



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:45 PM UTC

PDB ID : 2ZQJ / pdb_00002zqj
Title : Substrate-Free Form of Cytochrome P450BSbeta
Authors : Shoji, O.; Fujishiro, T.; Nagano, S.; Hirose, T.; Shiro, Y.; Watanabe, Y.
Deposited on : 2008-08-11
Resolution : 2.90 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

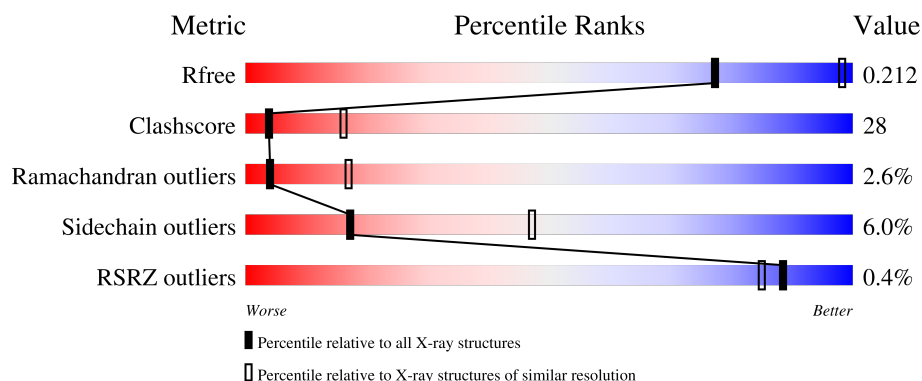
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	417	
1	B	417	
1	C	417	

2 Entry composition [i](#)

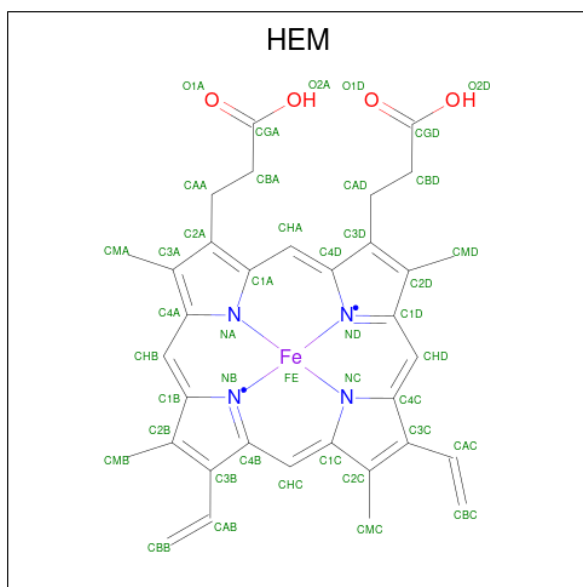
There are 3 unique types of molecules in this entry. The entry contains 10203 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cytochrome P450 152A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3339	2125	594	601	19			
1	B	411	Total	C	N	O	S	0	0	0
			3339	2125	594	601	19			
1	C	411	Total	C	N	O	S	0	0	0
			3339	2125	594	601	19			

- 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	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

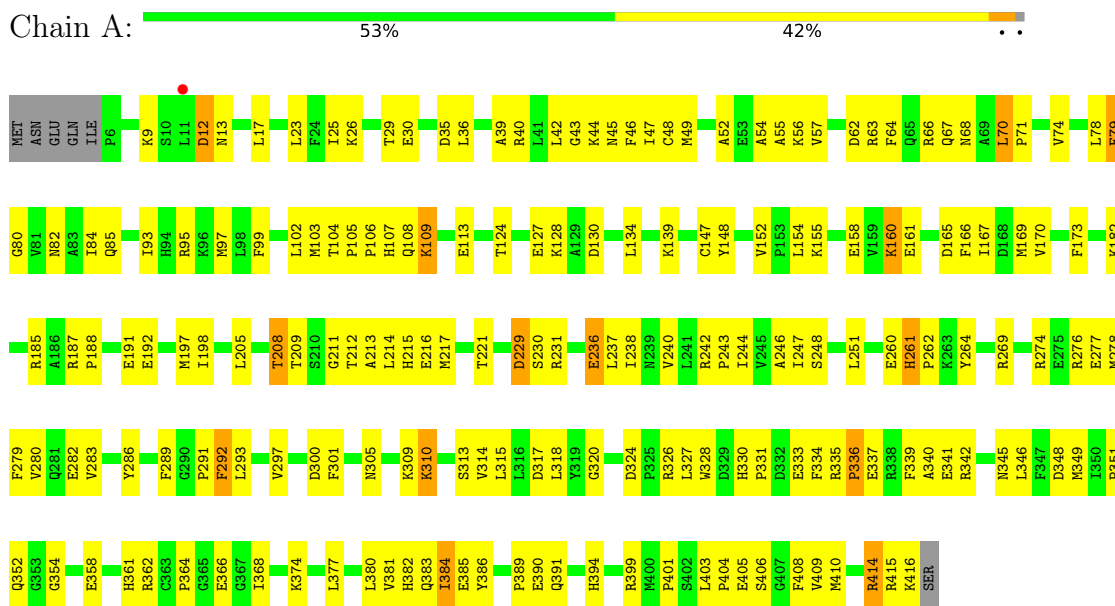
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total 28	O 28	0	0
3	B	17	Total 17	O 17	0	0
3	C	12	Total 12	O 12	0	0

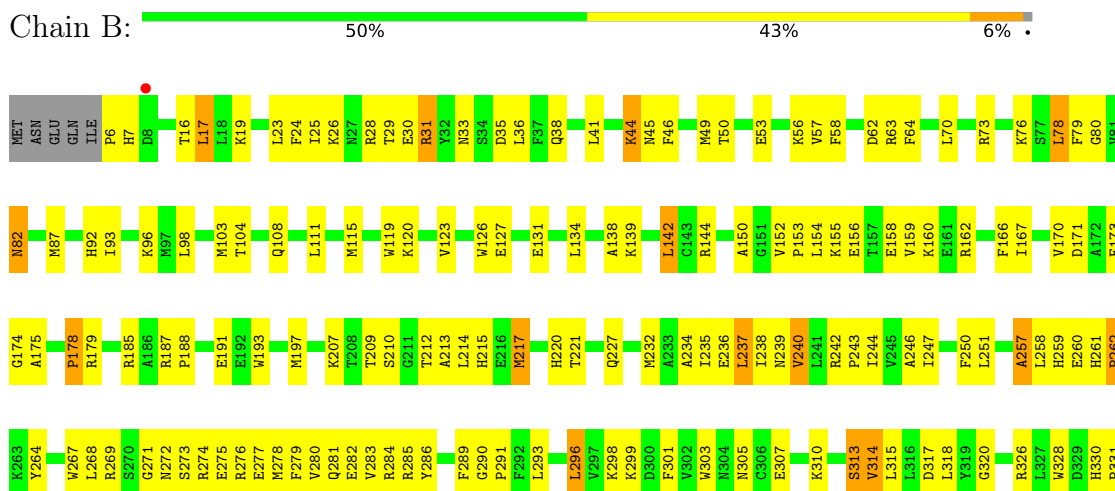
3 Residue-property plots

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

• Molecule 1: Cytochrome P450 152A1

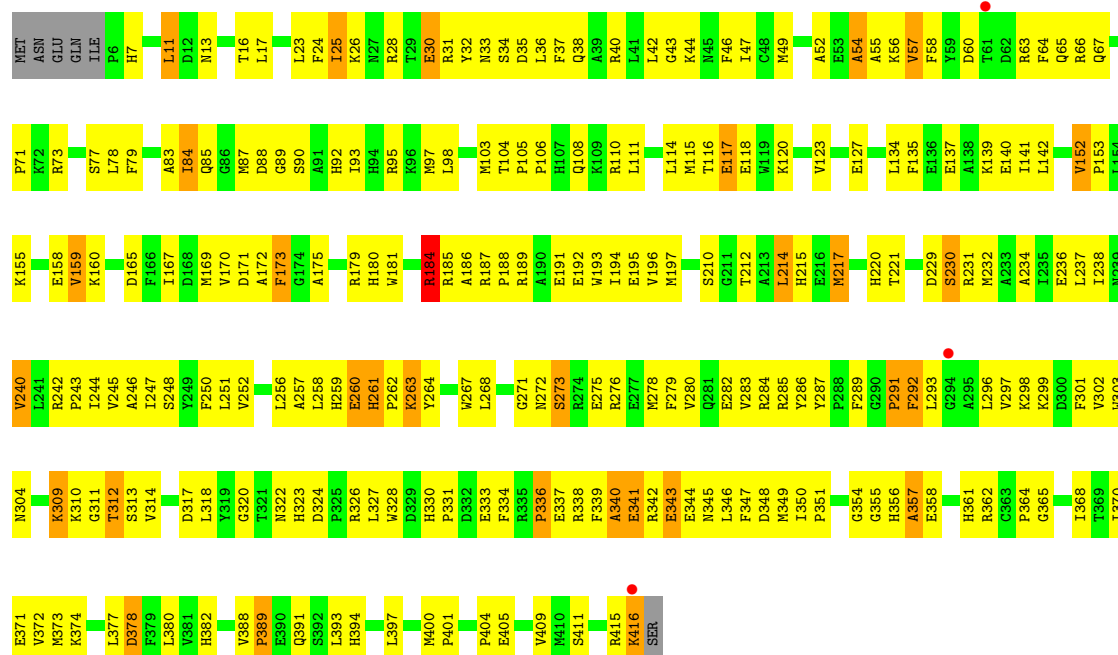
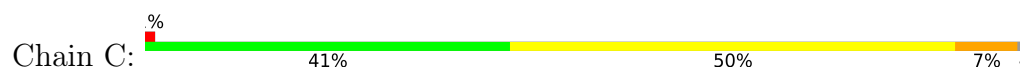


• Molecule 1: Cytochrome P450 152A1





• Molecule 1: Cytochrome P450 152A1



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	173.08Å 173.08Å 279.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.60 – 2.90 46.60 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.0 (46.60-2.90) 95.0 (46.60-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.97 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.221 , 0.286 0.215 , 0.212	Depositor DCC
R_{free} test set	1704 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10203	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.46% 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

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	0.50	0/3422	0.96	11/4614 (0.2%)
1	B	0.54	0/3422	1.00	13/4614 (0.3%)
1	C	0.44	0/3422	0.91	9/4614 (0.2%)
All	All	0.49	0/10266	0.95	33/13842 (0.2%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	240	VAL	N-CA-C	-8.50	104.90	111.62
1	B	79	PHE	N-CA-C	8.02	121.55	111.69
1	B	286	TYR	N-CA-C	7.51	120.56	111.40
1	B	240	VAL	N-CA-C	-7.37	105.80	111.62
1	A	80	GLY	N-CA-C	-7.19	104.23	112.29
1	B	82	ASN	N-CA-C	7.10	121.24	112.58
1	B	70	LEU	CA-C-N	6.90	126.92	119.89
1	B	70	LEU	C-N-CA	6.90	126.92	119.89
1	C	357	ALA	N-CA-C	-6.83	104.04	112.38
1	A	286	TYR	N-CA-C	6.34	118.27	111.36
1	B	78	LEU	N-CA-C	6.08	119.08	111.24
1	A	62	ASP	N-CA-C	-5.85	106.10	113.18
1	A	130	ASP	N-CA-C	-5.84	103.63	112.04
1	A	383	GLN	N-CA-C	5.81	117.69	111.36
1	B	290	GLY	CA-C-N	5.80	127.09	119.84
1	B	290	GLY	C-N-CA	5.80	127.09	119.84
1	C	173	PHE	N-CA-C	5.70	118.26	111.71
1	C	54	ALA	N-CA-C	-5.70	105.15	111.36
1	C	382	HIS	N-CA-C	5.60	119.38	112.54
1	B	384	ILE	N-CA-C	5.38	115.39	108.82
1	B	80	GLY	N-CA-C	-5.34	104.73	111.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	VAL	CB-CA-C	-5.33	106.31	111.05
1	C	184	ARG	N-CA-C	-5.31	106.07	112.54
1	B	407	GLY	N-CA-C	-5.26	107.27	114.64
1	A	79	PHE	N-CA-C	5.25	118.15	111.69
1	A	261	HIS	CA-C-N	5.24	126.39	119.84
1	A	261	HIS	C-N-CA	5.24	126.39	119.84
1	C	152	VAL	CA-C-N	5.19	126.00	119.98
1	C	152	VAL	C-N-CA	5.19	126.00	119.98
1	A	70	LEU	CA-C-N	5.11	125.10	119.89
1	A	70	LEU	C-N-CA	5.11	125.10	119.89
1	A	29	THR	N-CA-C	-5.10	107.01	113.18
1	C	273	SER	N-CA-C	-5.04	107.27	113.41

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	3339	0	3290	148	0
1	B	3339	0	3290	170	0
1	C	3339	0	3290	254	0
2	A	43	0	30	5	0
2	B	43	0	30	7	0
2	C	43	0	30	7	0
3	A	28	0	0	2	0
3	B	17	0	0	2	0
3	C	12	0	0	0	0
All	All	10203	0	9960	572	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 28.

All (572) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:ARG:HH11	1:C:370:ILE:HD11	1.19	1.05
1:A:109:LYS:HA	1:A:109:LYS:HE3	1.43	0.99
1:C:250:PHE:HB3	1:C:373:MET:HE3	1.43	0.98
1:B:391:GLN:HE22	1:B:409:VAL:H	1.09	0.96
1:C:25:ILE:HD12	1:C:26:LYS:H	1.30	0.95
1:B:44:LYS:HE2	1:B:45:ASN:H	1.31	0.94
1:C:345:ASN:HD22	1:C:348:ASP:HB3	1.32	0.94
1:B:153:PRO:HD2	1:B:197:MET:SD	2.11	0.90
1:A:160:LYS:HD3	1:A:161:GLU:H	1.37	0.89
1:A:391:GLN:HE22	1:A:409:VAL:H	1.16	0.87
1:C:84:ILE:HD13	1:C:95:ARG:HB3	1.57	0.86
1:C:65:GLN:NE2	1:C:67:GLN:HB2	1.91	0.86
1:B:280:VAL:HG21	1:B:374:LYS:HG2	1.56	0.85
1:B:328:TRP:O	1:B:331:PRO:HD3	1.77	0.85
1:B:272:ASN:CG	1:B:273:SER:H	1.85	0.84
1:C:11:LEU:HD22	1:C:40:ARG:HG2	1.59	0.82
1:B:342:ARG:HG3	1:B:342:ARG:HH11	1.44	0.82
1:C:127:GLU:CD	1:C:415:ARG:HG2	2.05	0.82
1:C:391:GLN:HE21	1:C:393:LEU:HD21	1.44	0.82
1:A:391:GLN:NE2	1:A:409:VAL:H	1.77	0.81
1:C:272:ASN:CG	1:C:273:SER:H	1.85	0.81
1:A:160:LYS:HE3	1:A:161:GLU:HG3	1.62	0.80
1:C:73:ARG:HB2	1:C:73:ARG:NH1	1.97	0.79
1:B:391:GLN:HE22	1:B:409:VAL:N	1.81	0.78
1:C:114:LEU:O	1:C:117:GLU:HG3	1.82	0.78
1:A:292:PHE:HA	1:A:318:LEU:HD13	1.64	0.78
1:A:403:LEU:HD12	1:A:404:PRO:HD2	1.66	0.78
1:A:391:GLN:HE22	1:A:409:VAL:N	1.81	0.77
1:C:49:MET:HE3	1:C:54:ALA:HB1	1.65	0.77
1:C:268:LEU:HD23	1:C:275:GLU:HB3	1.66	0.77
1:B:150:ALA:HB1	1:B:213:ALA:HB3	1.66	0.76
1:C:275:GLU:HA	1:C:278:MET:HE3	1.67	0.76
1:A:160:LYS:CE	1:A:161:GLU:HG3	2.17	0.75
1:C:260:GLU:O	1:C:262:PRO:HD3	1.87	0.75
1:C:54:ALA:O	1:C:57:VAL:HG23	1.87	0.75
1:C:264:TYR:CZ	1:C:336:PRO:HD2	2.22	0.74
1:C:73:ARG:CB	1:C:73:ARG:HH11	2.00	0.74
1:B:242:ARG:HB3	1:B:243:PRO:HD3	1.69	0.74
1:C:328:TRP:O	1:C:331:PRO:HD3	1.88	0.74
1:B:26:LYS:O	1:B:30:GLU:HG3	1.88	0.74
1:C:181:TRP:HB3	1:C:185:ARG:NH1	2.03	0.73
1:C:343:GLU:HG3	1:C:344:GLU:H	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:ARG:HB3	1:C:188:PRO:HD3	1.69	0.73
1:C:247:ILE:HA	2:C:501:HEM:HBB1	1.71	0.73
1:A:385:GLU:HB2	1:A:414:ARG:NH1	2.03	0.73
1:A:52:ALA:O	1:A:56:LYS:HG3	1.88	0.72
1:C:279:PHE:O	1:C:283:VAL:HG23	1.89	0.72
1:C:232:MET:HE3	1:C:236:GLU:HG2	1.70	0.72
1:B:264:TYR:CZ	1:B:336:PRO:HD2	2.25	0.72
1:A:213:ALA:O	1:A:217:MET:HG2	1.88	0.72
1:B:104:THR:O	1:B:108:GLN:HG3	1.89	0.72
1:B:139:LYS:HE2	1:B:167:ILE:HG13	1.71	0.71
1:A:280:VAL:HG21	1:A:374:LYS:HG2	1.72	0.71
1:B:243:PRO:O	1:B:246:ALA:HB3	1.91	0.71
1:C:95:ARG:HG2	1:C:95:ARG:HH11	1.56	0.71
1:B:210:SER:HA	1:B:215:HIS:CD2	2.26	0.71
1:B:44:LYS:CE	1:B:45:ASN:H	2.01	0.70
1:A:26:LYS:O	1:A:30:GLU:HG3	1.91	0.70
1:B:44:LYS:HE2	1:B:45:ASN:N	2.05	0.70
1:C:191:GLU:HB3	1:C:231:ARG:HH11	1.57	0.69
1:C:210:SER:HA	1:C:215:HIS:CD2	2.27	0.69
1:A:187:ARG:HB3	1:A:188:PRO:HD3	1.75	0.69
1:B:279:PHE:O	1:B:283:VAL:HG23	1.92	0.69
1:B:385:GLU:HG2	1:B:416:LYS:HD3	1.74	0.69
1:A:274:ARG:HG2	1:A:278:MET:HE2	1.73	0.69
1:A:382:HIS:O	1:A:416:LYS:HD3	1.93	0.69
1:A:264:TYR:CE1	1:A:336:PRO:HD2	2.27	0.68
1:B:385:GLU:OE2	1:B:416:LYS:HD3	1.93	0.68
1:C:67:GLN:NE2	1:C:298:LYS:NZ	2.42	0.68
1:B:150:ALA:CB	1:B:213:ALA:HB3	2.22	0.68
1:C:25:ILE:CD1	1:C:26:LYS:H	2.04	0.68
1:C:391:GLN:NE2	1:C:393:LEU:HD21	2.08	0.68
1:C:191:GLU:HB3	1:C:231:ARG:NH1	2.09	0.68
1:A:70:LEU:HD22	1:A:71:PRO:HD2	1.77	0.67
1:B:217:MET:HE2	1:B:237:LEU:HD23	1.75	0.67
1:C:345:ASN:HB3	1:C:348:ASP:OD1	1.94	0.67
1:A:242:ARG:HB3	1:A:243:PRO:HD3	1.77	0.67
1:C:317:ASP:OD2	1:C:320:GLY:HA3	1.94	0.67
1:B:17:LEU:O	1:B:17:LEU:HD12	1.95	0.66
1:B:144:ARG:NH1	1:B:156:GLU:OE2	2.28	0.66
1:C:139:LYS:HE3	1:C:167:ILE:HG13	1.77	0.66
1:B:103:MET:HE2	2:B:501:HEM:HAC	1.78	0.66
1:A:127:GLU:OE1	1:A:415:ARG:HB2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:THR:O	1:A:212:THR:HG23	1.96	0.66
1:B:25:ILE:O	1:B:29:THR:HG23	1.96	0.66
1:A:49:MET:HE3	1:A:54:ALA:HB1	1.77	0.65
1:C:293:LEU:HD21	2:C:501:HEM:HAA2	1.78	0.65
1:C:244:ILE:HG12	2:C:501:HEM:HMC2	1.78	0.65
1:B:269:ARG:HA	1:B:382:HIS:HE1	1.62	0.65
1:C:17:LEU:C	1:C:17:LEU:HD23	2.21	0.64
1:C:397:LEU:N	1:C:397:LEU:HD12	2.12	0.64
1:C:339:PHE:HE2	1:C:349:MET:HE1	1.63	0.64
1:B:391:GLN:NE2	1:B:409:VAL:H	1.88	0.64
1:C:240:VAL:O	1:C:243:PRO:HD2	1.97	0.64
1:B:250:PHE:HB3	1:B:373:MET:HE3	1.78	0.64
1:B:78:LEU:CD1	1:B:170:VAL:HA	2.29	0.63
1:A:380:LEU:HA	1:A:384:ILE:HD11	1.79	0.63
1:B:28:ARG:HG3	1:B:28:ARG:HH11	1.63	0.63
1:B:272:ASN:CG	1:B:273:SER:N	2.56	0.63
1:C:7:HIS:HA	1:C:38:GLN:HB2	1.81	0.63
1:B:16:THR:HG22	1:B:19:LYS:HZ2	1.63	0.63
1:A:349:MET:HG2	1:A:351:PRO:HD3	1.80	0.63
1:C:272:ASN:CG	1:C:273:SER:N	2.57	0.63
1:A:277:GLU:HG2	1:A:374:LYS:HD3	1.80	0.62
1:A:109:LYS:HA	1:A:109:LYS:CE	2.24	0.62
1:B:28:ARG:HG3	1:B:28:ARG:NH1	2.15	0.62
1:B:138:ALA:O	1:B:142:LEU:HB2	1.99	0.62
1:B:175:ALA:HB2	1:B:179:ARG:NH1	2.15	0.62
1:A:328:TRP:O	1:A:331:PRO:HD3	2.00	0.62
1:C:180:HIS:NE2	1:C:184:ARG:NH1	2.47	0.62
1:C:240:VAL:C	1:C:243:PRO:HD2	2.25	0.62
1:C:79:PHE:HB3	1:C:85:GLN:OE1	2.00	0.61
1:A:385:GLU:HB2	1:A:414:ARG:HH12	1.64	0.61
1:A:64:PHE:CE1	1:A:314:VAL:HG21	2.36	0.61
1:C:25:ILE:HD12	1:C:26:LYS:N	2.11	0.61
1:C:236:GLU:OE2	1:C:236:GLU:HA	1.99	0.61
1:C:256:LEU:HD12	1:C:287:TYR:OH	1.99	0.61
1:A:279:PHE:O	1:A:283:VAL:HG23	2.01	0.61
1:C:260:GLU:C	1:C:262:PRO:HD3	2.25	0.61
1:C:397:LEU:HD12	1:C:397:LEU:H	1.66	0.61
1:C:370:ILE:HG22	1:C:374:LYS:HE2	1.82	0.61
1:B:250:PHE:HB3	1:B:373:MET:CE	2.30	0.61
1:C:73:ARG:HB2	1:C:73:ARG:HH11	1.62	0.61
1:C:284:ARG:NH1	1:C:370:ILE:HD11	2.03	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:GLU:OE2	1:C:30:GLU:N	2.34	0.61
1:C:291:PRO:HB3	1:C:400:MET:HE2	1.83	0.61
1:C:250:PHE:HB3	1:C:373:MET:CE	2.27	0.60
1:B:76:LYS:O	1:B:187:ARG:HD2	2.00	0.60
1:C:324:ASP:HB3	1:C:327:LEU:HD12	1.84	0.60
1:B:119:TRP:HB3	1:B:379:PHE:CD1	2.36	0.60
1:A:293:LEU:HG	1:A:318:LEU:HD11	1.83	0.60
1:C:17:LEU:HD23	1:C:17:LEU:O	2.02	0.60
1:B:277:GLU:HA	1:B:374:LYS:HD3	1.83	0.60
1:B:31:ARG:O	1:B:31:ARG:HG2	2.01	0.60
1:A:67:GLN:O	1:A:68:ASN:HB2	2.01	0.60
1:B:63:ARG:HG2	1:B:301:PHE:CD1	2.37	0.59
1:C:104:THR:HB	1:C:105:PRO:CD	2.33	0.59
1:C:63:ARG:HD3	1:C:301:PHE:CE2	2.38	0.59
1:C:64:PHE:HA	1:C:296:LEU:O	2.02	0.59
1:B:239:ASN:HD22	1:B:242:ARG:HH12	1.50	0.59
1:A:17:LEU:HD12	1:A:17:LEU:O	2.03	0.59
1:C:110:ARG:NH1	1:C:114:LEU:HD21	2.18	0.59
1:C:104:THR:HB	1:C:105:PRO:HD2	1.84	0.58
1:B:272:ASN:HB3	1:B:275:GLU:OE2	2.02	0.58
1:C:52:ALA:O	1:C:55:ALA:HB3	2.03	0.58
1:C:191:GLU:HA	1:C:238:ILE:HD11	1.84	0.58
1:C:73:ARG:NH1	1:C:73:ARG:CB	2.62	0.58
1:C:192:GLU:O	1:C:196:VAL:HG23	2.04	0.58
1:B:342:ARG:HH11	1:B:342:ARG:CG	2.14	0.58
1:B:217:MET:HE1	1:B:240:VAL:HG21	1.85	0.58
1:C:194:ILE:CG2	1:C:237:LEU:HD23	2.34	0.58
1:A:345:ASN:HB3	1:A:348:ASP:OD1	2.04	0.57
1:B:152:VAL:HG13	1:B:197:MET:SD	2.44	0.57
1:B:272:ASN:ND2	1:B:273:SER:H	2.02	0.57
1:C:127:GLU:OE1	1:C:415:ARG:HG2	2.03	0.57
1:C:11:LEU:CD2	1:C:40:ARG:HG2	2.30	0.57
1:C:123:VAL:CG1	1:C:415:ARG:HB3	2.33	0.57
1:C:280:VAL:HG21	1:C:374:LYS:HG2	1.86	0.57
1:B:166:PHE:HE1	1:B:238:ILE:HG23	1.68	0.57
1:C:93:ILE:O	1:C:97:MET:HG2	2.05	0.57
1:C:95:ARG:HG2	1:C:95:ARG:NH1	2.19	0.57
1:C:309:LYS:HG2	1:C:310:LYS:H	1.69	0.57
1:C:391:GLN:OE1	1:C:409:VAL:HB	2.04	0.57
1:B:87:MET:HE2	1:B:92:HIS:HA	1.87	0.57
1:B:317:ASP:OD1	1:B:320:GLY:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:GLU:CG	1:B:416:LYS:HD3	2.34	0.57
1:A:300:ASP:OD2	1:A:309:LYS:HD3	2.05	0.57
1:B:7:HIS:CD2	1:B:38:GLN:HG3	2.39	0.57
1:C:67:GLN:HE22	1:C:298:LYS:NZ	2.01	0.57
1:C:78:LEU:O	1:C:78:LEU:HG	2.04	0.56
1:B:368:ILE:O	1:B:372:VAL:HG23	2.04	0.56
1:C:60:ASP:HB3	1:C:63:ARG:HB2	1.86	0.56
1:C:110:ARG:O	1:C:114:LEU:HG	2.04	0.56
1:C:155:LYS:O	1:C:159:VAL:HG23	2.06	0.56
1:C:337:GLU:CD	1:C:337:GLU:H	2.14	0.56
1:B:272:ASN:ND2	1:B:273:SER:N	2.53	0.56
1:C:292:PHE:CZ	1:C:400:MET:HE1	2.41	0.56
1:A:208:THR:HG22	1:A:215:HIS:HB2	1.88	0.56
1:B:345:ASN:ND2	1:B:346:LEU:H	2.04	0.56
1:B:73:ARG:NH2	1:B:175:ALA:O	2.39	0.55
1:B:369:THR:O	1:B:373:MET:HG3	2.05	0.55
1:C:186:ALA:O	1:C:189:ARG:HB2	2.06	0.55
1:C:339:PHE:CE2	1:C:349:MET:HE1	2.40	0.55
1:B:232:MET:HE3	1:B:235:ILE:HB	1.86	0.55
1:B:56:LYS:HD3	1:B:347:PHE:CD2	2.41	0.55
1:C:194:ILE:HG23	1:C:237:LEU:HD23	1.87	0.55
1:B:274:ARG:HH12	1:B:278:MET:HG3	1.72	0.55
1:B:415:ARG:HG2	1:B:416:LYS:H	1.72	0.55
1:C:46:PHE:HA	1:C:313:SER:O	2.06	0.55
1:C:302:VAL:HG12	1:C:303:TRP:N	2.21	0.55
1:A:66:ARG:HG3	1:A:361:HIS:CD2	2.42	0.55
1:B:274:ARG:NH1	1:B:274:ARG:O	2.40	0.55
1:B:258:LEU:HD11	1:B:268:LEU:HD12	1.89	0.55
1:C:309:LYS:HG2	1:C:310:LYS:N	2.22	0.55
1:C:114:LEU:HA	1:C:117:GLU:CG	2.37	0.55
1:B:284:ARG:HH12	1:B:352:GLN:HG3	1.72	0.54
1:C:118:GLU:HG3	1:C:141:ILE:HG23	1.89	0.54
1:C:92:HIS:CD2	1:C:361:HIS:CE1	2.95	0.54
1:C:272:ASN:HB3	1:C:275:GLU:OE1	2.07	0.54
1:C:282:GLU:O	1:C:286:TYR:HB3	2.07	0.54
1:A:109:LYS:O	1:A:113:GLU:HG3	2.08	0.54
1:B:29:THR:HG21	1:B:50:THR:CG2	2.38	0.54
1:C:272:ASN:ND2	1:C:273:SER:H	2.04	0.54
1:A:165:ASP:O	1:A:169:MET:HG3	2.07	0.54
1:A:384:ILE:HD13	1:A:384:ILE:H	1.73	0.54
1:C:330:HIS:N	1:C:331:PRO:CD	2.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:THR:HG21	1:C:28:ARG:NH2	2.22	0.54
1:A:109:LYS:HE3	1:A:109:LYS:CA	2.26	0.54
1:B:16:THR:HA	1:B:19:LYS:HG2	1.89	0.54
1:B:276:ARG:CB	1:B:276:ARG:HH11	2.21	0.54
1:A:139:LYS:HD2	1:A:167:ILE:HG13	1.90	0.54
1:A:385:GLU:HA	3:A:518:HOH:O	2.08	0.54
1:B:24:PHE:HE2	1:B:41:LEU:HD11	1.73	0.54
1:B:98:LEU:HD22	1:B:220:HIS:CG	2.43	0.54
1:B:275:GLU:HA	1:B:278:MET:HE3	1.88	0.54
1:C:105:PRO:HB2	1:C:106:PRO:HD3	1.89	0.54
1:C:116:THR:CG2	1:C:120:LYS:HE3	2.38	0.54
1:C:328:TRP:HB2	1:C:331:PRO:HB3	1.90	0.54
1:B:394:HIS:HB3	1:B:405:GLU:OE1	2.08	0.54
1:C:89:GLY:O	1:C:93:ILE:HG12	2.08	0.54
1:C:181:TRP:HE3	1:C:185:ARG:HD3	1.72	0.54
1:C:229:ASP:O	1:C:232:MET:N	2.40	0.54
1:C:263:LYS:H	1:C:263:LYS:HD3	1.73	0.54
1:C:111:LEU:HD12	1:C:368:ILE:HD12	1.89	0.53
1:A:160:LYS:HD3	1:A:161:GLU:N	2.15	0.53
1:B:269:ARG:HA	1:B:382:HIS:CE1	2.43	0.53
1:C:282:GLU:HG3	1:C:334:PHE:CE1	2.42	0.53
1:C:343:GLU:HG3	1:C:344:GLU:N	2.22	0.53
1:A:293:LEU:HD13	2:A:501:HEM:CGA	2.37	0.53
1:B:23:LEU:HD21	1:B:397:LEU:HD13	1.90	0.53
1:B:24:PHE:CE2	1:B:41:LEU:HD11	2.43	0.53
1:C:246:ALA:C	1:C:248:SER:H	2.15	0.53
1:C:389:PRO:HD3	1:C:411:SER:HB3	1.89	0.53
1:A:185:ARG:C	1:A:188:PRO:HD2	2.32	0.53
1:B:281:GLN:OE1	1:B:281:GLN:HA	2.07	0.53
1:C:11:LEU:HD13	1:C:40:ARG:HG2	1.89	0.53
1:C:282:GLU:HG3	1:C:334:PHE:CD1	2.43	0.53
1:C:123:VAL:CG1	1:C:415:ARG:NH1	2.72	0.53
1:C:36:LEU:HD22	1:C:303:TRP:HZ3	1.74	0.53
1:B:285:ARG:HB2	1:B:349:MET:SD	2.48	0.53
1:C:371:GLU:OE2	1:C:371:GLU:HA	2.08	0.53
1:A:36:LEU:C	1:A:36:LEU:HD12	2.34	0.53
1:C:283:VAL:HG13	1:C:287:TYR:CD2	2.44	0.53
1:A:191:GLU:HB3	1:A:231:ARG:NH2	2.24	0.52
1:A:352:GLN:HE22	1:A:366:GLU:HA	1.73	0.52
1:C:246:ALA:C	1:C:248:SER:N	2.65	0.52
1:A:247:ILE:HA	2:A:501:HEM:HBB1	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:GLU:O	1:B:162:ARG:HG2	2.09	0.52
1:C:170:VAL:C	1:C:172:ALA:H	2.17	0.52
1:B:239:ASN:ND2	1:B:242:ARG:HH12	2.07	0.52
1:C:63:ARG:HD3	1:C:301:PHE:CD2	2.45	0.52
1:A:269:ARG:HD3	1:A:416:LYS:HZ1	1.75	0.52
1:B:155:LYS:HB2	1:B:158:GLU:HG2	1.91	0.52
1:B:155:LYS:O	1:B:159:VAL:HG23	2.09	0.52
1:C:191:GLU:O	1:C:195:GLU:HB2	2.10	0.52
1:C:283:VAL:HG13	1:C:287:TYR:HD2	1.74	0.52
1:C:416:LYS:NZ	1:C:416:LYS:HB3	2.25	0.52
1:A:335:ARG:HB3	1:A:337:GLU:OE1	2.09	0.51
1:B:264:TYR:CE1	1:B:336:PRO:HD2	2.44	0.51
1:C:338:ARG:O	1:C:342:ARG:NH1	2.43	0.51
1:B:247:ILE:HA	2:B:501:HEM:HBB1	1.91	0.51
1:A:71:PRO:HG2	1:A:74:VAL:HG23	1.93	0.51
1:B:103:MET:HE2	2:B:501:HEM:CAC	2.39	0.51
1:B:187:ARG:HB3	1:B:188:PRO:HD3	1.92	0.51
1:C:355:GLY:O	1:C:362:ARG:HD3	2.10	0.51
1:C:73:ARG:HH11	1:C:73:ARG:HB3	1.75	0.51
1:A:261:HIS:HB3	1:A:264:TYR:HD2	1.75	0.51
1:B:244:ILE:HG13	2:B:501:HEM:HBC2	1.93	0.51
1:C:181:TRP:HE3	1:C:185:ARG:CD	2.23	0.51
1:C:394:HIS:O	1:C:404:PRO:HA	2.11	0.51
1:B:57:VAL:HG12	1:B:64:PHE:HE2	1.75	0.50
1:B:259:HIS:O	1:B:262:PRO:HD3	2.10	0.50
1:C:283:VAL:O	1:C:287:TYR:HB2	2.11	0.50
1:C:327:LEU:HB2	1:C:328:TRP:CD1	2.46	0.50
1:C:28:ARG:HB2	1:C:37:PHE:CE2	2.47	0.50
1:C:79:PHE:CG	1:C:85:GLN:HG2	2.46	0.50
1:C:173:PHE:CE2	1:C:401:PRO:HD3	2.45	0.50
1:B:274:ARG:CZ	1:B:278:MET:HE2	2.42	0.50
1:B:274:ARG:NH2	1:B:278:MET:HE2	2.27	0.50
1:A:103:MET:SD	1:A:364:PRO:HG2	2.51	0.50
1:A:406:SER:C	1:A:408:PHE:H	2.20	0.50
1:B:293:LEU:O	1:B:315:LEU:HA	2.12	0.50
1:C:285:ARG:HB2	1:C:349:MET:SD	2.51	0.50
1:B:268:LEU:HD22	1:B:276:ARG:HG2	1.93	0.50
1:C:65:GLN:HB3	1:C:298:LYS:HD3	1.92	0.50
1:C:158:GLU:O	1:C:159:VAL:C	2.55	0.50
1:A:198:ILE:HG21	1:A:230:SER:HA	1.92	0.50
1:A:277:GLU:HG2	1:A:374:LYS:CD	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:GLN:NE2	1:C:298:LYS:HZ2	2.10	0.50
1:C:272:ASN:ND2	1:C:273:SER:N	2.59	0.50
1:A:297:VAL:HG12	1:A:310:LYS:HA	1.94	0.50
1:C:114:LEU:HA	1:C:117:GLU:HG2	1.94	0.50
1:C:87:MET:HB3	1:C:92:HIS:HB2	1.94	0.49
1:C:244:ILE:CG1	2:C:501:HEM:HMC2	2.40	0.49
1:C:391:GLN:HE21	1:C:393:LEU:CD2	2.20	0.49
1:B:96:LYS:HE3	1:B:364:PRO:HD3	1.94	0.49
1:B:298:LYS:O	1:B:310:LYS:HG3	2.13	0.49
1:C:312:THR:O	1:C:314:VAL:HG13	2.13	0.49
1:B:276:ARG:NH1	1:B:276:ARG:HB2	2.28	0.49
1:B:49:MET:HE3	1:B:314:VAL:HG21	1.93	0.49
1:A:95:ARG:NH1	1:A:236:GLU:OE2	2.46	0.49
1:A:25:ILE:HG21	1:A:317:ASP:HB2	1.93	0.49
1:C:118:GLU:CG	1:C:141:ILE:HG23	2.42	0.49
1:B:162:ARG:HD2	1:B:193:TRP:CZ3	2.48	0.49
1:C:416:LYS:HB3	1:C:416:LYS:HZ2	1.78	0.49
1:A:147:CYS:SG	1:A:154:LEU:HD22	2.53	0.48
1:B:342:ARG:HD3	1:B:343:GLU:O	2.13	0.48
1:B:404:PRO:O	1:B:405:GLU:C	2.55	0.48
1:A:317:ASP:OD2	1:A:320:GLY:HA3	2.13	0.48
1:A:368:ILE:HD12	2:A:501:HEM:HBC2	1.94	0.48
1:C:210:SER:C	1:C:212:THR:H	2.21	0.48
1:C:242:ARG:HB3	1:C:243:PRO:HD3	1.94	0.48
1:A:381:VAL:HG12	1:A:382:HIS:ND1	2.28	0.48
1:C:56:LYS:HG2	1:C:347:PHE:CD2	2.48	0.48
1:C:221:THR:HG23	1:C:221:THR:O	2.13	0.48
1:A:244:ILE:HG12	2:A:501:HEM:HMC2	1.95	0.48
1:A:328:TRP:CE3	1:A:342:ARG:NH1	2.82	0.48
1:B:73:ARG:HD2	3:B:503:HOH:O	2.14	0.48
1:B:250:PHE:HE2	1:B:352:GLN:NE2	2.12	0.48
1:C:77:SER:O	1:C:169:MET:HB3	2.14	0.48
1:A:327:LEU:HB2	1:A:328:TRP:CD1	2.48	0.48
1:B:247:ILE:HG22	1:B:247:ILE:O	2.14	0.48
1:B:409:VAL:HG12	1:B:410:MET:N	2.28	0.48
1:C:43:GLY:O	1:C:44:LYS:HG2	2.14	0.48
1:C:165:ASP:HB3	1:C:186:ALA:HB1	1.95	0.48
1:C:25:ILE:CD1	1:C:26:LYS:N	2.73	0.48
1:C:95:ARG:NH1	1:C:236:GLU:OE1	2.47	0.48
1:C:135:PHE:HD1	1:C:252:VAL:HG21	1.78	0.48
1:A:406:SER:C	1:A:408:PHE:N	2.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:PHE:HA	1:B:313:SER:O	2.14	0.48
1:B:126:TRP:HB3	1:B:413:ILE:HD12	1.95	0.48
1:A:354:GLY:HA2	1:A:362:ARG:NH1	2.29	0.48
1:C:247:ILE:HD11	2:C:501:HEM:HMC1	1.96	0.47
1:A:282:GLU:HG3	1:A:334:PHE:CE1	2.49	0.47
1:C:262:PRO:O	1:C:263:LYS:C	2.57	0.47
1:A:63:ARG:CZ	1:A:301:PHE:CD2	2.96	0.47
1:A:385:GLU:CB	1:A:414:ARG:HH12	2.26	0.47
1:B:93:ILE:HD12	1:B:358:GLU:O	2.14	0.47
1:A:337:GLU:CD	1:A:337:GLU:H	2.22	0.47
1:A:337:GLU:C	1:A:339:PHE:N	2.70	0.47
1:B:261:HIS:CE1	1:B:334:PHE:HB3	2.50	0.47
1:B:162:ARG:HD2	1:B:193:TRP:CH2	2.49	0.47
1:B:221:THR:HA	1:B:227:GLN:HA	1.96	0.47
1:C:339:PHE:O	1:C:341:GLU:N	2.48	0.47
1:C:345:ASN:O	1:C:348:ASP:OD1	2.33	0.47
1:A:104:THR:HB	1:A:105:PRO:HD2	1.95	0.47
1:A:107:HIS:O	1:A:108:GLN:C	2.56	0.47
1:A:185:ARG:O	1:A:188:PRO:HD2	2.14	0.47
1:A:276:ARG:HG2	1:A:377:LEU:HD23	1.95	0.47
1:B:232:MET:HE3	1:B:232:MET:HA	1.97	0.47
1:B:240:VAL:O	1:B:244:ILE:HG13	2.15	0.47
1:B:244:ILE:CG1	2:B:501:HEM:HBC2	2.45	0.47
1:B:377:LEU:O	1:B:378:ASP:C	2.57	0.47
1:C:65:GLN:HE21	1:C:67:GLN:HB2	1.77	0.47
1:C:67:GLN:HG3	1:C:88:ASP:OD2	2.14	0.47
1:B:250:PHE:HE2	1:B:352:GLN:HE22	1.63	0.47
1:B:154:LEU:HD12	1:B:158:GLU:HG3	1.96	0.47
1:C:47:ILE:HB	1:C:314:VAL:HG12	1.95	0.47
1:C:64:PHE:CE1	1:C:314:VAL:HG21	2.50	0.47
1:C:247:ILE:HG22	1:C:251:LEU:HD13	1.97	0.47
1:C:268:LEU:HD13	1:C:377:LEU:HD21	1.95	0.47
1:C:311:GLY:O	1:C:312:THR:C	2.58	0.47
1:A:337:GLU:C	1:A:339:PHE:H	2.23	0.47
1:C:217:MET:HE2	1:C:236:GLU:O	2.14	0.47
1:B:6:PRO:HD2	1:B:36:LEU:O	2.15	0.46
1:C:32:TYR:O	1:C:34:SER:N	2.48	0.46
1:C:98:LEU:HB2	1:C:220:HIS:CE1	2.51	0.46
1:C:123:VAL:HG11	1:C:415:ARG:NH1	2.31	0.46
1:A:394:HIS:O	1:A:405:GLU:HG3	2.16	0.46
1:B:187:ARG:NH1	1:B:191:GLU:OE2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:ARG:C	1:B:271:GLY:N	2.73	0.46
1:B:345:ASN:HB3	1:B:348:ASP:OD1	2.15	0.46
1:C:214:LEU:O	1:C:214:LEU:HD22	2.16	0.46
1:C:297:VAL:HG23	1:C:312:THR:O	2.16	0.46
1:A:99:PHE:CZ	1:A:236:GLU:HG3	2.50	0.46
1:A:264:TYR:CZ	1:A:336:PRO:HD2	2.51	0.46
1:B:330:HIS:HB3	1:B:333:GLU:HB2	1.97	0.46
1:C:247:ILE:HG22	1:C:247:ILE:O	2.15	0.46
1:C:267:TRP:CZ2	1:C:275:GLU:HG3	2.51	0.46
1:A:152:VAL:HG13	1:A:197:MET:SD	2.56	0.46
1:B:234:ALA:O	1:B:238:ILE:HG12	2.16	0.46
1:B:282:GLU:HG3	1:B:334:PHE:CE1	2.51	0.46
1:C:127:GLU:OE2	1:C:415:ARG:HG2	2.13	0.46
1:C:374:LYS:O	1:C:377:LEU:HB3	2.16	0.46
1:A:13:ASN:OD1	1:A:39:ALA:HB1	2.16	0.45
1:B:276:ARG:HH11	1:B:276:ARG:HB2	1.81	0.45
1:C:167:ILE:HD11	1:C:245:VAL:HG12	1.97	0.45
1:A:54:ALA:O	1:A:57:VAL:N	2.48	0.45
1:B:111:LEU:HD12	1:B:368:ILE:HD13	1.97	0.45
1:B:269:ARG:C	1:B:271:GLY:H	2.22	0.45
1:C:345:ASN:C	1:C:347:PHE:H	2.23	0.45
1:C:356:HIS:C	1:C:358:GLU:N	2.71	0.45
1:C:229:ASP:O	1:C:231:ARG:N	2.50	0.45
1:A:46:PHE:CZ	1:A:313:SER:HB3	2.52	0.45
1:B:342:ARG:HG3	1:B:342:ARG:NH1	2.21	0.45
1:B:365:GLY:HA3	2:B:501:HEM:C3C	2.51	0.45
1:C:280:VAL:HG21	1:C:374:LYS:CG	2.45	0.45
1:C:340:ALA:O	1:C:341:GLU:C	2.59	0.45
1:A:47:ILE:HB	1:A:314:VAL:HG12	1.99	0.45
1:A:330:HIS:HB3	1:A:333:GLU:HG3	1.98	0.45
1:B:96:LYS:HE3	1:B:364:PRO:HB3	1.99	0.45
1:B:160:LYS:CD	1:B:160:LYS:H	2.30	0.45
1:C:32:TYR:C	1:C:34:SER:N	2.73	0.45
1:B:277:GLU:HG2	1:B:374:LYS:HE2	1.99	0.45
1:B:335:ARG:O	1:B:336:PRO:C	2.57	0.45
1:B:354:GLY:HA2	1:B:362:ARG:NH1	2.32	0.45
1:C:71:PRO:HB2	1:C:73:ARG:HG2	1.98	0.45
1:C:111:LEU:CD1	1:C:368:ILE:HD12	2.47	0.45
1:C:365:GLY:O	1:C:368:ILE:HB	2.16	0.45
1:B:378:ASP:O	1:B:379:PHE:C	2.59	0.45
1:A:93:ILE:O	1:A:97:MET:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ASP:OD2	1:A:229:ASP:N	2.45	0.44
1:C:175:ALA:HB2	1:C:179:ARG:NH1	2.32	0.44
1:A:403:LEU:CD1	1:A:404:PRO:HD2	2.43	0.44
1:A:324:ASP:OD2	1:A:326:ARG:HB2	2.17	0.44
1:C:67:GLN:NE2	1:C:298:LYS:HZ3	2.16	0.44
1:C:152:VAL:HG13	1:C:197:MET:SD	2.58	0.44
1:C:195:GLU:HA	1:C:234:ALA:HB2	1.99	0.44
1:A:269:ARG:HE	1:A:269:ARG:HB2	1.61	0.44
1:A:282:GLU:HG3	1:A:334:PHE:CD1	2.53	0.44
1:B:264:TYR:HA	1:B:267:TRP:HB3	1.99	0.44
1:A:84:ILE:HG23	1:A:85:GLN:N	2.33	0.44
1:B:349:MET:HE3	1:B:351:PRO:HG3	1.99	0.44
1:C:115:MET:HG3	1:C:372:VAL:HG13	2.00	0.44
1:A:269:ARG:NH1	1:A:416:LYS:NZ	2.66	0.43
1:B:36:LEU:HD22	1:B:303:TRP:HZ3	1.81	0.43
1:B:115:MET:HG3	1:B:372:VAL:HG13	2.00	0.43
1:C:87:MET:C	1:C:92:HIS:HB2	2.43	0.43
1:B:173:PHE:CD1	1:B:174:GLY:N	2.87	0.43
1:C:296:LEU:HG	1:C:311:GLY:HA2	2.00	0.43
1:C:304:ASN:OD1	1:C:304:ASN:O	2.36	0.43
1:C:349:MET:HG3	1:C:351:PRO:HD3	2.00	0.43
1:A:78:LEU:HD23	1:A:79:PHE:CE1	2.53	0.43
1:A:340:ALA:O	1:A:341:GLU:HB2	2.18	0.43
1:B:103:MET:CE	2:B:501:HEM:HAC	2.47	0.43
1:C:191:GLU:HA	1:C:238:ILE:CD1	2.47	0.43
1:C:247:ILE:HD11	2:C:501:HEM:CMC	2.48	0.43
1:C:276:ARG:CZ	1:C:378:ASP:OD1	2.66	0.43
1:A:261:HIS:N	1:A:262:PRO:HD3	2.34	0.43
1:C:83:ALA:O	1:C:85:GLN:N	2.51	0.43
1:A:42:LEU:C	1:A:44:LYS:H	2.27	0.43
1:B:35:ASP:CG	1:B:326:ARG:HH12	2.27	0.43
1:B:62:ASP:O	1:B:299:LYS:HE3	2.19	0.43
1:B:78:LEU:HD13	1:B:170:VAL:HA	2.00	0.43
1:B:209:THR:O	1:B:212:THR:HG23	2.18	0.43
1:C:11:LEU:HD22	1:C:40:ARG:CG	2.40	0.43
1:A:104:THR:HB	1:A:105:PRO:CD	2.48	0.43
1:C:13:ASN:HB2	1:C:40:ARG:O	2.18	0.43
1:C:56:LYS:HG2	1:C:347:PHE:CE2	2.54	0.43
1:A:345:ASN:ND2	1:A:346:LEU:H	2.17	0.43
1:B:58:PHE:HA	1:B:64:PHE:CD2	2.54	0.43
1:C:104:THR:OG1	1:C:106:PRO:HD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:HIS:HD2	1:C:333:GLU:HG3	1.83	0.43
1:A:36:LEU:HD12	1:A:36:LEU:O	2.19	0.43
1:A:54:ALA:O	1:A:55:ALA:C	2.62	0.43
1:A:292:PHE:O	1:A:293:LEU:HD23	2.19	0.43
1:B:119:TRP:HA	1:B:119:TRP:CE3	2.54	0.43
1:C:324:ASP:OD2	1:C:326:ARG:HB2	2.19	0.43
1:A:134:LEU:C	1:A:134:LEU:HD13	2.44	0.43
1:A:170:VAL:O	1:A:173:PHE:CD2	2.72	0.43
1:A:214:LEU:HD23	1:A:214:LEU:O	2.18	0.43
1:A:261:HIS:HB3	1:A:264:TYR:CD2	2.54	0.43
1:B:257:ALA:O	1:B:258:LEU:C	2.62	0.43
1:A:102:LEU:HD21	1:A:216:GLU:HG3	2.00	0.43
1:A:260:GLU:C	1:A:262:PRO:HD3	2.43	0.43
1:B:296:LEU:HD12	1:B:296:LEU:HA	1.75	0.43
1:B:318:LEU:HG	1:B:350:ILE:O	2.19	0.43
1:C:49:MET:HE2	1:C:58:PHE:HB2	2.00	0.43
1:C:322:ASN:O	1:C:323:HIS:HD2	2.02	0.43
1:C:357:ALA:HA	1:C:362:ARG:HB3	2.01	0.43
1:C:330:HIS:HB3	1:C:333:GLU:HB2	2.01	0.42
1:C:140:GLU:OE2	1:C:160:LYS:HG3	2.19	0.42
1:A:261:HIS:CD2	1:A:334:PHE:CD2	3.06	0.42
1:B:7:HIS:CG	1:B:38:GLN:HG3	2.53	0.42
1:B:33:ASN:OD1	3:B:504:HOH:O	2.21	0.42
1:C:30:GLU:C	1:C:32:TYR:N	2.77	0.42
1:C:361:HIS:HA	2:C:501:HEM:O1D	2.19	0.42
1:A:70:LEU:CD2	1:A:71:PRO:HD2	2.48	0.42
1:A:155:LYS:O	1:A:158:GLU:HB3	2.19	0.42
1:A:337:GLU:O	1:A:339:PHE:N	2.52	0.42
1:A:386:TYR:N	1:A:386:TYR:CD2	2.87	0.42
1:B:207:LYS:HD2	1:B:207:LYS:C	2.44	0.42
1:C:84:ILE:HD13	1:C:95:ARG:CB	2.40	0.42
1:C:232:MET:O	1:C:236:GLU:HG2	2.19	0.42
1:C:309:LYS:CG	1:C:310:LYS:H	2.28	0.42
1:A:399:ARG:NH1	1:A:401:PRO:O	2.53	0.42
1:C:88:ASP:N	1:C:92:HIS:HB2	2.35	0.42
1:A:246:ALA:C	1:A:248:SER:N	2.76	0.42
1:A:12:ASP:N	3:A:520:HOH:O	2.52	0.42
1:A:229:ASP:O	1:A:230:SER:C	2.61	0.42
1:B:123:VAL:O	1:B:127:GLU:HG3	2.19	0.42
1:C:36:LEU:HD23	1:C:36:LEU:N	2.35	0.42
1:C:261:HIS:HA	1:C:263:LYS:HE3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:GLY:HA2	1:C:362:ARG:HH11	1.84	0.42
1:A:42:LEU:O	1:A:44:LYS:N	2.53	0.42
1:B:49:MET:CE	1:B:314:VAL:HG21	2.50	0.42
1:B:280:VAL:O	1:B:284:ARG:HG3	2.20	0.42
1:C:92:HIS:NE2	1:C:361:HIS:CE1	2.87	0.42
1:C:152:VAL:HA	1:C:153:PRO:HD3	1.83	0.42
1:C:229:ASP:O	1:C:230:SER:C	2.62	0.42
1:C:257:ALA:C	1:C:259:HIS:N	2.78	0.42
1:A:236:GLU:OE1	1:A:236:GLU:HA	2.19	0.42
1:B:53:GLU:O	1:B:57:VAL:HG23	2.20	0.42
1:C:26:LYS:HG2	1:C:26:LYS:O	2.20	0.42
1:C:92:HIS:ND1	1:C:92:HIS:C	2.78	0.42
1:A:105:PRO:HB2	1:A:106:PRO:HD3	2.02	0.42
1:A:352:GLN:NE2	1:A:366:GLU:HA	2.34	0.42
1:A:389:PRO:O	1:A:390:GLU:C	2.63	0.42
1:B:29:THR:HG21	1:B:50:THR:HG21	2.01	0.42
1:C:187:ARG:NH1	1:C:187:ARG:HG3	2.34	0.42
1:C:282:GLU:O	1:C:282:GLU:HG3	2.20	0.42
1:A:40:ARG:NH2	1:A:45:ASN:OD1	2.53	0.41
1:A:46:PHE:CE1	1:A:313:SER:HB3	2.55	0.41
1:A:124:THR:O	1:A:128:LYS:HE3	2.19	0.41
1:A:364:PRO:HD2	2:A:501:HEM:C1D	2.55	0.41
1:C:173:PHE:CD1	1:C:173:PHE:C	2.98	0.41
1:C:302:VAL:CG1	1:C:303:TRP:N	2.83	0.41
1:C:328:TRP:CZ3	1:C:342:ARG:NH1	2.88	0.41
1:A:66:ARG:HG3	1:A:66:ARG:NH1	2.35	0.41
1:C:30:GLU:C	1:C:32:TYR:H	2.28	0.41
1:C:139:LYS:HE3	1:C:167:ILE:CG1	2.49	0.41
1:C:291:PRO:O	1:C:318:LEU:HB2	2.20	0.41
1:B:284:ARG:NH1	1:B:352:GLN:HG3	2.33	0.41
1:C:31:ARG:C	1:C:32:TYR:HD2	2.28	0.41
1:C:280:VAL:HG13	1:C:373:MET:SD	2.60	0.41
1:A:17:LEU:HD12	1:A:17:LEU:C	2.44	0.41
1:A:36:LEU:HA	1:A:48:CYS:O	2.20	0.41
1:B:342:ARG:CG	1:B:342:ARG:NH1	2.74	0.41
1:C:388:VAL:O	1:C:389:PRO:O	2.38	0.41
1:A:35:ASP:O	1:A:49:MET:HA	2.20	0.41
1:B:385:GLU:HG2	1:B:416:LYS:CD	2.47	0.41
1:C:24:PHE:CE1	1:C:28:ARG:CZ	3.03	0.41
1:C:170:VAL:C	1:C:172:ALA:N	2.78	0.41
1:A:160:LYS:HE3	1:A:161:GLU:CG	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ILE:C	1:A:240:VAL:H	2.29	0.41
1:B:36:LEU:HD22	1:B:303:TRP:CZ3	2.55	0.41
1:B:232:MET:HE1	1:B:235:ILE:HG21	2.02	0.41
1:B:236:GLU:HA	1:B:236:GLU:OE1	2.21	0.41
1:B:280:VAL:CG2	1:B:374:LYS:HG2	2.40	0.41
1:C:137:GLU:O	1:C:141:ILE:HG13	2.21	0.41
1:C:350:ILE:N	1:C:351:PRO:CD	2.84	0.41
1:A:12:ASP:O	1:A:13:ASN:C	2.62	0.41
1:A:103:MET:HG2	1:A:368:ILE:HD12	2.03	0.41
1:A:328:TRP:CZ3	1:A:342:ARG:NH1	2.89	0.40
1:B:191:GLU:OE2	1:B:235:ILE:HG12	2.21	0.40
1:C:108:GLN:HB3	1:C:371:GLU:HG3	2.03	0.40
1:C:296:LEU:HG	1:C:311:GLY:O	2.21	0.40
1:C:297:VAL:HG12	1:C:299:LYS:O	2.21	0.40
1:C:380:LEU:HD23	1:C:380:LEU:HA	1.80	0.40
1:A:147:CYS:O	1:A:148:TYR:C	2.63	0.40
1:A:166:PHE:HD1	1:A:169:MET:HE3	1.86	0.40
1:A:280:VAL:HG21	1:A:374:LYS:CG	2.46	0.40
1:A:386:TYR:CG	1:A:410:MET:HE3	2.55	0.40
1:B:29:THR:HG21	1:B:50:THR:HG22	2.03	0.40
1:B:120:LYS:O	1:B:123:VAL:HG23	2.21	0.40
1:B:385:GLU:CD	1:B:416:LYS:HD3	2.45	0.40
1:C:34:SER:OG	1:C:35:ASP:N	2.53	0.40
1:C:103:MET:SD	1:C:364:PRO:O	2.80	0.40
1:C:36:LEU:HG	1:C:36:LEU:O	2.21	0.40
1:A:205:LEU:HD23	1:A:205:LEU:HA	1.90	0.40
1:B:185:ARG:O	1:B:188:PRO:HD2	2.21	0.40
1:C:11:LEU:CD1	1:C:40:ARG:HG2	2.51	0.40
1:C:279:PHE:CE2	1:C:334:PHE:HE2	2.39	0.40
1:C:296:LEU:HD12	1:C:313:SER:HA	2.04	0.40
1:C:388:VAL:HA	1:C:389:PRO:HD2	1.87	0.40
1:A:211:GLY:N	1:A:216:GLU:OE2	2.47	0.40
1:A:246:ALA:C	1:A:248:SER:H	2.28	0.40
1:A:293:LEU:O	1:A:315:LEU:HA	2.22	0.40
1:B:171:ASP:HA	1:B:401:PRO:HD2	2.04	0.40
1:C:66:ARG:HD3	1:C:66:ARG:HA	1.81	0.40
1:C:349:MET:HG2	1:C:351:PRO:CD	2.51	0.40
1:C:368:ILE:O	1:C:372:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	409/417 (98%)	372 (91%)	33 (8%)	4 (1%)	12	39
1	B	409/417 (98%)	375 (92%)	24 (6%)	10 (2%)	4	18
1	C	409/417 (98%)	349 (85%)	42 (10%)	18 (4%)	2	8
All	All	1227/1251 (98%)	1096 (89%)	99 (8%)	32 (3%)	4	17

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASP
1	C	159	VAL
1	C	289	PHE
1	C	309	LYS
1	C	340	ALA
1	C	389	PRO
1	B	343	GLU
1	C	33	ASN
1	C	84	ILE
1	C	230	SER
1	B	257	ALA
1	B	260	GLU
1	B	405	GLU
1	C	171	ASP
1	C	271	GLY
1	C	291	PRO
1	C	346	LEU
1	B	289	PHE
1	C	193	TRP
1	C	258	LEU
1	C	343	GLU
1	C	405	GLU
1	A	43	GLY
1	B	291	PRO

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Mol	Chain	Res	Type
1	B	389	PRO
1	C	312	THR
1	A	289	PHE
1	A	291	PRO
1	B	178	PRO
1	B	262	PRO
1	B	404	PRO
1	C	261	HIS

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	352/358 (98%)	332 (94%)	20 (6%)	18	49
1	B	352/358 (98%)	329 (94%)	23 (6%)	15	44
1	C	352/358 (98%)	332 (94%)	20 (6%)	18	49
All	All	1056/1074 (98%)	993 (94%)	63 (6%)	17	47

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	23	LEU
1	A	82	ASN
1	A	109	LYS
1	A	160	LYS
1	A	182	LYS
1	A	192	GLU
1	A	208	THR
1	A	221	THR
1	A	229	ASP
1	A	236	GLU
1	A	237	LEU
1	A	251	LEU
1	A	292	PHE

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Mol	Chain	Res	Type
1	A	305	ASN
1	A	310	LYS
1	A	336	PRO
1	A	358	GLU
1	A	384	ILE
1	A	414	ARG
1	B	17	LEU
1	B	31	ARG
1	B	44	LYS
1	B	82	ASN
1	B	131	GLU
1	B	134	LEU
1	B	142	LEU
1	B	178	PRO
1	B	214	LEU
1	B	217	MET
1	B	237	LEU
1	B	251	LEU
1	B	296	LEU
1	B	305	ASN
1	B	307	GLU
1	B	313	SER
1	B	314	VAL
1	B	333	GLU
1	B	342	ARG
1	B	346	LEU
1	B	352	GLN
1	B	368	ILE
1	B	383	GLN
1	C	11	LEU
1	C	23	LEU
1	C	25	ILE
1	C	30	GLU
1	C	42	LEU
1	C	57	VAL
1	C	90	SER
1	C	117	GLU
1	C	134	LEU
1	C	142	LEU
1	C	184	ARG
1	C	214	LEU
1	C	217	MET

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Mol	Chain	Res	Type
1	C	260	GLU
1	C	263	LYS
1	C	292	PHE
1	C	336	PRO
1	C	341	GLU
1	C	378	ASP
1	C	416	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	HIS
1	A	107	HIS
1	A	305	ASN
1	A	323	HIS
1	A	330	HIS
1	A	352	GLN
1	A	391	GLN
1	B	65	GLN
1	B	227	GLN
1	B	239	ASN
1	B	261	HIS
1	B	272	ASN
1	B	304	ASN
1	B	305	ASN
1	B	345	ASN
1	B	382	HIS
1	B	391	GLN
1	C	65	GLN
1	C	67	GLN
1	C	107	HIS
1	C	108	GLN
1	C	215	HIS
1	C	272	ASN
1	C	304	ASN
1	C	345	ASN
1	C	361	HIS

5.3.3 RNA ⓘ

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](#)

3 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	501	1	50,50,50	3.43	9 (18%)	67,82,82	1.89	13 (19%)
2	HEM	B	501	1	50,50,50	3.54	13 (26%)	67,82,82	1.94	15 (22%)
2	HEM	C	501	1	50,50,50	3.82	14 (28%)	67,82,82	1.99	15 (22%)

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	501	1	-	1/14/54/54	-
2	HEM	B	501	1	-	6/14/54/54	-
2	HEM	C	501	1	-	5/14/54/54	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	FE-NC	23.45	2.72	1.95
2	B	501	HEM	FE-NC	21.61	2.66	1.95
2	A	501	HEM	FE-NC	21.56	2.66	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	CHD-C1D	4.79	1.50	1.39
2	C	501	HEM	CHD-C4C	4.71	1.47	1.38
2	C	501	HEM	CHA-C4D	4.46	1.47	1.38
2	B	501	HEM	CAC-C3C	-4.21	1.36	1.47
2	B	501	HEM	CHD-C4C	4.12	1.46	1.38
2	C	501	HEM	CAC-C3C	-3.94	1.36	1.47
2	A	501	HEM	CAC-C3C	-3.84	1.37	1.47
2	B	501	HEM	CHA-C4D	3.38	1.45	1.38
2	A	501	HEM	CHA-C4D	3.30	1.45	1.38
2	B	501	HEM	C1C-NC	-3.27	1.33	1.39
2	B	501	HEM	CAB-C3B	-3.23	1.38	1.47
2	C	501	HEM	C1C-NC	-3.13	1.33	1.39
2	C	501	HEM	FE-NB	3.13	2.04	1.94
2	A	501	HEM	C4C-NC	-3.07	1.33	1.39
2	A	501	HEM	CHD-C1D	3.06	1.46	1.39
2	B	501	HEM	C4B-NB	3.05	1.44	1.38
2	A	501	HEM	CHD-C4C	2.96	1.44	1.38
2	B	501	HEM	C4C-NC	-2.79	1.34	1.39
2	B	501	HEM	CHD-C1D	2.76	1.45	1.39
2	A	501	HEM	CHC-C4B	2.68	1.45	1.39
2	C	501	HEM	CAB-C3B	-2.66	1.40	1.47
2	C	501	HEM	C4C-NC	-2.64	1.34	1.39
2	B	501	HEM	C3C-C2C	2.50	1.42	1.37
2	A	501	HEM	CHB-C1B	2.47	1.43	1.38
2	C	501	HEM	C1D-ND	2.46	1.43	1.38
2	C	501	HEM	CHA-C1A	2.43	1.44	1.39
2	B	501	HEM	CMB-C2B	2.31	1.55	1.50
2	B	501	HEM	CHC-C4B	2.22	1.44	1.39
2	B	501	HEM	C1A-NA	-2.16	1.35	1.39
2	C	501	HEM	CHC-C4B	2.15	1.44	1.39
2	C	501	HEM	C4D-ND	2.10	1.43	1.40
2	C	501	HEM	CHB-C1B	2.08	1.42	1.38
2	A	501	HEM	C1B-NB	2.03	1.43	1.40

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	CHD-C4C-C3C	6.53	136.22	125.21
2	C	501	HEM	CHD-C4C-C3C	6.42	136.03	125.21
2	B	501	HEM	CHD-C4C-C3C	5.81	135.00	125.21
2	A	501	HEM	CHD-C4C-NC	-5.49	118.48	124.45
2	B	501	HEM	CHC-C1C-NC	-5.46	118.51	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	HEM	CHD-C4C-NC	-5.35	118.62	124.45
2	B	501	HEM	C4C-NC-C1C	4.90	113.80	105.82
2	C	501	HEM	CHD-C1D-ND	4.72	129.50	124.42
2	C	501	HEM	CHC-C1C-NC	-4.57	119.47	124.45
2	C	501	HEM	C4C-NC-C1C	4.53	113.20	105.82
2	A	501	HEM	C4C-NC-C1C	4.20	112.67	105.82
2	A	501	HEM	CHC-C1C-NC	-3.98	120.12	124.45
2	B	501	HEM	CHC-C4B-NB	3.88	128.59	124.42
2	C	501	HEM	C2D-C1D-ND	-3.77	105.55	109.90
2	B	501	HEM	CHC-C1C-C2C	3.72	133.23	125.49
2	A	501	HEM	CBA-CAA-C2A	3.70	122.76	112.53
2	B	501	HEM	C4C-CHD-C1D	3.61	133.68	126.02
2	A	501	HEM	CHC-C4B-NB	3.46	128.14	124.42
2	B	501	HEM	CHD-C4C-NC	-3.42	120.72	124.45
2	A	501	HEM	CHD-C1D-ND	3.39	128.07	124.42
2	C	501	HEM	CHC-C4B-NB	3.34	128.02	124.42
2	A	501	HEM	C4C-CHD-C1D	3.31	133.04	126.02
2	B	501	HEM	CMD-C2D-C1D	3.22	130.06	125.03
2	C	501	HEM	C1D-C2D-C3D	3.17	110.32	106.98
2	C	501	HEM	C1C-CHC-C4B	3.15	132.72	126.02
2	B	501	HEM	C3C-C2C-C1C	-3.06	104.15	107.05
2	C	501	HEM	C4C-CHD-C1D	2.99	132.38	126.02
2	C	501	HEM	CHC-C1C-C2C	2.98	131.68	125.49
2	A	501	HEM	CHC-C1C-C2C	2.83	131.38	125.49
2	A	501	HEM	C1C-CHC-C4B	2.55	131.44	126.02
2	A	501	HEM	C3B-C4B-NB	-2.51	107.67	109.47
2	B	501	HEM	C4C-C3C-C2C	2.46	108.94	106.81
2	C	501	HEM	CMD-C2D-C1D	2.45	128.86	125.03
2	B	501	HEM	CBD-CAD-C3D	2.40	119.18	112.53
2	B	501	HEM	C2D-C1D-ND	-2.38	107.15	109.90
2	B	501	HEM	C1D-C2D-C3D	2.29	109.39	106.98
2	A	501	HEM	C2D-C1D-ND	-2.27	107.28	109.90
2	B	501	HEM	CMD-C2D-C3D	-2.20	120.21	126.15
2	C	501	HEM	C4D-ND-C1D	2.19	107.80	105.21
2	C	501	HEM	CHA-C1A-C2A	2.15	130.01	125.30
2	B	501	HEM	CHA-C1A-NA	-2.09	120.08	123.86
2	A	501	HEM	CMA-C3A-C2A	2.06	130.00	125.62
2	C	501	HEM	CMD-C2D-C3D	-2.00	120.73	126.15

There are no chirality outliers.

All (12) torsion outliers are listed below:

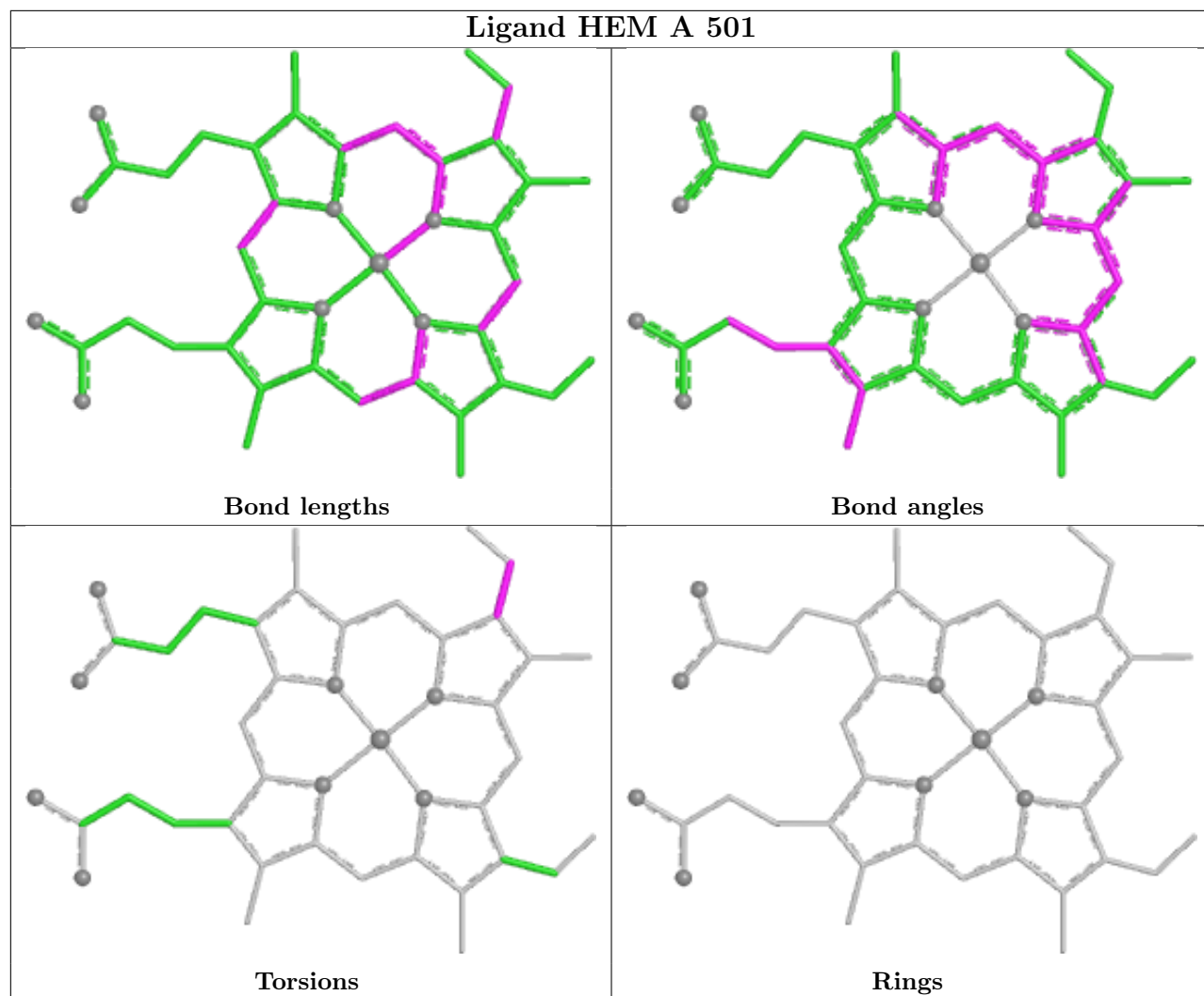
Mol	Chain	Res	Type	Atoms
2	B	501	HEM	C2B-C3B-CAB-CBB
2	C	501	HEM	C4C-C3C-CAC-CBC
2	B	501	HEM	C2C-C3C-CAC-CBC
2	C	501	HEM	C2B-C3B-CAB-CBB
2	C	501	HEM	C2C-C3C-CAC-CBC
2	B	501	HEM	C4B-C3B-CAB-CBB
2	C	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	CAA-CBA-CGA-O2A
2	B	501	HEM	CAA-CBA-CGA-O1A
2	A	501	HEM	C2C-C3C-CAC-CBC
2	B	501	HEM	CAD-CBD-CGD-O2D
2	C	501	HEM	CAD-CBD-CGD-O2D

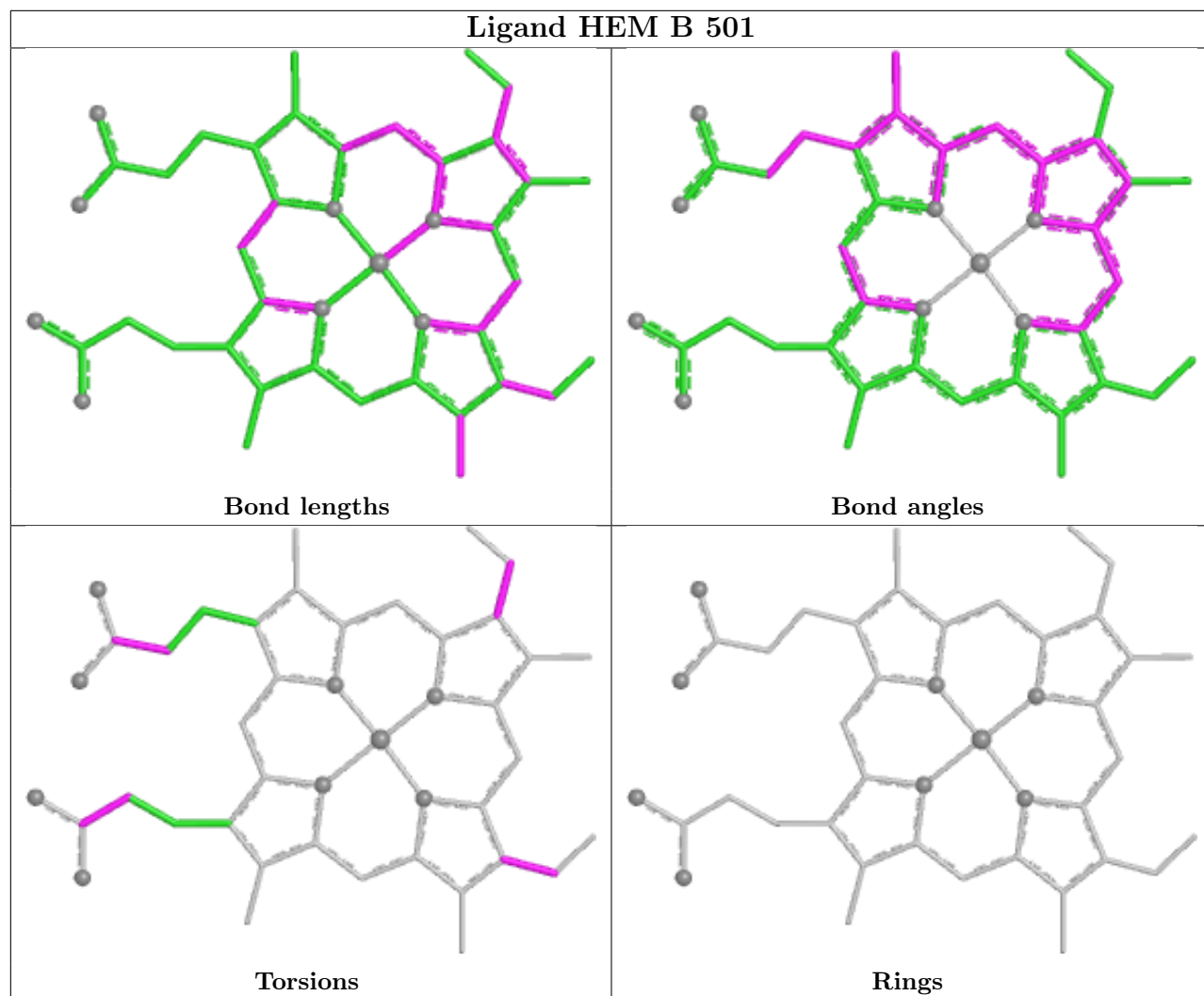
There are no ring outliers.

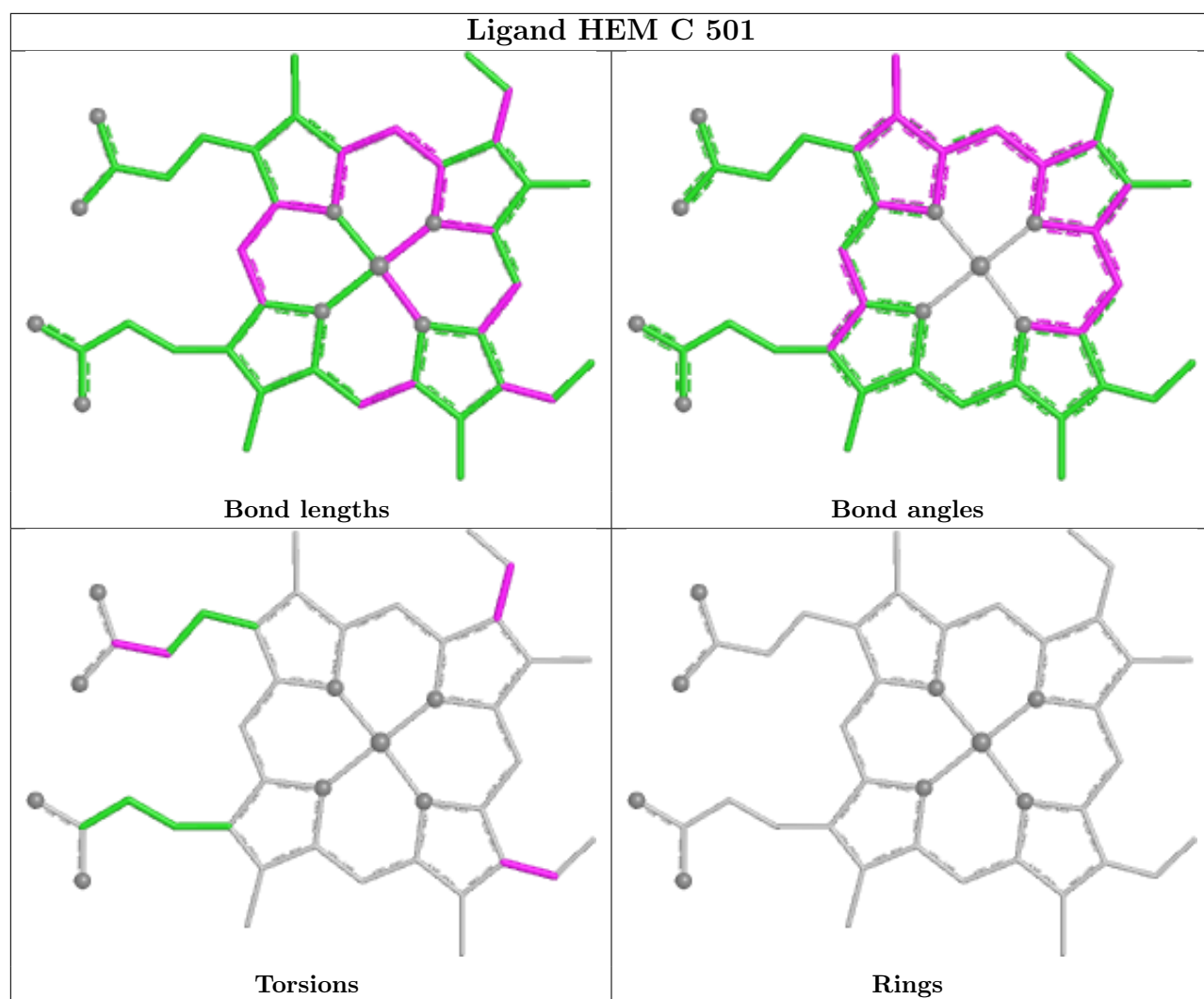
3 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	5	0
2	B	501	HEM	7	0
2	C	501	HEM	7	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	411/417 (98%)	-0.21	1 (0%) 91 89	20, 36, 58, 72	0
1	B	411/417 (98%)	-0.20	1 (0%) 91 89	16, 37, 62, 74	0
1	C	411/417 (98%)	0.21	3 (0%) 84 79	33, 56, 72, 80	0
All	All	1233/1251 (98%)	-0.07	5 (0%) 88 85	16, 43, 68, 80	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	61	THR	2.6
1	C	294	GLY	2.5
1	A	11	LEU	2.2
1	C	416	LYS	2.2
1	B	8	ASP	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](#)

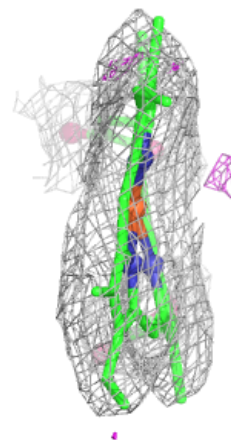
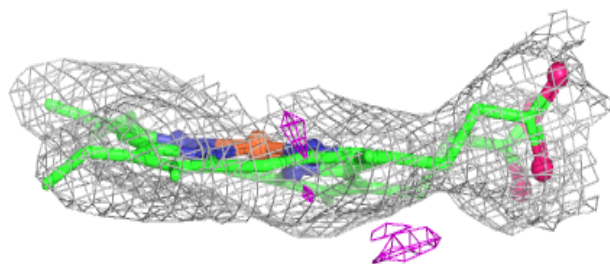
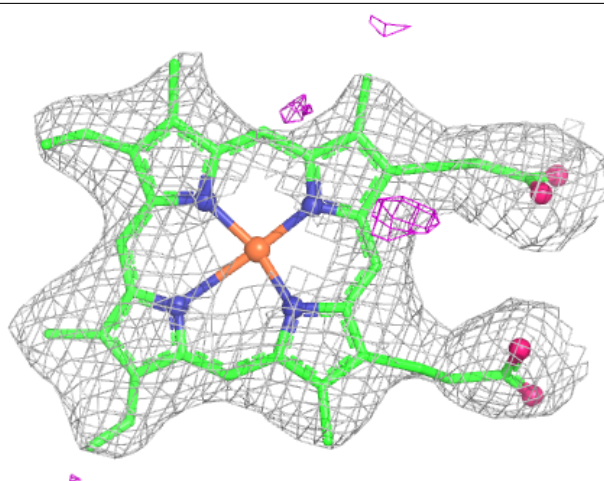
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
2	HEM	B	501	43/43	0.97	0.08	20,24,27,29	0
2	HEM	C	501	43/43	0.97	0.08	35,41,47,50	0
2	HEM	A	501	43/43	0.98	0.07	15,21,26,31	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.

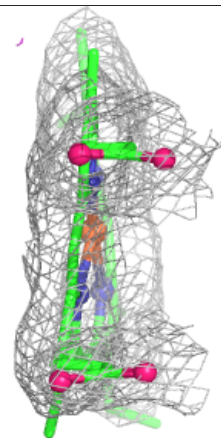
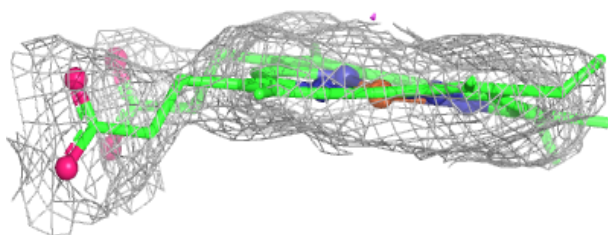
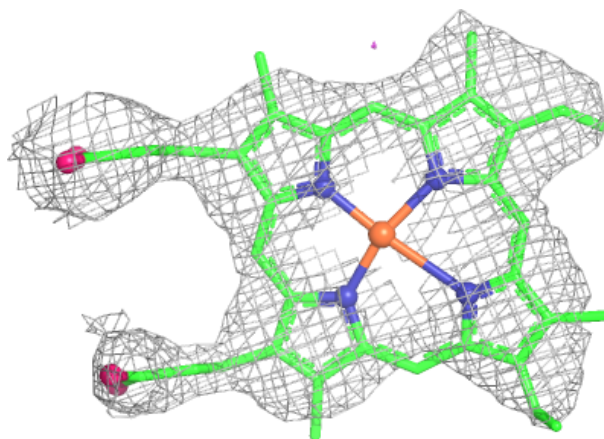
Electron density around HEM B 501:

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



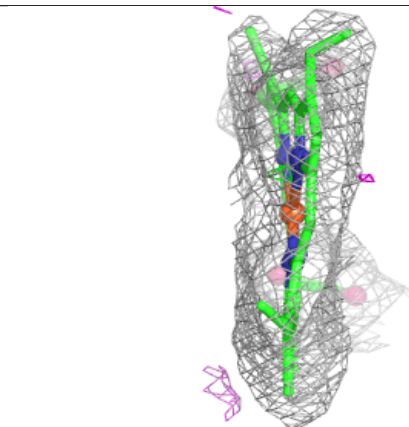
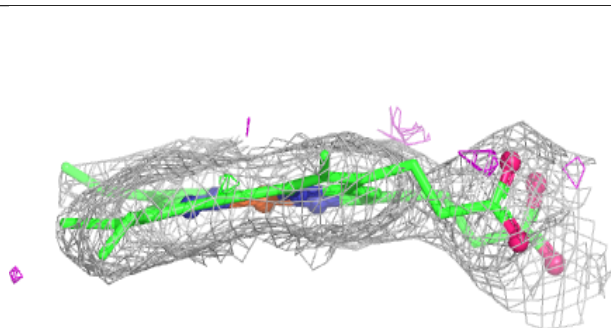
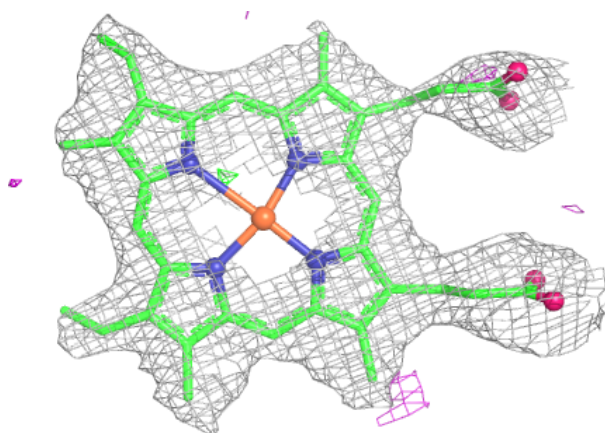
Electron density around HEM C 501:

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



Electron density around HEM A 501:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.