



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:55 PM UTC

PDB ID : 3VLL / pdb_00003vll
Title : Crystal Structure Analysis of the Ser305Ala variant of KatG from HALOAR-CULA MARISMORTUI Complexes with Inhibitor SHA
Authors : Sato, T.; Higuchi, W.; Yoshimatsu, K.; Fujiwara, T.
Deposited on : 2011-12-01
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

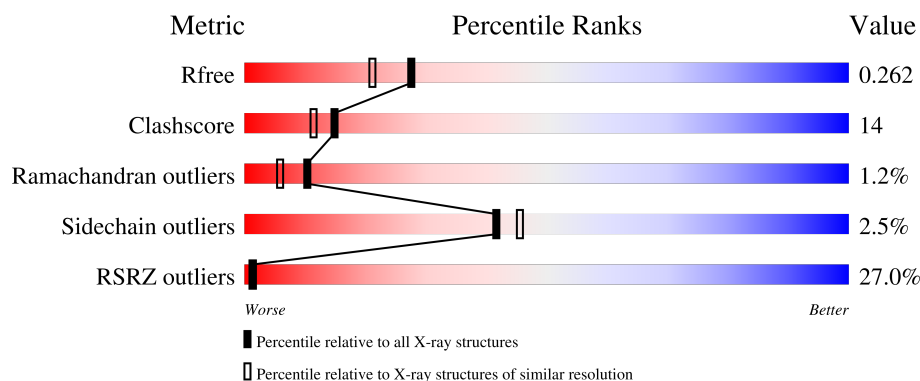
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	737	21% 74% 19% • 5%
1	B	737	31% 68% 26% • •

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	SHA	A	801	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11483 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-peroxidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	703	Total	C	N	O	S	0	0	0
			5542	3469	929	1126	18			
1	B	710	Total	C	N	O	S	0	0	0
			5591	3497	941	1134	19			

There are 14 discrepancies between the modelled and reference sequences:

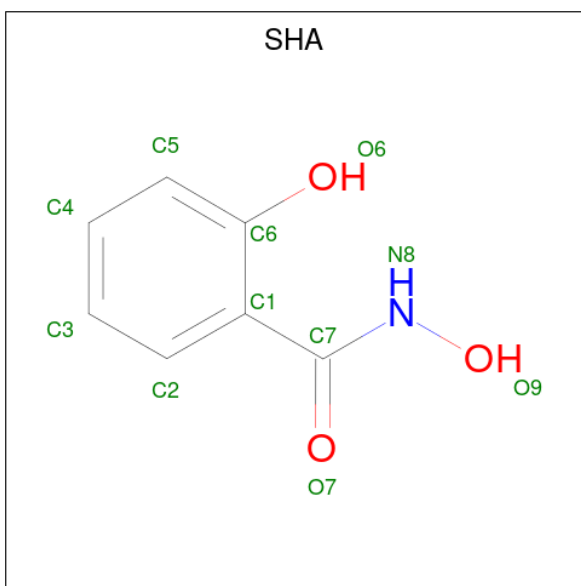
Chain	Residue	Modelled	Actual	Comment	Reference
A	305	ALA	SER	engineered mutation	UNP O59651
A	732	HIS	-	expression tag	UNP O59651
A	733	HIS	-	expression tag	UNP O59651
A	734	HIS	-	expression tag	UNP O59651
A	735	HIS	-	expression tag	UNP O59651
A	736	HIS	-	expression tag	UNP O59651
A	737	HIS	-	expression tag	UNP O59651
B	305	ALA	SER	engineered mutation	UNP O59651
B	732	HIS	-	expression tag	UNP O59651
B	733	HIS	-	expression tag	UNP O59651
B	734	HIS	-	expression tag	UNP O59651
B	735	HIS	-	expression tag	UNP O59651
B	736	HIS	-	expression tag	UNP O59651
B	737	HIS	-	expression tag	UNP O59651

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 3 is SALICYLHYDROXAMIC ACID (CCD ID: SHA) (formula: $C_7H_7NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 11	C 7	N 1	O 3	0	0
3	B	1	Total 11	C 7	N 1	O 3	0	0

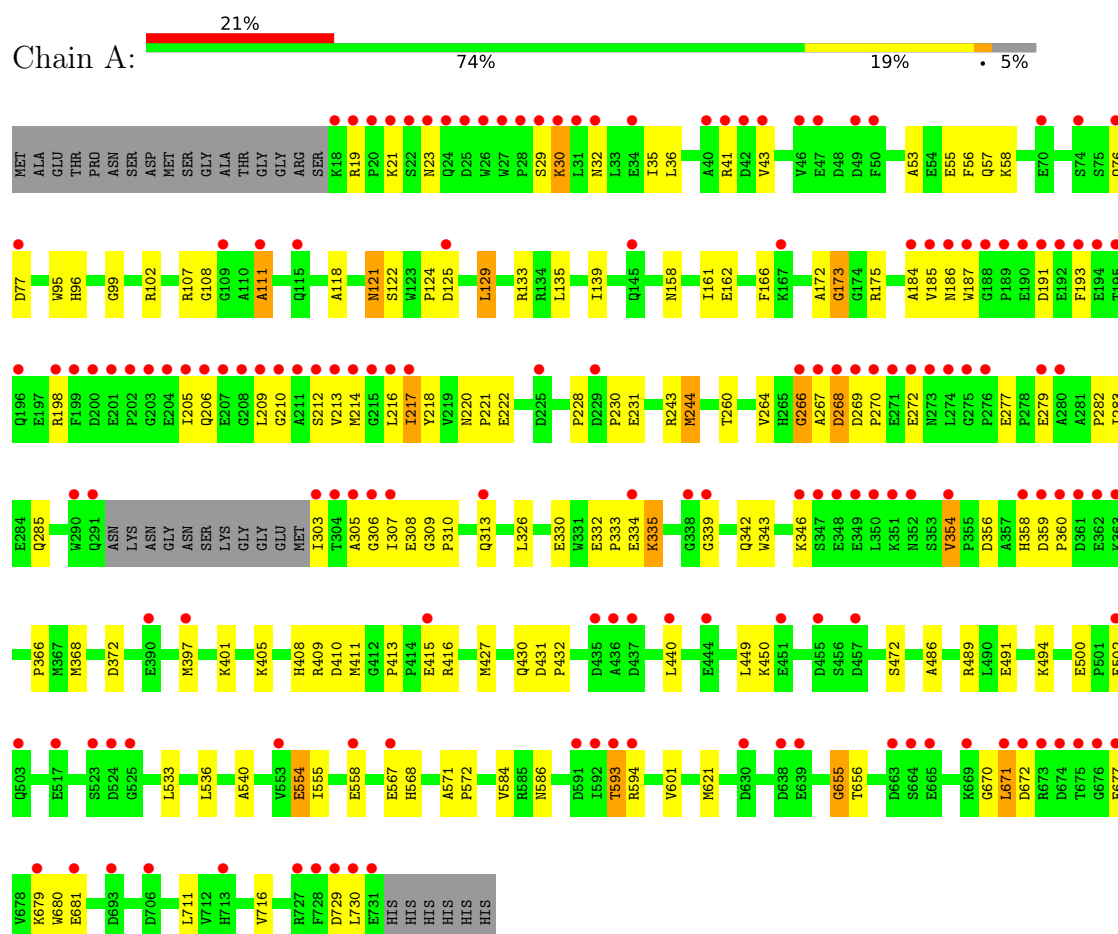
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	149	Total 149	O 149	0	0
4	B	93	Total 93	O 93	0	0

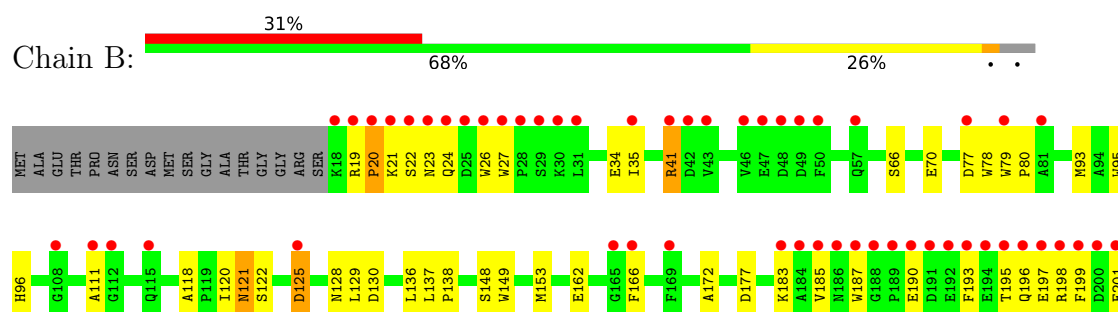
3 Residue-property plots [i](#)

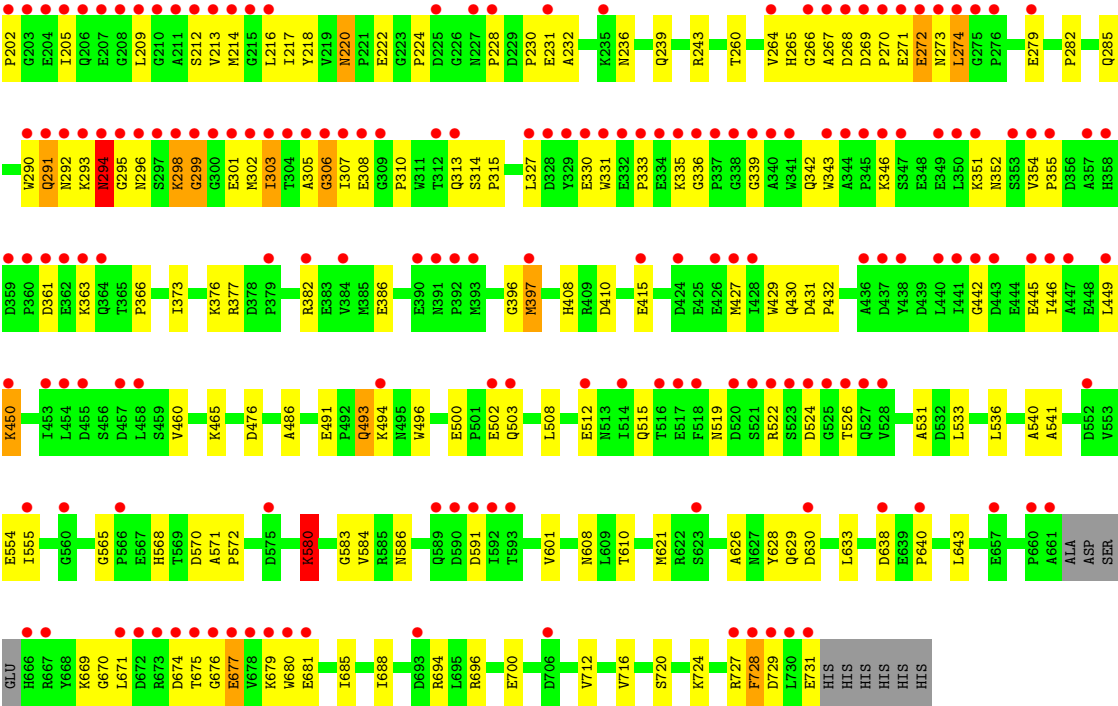
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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-peroxidase 2



• Molecule 1: Catalase-peroxidase 2





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	150.19Å 76.32Å 140.24Å 90.00° 92.32° 90.00°	Depositor
Resolution (Å)	48.36 – 2.00 48.36 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.36-2.00) 98.6 (48.36-2.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 1.79Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.247 , 0.271 (Not available) , 0.262	Depositor DCC
R_{free} test set	7133 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11483	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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, SHA

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	0.48	1/5677 (0.0%)	0.91	14/7716 (0.2%)
1	B	0.36	0/5726	0.85	13/7778 (0.2%)
All	All	0.43	1/11403 (0.0%)	0.88	27/15494 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	217	ILE	C-N	17.08	1.57	1.33

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	500	GLU	CA-C-N	7.14	128.76	119.84
1	A	500	GLU	C-N-CA	7.14	128.76	119.84
1	A	260	THR	N-CA-C	-6.99	104.01	112.54
1	A	217	ILE	CA-C-N	-6.79	110.25	122.46
1	A	217	ILE	C-N-CA	-6.79	110.25	122.46
1	B	728	PHE	N-CA-C	-6.66	105.31	113.50
1	B	260	THR	N-CA-C	-6.35	105.02	112.89
1	A	129	LEU	N-CA-C	-5.96	105.96	113.18
1	A	332	GLU	CA-C-N	5.90	125.86	119.78
1	A	332	GLU	C-N-CA	5.90	125.86	119.78
1	B	580	LYS	N-CA-C	-5.63	106.25	113.23
1	B	500	GLU	CA-C-N	5.63	126.87	119.84
1	B	500	GLU	C-N-CA	5.63	126.87	119.84
1	A	671	LEU	N-CA-C	5.36	120.48	113.30
1	B	197	GLU	N-CA-C	-5.35	104.54	111.71
1	A	173	GLY	N-CA-C	-5.31	104.19	112.58
1	A	472	SER	N-CA-C	5.24	119.29	113.01
1	A	655	GLY	N-CA-C	-5.18	108.54	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	610	THR	N-CA-C	-5.18	102.80	110.46
1	B	303	ILE	N-CA-C	5.17	116.09	108.45
1	A	108	GLY	N-CA-C	-5.15	104.08	112.83
1	A	354	VAL	N-CA-C	5.07	113.65	107.61
1	B	129	LEU	N-CA-C	-5.07	106.93	113.01
1	B	185	VAL	N-CA-C	5.04	114.88	108.12
1	B	493	GLN	N-CA-C	5.02	117.41	111.33
1	B	314	SER	CA-C-N	5.01	126.10	119.84
1	B	314	SER	C-N-CA	5.01	126.10	119.84

There are no chirality outliers.

There are no planarity outliers.

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	5542	0	5191	139	0
1	B	5591	0	5244	171	0
2	A	43	0	30	0	0
2	B	43	0	30	0	0
3	A	11	0	6	1	0
3	B	11	0	6	1	0
4	A	149	0	0	1	0
4	B	93	0	0	1	0
All	All	11483	0	10507	301	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 14.

All (301) 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:A:95:TRP:CH2	1:A:218:TYR:HE1	1.08	1.66
1:B:95:TRP:CH2	1:B:218:TYR:HE1	1.10	1.62
1:A:95:TRP:HH2	1:A:218:TYR:CE1	1.01	1.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:TRP:HH2	1:B:218:TYR:CE1	1.11	1.60
1:A:95:TRP:CH2	1:A:218:TYR:CE1	1.87	1.46
1:B:95:TRP:CH2	1:B:218:TYR:CE1	1.96	1.22
1:B:584:VAL:HG13	1:B:621:MET:HG2	1.41	0.98
1:B:35:ILE:HD11	1:B:601:VAL:HG12	1.45	0.97
1:A:270:PRO:HG3	1:A:305:ALA:HA	1.48	0.94
1:A:310:PRO:HG3	1:A:354:VAL:HG11	1.51	0.92
1:A:35:ILE:HD11	1:A:601:VAL:HG12	1.49	0.92
1:A:397:MET:HE2	1:A:401:LYS:HG3	1.48	0.92
1:A:95:TRP:HH2	1:A:218:TYR:CD1	1.87	0.91
1:A:427:MET:H	1:A:430:GLN:HE21	1.17	0.91
1:A:584:VAL:HG13	1:A:621:MET:HG2	1.52	0.90
1:A:267:ALA:H	1:A:303:ILE:HG12	1.36	0.88
1:A:95:TRP:CZ3	1:A:218:TYR:HE1	1.91	0.86
1:A:427:MET:H	1:A:430:GLN:NE2	1.74	0.85
1:A:672:ASP:HB2	1:A:679:LYS:HD3	1.56	0.84
1:A:266:GLY:HA2	1:A:303:ILE:HA	1.59	0.83
1:A:172:ALA:H	1:A:408:HIS:HE1	1.27	0.81
1:B:310:PRO:HG3	1:B:354:VAL:HG11	1.61	0.81
1:B:19:ARG:HD3	1:B:19:ARG:H	1.47	0.80
1:A:95:TRP:CH2	1:A:218:TYR:CD1	2.68	0.77
1:B:313:GLN:HA	1:B:354:VAL:HG22	1.67	0.77
1:A:313:GLN:HA	1:A:354:VAL:HG22	1.66	0.76
1:B:670:GLY:O	1:B:679:LYS:HB3	1.84	0.76
1:B:270:PRO:HB3	1:B:306:GLY:HA3	1.67	0.76
1:A:43:VAL:HG21	1:B:694:ARG:NH2	2.00	0.76
1:A:326:LEU:HD13	1:A:368:MET:HE2	1.68	0.75
1:B:282:PRO:HD2	1:B:285:GLN:NE2	2.02	0.74
1:B:95:TRP:CZ2	1:B:218:TYR:CE1	2.72	0.74
1:A:217:ILE:HG23	1:A:218:TYR:N	2.02	0.74
1:B:274:LEU:H	1:B:274:LEU:HD12	1.52	0.74
1:A:264:VAL:HG21	1:A:307:ILE:HG22	1.68	0.73
1:B:269:ASP:HB3	1:B:272:GLU:HB2	1.70	0.73
1:A:267:ALA:N	1:A:303:ILE:HG12	2.04	0.72
1:B:679:LYS:HG2	1:B:680:TRP:H	1.54	0.72
1:A:191:ASP:HA	1:B:21:LYS:NZ	2.03	0.72
1:B:266:GLY:HA2	1:B:303:ILE:HG23	1.74	0.70
1:B:565:GLY:H	1:B:568:HIS:HD2	1.39	0.70
1:B:583:GLY:HA2	1:B:685:ILE:HD13	1.73	0.70
1:A:571:ALA:HB3	1:A:572:PRO:HD3	1.74	0.69
1:A:269:ASP:HB3	1:A:272:GLU:OE1	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:ALA:H	1:B:408:HIS:HE1	1.41	0.69
1:B:265:HIS:HB3	1:B:303:ILE:HA	1.74	0.69
1:B:273:ASN:HB3	1:B:293:LYS:H	1.58	0.68
1:B:491:GLU:CD	1:B:494:LYS:HE2	2.18	0.68
1:A:326:LEU:HD13	1:A:368:MET:CE	2.23	0.67
1:B:397:MET:HE3	1:B:397:MET:HA	1.76	0.67
1:A:567:GLU:HG2	1:A:568:HIS:CD2	2.31	0.66
1:B:190:GLU:HG2	1:B:196:GLN:HA	1.77	0.65
1:A:41:ARG:HG2	1:B:41:ARG:HD2	1.79	0.65
1:A:671:LEU:O	1:A:672:ASP:HB3	1.96	0.65
1:B:633:LEU:HD23	1:B:681:GLU:HG3	1.79	0.65
1:A:23:ASN:HD22	1:A:30:LYS:HD3	1.62	0.65
1:B:121:ASN:HD22	1:B:122:SER:N	1.95	0.64
1:B:727:ARG:HB3	1:B:727:ARG:HH21	1.62	0.64
1:A:53:ALA:O	1:A:57:GLN:HG3	1.98	0.64
1:A:593:THR:HG23	1:A:594:ARG:H	1.61	0.64
1:B:580:LYS:HD3	1:B:580:LYS:H	1.64	0.63
1:A:99:GLY:C	1:A:217:ILE:HD11	2.24	0.63
1:A:656:THR:HA	1:A:672:ASP:HA	1.80	0.62
1:A:335:LYS:HZ3	1:A:339:GLY:HA2	1.65	0.62
1:B:198:ARG:HD2	1:B:212:SER:C	2.25	0.62
1:A:191:ASP:HA	1:B:21:LYS:HZ1	1.63	0.61
1:B:220:ASN:HD22	1:B:222:GLU:H	1.45	0.61
1:B:239:GLN:HE21	1:B:243:ARG:HH21	1.47	0.61
1:B:460:VAL:HG13	1:B:541:ALA:HB1	1.82	0.60
1:A:655:GLY:O	1:A:672:ASP:HA	2.01	0.60
1:A:111:ALA:O	1:A:175:ARG:HB3	2.02	0.60
1:B:727:ARG:HB3	1:B:727:ARG:NH2	2.17	0.60
1:A:186:ASN:HB2	1:B:20:PRO:HG3	1.83	0.60
1:B:580:LYS:HD3	1:B:580:LYS:N	2.16	0.60
1:B:580:LYS:H	1:B:580:LYS:CD	2.15	0.60
1:B:290:TRP:O	1:B:292:ASN:N	2.35	0.59
1:A:205:ILE:HB	1:A:243:ARG:HH12	1.67	0.59
1:A:220:ASN:HD22	1:A:220:ASN:C	2.10	0.59
1:A:266:GLY:O	1:A:308:GLU:HB2	2.03	0.58
1:B:376:LYS:O	1:B:382:ARG:HD3	2.02	0.58
1:B:294:ASN:O	1:B:302:MET:HA	2.03	0.58
1:B:571:ALA:HB3	1:B:572:PRO:HD3	1.84	0.58
1:A:270:PRO:HD3	1:A:306:GLY:H	1.69	0.58
1:A:368:MET:CE	1:A:372:ASP:HB3	2.34	0.58
1:B:196:GLN:HB3	1:B:213:VAL:HG22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:GLY:O	1:B:308:GLU:HB2	2.03	0.58
1:B:327:LEU:HD22	1:B:382:ARG:NH2	2.18	0.57
1:B:503:GLN:HG3	4:B:954:HOH:O	2.03	0.57
1:A:121:ASN:HD22	1:A:122:SER:N	2.01	0.57
1:B:476:ASP:CG	1:B:608:ASN:HD21	2.13	0.57
1:B:231:GLU:OE1	1:B:377:ARG:HD2	2.05	0.56
1:B:335:LYS:HD2	1:B:339:GLY:HA2	1.86	0.56
1:B:354:VAL:HG21	1:B:366:PRO:HG3	1.86	0.56
1:B:111:ALA:HB2	1:B:410:ASP:OD2	2.05	0.56
1:B:213:VAL:HB	1:B:216:LEU:CD1	2.35	0.56
1:A:95:TRP:CZ3	1:A:218:TYR:CE1	2.76	0.56
1:A:107:ARG:HD3	1:A:185:VAL:HG22	1.87	0.56
1:A:111:ALA:HB2	1:A:410:ASP:OD2	2.06	0.56
1:B:149:TRP:O	1:B:153:MET:HG3	2.05	0.56
1:B:570:ASP:OD1	1:B:572:PRO:HD2	2.05	0.56
1:B:427:MET:HG2	1:B:430:GLN:HE21	1.71	0.55
1:A:213:VAL:HB	1:A:216:LEU:HD12	1.88	0.55
1:B:118:ALA:HB2	1:B:279:GLU:CD	2.31	0.55
1:B:450:LYS:HB2	1:B:450:LYS:HZ2	1.72	0.54
1:B:431:ASP:N	1:B:432:PRO:HD3	2.22	0.54
1:A:567:GLU:HG2	1:A:568:HIS:HD2	1.71	0.54
1:B:230:PRO:HB2	1:B:377:ARG:HG3	1.90	0.54
1:B:95:TRP:CH2	1:B:218:TYR:CD1	2.86	0.54
1:B:125:ASP:CG	1:B:216:LEU:HA	2.32	0.54
1:B:199:PHE:HB3	1:B:205:ILE:HA	1.90	0.54
1:B:120:ILE:HD11	1:B:187:TRP:CZ2	2.43	0.54
1:B:580:LYS:H	1:B:580:LYS:HZ2	1.55	0.54
1:A:270:PRO:HG3	1:A:305:ALA:CA	2.30	0.53
1:A:43:VAL:HG21	1:B:694:ARG:HH22	1.72	0.53
1:B:450:LYS:HZ2	1:B:536:LEU:HD11	1.73	0.53
1:B:273:ASN:O	1:B:292:ASN:HA	2.09	0.53
1:B:427:MET:HG2	1:B:430:GLN:NE2	2.23	0.53
1:B:220:ASN:ND2	1:B:222:GLU:H	2.06	0.53
1:B:34:GLU:CD	1:B:183:LYS:HE2	2.33	0.53
1:A:76:GLN:HG3	1:A:135:LEU:CD2	2.40	0.52
1:A:96:HIS:CE1	1:A:125:ASP:O	2.62	0.52
1:A:217:ILE:CG2	1:A:218:TYR:N	2.69	0.52
1:A:670:GLY:O	1:A:679:LYS:O	2.26	0.52
1:A:405:LYS:O	1:A:409:ARG:HB2	2.09	0.52
1:B:307:ILE:N	1:B:307:ILE:HD12	2.25	0.52
1:B:450:LYS:HG3	1:B:540:ALA:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ASN:ND2	1:A:35:ILE:HG23	2.24	0.52
1:B:125:ASP:OD2	1:B:217:ILE:HG12	2.09	0.51
1:A:415:GLU:H	1:A:415:GLU:CD	2.19	0.51
1:A:124:PRO:HG2	1:A:193:PHE:HB3	1.93	0.51
1:B:450:LYS:NZ	1:B:536:LEU:HD11	2.25	0.51
1:B:676:GLY:O	1:B:677:GLU:HB2	2.10	0.51
1:A:282:PRO:HD2	1:A:285:GLN:NE2	2.25	0.50
1:B:333:PRO:HG3	1:B:343:TRP:CZ2	2.46	0.50
1:B:354:VAL:CG2	1:B:366:PRO:HG3	2.41	0.50
1:A:216:LEU:HD22	3:A:801:SHA:O6	2.11	0.50
1:A:268:ASP:O	1:A:306:GLY:HA2	2.12	0.50
1:A:308:GLU:H	1:A:342:GLN:HE22	1.59	0.50
1:B:427:MET:CG	1:B:430:GLN:HE21	2.25	0.50
1:B:508:LEU:O	1:B:512:GLU:HG3	2.10	0.50
1:A:214:MET:C	1:A:216:LEU:H	2.20	0.50
1:B:555:ILE:HG12	1:B:716:VAL:HG13	1.94	0.50
1:A:139:ILE:HG13	4:A:1025:HOH:O	2.12	0.49
1:A:558:GLU:OE1	1:A:730:LEU:HD22	2.12	0.49
1:A:217:ILE:HG23	1:A:218:TYR:H	1.73	0.49
1:A:397:MET:CE	1:A:401:LYS:HG3	2.32	0.49
1:B:307:ILE:HG23	1:B:342:GLN:CD	2.38	0.49
1:B:313:GLN:C	1:B:315:PRO:HD3	2.37	0.49
1:B:696:ARG:O	1:B:700:GLU:HG3	2.12	0.49
1:A:335:LYS:HB3	1:A:335:LYS:NZ	2.27	0.49
1:B:330:GLU:HB3	1:B:346:LYS:HD3	1.93	0.49
1:A:35:ILE:HB	1:A:184:ALA:HB2	1.95	0.49
1:B:162:GLU:HA	1:B:166:PHE:O	2.11	0.49
1:B:291:GLN:O	1:B:293:LYS:HE3	2.13	0.49
1:B:728:PHE:HA	1:B:731:GLU:CD	2.39	0.48
1:A:220:ASN:ND2	1:A:222:GLU:H	2.11	0.48
1:A:307:ILE:HA	1:A:342:GLN:NE2	2.29	0.48
1:A:554:GLU:OE1	1:A:554:GLU:HA	2.13	0.48
1:B:230:PRO:CB	1:B:377:ARG:HG3	2.43	0.48
1:A:102:ARG:HD3	1:A:107:ARG:O	2.14	0.48
1:A:122:SER:HB3	1:A:277:GLU:HG3	1.95	0.48
1:B:193:PHE:O	1:B:195:THR:HG23	2.13	0.48
1:A:121:ASN:HD22	1:A:121:ASN:C	2.19	0.47
1:B:220:ASN:HD22	1:B:220:ASN:C	2.22	0.47
1:B:121:ASN:HD22	1:B:121:ASN:C	2.19	0.47
1:B:351:LYS:HG2	1:B:352:ASN:ND2	2.28	0.47
1:B:382:ARG:NH2	1:B:386:GLU:OE1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ASN:C	1:B:121:ASN:ND2	2.72	0.47
1:B:679:LYS:HG2	1:B:680:TRP:N	2.25	0.47
1:A:198:ARG:NH1	1:A:209:LEU:HD13	2.30	0.47
1:A:264:VAL:HG22	1:A:309:GLY:O	2.15	0.47
1:A:413:PRO:HB2	1:A:415:GLU:OE1	2.14	0.47
1:A:431:ASP:N	1:A:432:PRO:HD3	2.30	0.47
1:A:335:LYS:HZ3	1:A:335:LYS:HB3	1.80	0.47
1:B:80:PRO:HD2	1:B:296:ASN:O	2.15	0.47
1:B:298:LYS:O	1:B:299:GLY:C	2.57	0.47
1:A:118:ALA:HB2	1:A:279:GLU:CD	2.39	0.46
1:A:161:ILE:CG2	1:A:166:PHE:HB3	2.45	0.46
1:A:220:ASN:HD22	1:A:221:PRO:N	2.12	0.46
1:A:270:PRO:HB3	1:A:303:ILE:HG22	1.97	0.46
1:A:161:ILE:HG22	1:A:166:PHE:HB3	1.96	0.46
1:A:567:GLU:H	1:A:567:GLU:CD	2.23	0.46
1:A:401:LYS:HE3	1:A:427:MET:CE	2.45	0.46
1:B:271:GLU:HA	1:B:274:LEU:HD13	1.96	0.46
1:B:213:VAL:HB	1:B:216:LEU:HD12	1.97	0.46
1:B:265:HIS:HB3	1:B:303:ILE:CA	2.45	0.46
1:A:32:ASN:ND2	1:A:35:ILE:CG2	2.78	0.46
1:B:486:ALA:HB2	1:B:531:ALA:HB2	1.98	0.46
1:B:676:GLY:O	1:B:677:GLU:CB	2.63	0.46
1:A:56:PHE:CZ	1:A:173:GLY:HA3	2.51	0.46
1:B:224:PRO:HG3	1:B:236:ASN:HD22	1.80	0.46
1:B:522:ARG:HG3	1:B:526:THR:O	2.15	0.46
1:A:41:ARG:HD2	1:A:41:ARG:O	2.16	0.46
1:A:55:GLU:HA	1:A:58:LYS:HD3	1.96	0.46
1:A:334:GLU:O	1:A:334:GLU:HG3	2.16	0.46
1:B:352:ASN:O	1:B:363:LYS:HD2	2.15	0.46
1:A:231:GLU:CD	1:A:231:GLU:H	2.24	0.46
1:A:440:LEU:HD22	1:A:440:LEU:N	2.31	0.46
1:B:22:SER:HB3	1:B:24:GLN:NE2	2.30	0.46
1:B:449:LEU:HD22	1:B:533:LEU:HD21	1.98	0.45
1:A:96:HIS:HE1	1:A:125:ASP:O	1.98	0.45
1:A:198:ARG:HD2	1:A:212:SER:C	2.42	0.45
1:B:720:SER:O	1:B:724:LYS:HG2	2.15	0.45
1:A:198:ARG:HG3	1:A:205:ILE:HG23	1.99	0.45
1:B:352:ASN:HB3	1:B:363:LYS:HB3	1.96	0.45
1:A:491:GLU:HG2	1:A:494:LYS:HE2	1.98	0.45
1:B:198:ARG:HD2	1:B:212:SER:O	2.17	0.45
1:A:335:LYS:NZ	1:A:339:GLY:HA2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:VAL:HG13	1:B:355:PRO:HD2	1.97	0.45
1:A:228:PRO:O	1:A:230:PRO:HD3	2.16	0.45
1:A:427:MET:N	1:A:430:GLN:HE21	1.99	0.45
1:A:711:LEU:HD13	1:A:711:LEU:C	2.42	0.45
1:B:148:SER:HB2	1:B:177:ASP:CG	2.42	0.45
1:B:638:ASP:C	1:B:640:PRO:HD3	2.42	0.45
1:B:19:ARG:HD3	1:B:19:ARG:N	2.25	0.44
1:B:515:GLN:HG2	1:B:519:ASN:ND2	2.32	0.44
1:B:628:TYR:CE1	1:B:629:GLN:HG3	2.51	0.44
1:B:95:TRP:CZ2	1:B:218:TYR:CD1	3.03	0.44
1:A:121:ASN:C	1:A:121:ASN:ND2	2.74	0.44
1:A:283:ILE:HD11	1:B:688:ILE:N	2.33	0.44
1:B:137:LEU:HB3	1:B:138:PRO:HD3	2.00	0.44
1:B:66:SER:O	1:B:70:GLU:HG3	2.18	0.44
1:B:202:PRO:HG2	1:B:232:ALA:HB1	1.99	0.44
1:B:209:LEU:O	1:B:243:ARG:HD3	2.18	0.44
1:B:267:ALA:H	1:B:303:ILE:CD1	2.30	0.44
1:A:354:VAL:CG2	1:A:366:PRO:HG3	2.48	0.44
1:A:449:LEU:HD22	1:A:533:LEU:HD21	1.99	0.44
1:B:23:ASN:HA	1:B:26:TRP:HD1	1.83	0.44
1:B:79:TRP:CE3	1:B:296:ASN:HA	2.53	0.44
1:B:228:PRO:O	1:B:230:PRO:HD3	2.18	0.44
1:A:118:ALA:HB2	1:A:279:GLU:HG3	1.99	0.44
1:A:368:MET:HE1	1:A:372:ASP:HB3	2.00	0.44
1:B:643:LEU:HD23	1:B:712:VAL:HG13	2.00	0.44
1:A:19:ARG:H	1:A:19:ARG:HD3	1.83	0.43
1:B:264:VAL:HG21	1:B:307:ILE:HG22	1.99	0.43
1:B:268:ASP:HB3	1:B:273:ASN:ND2	2.33	0.43
1:B:196:GLN:CG	1:B:213:VAL:HG22	2.48	0.43
1:B:213:VAL:HB	1:B:216:LEU:HG	2.00	0.43
1:A:415:GLU:CD	1:A:415:GLU:N	2.77	0.43
1:B:128:ASN:HA	1:B:130:ASP:OD2	2.17	0.43
1:A:205:ILE:HG22	1:A:206:GLN:N	2.33	0.43
1:B:669:LYS:HA	1:B:669:LYS:HD3	1.86	0.43
1:A:356:ASP:HB3	1:A:359:ASP:O	2.18	0.43
1:B:427:MET:HB3	1:B:429:TRP:CD1	2.54	0.43
1:B:310:PRO:CG	1:B:354:VAL:HG11	2.39	0.43
1:A:118:ALA:HB2	1:A:279:GLU:CG	2.49	0.43
1:A:679:LYS:O	1:A:680:TRP:CB	2.66	0.43
1:B:415:GLU:HG2	1:B:729:ASP:HA	2.01	0.43
1:B:442:GLY:O	1:B:446:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:493:GLN:HG2	1:B:496:TRP:CH2	2.54	0.43
1:B:502:GLU:H	1:B:502:GLU:CD	2.25	0.42
1:A:555:ILE:HG12	1:A:716:VAL:HG13	2.01	0.42
1:B:427:MET:HB3	1:B:429:TRP:NE1	2.34	0.42
1:A:43:VAL:HG21	1:B:694:ARG:HH21	1.78	0.42
1:A:502:GLU:H	1:A:502:GLU:CD	2.24	0.42
1:B:190:GLU:OE2	1:B:196:GLN:HA	2.20	0.42
1:B:224:PRO:HG3	1:B:236:ASN:ND2	2.34	0.42
1:B:331:TRP:HB3	1:B:343:TRP:HB3	2.00	0.42
1:A:41:ARG:HB3	1:B:41:ARG:HB3	2.01	0.42
1:A:401:LYS:HE3	1:A:427:MET:HE2	2.02	0.42
1:B:580:LYS:CD	1:B:580:LYS:N	2.80	0.42
1:A:129:LEU:O	1:A:133:ARG:HG3	2.19	0.42
1:A:536:LEU:HD23	1:A:536:LEU:O	2.20	0.42
1:B:26:TRP:HB2	1:B:27:TRP:CE3	2.54	0.42
1:B:291:GLN:OE1	1:B:291:GLN:HA	2.19	0.42
1:B:96:HIS:NE2	3:B:801:SHA:N8	2.68	0.42
1:B:198:ARG:CZ	1:B:209:LEU:HD13	2.49	0.42
1:B:445:GLU:OE1	1:B:526:THR:HG21	2.19	0.42
1:A:185:VAL:HG11	1:A:187:TRP:CZ2	2.55	0.42
1:B:515:GLN:HG2	1:B:519:ASN:HD21	1.85	0.42
1:A:486:ALA:O	1:A:489:ARG:HG2	2.20	0.41
1:B:301:GLU:H	1:B:301:GLU:HG2	1.61	0.41
1:B:93:MET:HE1	1:B:136:LEU:HD11	2.01	0.41
1:B:172:ALA:N	1:B:408:HIS:HE1	2.13	0.41
1:B:352:ASN:HB3	1:B:363:LYS:CB	2.51	0.41
1:A:118:ALA:HA	1:A:121:ASN:ND2	2.35	0.41
1:A:220:ASN:HD22	1:A:222:GLU:H	1.69	0.41
1:A:368:MET:HE3	1:A:372:ASP:HB3	2.01	0.41
1:A:411:MET:O	1:A:416:ARG:HD3	2.20	0.41
1:B:343:TRP:CD2	1:B:373:ILE:HG13	2.56	0.41
1:B:465:LYS:NZ	1:B:630:ASP:OD2	2.54	0.41
1:B:502:GLU:HG2	1:B:503:GLN:N	2.36	0.41
1:A:330:GLU:HB2	1:A:346:LYS:HD2	2.02	0.41
1:A:333:PRO:HG3	1:A:343:TRP:CH2	2.56	0.41
1:A:358:HIS:O	1:A:360:PRO:HD3	2.21	0.41
1:B:196:GLN:HG2	1:B:213:VAL:HG22	2.03	0.41
1:B:310:PRO:O	1:B:366:PRO:HA	2.21	0.41
1:B:274:LEU:H	1:B:274:LEU:CD1	2.29	0.41
1:B:330:GLU:CB	1:B:346:LYS:HD3	2.50	0.41
1:B:674:ASP:O	1:B:677:GLU:OE1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ILE:CG2	1:A:218:TYR:H	2.32	0.41
1:A:450:LYS:HG3	1:A:540:ALA:HB2	2.02	0.41
1:A:35:ILE:HG13	1:A:36:LEU:N	2.35	0.40
1:A:158:ASN:O	1:A:162:GLU:HG3	2.22	0.40
1:B:78:TRP:CD1	1:B:78:TRP:H	2.39	0.40
1:A:270:PRO:HD3	1:A:306:GLY:N	2.34	0.40
1:B:294:ASN:HD22	1:B:294:ASN:HA	1.56	0.40
1:B:282:PRO:HD2	1:B:285:GLN:CD	2.45	0.40
1:B:621:MET:HG3	1:B:626:ALA:HB3	2.04	0.40
1:B:166:PHE:HZ	1:B:396:GLY:O	2.05	0.40
1:A:210:GLY:O	1:A:244:MET:HE3	2.21	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	699/737 (95%)	665 (95%)	30 (4%)	4 (1%)	21	17
1	B	706/737 (96%)	650 (92%)	43 (6%)	13 (2%)	6	3
All	All	1405/1474 (95%)	1315 (94%)	73 (5%)	17 (1%)	10	6

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	298	LYS
1	B	305	ALA
1	A	268	ASP
1	B	291	GLN
1	B	591	ASP
1	B	677	GLU
1	A	111	ALA

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Mol	Chain	Res	Type
1	B	294	ASN
1	B	299	GLY
1	B	524	ASP
1	B	274	LEU
1	B	306	GLY
1	A	29	SER
1	B	20	PRO
1	B	336	GLY
1	B	295	GLY
1	A	266	GLY

5.3.2 Protein sidechains [i](#)

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	581/607 (96%)	569 (98%)	12 (2%)	47	52
1	B	586/607 (96%)	569 (97%)	17 (3%)	37	40
All	All	1167/1214 (96%)	1138 (98%)	29 (2%)	42	45

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	30	LYS
1	A	77	ASP
1	A	121	ASN
1	A	244	MET
1	A	335	LYS
1	A	554	GLU
1	A	586	ASN
1	A	593	THR
1	A	677	GLU
1	A	681	GLU
1	A	729	ASP
1	B	41	ARG

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Mol	Chain	Res	Type
1	B	77	ASP
1	B	121	ASN
1	B	125	ASP
1	B	201	GLU
1	B	214	MET
1	B	220	ASN
1	B	272	GLU
1	B	294	ASN
1	B	361	ASP
1	B	397	MET
1	B	450	LYS
1	B	554	GLU
1	B	580	LYS
1	B	586	ASN
1	B	671	LEU
1	B	675	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	57	GLN
1	A	121	ASN
1	A	141	GLN
1	A	145	GLN
1	A	196	GLN
1	A	220	ASN
1	A	227	ASN
1	A	285	GLN
1	A	286	GLN
1	A	313	GLN
1	A	324	ASN
1	A	342	GLN
1	A	352	ASN
1	A	389	GLN
1	A	391	ASN
1	A	408	HIS
1	A	430	GLN
1	A	513	ASN
1	A	515	GLN
1	A	527	GLN
1	A	544	GLN

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Mol	Chain	Res	Type
1	A	568	HIS
1	A	713	HIS
1	B	121	ASN
1	B	196	GLN
1	B	220	ASN
1	B	285	GLN
1	B	286	GLN
1	B	296	ASN
1	B	313	GLN
1	B	324	ASN
1	B	342	GLN
1	B	352	ASN
1	B	358	HIS
1	B	389	GLN
1	B	408	HIS
1	B	430	GLN
1	B	513	ASN
1	B	515	GLN
1	B	568	HIS
1	B	586	ASN
1	B	603	ASN
1	B	608	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](#)

4 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	$\# Z > 2$
2	HEM	A	800	1	50,50,50	2.59	12 (24%)	67,82,82	7.06	51 (76%)
3	SHA	A	801	-	11,11,11	1.77	3 (27%)	13,14,14	0.57	0
3	SHA	B	801	-	11,11,11	1.65	2 (18%)	13,14,14	0.61	0
2	HEM	B	800	1	50,50,50	3.38	12 (24%)	67,82,82	7.87	49 (73%)

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	A	800	1	-	2/14/54/54	-
3	SHA	A	801	-	-	0/6/6/6	0/1/1/1
3	SHA	B	801	-	-	0/6/6/6	0/1/1/1
2	HEM	B	800	1	-	4/14/54/54	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	800	HEM	FE-NB	14.08	2.38	1.94
2	B	800	HEM	FE-NC	10.82	2.30	1.95
2	B	800	HEM	FE-ND	8.17	2.20	1.94
2	A	800	HEM	FE-ND	7.50	2.18	1.94
2	B	800	HEM	FE-NA	7.16	2.18	1.95
2	A	800	HEM	FE-NB	7.11	2.16	1.94
2	A	800	HEM	FE-NC	7.01	2.18	1.95
2	A	800	HEM	FE-NA	6.46	2.16	1.95
2	B	800	HEM	CBC-CAC	5.38	1.56	1.30
2	A	800	HEM	CBC-CAC	5.35	1.56	1.30
2	A	800	HEM	CBB-CAB	5.35	1.56	1.30
2	B	800	HEM	CBB-CAB	5.08	1.54	1.30
2	B	800	HEM	CBD-CGD	-4.15	1.41	1.50
2	A	800	HEM	CBD-CGD	-4.11	1.41	1.50
2	B	800	HEM	CBA-CGA	-4.00	1.41	1.50
2	A	800	HEM	CBA-CGA	-3.86	1.41	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	SHA	C1-C6	3.40	1.46	1.40
3	A	801	SHA	C1-C6	3.37	1.46	1.40
3	B	801	SHA	C7-N8	3.25	1.36	1.32
3	A	801	SHA	C7-N8	2.97	1.36	1.32
2	A	800	HEM	O1A-CGA	2.53	1.30	1.22
2	B	800	HEM	C4D-ND	-2.34	1.36	1.40
2	B	800	HEM	O1A-CGA	2.32	1.29	1.22
3	A	801	SHA	C2-C1	2.19	1.43	1.39
2	B	800	HEM	CBD-CAD	2.12	1.59	1.51
2	B	800	HEM	CAC-C3C	2.11	1.53	1.47
2	A	800	HEM	C4D-ND	-2.10	1.36	1.40
2	A	800	HEM	CBD-CAD	2.08	1.59	1.51
2	A	800	HEM	CAC-C3C	2.00	1.52	1.47

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	HEM	C1C-CHC-C4B	19.18	166.77	126.02
2	B	800	HEM	CHC-C4B-NB	-18.40	104.62	124.42
2	A	800	HEM	CHC-C4B-NB	-17.26	105.85	124.42
2	B	800	HEM	C4C-CHD-C1D	16.48	161.04	126.02
2	A	800	HEM	CHD-C4C-NC	-16.33	106.67	124.45
2	B	800	HEM	CHD-C4C-NC	-16.05	106.98	124.45
2	B	800	HEM	CHB-C1B-NB	-15.92	104.68	124.37
2	B	800	HEM	CHC-C1C-NC	-15.83	107.22	124.45
2	B	800	HEM	CHD-C1D-ND	-15.62	107.61	124.42
2	A	800	HEM	CHA-C4D-ND	-15.49	105.21	124.37
2	B	800	HEM	C4A-CHB-C1B	14.99	161.49	126.25
2	A	800	HEM	C4C-CHD-C1D	14.10	155.99	126.02
2	A	800	HEM	CHB-C1B-NB	-13.47	107.70	124.37
2	A	800	HEM	C1C-CHC-C4B	13.45	154.61	126.02
2	B	800	HEM	CHC-C4B-C3B	13.32	151.66	125.07
2	A	800	HEM	CHD-C1D-ND	-12.62	110.85	124.42
2	A	800	HEM	CHC-C1C-NC	-12.33	111.03	124.45
2	B	800	HEM	C1A-CHA-C4D	12.06	154.60	126.25
2	A	800	HEM	CHA-C4D-C3D	11.94	147.24	125.23
2	A	800	HEM	C1A-CHA-C4D	11.78	153.95	126.25
2	B	800	HEM	CHA-C4D-ND	-11.61	110.00	124.37
2	A	800	HEM	C4A-CHB-C1B	11.30	152.81	126.25
2	B	800	HEM	CHA-C4D-C3D	11.17	145.82	125.23
2	B	800	HEM	CHD-C1D-C2D	11.12	142.58	125.03
2	B	800	HEM	CHB-C4A-NA	-10.52	104.78	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	HEM	CHD-C4C-C3C	10.35	142.65	125.21
2	B	800	HEM	CHC-C1C-C2C	10.24	146.78	125.49
2	A	800	HEM	C3B-C2B-C1B	-10.16	98.78	106.41
2	A	800	HEM	CHA-C1A-C2A	9.29	145.62	125.30
2	A	800	HEM	C2A-C1A-NA	-9.03	100.13	110.15
2	A	800	HEM	C2B-C1B-NB	8.81	119.97	109.84
2	A	800	HEM	CHD-C4C-C3C	8.79	140.03	125.21
2	B	800	HEM	O2D-CGD-O1D	-8.47	101.56	123.33
2	A	800	HEM	CHC-C4B-C3B	8.40	141.83	125.07
2	B	800	HEM	CHA-C1A-C2A	8.26	143.37	125.30
2	B	800	HEM	C3B-C4B-NB	-8.11	103.64	109.47
2	A	800	HEM	CAD-C3D-C4D	-7.82	111.07	124.70
2	A	800	HEM	C1D-C2D-C3D	-7.52	99.07	106.98
2	B	800	HEM	C4B-C3B-C2B	7.10	113.80	107.28
2	B	800	HEM	C3D-C4D-ND	-7.04	102.45	110.17
2	B	800	HEM	O1D-CGD-CBD	6.92	145.05	123.09
2	B	800	HEM	CAD-C3D-C4D	-6.92	112.64	124.70
2	A	800	HEM	C1A-C2A-C3A	6.64	117.14	106.87
2	A	800	HEM	CHB-C4A-NA	-6.53	112.02	123.86
2	A	800	HEM	CAA-C2A-C1A	-6.39	112.45	124.94
2	B	800	HEM	CHB-C4A-C3A	6.31	145.74	127.43
2	B	800	HEM	C2A-C1A-NA	-6.25	103.21	110.15
2	A	800	HEM	CMD-C2D-C1D	6.19	134.70	125.03
2	B	800	HEM	CHA-C1A-NA	-5.95	113.08	123.86
2	A	800	HEM	CHC-C1C-C2C	5.81	137.56	125.49
2	A	800	HEM	O2A-CGA-O1A	-5.80	108.41	123.33
2	B	800	HEM	C3B-C2B-C1B	-5.67	102.15	106.41
2	B	800	HEM	CHB-C1B-C2B	5.63	142.94	126.95
2	A	800	HEM	C4A-C3A-C2A	-5.42	100.61	106.82
2	A	800	HEM	O2A-CGA-CBA	5.40	131.05	114.00
2	B	800	HEM	O2A-CGA-O1A	-5.39	109.46	123.33
2	A	800	HEM	CHA-C1A-NA	-5.32	114.22	123.86
2	A	800	HEM	CHD-C1D-C2D	5.28	133.37	125.03
2	A	800	HEM	O2D-CGD-O1D	-5.25	109.82	123.33
2	B	800	HEM	C4D-C3D-C2D	5.17	114.42	106.89
2	B	800	HEM	C4D-ND-C1D	5.06	111.19	105.21
2	A	800	HEM	C1B-NB-C4B	-5.05	99.23	105.21
2	A	800	HEM	C4D-C3D-C2D	4.89	114.01	106.89
2	A	800	HEM	C2D-C1D-ND	4.70	115.34	109.90
2	B	800	HEM	CMC-C2C-C1C	-4.69	116.47	124.73
2	B	800	HEM	C1D-C2D-C3D	-4.62	102.12	106.98
2	B	800	HEM	C1A-C2A-C3A	4.61	114.00	106.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	HEM	CAA-C2A-C1A	-4.60	115.95	124.94
2	A	800	HEM	CAA-CBA-CGA	-4.27	102.35	113.67
2	A	800	HEM	C4A-NA-C1A	4.22	112.70	105.82
2	A	800	HEM	CAC-C3C-C4C	-4.15	114.92	124.82
2	A	800	HEM	C4B-C3B-C2B	4.02	110.98	107.28
2	B	800	HEM	CMA-C3A-C2A	3.85	133.78	125.62
2	B	800	HEM	C4A-C3A-C2A	-3.75	102.53	106.82
2	A	800	HEM	CAD-C3D-C2D	3.71	134.82	127.87
2	A	800	HEM	CHB-C4A-C3A	3.59	137.85	127.43
2	B	800	HEM	CMB-C2B-C3B	3.52	136.95	128.43
2	A	800	HEM	C3D-C4D-ND	-3.50	106.34	110.17
2	B	800	HEM	C1B-NB-C4B	3.39	109.22	105.21
2	B	800	HEM	CAA-CBA-CGA	-3.28	104.97	113.67
2	A	800	HEM	CMC-C2C-C1C	-3.27	118.97	124.73
2	B	800	HEM	CAC-C3C-C4C	-3.27	117.02	124.82
2	B	800	HEM	CMB-C2B-C1B	-3.24	119.97	125.03
2	A	800	HEM	CMB-C2B-C3B	3.23	136.24	128.43
2	B	800	HEM	C3C-C2C-C1C	3.13	110.01	107.05
2	B	800	HEM	C4A-NA-C1A	3.05	110.79	105.82
2	A	800	HEM	O1D-CGD-CBD	2.95	132.46	123.09
2	B	800	HEM	CMD-C2D-C1D	2.72	129.28	125.03
2	B	800	HEM	O2A-CGA-CBA	2.70	122.53	114.00
2	A	800	HEM	CBC-CAC-C3C	-2.67	114.21	127.53
2	B	800	HEM	CAD-C3D-C2D	2.65	132.84	127.87
2	A	800	HEM	CAC-C3C-C2C	2.61	136.93	128.43
2	B	800	HEM	CAC-C3C-C2C	2.44	136.37	128.43
2	A	800	HEM	CMA-C3A-C4A	2.44	129.13	125.42
2	A	800	HEM	C3B-C4B-NB	2.20	111.05	109.47
2	A	800	HEM	CMA-C3A-C2A	2.16	130.19	125.62
2	A	800	HEM	CMC-C2C-C3C	2.15	133.63	128.43
2	A	800	HEM	CBB-CAB-C3B	2.08	137.90	127.53
2	A	800	HEM	C4C-NC-C1C	-2.01	102.55	105.82
2	B	800	HEM	C2C-C1C-NC	-2.00	105.93	109.64

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	800	HEM	CAA-CBA-CGA-O1A
2	B	800	HEM	CAA-CBA-CGA-O2A
2	A	800	HEM	CAA-CBA-CGA-O2A
2	A	800	HEM	CAA-CBA-CGA-O1A

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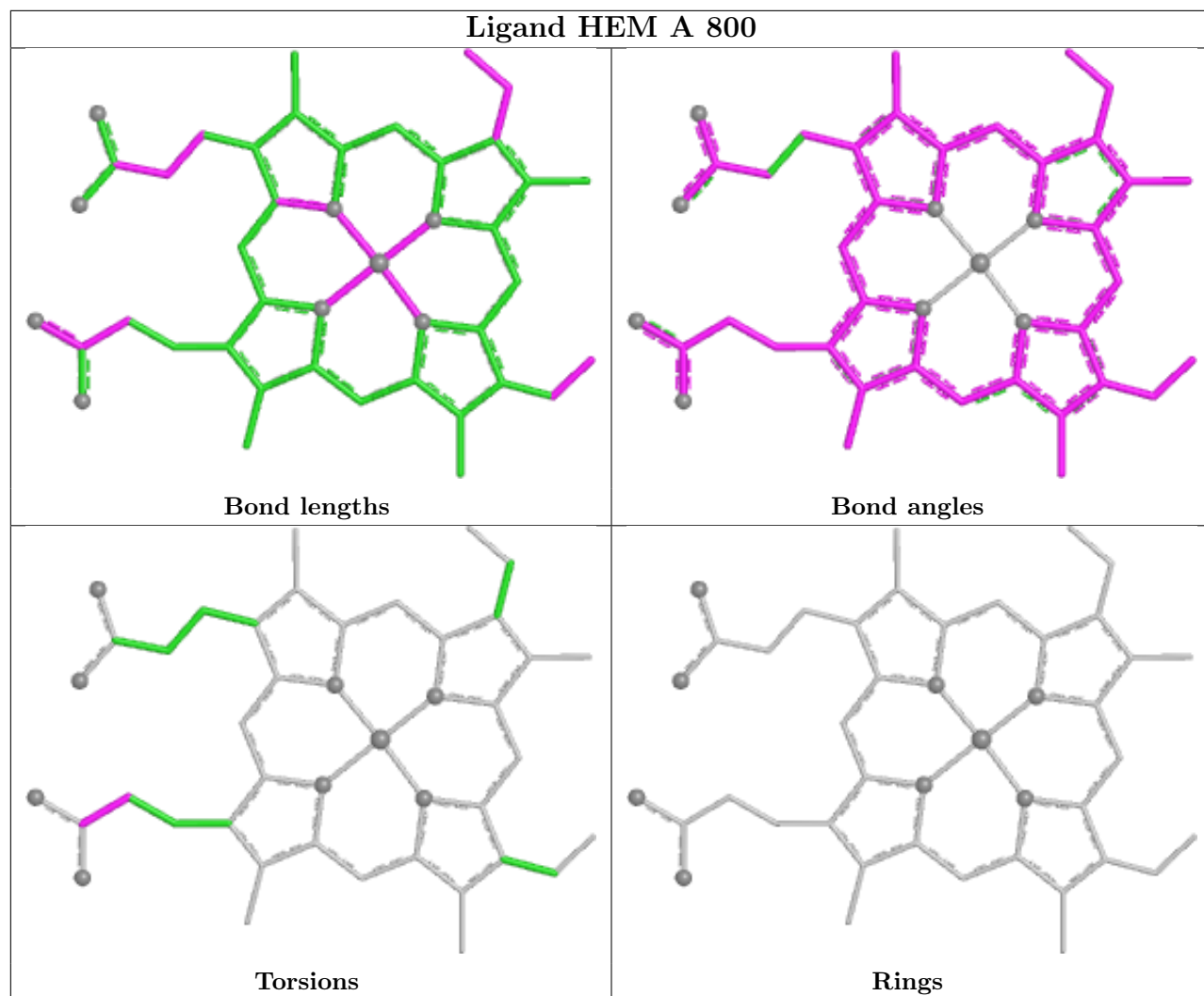
Mol	Chain	Res	Type	Atoms
2	B	800	HEM	C2B-C3B-CAB-CBB
2	B	800	HEM	C2C-C3C-CAC-CBC

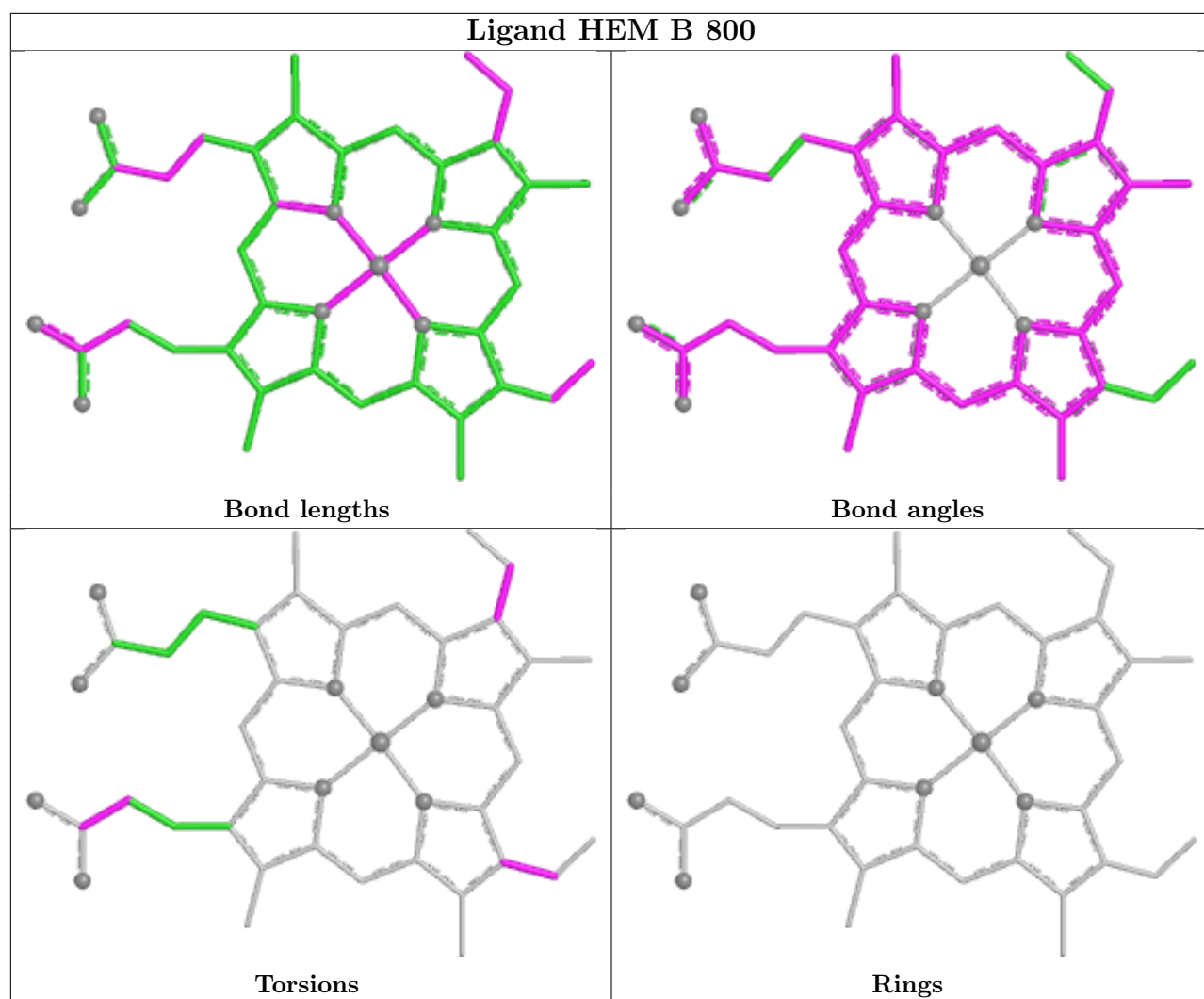
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	SHA	1	0
3	B	801	SHA	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

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	703/737 (95%)	1.20	155 (22%) 2 2	16, 27, 68, 78	0
1	B	710/737 (96%)	1.71	227 (31%) 1 1	17, 35, 72, 80	0
All	All	1413/1474 (95%)	1.46	382 (27%) 1 1	16, 31, 70, 80	0

All (382) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	297	SER	11.6
1	B	305	ALA	10.8
1	B	303	ILE	10.2
1	B	296	ASN	10.2
1	B	300	GLY	9.8
1	A	305	ALA	9.6
1	B	20	PRO	9.3
1	B	307	ILE	9.3
1	A	267	ALA	9.1
1	B	730	LEU	8.7
1	B	299	GLY	8.6
1	B	675	THR	8.5
1	B	678	VAL	8.4
1	A	272	GLU	8.4
1	B	189	PRO	8.3
1	A	270	PRO	8.3
1	B	295	GLY	8.2
1	A	273	ASN	8.2
1	A	274	LEU	8.2
1	A	26	TRP	8.1
1	A	187	TRP	8.1
1	B	270	PRO	8.1
1	A	675	THR	8.0
1	B	193	PHE	8.0

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Mol	Chain	Res	Type	RSRZ
1	A	303	ILE	7.8
1	A	20	PRO	7.5
1	A	188	GLY	7.5
1	A	210	GLY	7.4
1	B	187	TRP	7.3
1	A	266	GLY	7.3
1	B	298	LYS	7.3
1	A	27	TRP	7.3
1	B	267	ALA	7.3
1	B	266	GLY	7.3
1	A	184	ALA	7.1
1	B	26	TRP	7.1
1	B	185	VAL	7.0
1	A	209	LEU	6.9
1	B	273	ASN	6.9
1	B	590	ASP	6.8
1	A	202	PRO	6.8
1	A	674	ASP	6.8
1	B	676	GLY	6.7
1	B	195	THR	6.5
1	B	437	ASP	6.4
1	B	27	TRP	6.4
1	B	677	GLU	6.3
1	A	193	PHE	6.3
1	B	274	LEU	6.3
1	A	213	VAL	6.2
1	A	673	ARG	6.1
1	B	304	THR	5.9
1	B	306	GLY	5.9
1	B	337	PRO	5.8
1	B	269	ASP	5.8
1	B	28	PRO	5.7
1	B	302	MET	5.7
1	A	185	VAL	5.7
1	B	214	MET	5.7
1	A	216	LEU	5.6
1	A	195	THR	5.6
1	A	192	GLU	5.6
1	A	25	ASP	5.6
1	A	730	LEU	5.5
1	A	28	PRO	5.5
1	B	293	LYS	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	638	ASP	5.5
1	A	189	PRO	5.4
1	A	437	ASP	5.4
1	A	19	ARG	5.4
1	A	517	GLU	5.4
1	A	672	ASP	5.3
1	B	294	ASN	5.3
1	A	271	GLU	5.2
1	B	334	GLU	5.2
1	A	306	GLY	5.2
1	B	209	LEU	5.2
1	A	663	ASP	5.2
1	A	206	GLN	5.1
1	A	211	ALA	5.0
1	B	23	ASN	5.0
1	B	212	SER	5.0
1	B	292	ASN	5.0
1	A	203	GLY	4.9
1	B	210	GLY	4.9
1	B	729	ASP	4.9
1	A	205	ILE	4.9
1	A	361	ASP	4.9
1	B	347	SER	4.9
1	B	213	VAL	4.9
1	B	268	ASP	4.8
1	B	21	LYS	4.8
1	A	22	SER	4.8
1	A	347	SER	4.7
1	A	593	THR	4.7
1	A	77	ASP	4.6
1	B	630	ASP	4.6
1	B	211	ALA	4.6
1	A	199	PHE	4.6
1	B	361	ASP	4.5
1	A	503	GLN	4.5
1	A	194	GLU	4.5
1	A	269	ASP	4.5
1	A	111	ALA	4.5
1	A	23	ASN	4.5
1	B	205	ILE	4.4
1	A	212	SER	4.4
1	B	191	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	200	ASP	4.4
1	B	360	PRO	4.3
1	A	18	LYS	4.3
1	B	22	SER	4.3
1	B	190	GLU	4.3
1	A	214	MET	4.3
1	A	207	GLU	4.3
1	B	354	VAL	4.2
1	A	592	ILE	4.2
1	B	49	ASP	4.2
1	A	42	ASP	4.2
1	A	204	GLU	4.2
1	A	731	GLU	4.2
1	B	186	ASN	4.2
1	B	192	GLU	4.2
1	B	593	THR	4.1
1	B	364	GLN	4.1
1	B	197	GLU	4.1
1	B	19	ARG	4.1
1	B	42	ASP	4.1
1	B	679	LYS	4.1
1	A	217	ILE	4.0
1	A	338	GLY	4.0
1	B	24	GLN	4.0
1	B	731	GLU	4.0
1	A	523	SER	4.0
1	B	279	GLU	3.9
1	A	291	GLN	3.9
1	A	208	GLY	3.9
1	B	301	GLU	3.9
1	B	341	TRP	3.9
1	B	393	MET	3.9
1	A	198	ARG	3.9
1	B	591	ASP	3.9
1	B	346	LYS	3.9
1	B	291	GLN	3.9
1	B	524	ASP	3.8
1	B	339	GLY	3.8
1	B	201	GLU	3.8
1	B	727	ARG	3.8
1	B	202	PRO	3.8
1	B	199	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	681	GLU	3.8
1	B	194	GLU	3.8
1	B	208	GLY	3.8
1	B	215	GLY	3.8
1	B	350	LEU	3.8
1	A	679	LYS	3.8
1	B	169	PHE	3.8
1	B	188	GLY	3.7
1	A	186	ASN	3.7
1	A	125	ASP	3.7
1	B	440	LEU	3.7
1	B	336	GLY	3.7
1	A	29	SER	3.7
1	B	25	ASP	3.7
1	A	558	GLU	3.7
1	A	304	THR	3.7
1	B	666	HIS	3.6
1	B	362	GLU	3.6
1	B	575	ASP	3.6
1	B	363	LYS	3.6
1	A	334	GLU	3.6
1	A	348	GLU	3.6
1	B	203	GLY	3.6
1	B	29	SER	3.6
1	B	592	ILE	3.6
1	B	454	LEU	3.6
1	B	18	LYS	3.6
1	B	196	GLN	3.6
1	A	43	VAL	3.5
1	A	21	LYS	3.5
1	B	503	GLN	3.5
1	A	31	LEU	3.5
1	B	48	ASP	3.5
1	A	307	ILE	3.5
1	B	338	GLY	3.4
1	B	359	ASP	3.4
1	A	47	GLU	3.4
1	B	661	ALA	3.4
1	B	671	LEU	3.4
1	A	455	ASP	3.4
1	B	207	GLU	3.4
1	B	358	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	329	TYR	3.4
1	A	397	MET	3.4
1	A	727	ARG	3.4
1	B	512	GLU	3.4
1	A	268	ASP	3.4
1	A	729	ASP	3.4
1	B	392	PRO	3.4
1	B	523	SER	3.4
1	A	350	LEU	3.4
1	B	518	PHE	3.3
1	A	390	GLU	3.3
1	B	424	ASP	3.3
1	A	360	PRO	3.3
1	B	345	PRO	3.3
1	A	40	ALA	3.3
1	B	184	ALA	3.3
1	A	671	LEU	3.3
1	A	50	PHE	3.3
1	A	190	GLU	3.3
1	A	349	GLU	3.3
1	B	517	GLU	3.3
1	A	191	ASP	3.3
1	B	125	ASP	3.3
1	A	280	ALA	3.3
1	B	349	GLU	3.3
1	B	351	LYS	3.3
1	B	290	TRP	3.2
1	B	41	ARG	3.2
1	B	443	ASP	3.2
1	A	713	HIS	3.2
1	A	352	ASN	3.2
1	A	200	ASP	3.2
1	A	41	ARG	3.2
1	B	673	ARG	3.2
1	B	335	LYS	3.2
1	A	630	ASP	3.2
1	B	667	ARG	3.2
1	B	216	LEU	3.1
1	B	728	PHE	3.1
1	A	30	LYS	3.1
1	A	275	GLY	3.1
1	A	201	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	665	GLU	3.1
1	B	231	GLU	3.1
1	B	525	GLY	3.1
1	A	591	ASP	3.1
1	A	639	GLU	3.1
1	B	415	GLU	3.1
1	B	31	LEU	3.1
1	B	446	ILE	3.1
1	B	30	LYS	3.1
1	B	331	TRP	3.1
1	A	676	GLY	3.1
1	B	672	ASP	3.1
1	A	664	SER	3.0
1	B	46	VAL	3.0
1	A	362	GLU	3.0
1	B	502	GLU	3.0
1	B	355	PRO	3.0
1	A	34	GLU	3.0
1	B	272	GLU	3.0
1	B	397	MET	3.0
1	B	453	ILE	2.9
1	B	514	ILE	2.9
1	B	206	GLN	2.9
1	B	332	GLU	2.9
1	B	275	GLY	2.9
1	B	441	ILE	2.9
1	B	706	ASP	2.9
1	A	145	GLN	2.9
1	B	108	GLY	2.9
1	A	49	ASP	2.9
1	B	674	ASP	2.9
1	B	198	ARG	2.9
1	B	333	PRO	2.9
1	B	438	TYR	2.9
1	B	560	GLY	2.9
1	B	379	PRO	2.8
1	B	527	GLN	2.8
1	B	81	ALA	2.8
1	A	354	VAL	2.8
1	B	228	PRO	2.8
1	B	623	SER	2.8
1	A	24	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	427	MET	2.8
1	B	77	ASP	2.8
1	B	552	ASP	2.8
1	B	340	ALA	2.8
1	B	271	GLU	2.7
1	B	165	GLY	2.7
1	A	567	GLU	2.7
1	B	47	GLU	2.7
1	A	457	ASP	2.7
1	A	351	LYS	2.7
1	B	516	THR	2.7
1	B	526	THR	2.7
1	B	111	ALA	2.6
1	A	346	LYS	2.6
1	A	502	GLU	2.6
1	A	677	GLU	2.6
1	B	50	PHE	2.6
1	A	363	LYS	2.6
1	A	435	ASP	2.6
1	A	276	PRO	2.6
1	A	359	ASP	2.6
1	A	76	GLN	2.5
1	B	264	VAL	2.5
1	B	449	LEU	2.5
1	B	308	GLU	2.5
1	B	112	GLY	2.5
1	A	196	GLN	2.5
1	A	279	GLU	2.5
1	B	382	ARG	2.5
1	B	225	ASP	2.4
1	B	344	ALA	2.4
1	A	115	GLN	2.4
1	B	330	GLU	2.4
1	A	524	ASP	2.4
1	A	669	LYS	2.4
1	B	357	ALA	2.4
1	B	447	ALA	2.4
1	B	227	ASN	2.4
1	B	166	PHE	2.4
1	A	46	VAL	2.4
1	A	440	LEU	2.4
1	A	109	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	442	GLY	2.4
1	A	728	PHE	2.4
1	A	553	VAL	2.4
1	A	358	HIS	2.4
1	B	312	THR	2.4
1	B	390	GLU	2.3
1	B	589	GLN	2.3
1	B	520	ASP	2.3
1	B	640	PRO	2.3
1	A	74	SER	2.3
1	B	313	GLN	2.3
1	A	290	TRP	2.3
1	B	343	TRP	2.3
1	B	680	TRP	2.3
1	B	693	ASP	2.3
1	A	70	GLU	2.3
1	A	444	GLU	2.3
1	A	451	GLU	2.3
1	B	522	ARG	2.3
1	A	339	GLY	2.3
1	B	183	LYS	2.3
1	B	235	LYS	2.3
1	B	328	ASP	2.3
1	B	457	ASP	2.3
1	B	327	LEU	2.3
1	B	458	LEU	2.3
1	B	57	GLN	2.2
1	B	521	SER	2.2
1	B	436	ALA	2.2
1	A	313	GLN	2.2
1	B	681	GLU	2.2
1	B	276	PRO	2.2
1	A	638	ASP	2.2
1	A	415	GLU	2.1
1	B	657	GLU	2.1
1	A	525	GLY	2.1
1	A	436	ALA	2.1
1	B	494	LYS	2.1
1	B	391	ASN	2.1
1	A	229	ASP	2.1
1	B	455	ASP	2.1
1	B	566	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	43	VAL	2.1
1	B	353	SER	2.1
1	B	204	GLU	2.1
1	B	115	GLN	2.1
1	A	594	ARG	2.1
1	B	35	ILE	2.1
1	B	428	ILE	2.1
1	A	167	LYS	2.1
1	B	426	GLU	2.1
1	B	445	GLU	2.1
1	B	660	PRO	2.1
1	B	309	GLY	2.1
1	B	450	LYS	2.1
1	B	384	VAL	2.1
1	B	79	TRP	2.1
1	A	32	ASN	2.0
1	A	693	ASP	2.0
1	A	706	ASP	2.0
1	B	555	ILE	2.0
1	B	528	VAL	2.0
1	A	225	ASP	2.0
1	A	215	GLY	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.

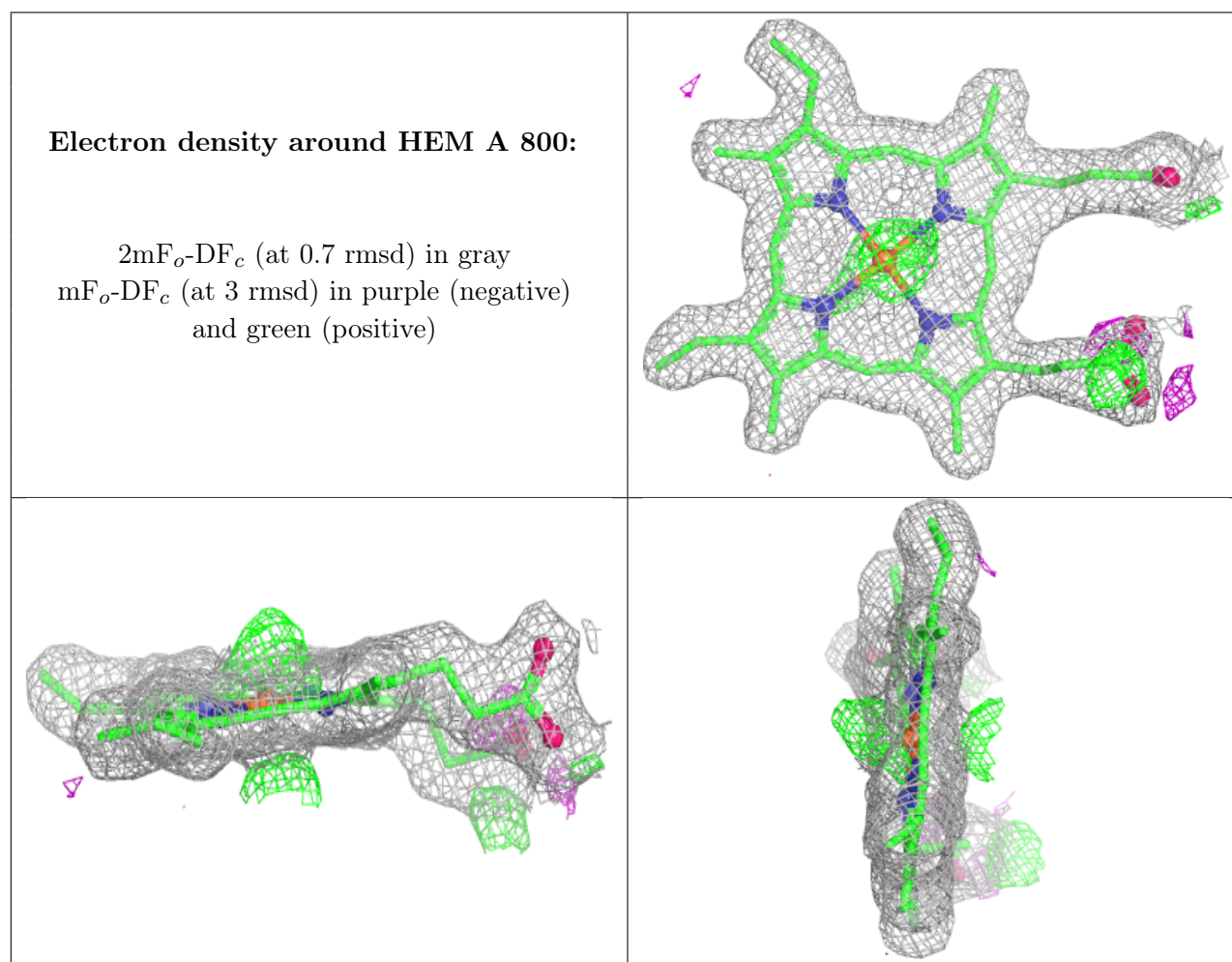
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SHA	A	801	11/11	0.50	0.43	52,52,52,53	11

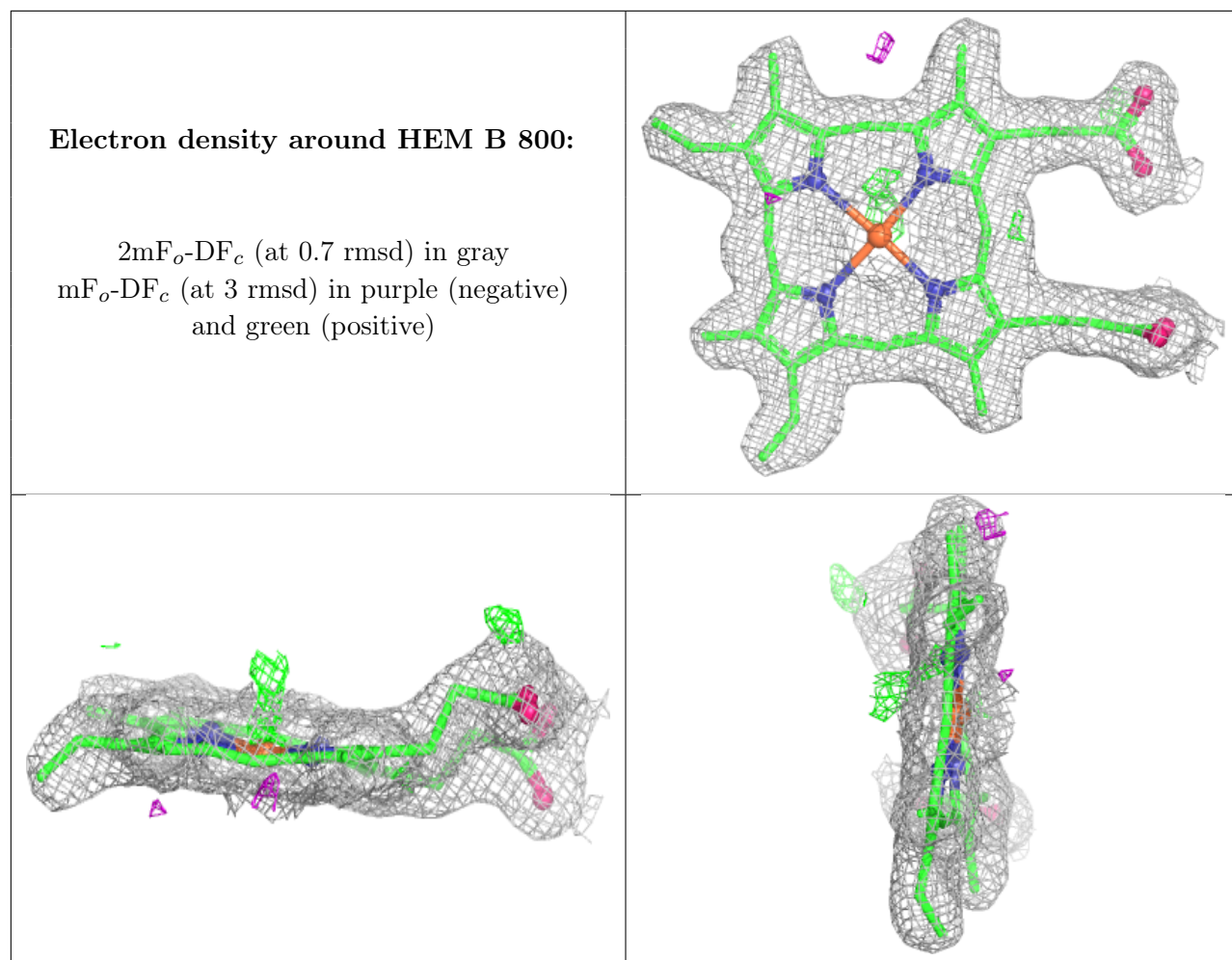
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SHA	B	801	11/11	0.65	0.26	49,51,51,51	11
2	HEM	A	800	43/43	0.96	0.10	15,21,30,39	0
2	HEM	B	800	43/43	0.96	0.09	21,29,36,39	0

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.





6.5 Other polymers [i](#)

There are no such residues in this entry.