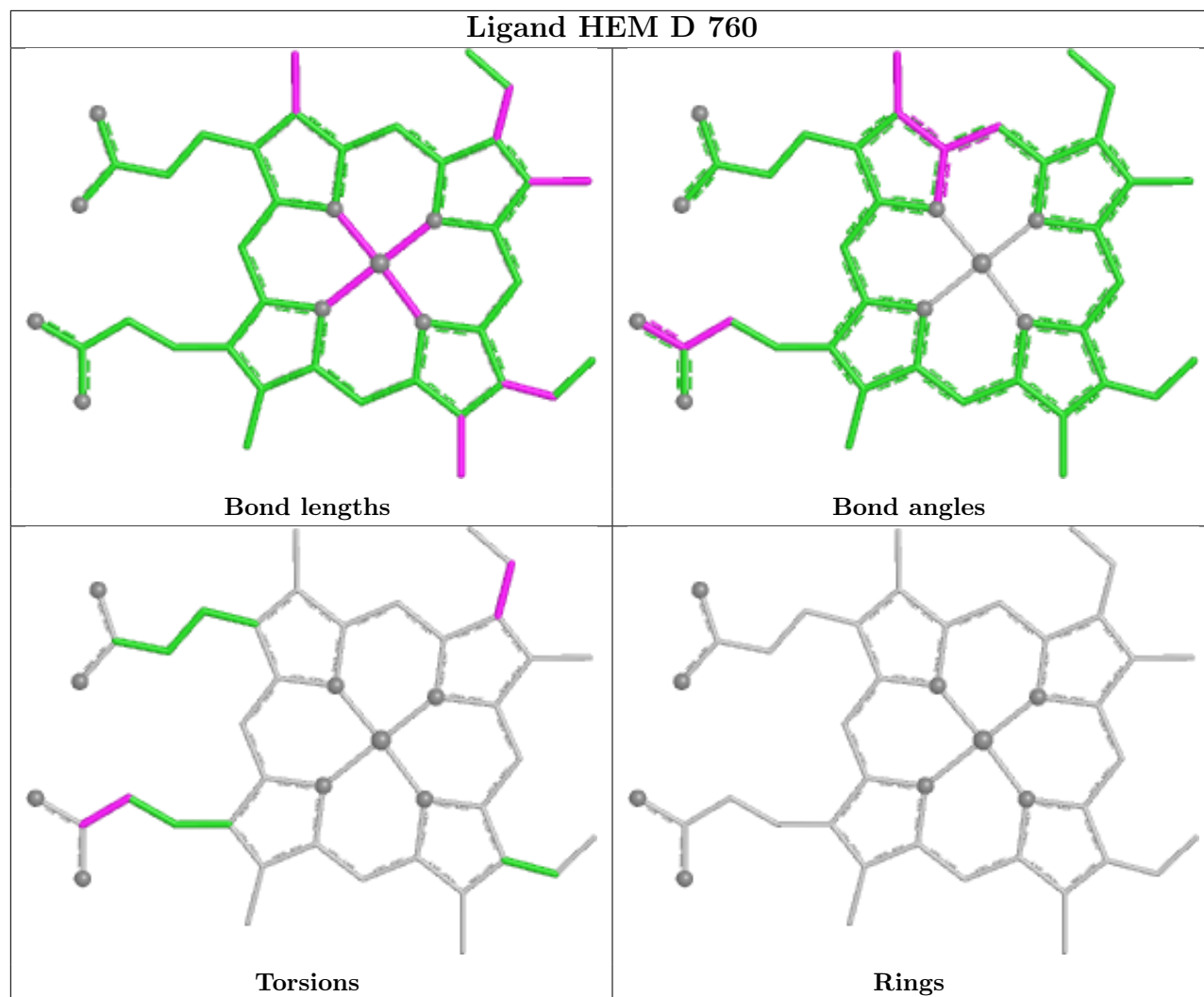
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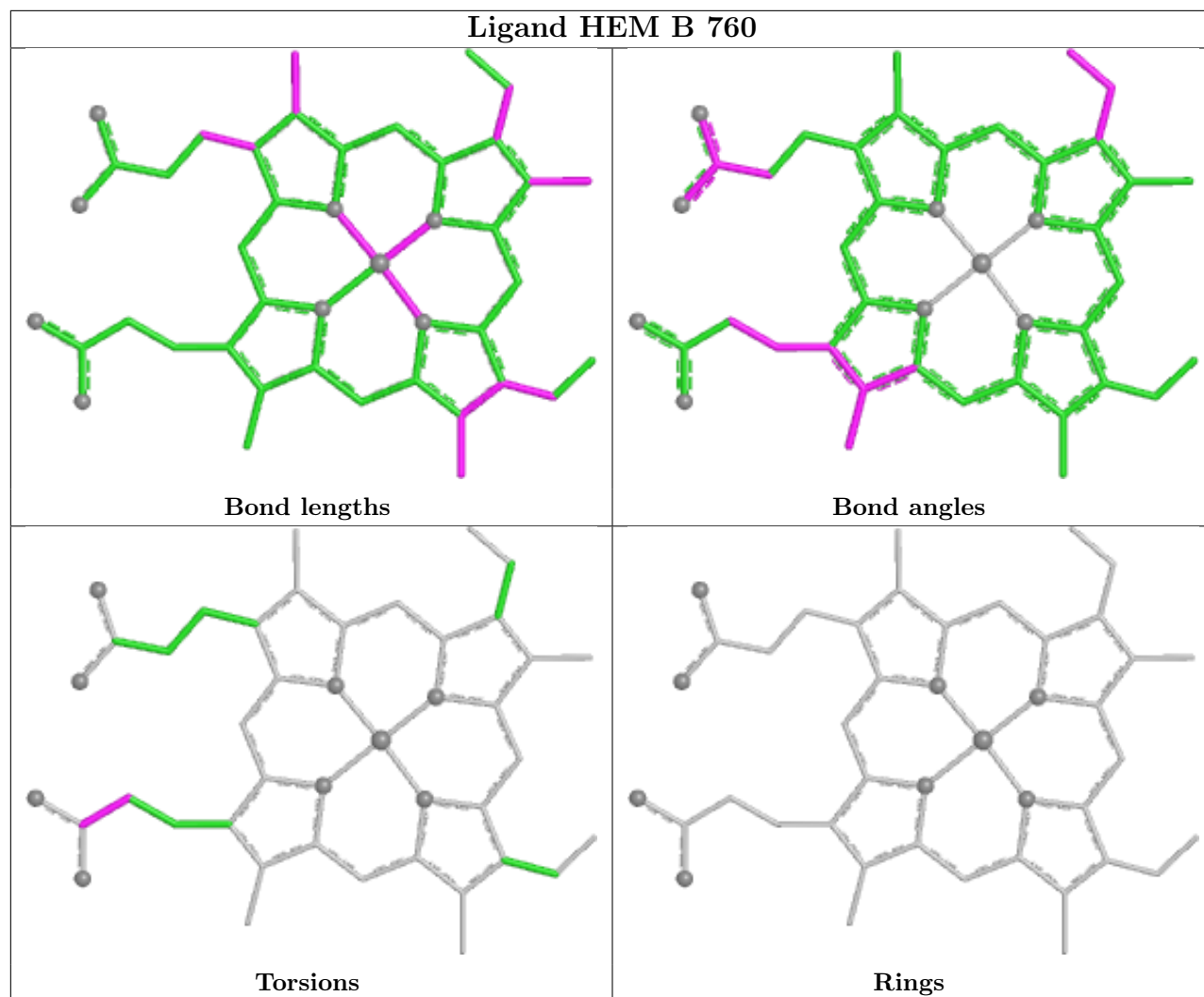
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	760	HEM	4	0
3	C	5003	PEO	1	0
2	B	760	HEM	3	0

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

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	727/753 (96%)	-0.28	13 (1%) 67 69	10, 20, 43, 91	1 (0%)
1	B	727/753 (96%)	-0.18	13 (1%) 67 69	13, 22, 46, 91	1 (0%)
1	C	727/753 (96%)	-0.18	9 (1%) 76 78	11, 22, 45, 90	1 (0%)
1	D	727/753 (96%)	-0.26	10 (1%) 73 75	11, 20, 44, 92	1 (0%)
All	All	2908/3012 (96%)	-0.23	45 (1%) 72 73	10, 21, 45, 92	4 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	726	GLY	7.6
1	D	27	ASP	6.5
1	A	29	LEU	5.9
1	B	27	ASP	5.7
1	A	27	ASP	5.1
1	D	29	LEU	4.9
1	A	751	ILE	4.1
1	C	29	LEU	3.9
1	B	29	LEU	3.8
1	D	28	SER	3.7
1	D	725	ASP	3.6
1	A	28	SER	3.5
1	B	28	SER	3.5
1	C	27	ASP	3.4
1	D	30	ALA	3.4
1	C	30	ALA	3.2
1	C	28	SER	3.1
1	A	34	GLY	3.1
1	B	751	ILE	3.0
1	B	31	PRO	3.0
1	A	710	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	750	LYS	2.7
1	A	30	ALA	2.7
1	D	31	PRO	2.7
1	B	30	ALA	2.7
1	A	749	ASP	2.7
1	D	751	ILE	2.6
1	A	725	ASP	2.6
1	B	726	GLY	2.5
1	B	37	ARG	2.5
1	C	726	GLY	2.5
1	D	36	HIS	2.5
1	B	724	ALA	2.5
1	A	31	PRO	2.5
1	C	31	PRO	2.4
1	D	32	GLU	2.4
1	C	34	GLY	2.3
1	B	369	ARG	2.2
1	A	37	ARG	2.1
1	C	751	ILE	2.1
1	A	724	ALA	2.1
1	B	36	HIS	2.1
1	B	61	ARG	2.0
1	B	711	ALA	2.0
1	C	711	ALA	2.0

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](#)

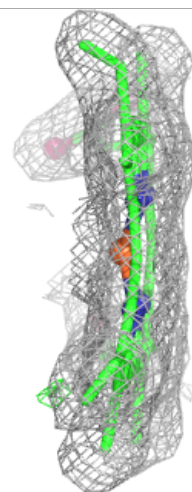
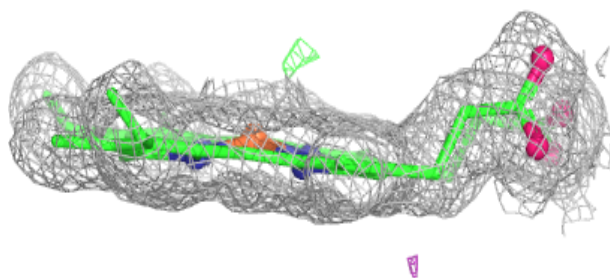
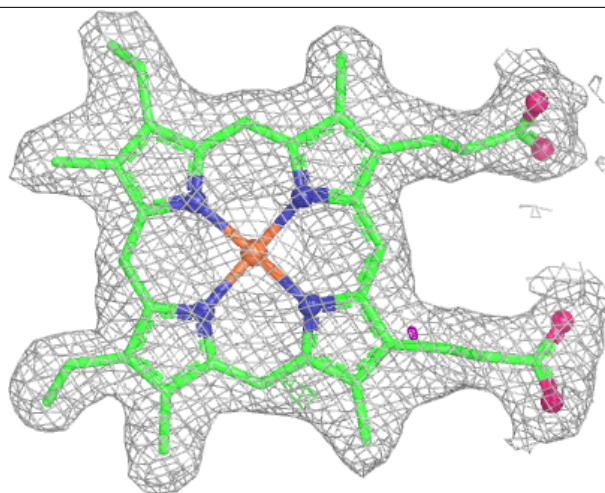
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	PEO	D	3004	2/2	0.83	0.14	33,33,33,34	0
3	PEO	B	4002	2/2	0.93	0.15	25,25,25,28	0
3	PEO	B	4003	2/2	0.95	0.06	31,31,31,32	0
3	PEO	A	3001	2/2	0.95	0.10	29,29,29,29	0
3	PEO	D	6002	2/2	0.95	0.09	18,18,18,18	0
3	PEO	D	6003	2/2	0.95	0.09	21,21,21,23	0
3	PEO	B	4001	2/2	0.96	0.06	17,17,17,19	0
3	PEO	D	6001	2/2	0.96	0.08	21,21,21,22	0
2	HEM	D	760	43/43	0.97	0.06	10,15,16,18	0
3	PEO	A	3002	2/2	0.97	0.07	13,13,13,16	0
3	PEO	A	3003	2/2	0.97	0.05	22,22,22,25	0
3	PEO	C	5003	2/2	0.97	0.07	18,18,18,18	0
2	HEM	B	760	43/43	0.98	0.05	12,16,18,18	0
2	HEM	C	760	43/43	0.98	0.06	16,18,19,21	0
2	HEM	A	760	43/43	0.98	0.05	9,14,16,18	0
3	PEO	C	5002	2/2	0.98	0.07	34,34,34,35	0
3	PEO	C	5001	2/2	0.98	0.05	20,20,20,21	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.

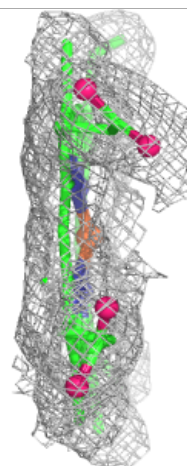
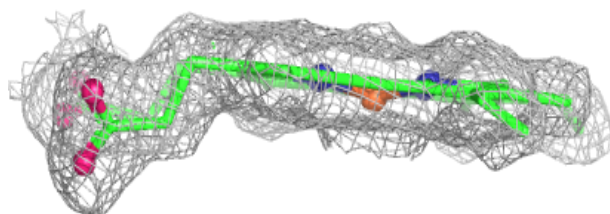
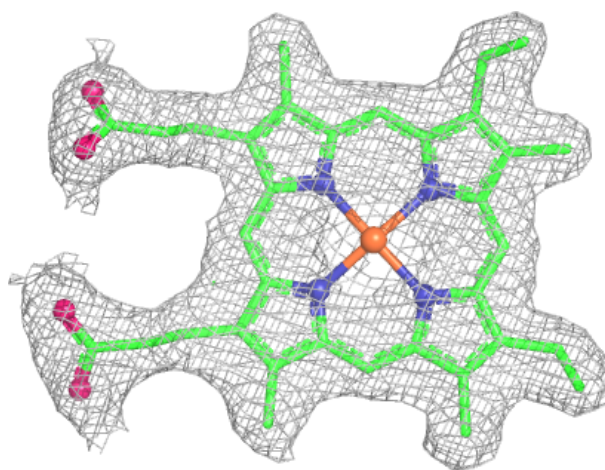
Electron density around HEM D 760:

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



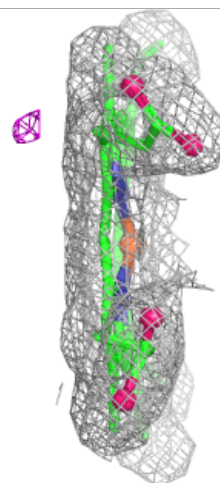
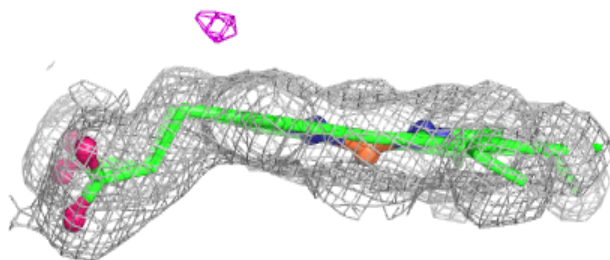
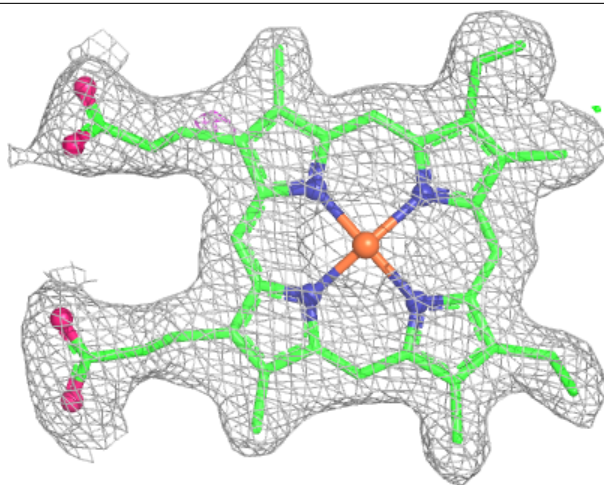
Electron density around HEM B 760:

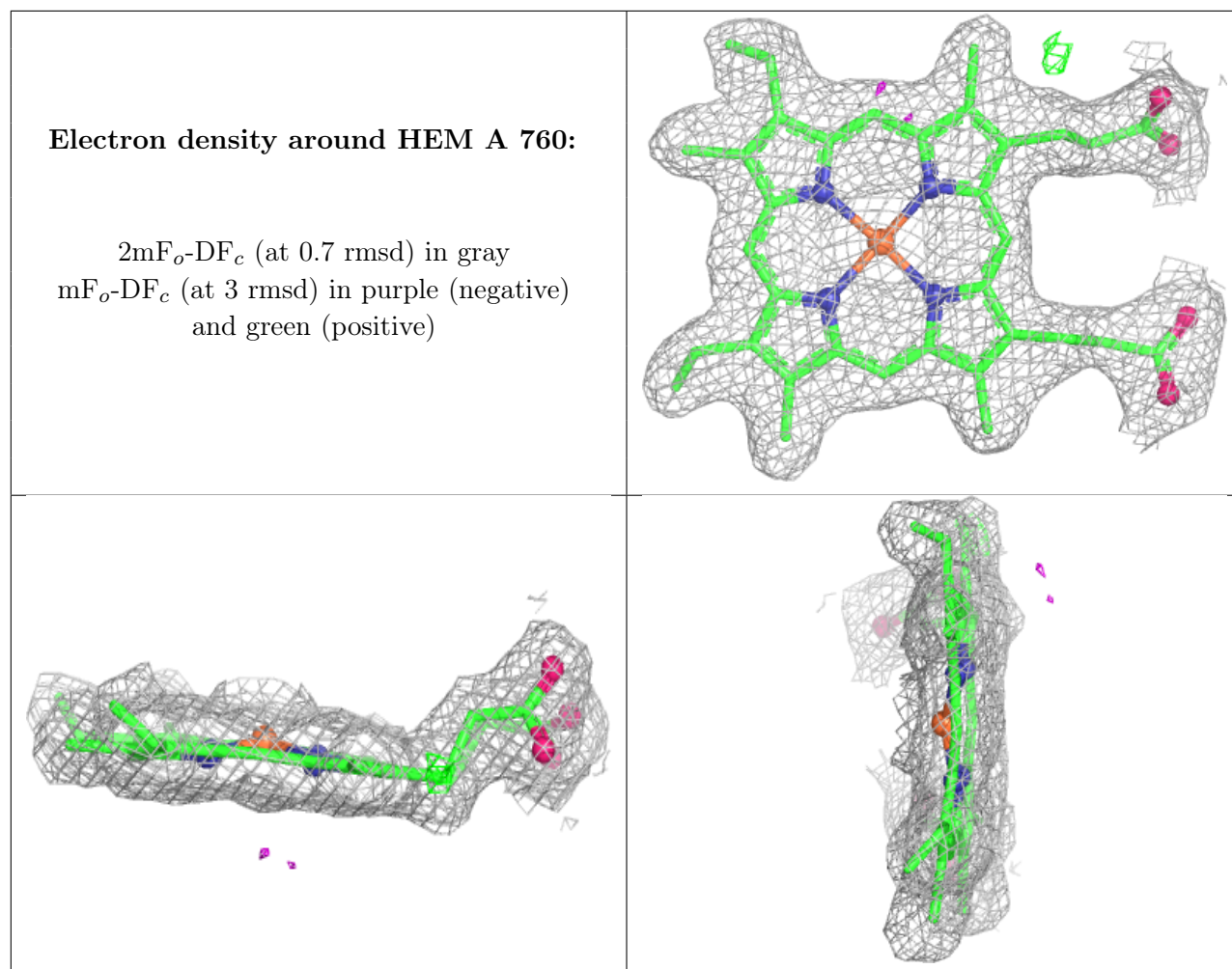
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 760:

$2mF_o-DF_c$ (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.