



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 03:18 AM UTC

PDB ID : 2PG5 / pdb_00002pg5
Title : Crystal Structure of Human Microsomal P450 2A6 N297Q
Authors : Sansen, S.; Hsu, M.H.; Stout, C.D.; Johnson, E.F.
Deposited on : 2007-04-06
Resolution : 1.95 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)
Xtrriage (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

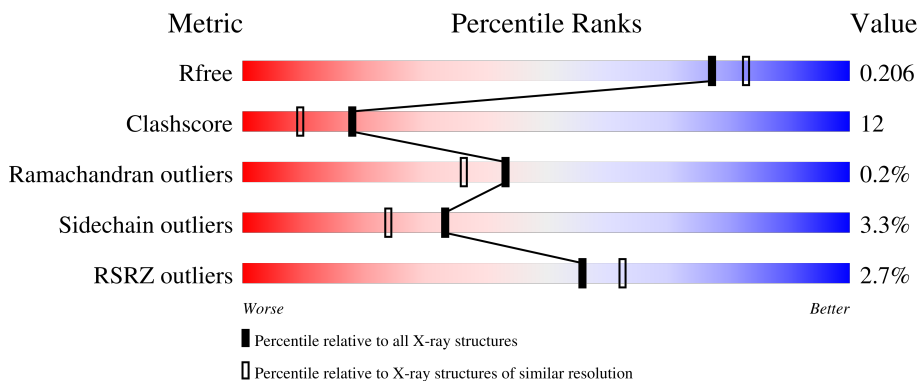
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	476	 76% 19% . .
1	B	476	 67% 26% . .
1	C	476	 75% 20% . .
1	D	476	 70% 25% . .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15846 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 2A6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	464	3752	2409	648	677	18	0	0	0
1	B	464	3758	2413	650	677	18	0	0	0
1	C	463	3748	2407	647	676	18	0	0	0
1	D	464	3752	2409	648	677	18	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

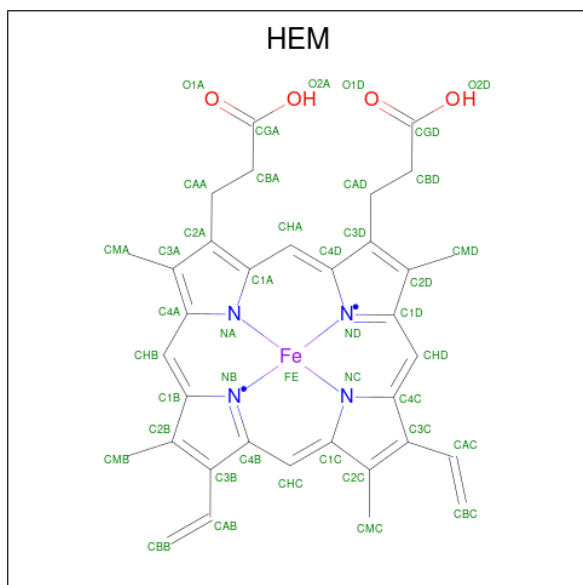
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	cloning artifact	UNP P11509
A	24	ALA	-	cloning artifact	UNP P11509
A	25	LYS	-	cloning artifact	UNP P11509
A	26	LYS	-	cloning artifact	UNP P11509
A	27	THR	-	cloning artifact	UNP P11509
A	28	SER	-	cloning artifact	UNP P11509
A	160	LEU	HIS	variant	UNP P11509
A	297	GLN	ASN	engineered mutation	UNP P11509
A	495	HIS	-	expression tag	UNP P11509
A	496	HIS	-	expression tag	UNP P11509
A	497	HIS	-	expression tag	UNP P11509
A	498	HIS	-	expression tag	UNP P11509
B	23	MET	-	cloning artifact	UNP P11509
B	24	ALA	-	cloning artifact	UNP P11509
B	25	LYS	-	cloning artifact	UNP P11509
B	26	LYS	-	cloning artifact	UNP P11509
B	27	THR	-	cloning artifact	UNP P11509
B	28	SER	-	cloning artifact	UNP P11509
B	160	LEU	HIS	variant	UNP P11509
B	297	GLN	ASN	engineered mutation	UNP P11509
B	495	HIS	-	expression tag	UNP P11509

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Chain	Residue	Modelled	Actual	Comment	Reference
B	496	HIS	-	expression tag	UNP P11509
B	497	HIS	-	expression tag	UNP P11509
B	498	HIS	-	expression tag	UNP P11509
C	23	MET	-	cloning artifact	UNP P11509
C	24	ALA	-	cloning artifact	UNP P11509
C	25	LYS	-	cloning artifact	UNP P11509
C	26	LYS	-	cloning artifact	UNP P11509
C	27	THR	-	cloning artifact	UNP P11509
C	28	SER	-	cloning artifact	UNP P11509
C	160	LEU	HIS	variant	UNP P11509
C	297	GLN	ASN	engineered mutation	UNP P11509
C	495	HIS	-	expression tag	UNP P11509
C	496	HIS	-	expression tag	UNP P11509
C	497	HIS	-	expression tag	UNP P11509
C	498	HIS	-	expression tag	UNP P11509
D	23	MET	-	cloning artifact	UNP P11509
D	24	ALA	-	cloning artifact	UNP P11509
D	25	LYS	-	cloning artifact	UNP P11509
D	26	LYS	-	cloning artifact	UNP P11509
D	27	THR	-	cloning artifact	UNP P11509
D	28	SER	-	cloning artifact	UNP P11509
D	160	LEU	HIS	variant	UNP P11509
D	297	GLN	ASN	engineered mutation	UNP P11509
D	495	HIS	-	expression tag	UNP P11509
D	496	HIS	-	expression tag	UNP P11509
D	497	HIS	-	expression tag	UNP P11509
D	498	HIS	-	expression tag	UNP P11509

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



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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

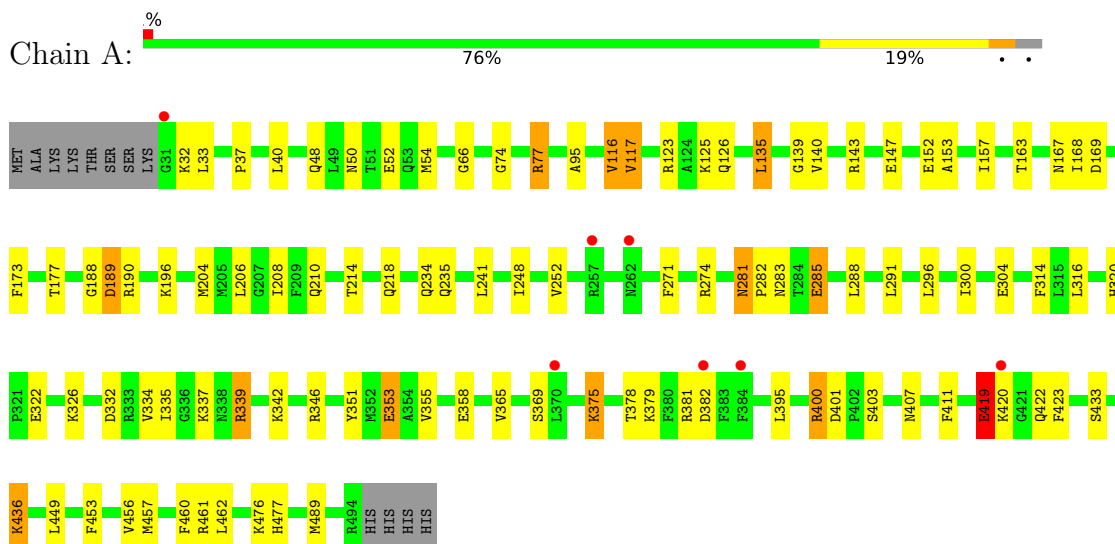
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	158	Total O 158 158	0	0
4	B	134	Total O 134 134	0	0
4	C	201	Total O 201 201	0	0
4	D	155	Total O 155 155	0	0

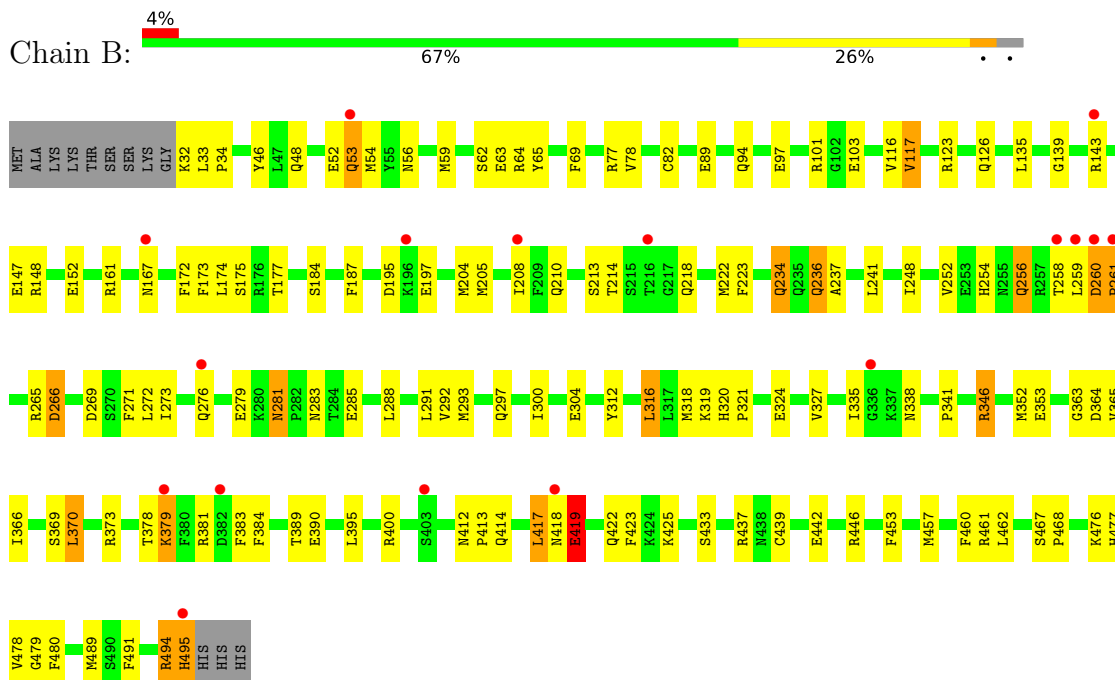
3 Residue-property plots [i](#)

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.

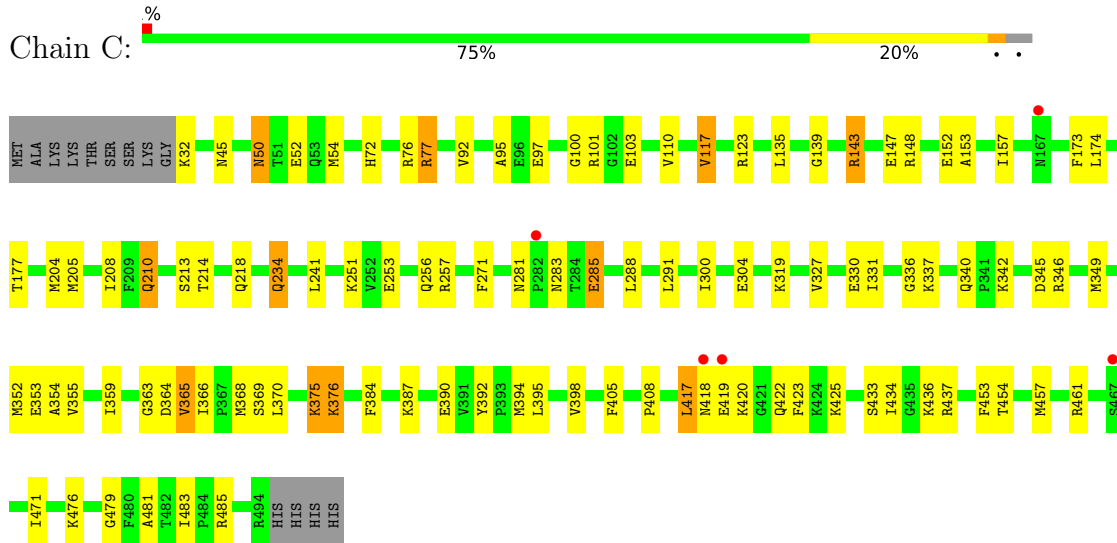
• Molecule 1: Cytochrome P450 2A6



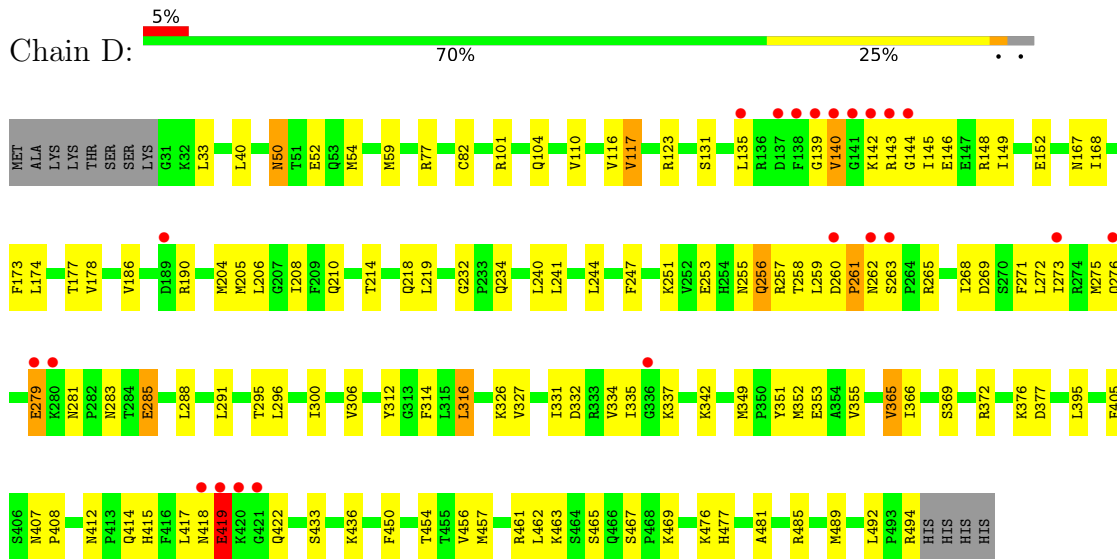
• Molecule 1: Cytochrome P450 2A6



• Molecule 1: Cytochrome P450 2A6



• Molecule 1: Cytochrome P450 2A6



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.85Å 157.97Å 103.74Å 90.00° 92.23° 90.00°	Depositor
Resolution (Å)	35.00 – 1.95 35.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.7 (35.00-1.95) 98.7 (35.00-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 1.95Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.215 , 0.239 0.208 , 0.206	Depositor DCC
R_{free} test set	8204 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtrriage
Anisotropy	0.425	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15846	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, 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	0.43	0/3843	0.97	24/5176 (0.5%)
1	B	0.43	0/3850	0.97	19/5186 (0.4%)
1	C	0.44	0/3839	0.95	13/5171 (0.3%)
1	D	0.44	0/3843	0.95	13/5176 (0.3%)
All	All	0.44	0/15375	0.96	69/20709 (0.3%)

There are no bond length outliers.

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	494	ARG	N-CA-C	-11.55	98.57	112.89
1	C	419	GLU	N-CA-C	-10.37	100.03	112.89
1	D	419	GLU	N-CA-C	-8.48	101.54	112.23
1	A	436	LYS	N-CA-C	7.73	119.71	111.28
1	B	173	PHE	N-CA-C	-7.68	102.84	111.14
1	D	117	VAL	N-CA-C	7.02	117.78	110.62
1	C	365	VAL	N-CA-C	6.94	117.70	110.62
1	D	365	VAL	N-CA-C	6.81	118.39	110.62
1	C	288	LEU	N-CA-C	6.80	119.28	111.11
1	B	419	GLU	N-CA-C	-6.79	104.46	112.89
1	D	335	ILE	N-CA-C	6.79	118.11	111.67
1	C	461	ARG	N-CA-C	-6.76	98.90	109.72
1	A	190	ARG	N-CA-C	6.68	119.57	110.55
1	B	461	ARG	N-CA-C	-6.56	99.52	109.95
1	D	436	LYS	N-CA-C	6.43	120.39	112.54
1	A	334	VAL	N-CA-C	6.42	116.56	110.53
1	A	461	ARG	N-CA-C	-6.37	99.82	109.95
1	D	461	ARG	N-CA-C	-6.25	100.02	109.95
1	A	407	ASN	CA-C-N	6.05	126.48	119.47
1	A	407	ASN	C-N-CA	6.05	126.48	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	366	ILE	CA-C-N	6.04	126.48	119.47
1	D	366	ILE	C-N-CA	6.04	126.48	119.47
1	A	320	HIS	CA-C-N	5.99	126.15	119.32
1	A	320	HIS	C-N-CA	5.99	126.15	119.32
1	A	117	VAL	N-CA-C	5.99	116.16	110.53
1	C	370	LEU	N-CA-C	-5.94	99.50	109.07
1	B	139	GLY	N-CA-C	5.92	121.74	114.69
1	C	398	VAL	N-CA-C	-5.92	105.94	111.45
1	D	104	GLN	N-CA-C	-5.91	96.04	107.44
1	A	116	VAL	N-CA-C	5.90	117.34	110.62
1	B	366	ILE	CA-C-N	5.90	126.04	119.32
1	B	366	ILE	C-N-CA	5.90	126.04	119.32
1	D	173	PHE	N-CA-C	-5.87	104.96	111.36
1	B	304	GLU	N-CA-C	5.86	117.75	111.36
1	A	335	ILE	N-CA-C	5.84	116.84	111.81
1	A	288	LEU	N-CA-C	5.84	118.11	111.11
1	A	173	PHE	N-CA-C	-5.78	104.90	111.14
1	A	365	VAL	N-CA-C	5.75	117.17	110.62
1	A	169	ASP	N-CA-C	-5.73	101.27	109.24
1	A	419	GLU	N-CA-C	5.70	117.30	111.14
1	A	74	GLY	N-CA-C	-5.68	100.75	112.34
1	B	365	VAL	N-CA-C	5.67	117.08	110.62
1	A	66	GLY	CA-C-N	5.66	125.34	119.56
1	A	66	GLY	C-N-CA	5.66	125.34	119.56
1	C	366	ILE	CA-C-N	5.64	126.01	119.47
1	C	366	ILE	C-N-CA	5.64	126.01	119.47
1	D	285	GLU	N-CA-C	-5.61	106.11	113.17
1	D	219	LEU	N-CA-C	-5.54	105.32	111.36
1	B	266	ASP	N-CA-C	5.53	115.42	108.45
1	B	117	VAL	N-CA-C	5.46	115.67	110.53
1	C	117	VAL	N-CA-C	5.42	116.19	110.72
1	B	288	LEU	N-CA-C	5.38	120.25	111.37
1	D	334	VAL	N-CA-C	5.38	116.86	111.00
1	A	139	GLY	N-CA-C	5.38	121.91	114.92
1	C	139	GLY	N-CA-C	5.36	121.06	114.69
1	C	173	PHE	N-CA-C	-5.35	105.45	111.28
1	A	339	ARG	N-CA-C	5.31	117.72	110.55
1	A	304	GLU	N-CA-C	5.30	117.06	111.28
1	C	304	GLU	N-CA-C	5.30	117.97	111.82
1	A	285	GLU	N-CA-C	-5.28	106.52	113.17
1	B	279	GLU	N-CA-C	5.23	118.45	111.75
1	B	116	VAL	N-CA-C	5.23	115.95	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	285	GLU	N-CA-C	-5.20	106.61	113.17
1	B	320	HIS	CA-C-N	5.20	125.50	119.47
1	B	320	HIS	C-N-CA	5.20	125.50	119.47
1	B	338	ASN	N-CA-C	5.17	118.62	112.72
1	A	460	PHE	N-CA-C	5.11	116.95	109.24
1	B	223	PHE	N-CA-C	5.10	119.06	111.87
1	B	78	VAL	N-CA-C	5.07	115.20	108.11

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	3752	0	3736	72	0
1	B	3758	0	3740	106	0
1	C	3748	0	3733	87	0
1	D	3752	0	3736	105	0
2	A	43	0	30	3	0
2	B	43	0	30	4	0
2	C	43	0	30	4	0
2	D	43	0	30	3	0
3	A	4	0	6	0	0
3	B	4	0	6	0	0
3	C	4	0	6	0	0
3	D	4	0	6	0	0
4	A	158	0	0	5	0
4	B	134	0	0	4	1
4	C	201	0	0	4	1
4	D	155	0	0	2	0
All	All	15846	0	15089	370	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (370) 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:418:ASN:HD22	1:C:422:GLN:HB2	1.14	1.11
1:B:234:GLN:H	1:B:234:GLN:HE21	1.02	0.97
1:C:45:ASN:HD22	1:C:72:HIS:H	1.02	0.95
1:D:457:MET:HE1	1:D:462:LEU:HD21	1.48	0.93
1:A:54:MET:HG3	1:A:218:GLN:HE21	1.32	0.91
1:C:234:GLN:H	1:C:234:GLN:HE21	1.12	0.91
1:C:375:LYS:HB3	1:C:376:LYS:HE2	1.53	0.90
1:D:259:LEU:HD11	1:D:273:ILE:HD11	1.54	0.90
1:D:142:LYS:HG3	1:D:144:GLY:H	1.38	0.89
1:C:392:TYR:HB3	1:C:394:MET:HE3	1.54	0.89
1:A:457:MET:HE1	1:A:462:LEU:HD21	1.56	0.88
1:B:236:GLN:HG2	4:B:619:HOH:O	1.73	0.88
1:C:32:LYS:HB3	1:C:384:PHE:HB3	1.54	0.87
1:C:77:ARG:HH11	1:C:77:ARG:HG2	1.39	0.87
1:A:314:PHE:HE2	1:A:457:MET:HE3	1.40	0.87
1:B:54:MET:HG3	1:B:218:GLN:HE21	1.43	0.84
1:B:234:GLN:H	1:B:234:GLN:NE2	1.75	0.84
1:A:32:LYS:HD2	1:A:33:LEU:H	1.42	0.84
1:D:54:MET:HG3	1:D:218:GLN:HE21	1.44	0.83
1:C:97:GLU:HG3	4:C:562:HOH:O	1.80	0.81
1:B:318:MET:HE1	1:B:489:MET:HB2	1.62	0.81
1:C:45:ASN:HD22	1:C:72:HIS:N	1.81	0.78
1:C:352:MET:HE3	1:C:454:THR:HG22	1.66	0.77
1:A:143:ARG:O	1:A:147:GLU:HG2	1.85	0.77
1:A:419:GLU:HA	1:A:419:GLU:OE1	1.84	0.76
1:C:143:ARG:NE	1:C:147:GLU:HG3	2.00	0.76
1:A:77:ARG:HG2	1:A:77:ARG:HH11	1.51	0.76
1:D:186:VAL:HG11	1:D:295:THR:HG23	1.65	0.76
1:B:234:GLN:HE21	1:B:234:GLN:N	1.83	0.76
1:C:418:ASN:HB2	1:C:422:GLN:H	1.49	0.76
1:B:64:ARG:HG2	1:B:64:ARG:HH11	1.50	0.76
1:C:32:LYS:HE2	1:C:384:PHE:HB2	1.68	0.75
1:B:161:ARG:HG3	1:B:161:ARG:HH11	1.51	0.75
1:D:101:ARG:HD3	1:D:117:VAL:O	1.87	0.75
1:A:339:ARG:NH1	1:A:342:LYS:HZ3	1.86	0.74
1:A:314:PHE:CE2	1:A:457:MET:HE3	2.22	0.73
1:C:418:ASN:ND2	1:C:422:GLN:HB2	1.98	0.73
1:D:352:MET:HE3	1:D:454:THR:HG22	1.70	0.72
1:D:314:PHE:HE2	1:D:457:MET:HE3	1.55	0.72
1:B:318:MET:HE3	1:B:489:MET:HE3	1.72	0.71
1:D:50:ASN:HD22	1:D:50:ASN:C	1.99	0.70
1:B:32:LYS:HG2	1:B:384:PHE:HB2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:GLN:H	1:C:234:GLN:NE2	1.90	0.69
1:C:123:ARG:HA	1:C:285:GLU:HG3	1.75	0.69
1:B:205:MET:HE2	1:B:300:ILE:HA	1.74	0.69
1:D:261:PRO:HA	1:D:273:ILE:HD12	1.75	0.69
1:A:337:LYS:HD2	1:A:337:LYS:N	2.09	0.68
1:D:419:GLU:H	1:D:419:GLU:CD	2.01	0.68
1:D:256:GLN:HE22	1:D:272:LEU:CD2	2.06	0.68
1:D:457:MET:HE2	1:D:457:MET:HA	1.75	0.68
1:D:208:ILE:HD11	1:D:240:LEU:HB2	1.76	0.68
1:B:423:PHE:HE1	1:B:425:LYS:HG2	1.59	0.67
1:B:210:GLN:HE21	1:B:477:HIS:HD2	1.39	0.67
1:A:456:VAL:HG12	1:A:457:MET:HE2	1.76	0.66
1:B:33:LEU:HD12	1:B:34:PRO:HD2	1.76	0.66
1:C:368:MET:HB3	1:C:394:MET:HE1	1.78	0.65
1:D:50:ASN:ND2	1:D:52:GLU:H	1.93	0.65
1:D:167:ASN:HD21	1:D:465:SER:HB3	1.62	0.64
1:C:392:TYR:HB3	1:C:394:MET:CE	2.27	0.64
1:C:205:MET:HE2	1:C:300:ILE:HG12	1.78	0.64
1:A:339:ARG:NH1	1:A:342:LYS:NZ	2.45	0.64
1:B:318:MET:HE3	1:B:462:LEU:HB3	1.79	0.64
1:C:423:PHE:HE1	1:C:425:LYS:HG2	1.62	0.64
1:C:418:ASN:HB3	1:C:420:LYS:H	1.63	0.64
1:B:77:ARG:HH12	1:B:389:THR:HG23	1.62	0.64
1:C:45:ASN:ND2	1:C:72:HIS:H	1.86	0.63
1:C:205:MET:HE2	1:C:300:ILE:CG1	2.28	0.63
1:D:256:GLN:HE22	1:D:272:LEU:HD22	1.62	0.63
1:A:353:GLU:HG2	1:A:423:PHE:CD2	2.34	0.63
1:D:205:MET:HE2	1:D:300:ILE:HA	1.79	0.63
1:D:256:GLN:HA	1:D:256:GLN:HE21	1.62	0.63
1:A:420:LYS:HG3	1:A:422:GLN:NE2	2.12	0.63
1:C:50:ASN:C	1:C:50:ASN:HD22	2.06	0.63
1:B:77:ARG:HG2	1:B:77:ARG:HH11	1.62	0.63
1:B:204:MET:O	1:B:208:ILE:HG13	1.98	0.63
1:B:259:LEU:HD21	1:B:273:ILE:HD13	1.81	0.62
1:B:210:GLN:HE21	1:B:477:HIS:CD2	2.17	0.62
1:A:420:LYS:CG	1:A:422:GLN:HE21	2.13	0.62
1:D:253:GLU:HG2	1:D:257:ARG:HH21	1.64	0.62
1:B:101:ARG:HD3	1:B:117:VAL:O	2.00	0.61
1:B:254:HIS:O	1:B:258:THR:HG22	2.00	0.61
1:C:54:MET:HG3	1:C:218:GLN:HE21	1.66	0.61
1:A:281:ASN:C	1:A:281:ASN:HD22	2.08	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:372:ARG:NH2	4:D:570:HOH:O	2.32	0.61
1:B:33:LEU:HD12	1:B:34:PRO:CD	2.31	0.61
1:B:346:ARG:HD2	1:B:353:GLU:OE2	2.01	0.61
1:D:247:PHE:O	1:D:251:LYS:HG2	2.00	0.61
1:B:281:ASN:C	1:B:281:ASN:HD22	2.09	0.60
1:C:257:ARG:HH11	1:C:257:ARG:HG2	1.65	0.60
1:B:101:ARG:NH2	1:B:370:LEU:HB3	2.17	0.60
1:A:123:ARG:HA	1:A:285:GLU:HG3	1.83	0.60
1:C:375:LYS:CB	1:C:376:LYS:HE2	2.29	0.60
1:A:188:GLY:O	1:A:189:ASP:HB3	2.00	0.60
1:D:204:MET:O	1:D:208:ILE:HG12	2.02	0.60
1:A:476:LYS:HE2	1:A:477:HIS:NE2	2.18	0.59
1:A:77:ARG:HG2	1:A:77:ARG:NH1	2.15	0.59
1:B:148:ARG:HH11	1:B:184:SER:HB3	1.67	0.59
1:D:281:ASN:ND2	1:D:283:ASN:H	2.01	0.59
1:A:346:ARG:HD2	1:A:353:GLU:OE1	2.02	0.59
1:C:77:ARG:HG2	1:C:77:ARG:NH1	2.10	0.59
1:B:46:TYR:HA	1:B:222:MET:HE1	1.85	0.58
1:A:339:ARG:CZ	1:A:342:LYS:HZ3	2.16	0.58
1:C:50:ASN:ND2	1:C:52:GLU:H	2.01	0.58
1:C:234:GLN:HE21	1:C:234:GLN:N	1.93	0.58
1:C:394:MET:HA	1:C:394:MET:HE2	1.85	0.58
1:B:59:MET:HE1	1:B:82:CYS:SG	2.44	0.58
1:C:210:GLN:NE2	4:C:617:HOH:O	2.37	0.58
1:D:456:VAL:HG12	1:D:457:MET:CE	2.33	0.58
1:B:423:PHE:CE1	1:B:425:LYS:HG2	2.38	0.57
1:D:117:VAL:HG22	2:D:500:HEM:HAD1	1.85	0.57
1:D:186:VAL:CG1	1:D:295:THR:HG23	2.33	0.57
1:C:253:GLU:HA	1:C:256:GLN:HE21	1.69	0.56
1:A:37:PRO:HB2	1:A:48:GLN:NE2	2.20	0.56
1:C:152:GLU:HG3	1:C:177:THR:HG23	1.87	0.56
1:A:369:SER:HB2	1:A:395:LEU:HG	1.88	0.56
1:D:206:LEU:HD12	4:D:647:HOH:O	2.06	0.56
1:C:103:GLU:HG2	1:C:390:GLU:OE2	2.05	0.56
1:D:261:PRO:HA	1:D:273:ILE:CD1	2.35	0.55
1:B:53:GLN:OE1	1:B:56:ASN:N	2.19	0.55
1:D:269:ASP:O	1:D:273:ILE:HG12	2.07	0.55
1:A:339:ARG:CZ	1:A:342:LYS:NZ	2.70	0.55
1:D:418:ASN:HD22	1:D:422:GLN:HB2	1.70	0.55
1:B:161:ARG:HG3	1:B:161:ARG:NH1	2.16	0.55
1:A:135:LEU:HG	1:A:140:VAL:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:433:SER:HB3	2:C:500:HEM:HBA1	1.90	0.54
1:B:143:ARG:O	1:B:147:GLU:HG3	2.08	0.54
1:A:117:VAL:HG22	2:A:500:HEM:HAD1	1.90	0.54
1:D:101:ARG:CD	1:D:117:VAL:O	2.56	0.54
1:D:50:ASN:C	1:D:50:ASN:ND2	2.66	0.54
1:C:117:VAL:HG22	2:C:500:HEM:HAD1	1.89	0.54
1:A:400:ARG:HB2	1:A:400:ARG:HH11	1.72	0.53
1:B:494:ARG:O	1:B:495:HIS:HB2	2.08	0.53
1:C:32:LYS:HE2	1:C:384:PHE:CB	2.38	0.53
1:D:50:ASN:HD22	1:D:52:GLU:H	1.54	0.53
1:D:412:ASN:HD21	1:D:414:GLN:HB2	1.72	0.53
1:B:281:ASN:C	1:B:281:ASN:ND2	2.66	0.53
1:A:50:ASN:ND2	1:A:52:GLU:H	2.07	0.53
1:C:369:SER:HB2	1:C:395:LEU:HG	1.89	0.53
1:B:89:GLU:CD	1:B:381:ARG:HH21	2.16	0.53
1:B:379:LYS:HD3	1:B:383:PHE:O	2.09	0.53
1:D:407:ASN:H	1:D:415:HIS:HE1	1.55	0.53
1:A:433:SER:HB3	2:A:500:HEM:HBA1	1.91	0.52
1:B:64:ARG:HG2	1:B:64:ARG:NH1	2.22	0.52
1:B:269:ASP:O	1:B:273:ILE:HG12	2.10	0.52
1:B:369:SER:HB2	1:B:395:LEU:HG	1.91	0.52
1:C:346:ARG:HG2	1:C:353:GLU:OE1	2.10	0.52
1:D:110:VAL:HG11	1:D:241:LEU:HD22	1.92	0.52
1:B:293:MET:O	1:B:297:GLN:HG3	2.09	0.52
1:D:450:PHE:O	1:D:454:THR:HG23	2.09	0.52
1:B:261:PRO:HA	1:B:273:ILE:HD12	1.92	0.52
1:B:489:MET:HE2	1:B:491:PHE:CZ	2.45	0.51
1:D:131:SER:O	1:D:135:LEU:HD13	2.10	0.51
1:D:271:PHE:HB3	1:D:291:LEU:HD13	1.92	0.51
1:D:271:PHE:CG	1:D:291:LEU:HD13	2.45	0.51
1:B:433:SER:HB3	2:B:500:HEM:HBA1	1.93	0.51
1:D:275:MET:HE3	1:D:288:LEU:N	2.25	0.51
1:A:50:ASN:C	1:A:50:ASN:HD22	2.17	0.51
1:A:196:LYS:HG3	4:A:613:HOH:O	2.11	0.51
1:B:123:ARG:HA	1:B:285:GLU:HG3	1.92	0.51
1:B:161:ARG:HG2	1:B:460:PHE:HZ	1.76	0.51
1:D:123:ARG:HA	1:D:285:GLU:HG3	1.93	0.51
1:D:433:SER:HB3	2:D:500:HEM:HBA1	1.93	0.51
1:B:281:ASN:ND2	1:B:283:ASN:H	2.08	0.51
1:C:210:GLN:HA	1:C:483:ILE:CD1	2.40	0.51
1:C:327:VAL:HG13	1:C:352:MET:HE2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:LYS:CG	1:A:422:GLN:NE2	2.73	0.51
1:B:442:GLU:O	1:B:446:ARG:HG2	2.10	0.51
1:B:53:GLN:HE21	1:B:478:VAL:HB	1.75	0.51
1:B:412:ASN:OD1	1:B:414:GLN:HB2	2.11	0.51
1:B:32:LYS:HG2	1:B:384:PHE:CB	2.40	0.51
1:D:256:GLN:HB3	1:D:257:ARG:NH1	2.26	0.51
1:D:467:SER:OG	1:D:469:LYS:HG2	2.11	0.50
1:B:62:SER:HB3	1:B:69:PHE:CE2	2.46	0.50
1:A:271:PHE:CD2	1:A:291:LEU:HB2	2.47	0.50
1:B:418:ASN:HD22	1:B:422:GLN:HB2	1.76	0.50
1:D:281:ASN:C	1:D:281:ASN:HD22	2.20	0.50
1:D:419:GLU:CD	1:D:419:GLU:N	2.69	0.50
1:B:259:LEU:HD11	1:B:273:ILE:HD11	1.92	0.50
1:D:276:GLN:O	1:D:279:GLU:HB2	2.12	0.50
1:A:33:LEU:HD21	1:A:77:ARG:NH1	2.26	0.50
1:B:205:MET:CE	1:B:300:ILE:HA	2.40	0.50
1:D:142:LYS:O	1:D:145:ILE:HG22	2.11	0.50
1:C:418:ASN:HB2	1:C:422:GLN:N	2.23	0.50
1:C:103:GLU:HG2	1:C:390:GLU:CD	2.37	0.49
1:D:232:GLY:HA3	1:D:234:GLN:HE22	1.77	0.49
1:D:376:LYS:O	1:D:377:ASP:C	2.55	0.49
1:B:258:THR:HG23	1:B:265:ARG:HH22	1.78	0.49
1:A:208:ILE:HD13	1:A:241:LEU:HD23	1.94	0.49
1:D:253:GLU:CG	1:D:257:ARG:HH21	2.26	0.49
1:D:457:MET:HE2	1:D:457:MET:CA	2.43	0.49
1:A:208:ILE:HD13	1:A:241:LEU:CD2	2.43	0.49
1:C:281:ASN:ND2	1:C:283:ASN:H	2.11	0.49
1:D:327:VAL:HG13	1:D:352:MET:HE2	1.95	0.49
1:B:195:ASP:OD1	1:B:195:ASP:C	2.56	0.49
1:B:261:PRO:HA	1:B:273:ILE:CD1	2.43	0.49
1:D:331:ILE:HG12	1:D:349:MET:HE1	1.95	0.49
1:D:351:TYR:O	1:D:355:VAL:HG23	2.13	0.49
1:A:32:LYS:HD2	1:A:33:LEU:N	2.19	0.48
1:B:318:MET:CE	1:B:489:MET:HB2	2.39	0.48
1:C:110:VAL:HG11	1:C:241:LEU:HD22	1.94	0.48
1:D:253:GLU:HG2	1:D:257:ARG:NH2	2.28	0.48
1:C:281:ASN:HD22	1:C:281:ASN:C	2.20	0.48
1:A:281:ASN:ND2	1:A:283:ASN:H	2.11	0.48
1:D:405:PHE:O	1:D:408:PRO:HD3	2.13	0.48
1:A:419:GLU:OE1	1:A:419:GLU:CA	2.58	0.48
1:D:210:GLN:O	1:D:214:THR:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:ASN:C	1:A:281:ASN:ND2	2.71	0.48
1:B:413:PRO:O	1:B:417:LEU:HD22	2.13	0.48
1:C:76:ARG:NH2	1:C:103:GLU:HG3	2.28	0.48
1:B:476:LYS:HE3	1:B:477:HIS:CD2	2.49	0.48
1:D:259:LEU:HD12	1:D:260:ASP:H	1.78	0.47
1:D:463:LYS:HD3	1:D:492:LEU:HD11	1.95	0.47
1:B:205:MET:HE2	1:B:300:ILE:CG1	2.44	0.47
1:C:355:VAL:O	1:C:359:ILE:HG13	2.14	0.47
1:D:260:ASP:O	1:D:262:ASN:N	2.47	0.47
1:D:418:ASN:ND2	1:D:422:GLN:HB2	2.29	0.47
1:B:259:LEU:HD12	1:B:260:ASP:H	1.79	0.47
1:B:97:GLU:OE1	1:B:378:THR:HG23	2.14	0.47
1:B:101:ARG:CD	1:B:117:VAL:O	2.63	0.47
1:B:319:LYS:C	1:B:321:PRO:HD3	2.40	0.47
1:D:268:ILE:O	1:D:272:LEU:HG	2.14	0.47
1:D:462:LEU:HD22	1:D:489:MET:HE1	1.96	0.47
1:B:77:ARG:HH11	1:B:77:ARG:CG	2.28	0.47
1:B:210:GLN:O	1:B:214:THR:HG23	2.15	0.47
1:B:400:ARG:NE	4:B:546:HOH:O	2.47	0.47
1:C:336:GLY:O	1:C:337:LYS:HG2	2.14	0.47
1:C:423:PHE:CE1	1:C:425:LYS:HG2	2.46	0.47
1:C:50:ASN:C	1:C:50:ASN:ND2	2.73	0.47
1:A:95:ALA:HB1	1:A:436:LYS:HG2	1.97	0.47
1:C:143:ARG:HD3	1:C:143:ARG:C	2.40	0.47
1:D:259:LEU:HD12	1:D:260:ASP:N	2.30	0.47
1:B:152:GLU:HG3	1:B:177:THR:HG23	1.96	0.46
1:A:381:ARG:O	1:A:382:ASP:HB2	2.15	0.46
1:B:419:GLU:CD	1:B:419:GLU:H	2.21	0.46
1:D:59:MET:HE1	1:D:82:CYS:SG	2.54	0.46
1:B:248:ILE:HG22	1:B:292:VAL:HG13	1.96	0.46
1:B:327:VAL:HG13	1:B:352:MET:CE	2.45	0.46
1:A:50:ASN:ND2	1:A:50:ASN:C	2.74	0.46
1:B:292:VAL:HG12	1:B:293:MET:HE2	1.98	0.46
1:C:153:ALA:O	1:C:157:ILE:HG12	2.15	0.46
1:D:33:LEU:HD11	1:D:77:ARG:NH1	2.30	0.46
1:C:204:MET:O	1:C:208:ILE:HG13	2.15	0.46
1:A:375:LYS:HE2	4:A:606:HOH:O	2.14	0.46
1:D:259:LEU:HD11	1:D:273:ILE:CD1	2.36	0.46
1:B:467:SER:O	1:B:468:PRO:C	2.59	0.46
1:D:312:TYR:O	1:D:316:LEU:HD22	2.16	0.46
1:C:50:ASN:HD22	1:C:52:GLU:H	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:ILE:HD13	1:B:341:PRO:HG3	1.99	0.45
1:C:271:PHE:CD2	1:C:291:LEU:HB2	2.50	0.45
1:D:253:GLU:CG	1:D:257:ARG:NH2	2.80	0.45
1:B:94:GLN:NE2	4:B:623:HOH:O	2.48	0.45
1:B:271:PHE:CG	1:B:291:LEU:HD13	2.51	0.45
1:D:281:ASN:ND2	1:D:281:ASN:C	2.73	0.45
1:D:326:LYS:HD2	1:D:351:TYR:CZ	2.52	0.45
1:A:462:LEU:HD22	1:A:489:MET:HE1	1.97	0.45
1:B:248:ILE:CG2	1:B:292:VAL:HG13	2.47	0.45
1:B:272:LEU:O	1:B:276:GLN:HG3	2.16	0.45
1:A:449:LEU:O	1:A:453:PHE:HB2	2.16	0.45
1:D:369:SER:HB2	1:D:395:LEU:HG	1.98	0.45
1:A:116:VAL:HG13	1:A:117:VAL:N	2.31	0.45
1:D:208:ILE:HD12	1:D:241:LEU:HG	1.97	0.45
1:D:332:ASP:CG	1:D:494:ARG:HH22	2.23	0.45
1:D:271:PHE:CB	1:D:291:LEU:HD13	2.46	0.45
1:D:152:GLU:HG3	1:D:177:THR:HG23	1.99	0.44
1:C:92:VAL:HG23	1:C:434:ILE:HD12	1.99	0.44
1:C:95:ALA:HB1	1:C:436:LYS:HD3	1.99	0.44
1:B:172:PHE:HA	1:B:175:SER:OG	2.16	0.44
1:B:324:GLU:HG3	1:B:457:MET:CE	2.47	0.44
1:C:210:GLN:O	1:C:214:THR:HG23	2.18	0.44
1:C:375:LYS:HD2	1:C:375:LYS:HA	1.81	0.44
1:A:332:ASP:OD1	1:A:337:LYS:HE3	2.18	0.44
1:C:437:ARG:HE	2:C:500:HEM:CGD	2.31	0.44
1:D:234:GLN:NE2	1:D:234:GLN:H	2.15	0.44
1:A:433:SER:CB	2:A:500:HEM:HBA1	2.48	0.44
1:B:208:ILE:HD13	1:B:241:LEU:CD2	2.47	0.44
1:C:405:PHE:O	1:C:408:PRO:HD3	2.17	0.44
1:D:259:LEU:HD21	1:D:273:ILE:HD13	1.99	0.44
1:D:433:SER:CB	2:D:500:HEM:HBA1	2.46	0.44
1:C:76:ARG:CZ	1:C:103:GLU:HG3	2.47	0.44
1:C:100:GLY:HA2	1:C:375:LYS:HE2	1.98	0.44
1:A:420:LYS:HB2	1:A:422:GLN:HE21	1.83	0.44
1:A:125:LYS:HD2	4:A:530:HOH:O	2.18	0.44
1:A:358:GLU:HG3	1:A:411:PHE:CD1	2.53	0.43
1:A:378:THR:HG22	1:A:379:LYS:N	2.33	0.43
1:A:204:MET:O	1:A:208:ILE:HG13	2.19	0.43
1:C:453:PHE:O	1:C:457:MET:HG2	2.17	0.43
1:D:365:VAL:O	1:D:481:ALA:HA	2.18	0.43
1:A:210:GLN:O	1:A:214:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:VAL:O	1:C:481:ALA:HA	2.18	0.43
1:B:53:GLN:NE2	1:B:478:VAL:HB	2.33	0.43
1:B:64:ARG:HH11	1:B:64:ARG:CG	2.25	0.43
1:B:103:GLU:HG2	1:B:390:GLU:OE2	2.19	0.43
1:C:354:ALA:HB2	1:C:417:LEU:HD13	1.99	0.43
1:D:273:ILE:O	1:D:276:GLN:HB2	2.18	0.43
1:D:476:LYS:HB2	1:D:485:ARG:HA	2.00	0.43
1:A:271:PHE:HB3	1:A:291:LEU:HD13	1.99	0.43
1:D:143:ARG:HA	1:D:146:GLU:HB3	2.01	0.43
1:D:168:ILE:C	1:D:168:ILE:HD12	2.43	0.43
1:D:210:GLN:HE21	1:D:477:HIS:HD2	1.67	0.43
1:A:351:TYR:O	1:A:355:VAL:HG23	2.19	0.43
1:B:370:LEU:HD12	1:B:480:PHE:HE1	1.83	0.43
1:D:178:VAL:HG11	1:D:306:VAL:HB	2.00	0.43
1:D:244:LEU:HB3	1:D:296:LEU:HD11	2.01	0.43
1:D:369:SER:HB2	1:D:395:LEU:CD1	2.49	0.43
1:D:258:THR:OG1	1:D:265:ARG:NH1	2.42	0.43
1:A:281:ASN:HD22	1:A:282:PRO:N	2.17	0.42
1:B:64:ARG:HD3	1:B:65:TYR:CE2	2.53	0.42
1:C:394:MET:HE2	1:C:394:MET:CA	2.49	0.42
1:C:52:GLU:O	1:C:52:GLU:HG2	2.19	0.42
1:B:97:GLU:HG3	4:B:533:HOH:O	2.19	0.42
1:C:143:ARG:HD3	1:C:143:ARG:O	2.18	0.42
1:C:213:SER:HA	1:C:479:GLY:HA3	2.02	0.42
1:D:476:LYS:HE2	1:D:477:HIS:NE2	2.34	0.42
1:D:148:ARG:NH2	1:D:190:ARG:HB3	2.34	0.42
1:B:205:MET:HE2	1:B:300:ILE:HG12	2.00	0.42
1:A:153:ALA:O	1:A:157:ILE:HG12	2.20	0.42
1:B:195:ASP:OD1	1:B:197:GLU:N	2.53	0.42
1:D:116:VAL:HG13	1:D:117:VAL:N	2.35	0.42
1:C:101:ARG:CD	1:C:117:VAL:O	2.68	0.42
1:C:327:VAL:O	1:C:331:ILE:HG13	2.19	0.42
1:A:206:LEU:HD12	4:A:592:HOH:O	2.18	0.42
1:B:161:ARG:HG2	1:B:460:PHE:CZ	2.53	0.42
1:B:236:GLN:HG3	1:B:237:ALA:N	2.33	0.42
1:C:257:ARG:HG2	1:C:257:ARG:NH1	2.32	0.42
1:A:126:GLN:NE2	4:A:571:HOH:O	2.52	0.41
1:A:152:GLU:HG3	1:A:177:THR:HG23	2.02	0.41
1:A:234:GLN:HG2	1:A:235:GLN:N	2.34	0.41
1:D:210:GLN:HE21	1:D:477:HIS:CD2	2.38	0.41
1:B:59:MET:O	1:B:63:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:ARG:NH1	1:B:400:ARG:HG3	2.34	0.41
1:B:312:TYR:O	1:B:316:LEU:HD22	2.20	0.41
1:D:148:ARG:HH21	1:D:190:ARG:HB3	1.84	0.41
1:A:322:GLU:OE2	1:A:322:GLU:N	2.34	0.41
1:D:255:ASN:HA	1:D:265:ARG:HH22	1.85	0.41
1:A:401:ASP:OD2	1:A:403:SER:HB3	2.20	0.41
1:C:281:ASN:ND2	1:C:281:ASN:C	2.78	0.41
1:C:476:LYS:HB2	1:C:485:ARG:HA	2.02	0.41
1:A:248:ILE:O	1:A:252:VAL:HG23	2.21	0.41
1:D:140:VAL:HA	1:D:145:ILE:HG21	2.02	0.41
1:D:145:ILE:O	1:D:149:ILE:HG13	2.21	0.41
1:D:412:ASN:ND2	1:D:414:GLN:HB2	2.33	0.41
1:B:439:CYS:HB2	2:B:500:HEM:NA	2.34	0.41
1:C:210:GLN:HA	1:C:483:ILE:HD12	2.03	0.41
1:C:375:LYS:O	1:C:387:LYS:HG3	2.20	0.41
1:D:342:LYS:HB2	1:D:342:LYS:HE3	1.85	0.41
1:D:260:ASP:C	1:D:262:ASN:N	2.79	0.41
1:A:296:LEU:HD11	1:A:300:ILE:HD11	2.03	0.41
1:B:77:ARG:CG	1:B:77:ARG:NH1	2.84	0.41
1:B:213:SER:HA	1:B:479:GLY:HA3	2.03	0.41
1:B:252:VAL:O	1:B:256:GLN:HG3	2.21	0.41
1:B:453:PHE:O	1:B:457:MET:HG2	2.21	0.41
1:C:101:ARG:HD2	1:C:117:VAL:O	2.20	0.41
1:C:330:GLU:OE1	1:C:349:MET:HB3	2.21	0.41
1:D:139:GLY:O	1:D:140:VAL:C	2.63	0.41
1:C:210:GLN:HG2	4:C:676:HOH:O	2.21	0.41
1:C:319:LYS:HD3	1:C:471:ILE:HB	2.03	0.41
1:A:274:ARG:HA	1:A:274:ARG:HD2	1.77	0.40
1:C:363:GLY:O	1:C:364:ASP:C	2.64	0.40
1:C:375:LYS:CE	4:C:585:HOH:O	2.68	0.40
1:B:363:GLY:O	1:B:364:ASP:C	2.64	0.40
1:B:187:PHE:C	1:B:266:ASP:OD2	2.64	0.40
1:B:346:ARG:HG2	1:B:353:GLU:CD	2.47	0.40
1:C:342:LYS:HG2	1:C:345:ASP:OD2	2.20	0.40
1:A:163:THR:HG21	1:A:168:ILE:HD13	2.02	0.40
1:A:326:LYS:HB2	1:A:351:TYR:CE2	2.56	0.40
1:A:420:LYS:CB	1:A:422:GLN:HE21	2.35	0.40
1:C:433:SER:CB	2:C:500:HEM:HBA1	2.51	0.40
1:D:208:ILE:CD1	1:D:240:LEU:HB2	2.48	0.40
1:B:433:SER:CB	2:B:500:HEM:HBA1	2.51	0.40
1:B:437:ARG:HE	2:B:500:HEM:CGD	2.34	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:609:HOH:O	4:C:671:HOH:O[1_554]	2.14	0.06

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	462/476 (97%)	448 (97%)	14 (3%)	0	100	100
1	B	462/476 (97%)	445 (96%)	16 (4%)	1 (0%)	43	36
1	C	461/476 (97%)	448 (97%)	13 (3%)	0	100	100
1	D	462/476 (97%)	442 (96%)	18 (4%)	2 (0%)	30	21
All	All	1847/1904 (97%)	1783 (96%)	61 (3%)	3 (0%)	43	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	140	VAL
1	D	261	PRO
1	B	261	PRO

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	411/422 (97%)	400 (97%)	11 (3%)	39	32
1	B	412/422 (98%)	392 (95%)	20 (5%)	22	11
1	C	411/422 (97%)	398 (97%)	13 (3%)	34	25
1	D	411/422 (97%)	400 (97%)	11 (3%)	39	32
All	All	1645/1688 (98%)	1590 (97%)	55 (3%)	33	24

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	77	ARG
1	A	135	LEU
1	A	167	ASN
1	A	189	ASP
1	A	281	ASN
1	A	316	LEU
1	A	353	GLU
1	A	375	LYS
1	A	400	ARG
1	A	419	GLU
1	B	48	GLN
1	B	52	GLU
1	B	53	GLN
1	B	126	GLN
1	B	135	LEU
1	B	167	ASN
1	B	174	LEU
1	B	234	GLN
1	B	236	GLN
1	B	256	GLN
1	B	260	ASP
1	B	281	ASN
1	B	316	LEU
1	B	346	ARG
1	B	370	LEU
1	B	373	ARG
1	B	379	LYS
1	B	417	LEU
1	B	419	GLU
1	B	495	HIS
1	C	50	ASN
1	C	77	ARG

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Mol	Chain	Res	Type
1	C	135	LEU
1	C	143	ARG
1	C	148	ARG
1	C	174	LEU
1	C	210	GLN
1	C	234	GLN
1	C	251	LYS
1	C	340	GLN
1	C	375	LYS
1	C	376	LYS
1	C	417	LEU
1	D	40	LEU
1	D	50	ASN
1	D	174	LEU
1	D	256	GLN
1	D	263	SER
1	D	279	GLU
1	D	316	LEU
1	D	337	LYS
1	D	353	GLU
1	D	417	LEU
1	D	419	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	53	GLN
1	A	56	ASN
1	A	126	GLN
1	A	218	GLN
1	A	276	GLN
1	A	281	ASN
1	A	283	ASN
1	A	407	ASN
1	A	422	GLN
1	B	48	GLN
1	B	50	ASN
1	B	72	HIS
1	B	94	GLN
1	B	126	GLN
1	B	167	ASN

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Mol	Chain	Res	Type
1	B	210	GLN
1	B	218	GLN
1	B	234	GLN
1	B	255	ASN
1	B	281	ASN
1	B	328	HIS
1	B	340	GLN
1	B	414	GLN
1	B	418	ASN
1	B	422	GLN
1	B	459	ASN
1	B	477	HIS
1	C	45	ASN
1	C	50	ASN
1	C	53	GLN
1	C	56	ASN
1	C	94	GLN
1	C	126	GLN
1	C	167	ASN
1	C	210	GLN
1	C	218	GLN
1	C	234	GLN
1	C	256	GLN
1	C	281	ASN
1	C	418	ASN
1	C	458	GLN
1	D	50	ASN
1	D	53	GLN
1	D	56	ASN
1	D	72	HIS
1	D	167	ASN
1	D	210	GLN
1	D	218	GLN
1	D	234	GLN
1	D	236	GLN
1	D	239	GLN
1	D	256	GLN
1	D	281	ASN
1	D	283	ASN
1	D	328	HIS
1	D	415	HIS
1	D	418	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](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	D	500	1,4	50,50,50	2.43	23 (46%)	67,82,82	1.37	12 (17%)
3	EDO	B	501	-	3,3,3	0.59	0	2,2,2	0.35	0
3	EDO	C	501	-	3,3,3	0.55	0	2,2,2	0.34	0
2	HEM	C	500	1,4	50,50,50	2.42	22 (44%)	67,82,82	1.39	11 (16%)
3	EDO	A	501	-	3,3,3	0.53	0	2,2,2	0.34	0
2	HEM	B	500	1,4	50,50,50	2.42	23 (46%)	67,82,82	1.35	13 (19%)
3	EDO	D	501	-	3,3,3	0.62	0	2,2,2	0.34	0
2	HEM	A	500	1,4	50,50,50	2.39	22 (44%)	67,82,82	1.38	12 (17%)

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	D	500	1,4	-	2/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	501	-	-	0/1/1/1	-
3	EDO	C	501	-	-	0/1/1/1	-
2	HEM	C	500	1,4	-	3/14/54/54	-
3	EDO	A	501	-	-	0/1/1/1	-
2	HEM	B	500	1,4	-	5/14/54/54	-
3	EDO	D	501	-	-	0/1/1/1	-
2	HEM	A	500	1,4	-	2/14/54/54	-

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	C1D-ND	-4.80	1.29	1.38
2	C	500	HEM	C1D-ND	-4.77	1.29	1.38
2	A	500	HEM	C1D-ND	-4.52	1.30	1.38
2	B	500	HEM	FE-ND	4.49	2.08	1.94
2	D	500	HEM	C1D-ND	-4.48	1.30	1.38
2	A	500	HEM	C1B-NB	-4.37	1.32	1.40
2	A	500	HEM	FE-ND	4.33	2.08	1.94
2	D	500	HEM	C4A-NA	-4.32	1.31	1.39
2	D	500	HEM	C1B-NB	-4.27	1.32	1.40
2	C	500	HEM	FE-ND	4.27	2.08	1.94
2	D	500	HEM	FE-ND	4.26	2.08	1.94
2	C	500	HEM	C4A-NA	-4.18	1.31	1.39
2	B	500	HEM	C1B-NB	-4.17	1.33	1.40
2	A	500	HEM	C4A-NA	-4.15	1.31	1.39
2	B	500	HEM	C1C-NC	-4.11	1.31	1.39
2	B	500	HEM	C4A-NA	-4.01	1.32	1.39
2	A	500	HEM	CAC-C3C	-4.01	1.36	1.47
2	C	500	HEM	C1C-NC	-4.00	1.32	1.39
2	A	500	HEM	FE-NB	3.93	2.07	1.94
2	A	500	HEM	C1C-NC	-3.93	1.32	1.39
2	C	500	HEM	C4D-ND	-3.91	1.33	1.40
2	B	500	HEM	CBB-CAB	3.90	1.49	1.30
2	D	500	HEM	FE-NB	3.90	2.06	1.94
2	D	500	HEM	CBB-CAB	3.87	1.49	1.30
2	A	500	HEM	C4D-ND	-3.84	1.33	1.40
2	D	500	HEM	CMA-C3A	3.83	1.58	1.50
2	D	500	HEM	C4D-ND	-3.83	1.33	1.40
2	C	500	HEM	C1B-NB	-3.82	1.33	1.40
2	B	500	HEM	FE-NB	3.80	2.06	1.94
2	D	500	HEM	C1C-NC	-3.78	1.32	1.39
2	A	500	HEM	CBB-CAB	3.77	1.48	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	CMA-C3A	3.72	1.58	1.50
2	C	500	HEM	FE-NB	3.71	2.06	1.94
2	C	500	HEM	CBB-CAB	3.70	1.48	1.30
2	D	500	HEM	CAC-C3C	-3.69	1.37	1.47
2	B	500	HEM	C4D-ND	-3.66	1.33	1.40
2	B	500	HEM	CAC-C3C	-3.63	1.37	1.47
2	C	500	HEM	C4B-NB	-3.62	1.31	1.38
2	B	500	HEM	C1C-C2C	-3.56	1.38	1.45
2	C	500	HEM	CAC-C3C	-3.56	1.37	1.47
2	B	500	HEM	FE-NA	3.53	2.06	1.95
2	A	500	HEM	C4B-NB	-3.52	1.31	1.38
2	C	500	HEM	CMA-C3A	3.51	1.58	1.50
2	C	500	HEM	FE-NA	3.51	2.06	1.95
2	B	500	HEM	C4B-NB	-3.46	1.32	1.38
2	D	500	HEM	C1C-C2C	-3.43	1.38	1.45
2	D	500	HEM	FE-NA	3.42	2.06	1.95
2	B	500	HEM	CMA-C3A	3.38	1.57	1.50
2	C	500	HEM	C1C-C2C	-3.32	1.38	1.45
2	A	500	HEM	FE-NA	3.21	2.05	1.95
2	D	500	HEM	C4B-NB	-3.17	1.32	1.38
2	D	500	HEM	CMC-C2C	3.11	1.57	1.50
2	A	500	HEM	C1C-C2C	-3.06	1.39	1.45
2	A	500	HEM	FE-NC	3.06	2.05	1.95
2	C	500	HEM	CMC-C2C	3.04	1.57	1.50
2	C	500	HEM	FE-NC	2.98	2.05	1.95
2	C	500	HEM	C3B-C2B	2.97	1.43	1.37
2	D	500	HEM	FE-NC	2.97	2.04	1.95
2	D	500	HEM	C3B-C2B	2.95	1.43	1.37
2	B	500	HEM	CMC-C2C	2.89	1.56	1.50
2	A	500	HEM	CMC-C2C	2.83	1.56	1.50
2	D	500	HEM	O2A-CGA	-2.74	1.21	1.30
2	B	500	HEM	FE-NC	2.73	2.04	1.95
2	B	500	HEM	O2A-CGA	-2.72	1.21	1.30
2	B	500	HEM	C4C-NC	-2.68	1.34	1.39
2	C	500	HEM	O2A-CGA	-2.65	1.22	1.30
2	C	500	HEM	C4C-NC	-2.64	1.34	1.39
2	D	500	HEM	C4C-NC	-2.60	1.34	1.39
2	A	500	HEM	C3B-C2B	2.49	1.42	1.37
2	D	500	HEM	C3C-C2C	2.49	1.42	1.37
2	D	500	HEM	C4D-C3D	-2.48	1.40	1.45
2	A	500	HEM	O2A-CGA	-2.46	1.22	1.30
2	C	500	HEM	CBC-CAC	2.46	1.42	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	CBC-CAC	2.42	1.42	1.30
2	D	500	HEM	CBC-CAC	2.40	1.41	1.30
2	A	500	HEM	CBC-CAC	2.37	1.41	1.30
2	B	500	HEM	C3B-C2B	2.37	1.42	1.37
2	A	500	HEM	C4C-NC	-2.35	1.35	1.39
2	B	500	HEM	C3C-C4C	-2.28	1.42	1.46
2	A	500	HEM	C4D-C3D	-2.27	1.41	1.45
2	A	500	HEM	CMD-C2D	2.27	1.55	1.50
2	B	500	HEM	CAD-C3D	2.21	1.57	1.51
2	C	500	HEM	C4D-C3D	-2.19	1.41	1.45
2	B	500	HEM	CBD-CGD	2.17	1.55	1.50
2	D	500	HEM	CMD-C2D	2.14	1.55	1.50
2	B	500	HEM	C4D-C3D	-2.13	1.41	1.45
2	C	500	HEM	C1D-C2D	-2.12	1.40	1.44
2	A	500	HEM	C1D-C2D	-2.10	1.40	1.44
2	D	500	HEM	C3C-C4C	-2.06	1.42	1.46
2	C	500	HEM	CAD-C3D	2.03	1.56	1.51

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	HEM	CHD-C4C-NC	-3.18	120.99	124.45
2	D	500	HEM	CHD-C4C-NC	-3.07	121.11	124.45
2	A	500	HEM	C3B-C4B-NB	3.01	111.63	109.47
2	A	500	HEM	CHD-C4C-NC	-2.96	121.23	124.45
2	D	500	HEM	C4B-C3B-C2B	-2.94	104.58	107.28
2	B	500	HEM	C3B-C4B-NB	2.88	111.54	109.47
2	A	500	HEM	C4B-C3B-C2B	-2.83	104.68	107.28
2	B	500	HEM	C4B-C3B-C2B	-2.82	104.69	107.28
2	C	500	HEM	C4B-C3B-C2B	-2.81	104.70	107.28
2	D	500	HEM	C3B-C4B-NB	2.75	111.44	109.47
2	A	500	HEM	C1C-CHC-C4B	2.73	131.82	126.02
2	C	500	HEM	C1C-CHC-C4B	2.73	131.81	126.02
2	D	500	HEM	C4C-C3C-C2C	-2.73	104.45	106.81
2	B	500	HEM	CHD-C4C-NC	-2.68	121.53	124.45
2	A	500	HEM	O2A-CGA-CBA	2.67	122.45	114.00
2	D	500	HEM	C1C-CHC-C4B	2.64	131.63	126.02
2	A	500	HEM	C3B-C2B-C1B	-2.59	104.47	106.41
2	C	500	HEM	C4D-ND-C1D	2.59	108.27	105.21
2	C	500	HEM	C3B-C2B-C1B	-2.59	104.47	106.41
2	D	500	HEM	C4D-ND-C1D	2.55	108.23	105.21
2	C	500	HEM	C4C-C3C-C2C	-2.55	104.60	106.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	HEM	C1B-NB-C4B	2.55	108.22	105.21
2	C	500	HEM	O2A-CGA-CBA	2.54	122.03	114.00
2	D	500	HEM	C3B-C2B-C1B	-2.51	104.53	106.41
2	D	500	HEM	O2A-CGA-CBA	2.48	121.85	114.00
2	B	500	HEM	C3B-C2B-C1B	-2.47	104.56	106.41
2	B	500	HEM	O2A-CGA-CBA	2.46	121.79	114.00
2	A	500	HEM	C4D-ND-C1D	2.46	108.12	105.21
2	B	500	HEM	C4D-ND-C1D	2.46	108.12	105.21
2	B	500	HEM	C1C-CHC-C4B	2.45	131.24	126.02
2	C	500	HEM	C3B-C4B-NB	2.45	111.23	109.47
2	B	500	HEM	C4C-C3C-C2C	-2.44	104.70	106.81
2	D	500	HEM	C1B-NB-C4B	2.43	108.08	105.21
2	A	500	HEM	C1B-NB-C4B	2.42	108.08	105.21
2	A	500	HEM	C4A-CHB-C1B	2.42	131.94	126.25
2	B	500	HEM	C4A-CHB-C1B	2.37	131.83	126.25
2	D	500	HEM	C4A-CHB-C1B	2.36	131.80	126.25
2	B	500	HEM	C4C-CHD-C1D	2.28	130.87	126.02
2	A	500	HEM	CHB-C1B-NB	-2.25	121.58	124.37
2	B	500	HEM	CHC-C1C-NC	-2.22	122.03	124.45
2	B	500	HEM	C1B-NB-C4B	2.20	107.82	105.21
2	A	500	HEM	C4C-C3C-C2C	-2.20	104.91	106.81
2	C	500	HEM	C4C-CHD-C1D	2.16	130.60	126.02
2	C	500	HEM	C4A-CHB-C1B	2.13	131.27	126.25
2	A	500	HEM	C4C-CHD-C1D	2.13	130.55	126.02
2	D	500	HEM	CHB-C1B-NB	-2.12	121.74	124.37
2	D	500	HEM	CHD-C4C-C3C	2.10	128.74	125.21
2	B	500	HEM	C4D-C3D-C2D	-2.02	103.96	106.89

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	HEM	C2C-C3C-CAC-CBC
2	B	500	HEM	C2C-C3C-CAC-CBC
2	A	500	HEM	C4C-C3C-CAC-CBC
2	B	500	HEM	C4C-C3C-CAC-CBC
2	C	500	HEM	C2C-C3C-CAC-CBC
2	C	500	HEM	C4C-C3C-CAC-CBC
2	B	500	HEM	CAA-CBA-CGA-O1A
2	D	500	HEM	CAA-CBA-CGA-O1A
2	B	500	HEM	CAD-CBD-CGD-O2D
2	B	500	HEM	CAA-CBA-CGA-O2A

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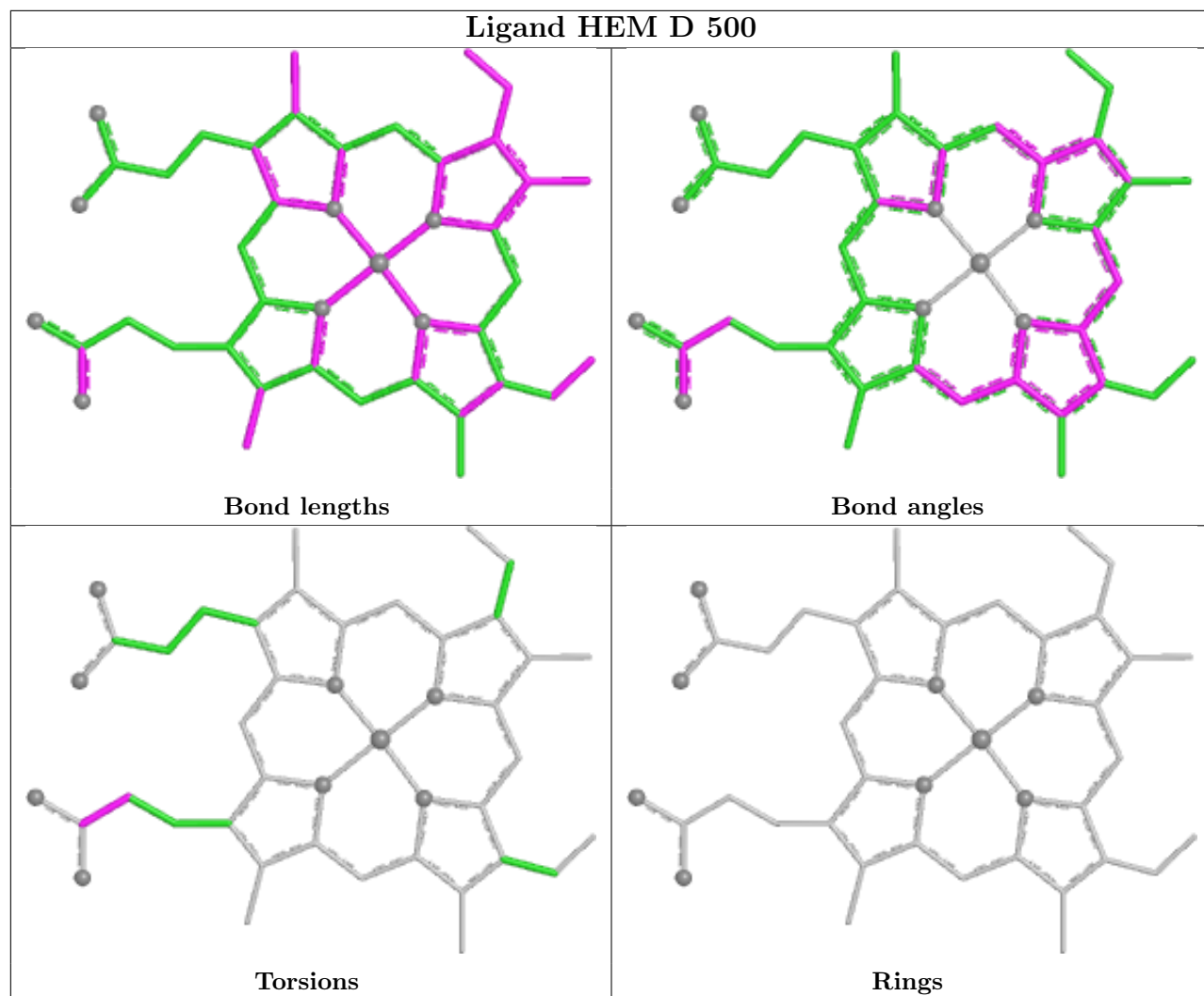
Mol	Chain	Res	Type	Atoms
2	C	500	HEM	CAD-CBD-CGD-O2D
2	D	500	HEM	CAA-CBA-CGA-O2A

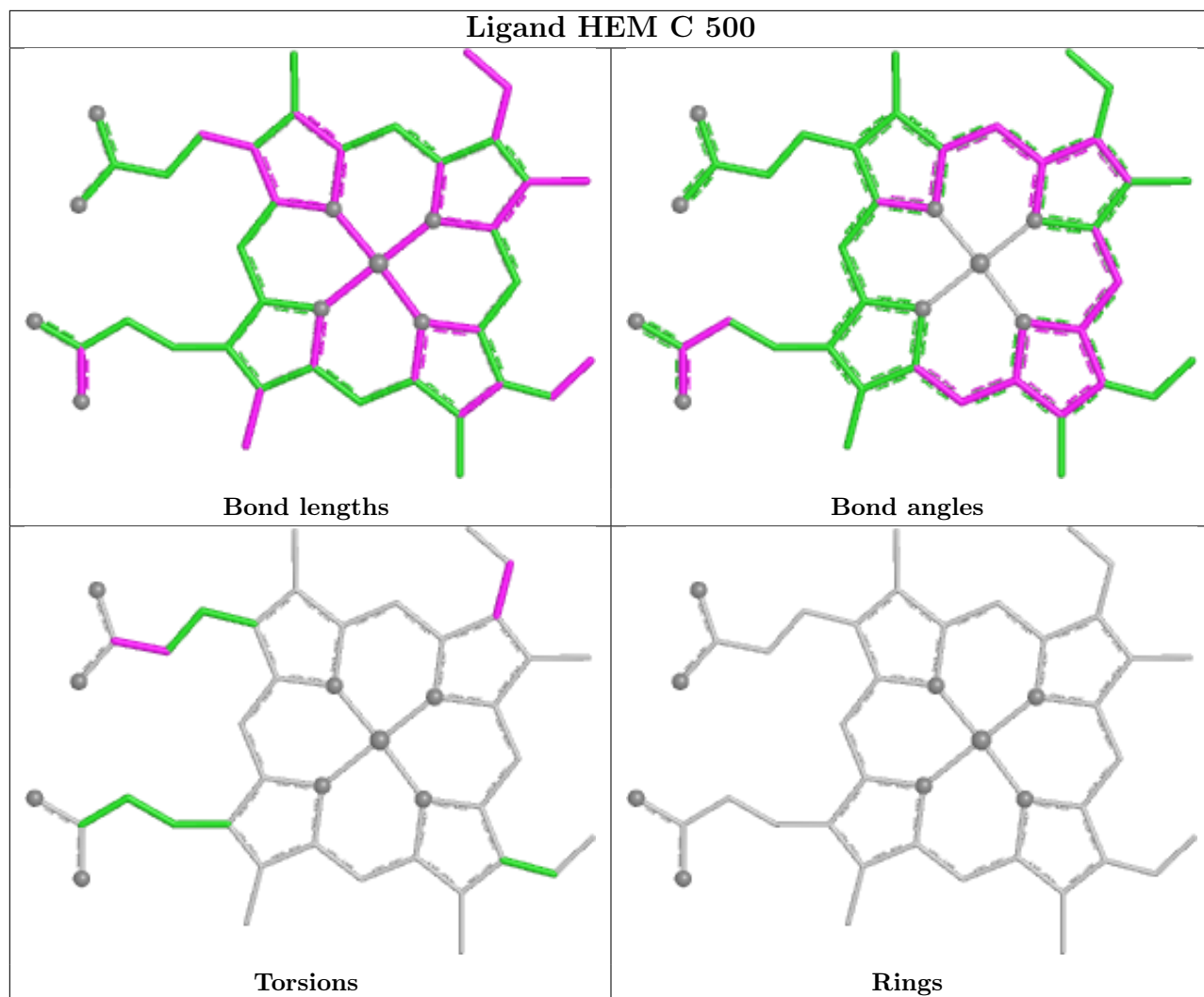
There are no ring outliers.

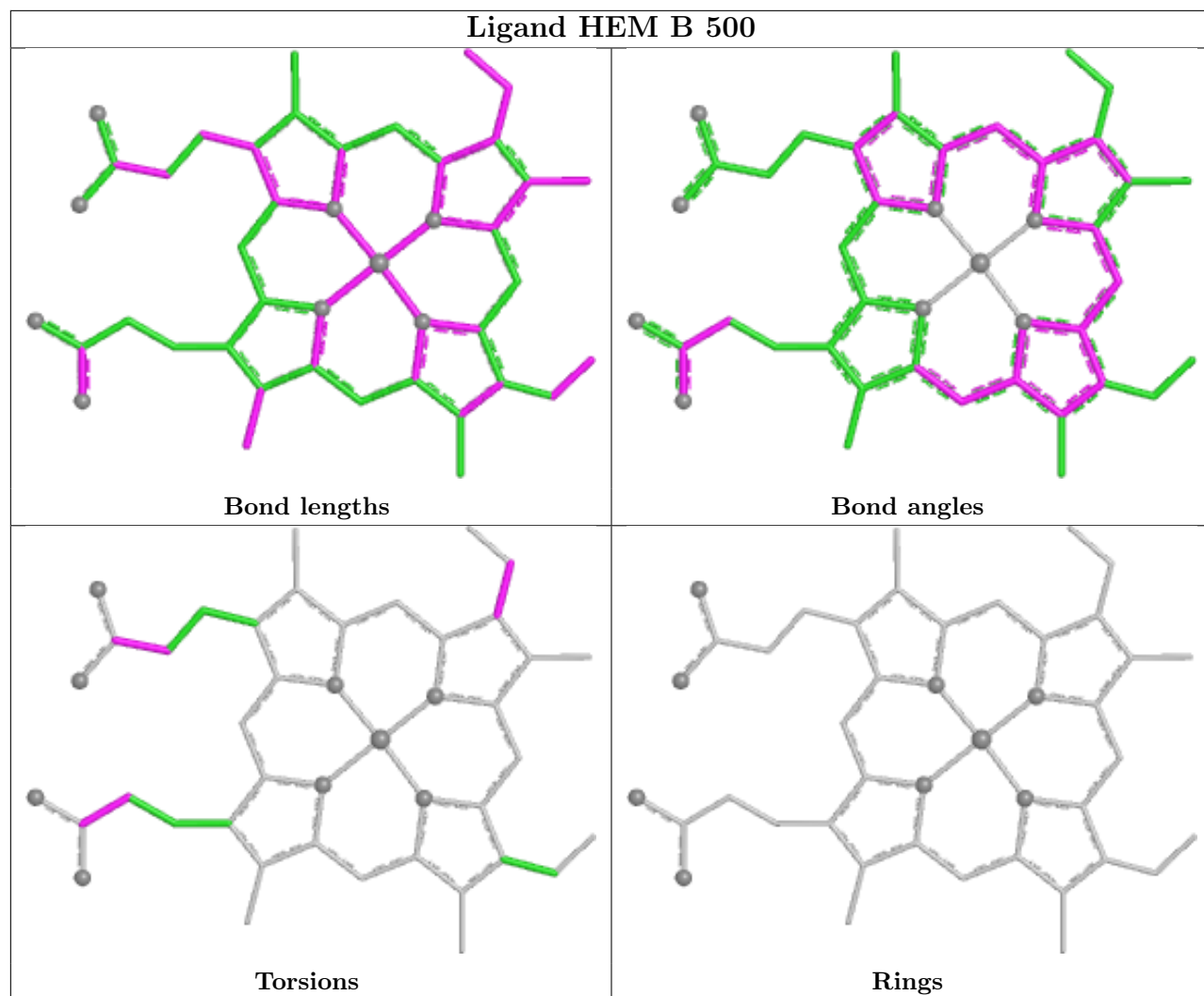
4 monomers are involved in 14 short contacts:

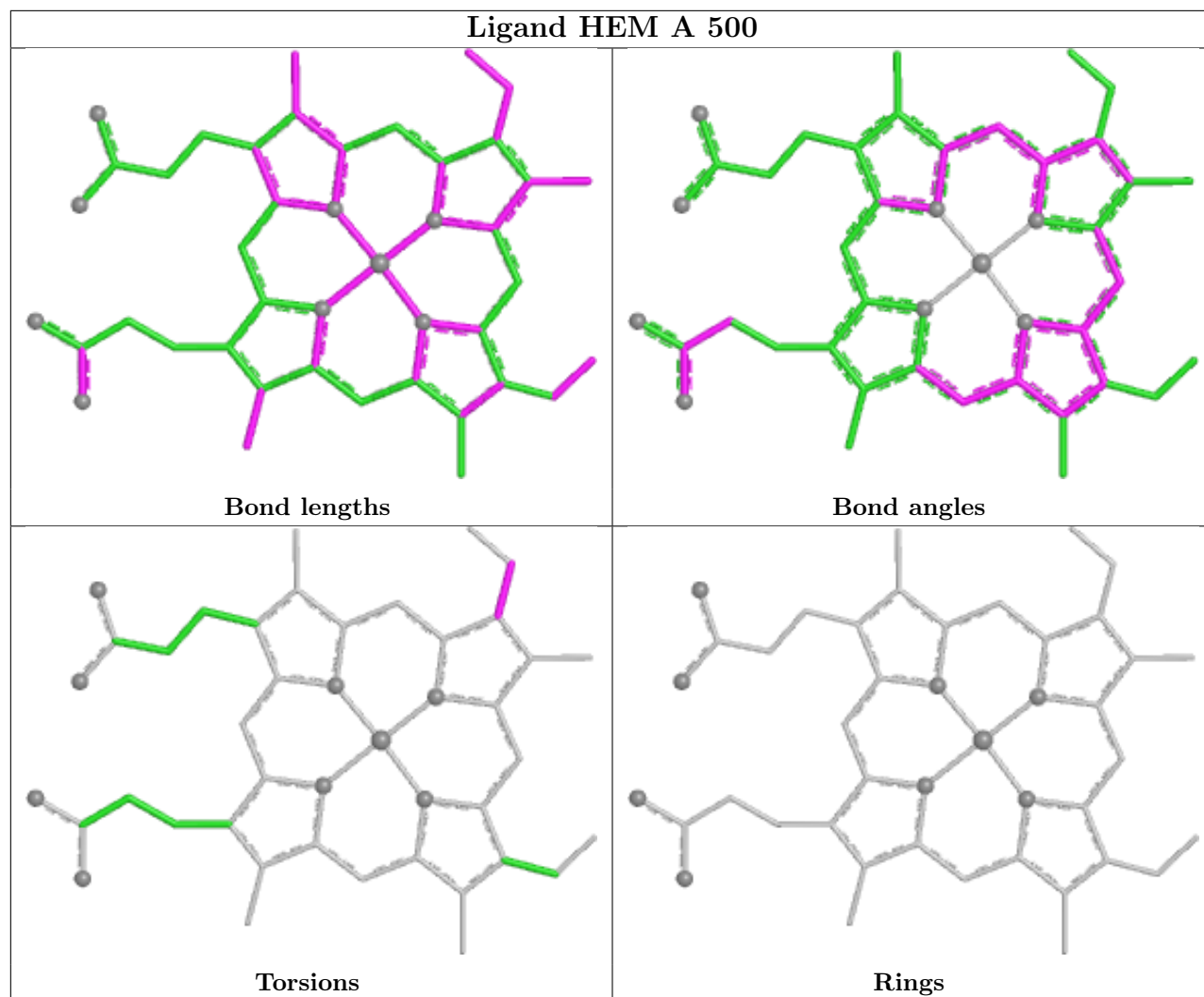
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	500	HEM	3	0
2	C	500	HEM	4	0
2	B	500	HEM	4	0
2	A	500	HEM	3	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	464/476 (97%)	0.29	7 (1%) 72 78	14, 34, 44, 50	1 (0%)
1	B	464/476 (97%)	0.48	17 (3%) 45 52	26, 36, 45, 50	0
1	C	463/476 (97%)	0.23	5 (1%) 78 83	22, 33, 44, 50	0
1	D	464/476 (97%)	0.42	22 (4%) 36 42	23, 35, 47, 51	0
All	All	1855/1904 (97%)	0.35	51 (2%) 56 62	14, 34, 45, 51	1 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	370	LEU	6.7
1	D	418	ASN	4.0
1	B	495	HIS	4.0
1	B	418	ASN	3.7
1	D	143	ARG	3.6
1	C	418	ASN	3.5
1	D	141	GLY	3.5
1	D	140	VAL	3.4
1	A	382	ASP	3.3
1	B	196	LYS	3.3
1	A	262	ASN	3.2
1	B	258	THR	3.2
1	D	138	PHE	3.0
1	B	143	ARG	3.0
1	D	135	LEU	3.0
1	B	260	ASP	3.0
1	D	144	GLY	2.9
1	C	282	PRO	2.9
1	B	276	GLN	2.9
1	D	137	ASP	2.9
1	D	139	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	142	LYS	2.7
1	D	273	ILE	2.6
1	B	167	ASN	2.6
1	A	31	GLY	2.5
1	A	257	ARG	2.5
1	D	336	GLY	2.4
1	A	384	PHE	2.4
1	D	419	GLU	2.4
1	B	53	GLN	2.4
1	D	420	LYS	2.4
1	D	189	ASP	2.3
1	D	276	GLN	2.3
1	D	260	ASP	2.3
1	B	208	ILE	2.2
1	B	216	THR	2.2
1	B	403	SER	2.2
1	A	420	LYS	2.2
1	D	263	SER	2.1
1	D	421	GLY	2.1
1	B	379	LYS	2.1
1	D	262	ASN	2.1
1	D	279	GLU	2.1
1	C	167	ASN	2.1
1	B	259	LEU	2.1
1	B	382	ASP	2.1
1	C	419	GLU	2.0
1	D	280	LYS	2.0
1	C	467	SER	2.0
1	B	336	GLY	2.0
1	B	261	PRO	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

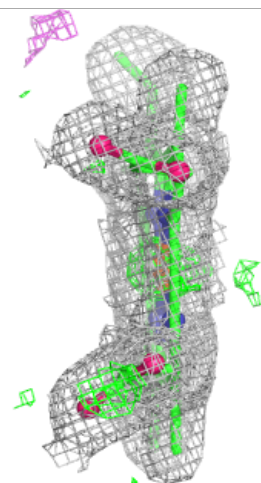
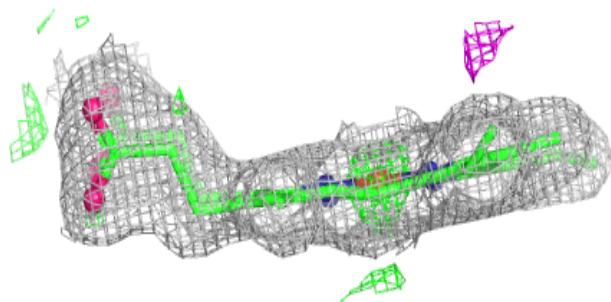
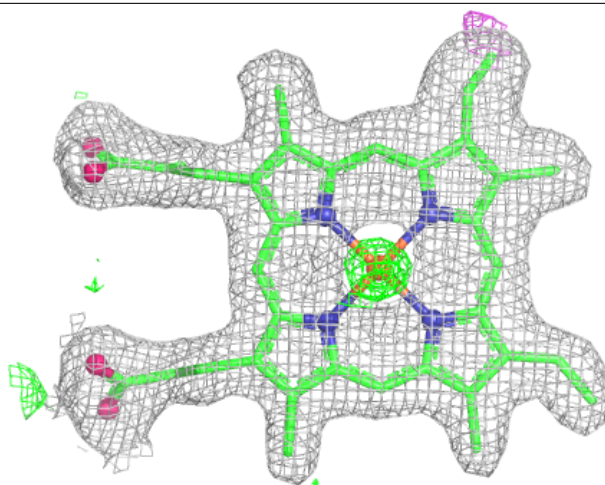
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

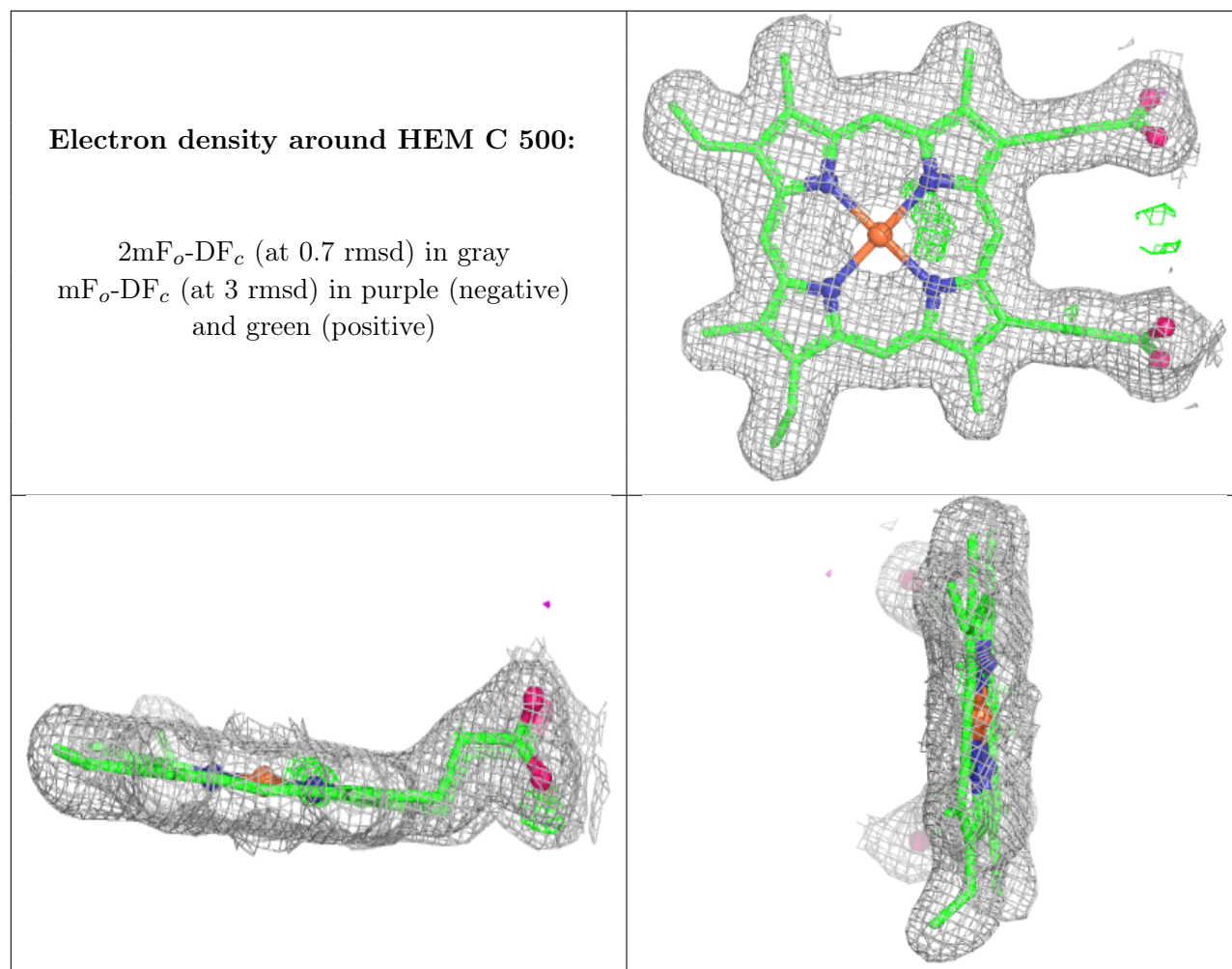
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	B	501	4/4	0.73	0.17	40,42,42,47	0
3	EDO	D	501	4/4	0.74	0.14	40,40,43,48	0
3	EDO	C	501	4/4	0.76	0.17	40,40,42,45	0
3	EDO	A	501	4/4	0.83	0.12	42,42,43,44	0
2	HEM	D	500	43/43	0.97	0.07	25,30,33,37	0
2	HEM	C	500	43/43	0.98	0.06	24,28,31,36	0
2	HEM	A	500	43/43	0.98	0.06	23,27,30,33	0
2	HEM	B	500	43/43	0.98	0.07	25,29,31,38	0

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

Electron density around HEM D 500:

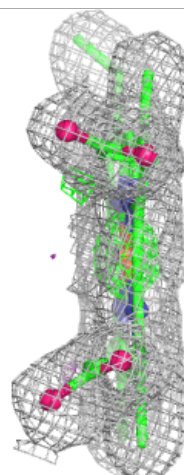
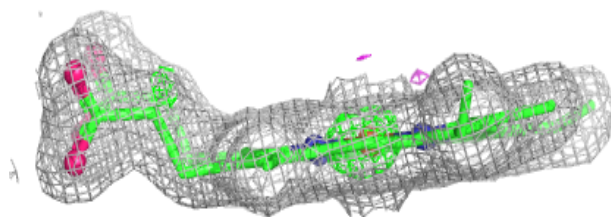
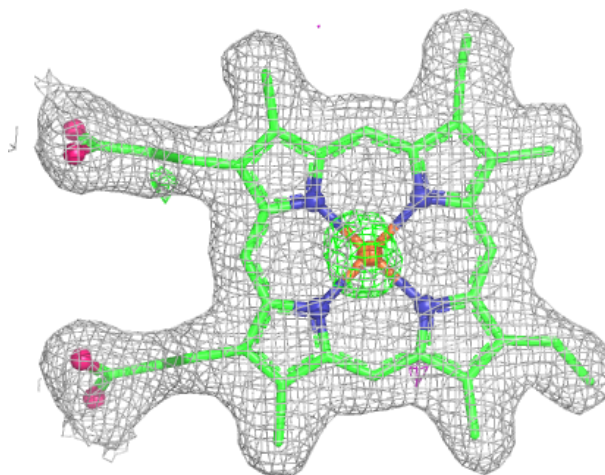
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

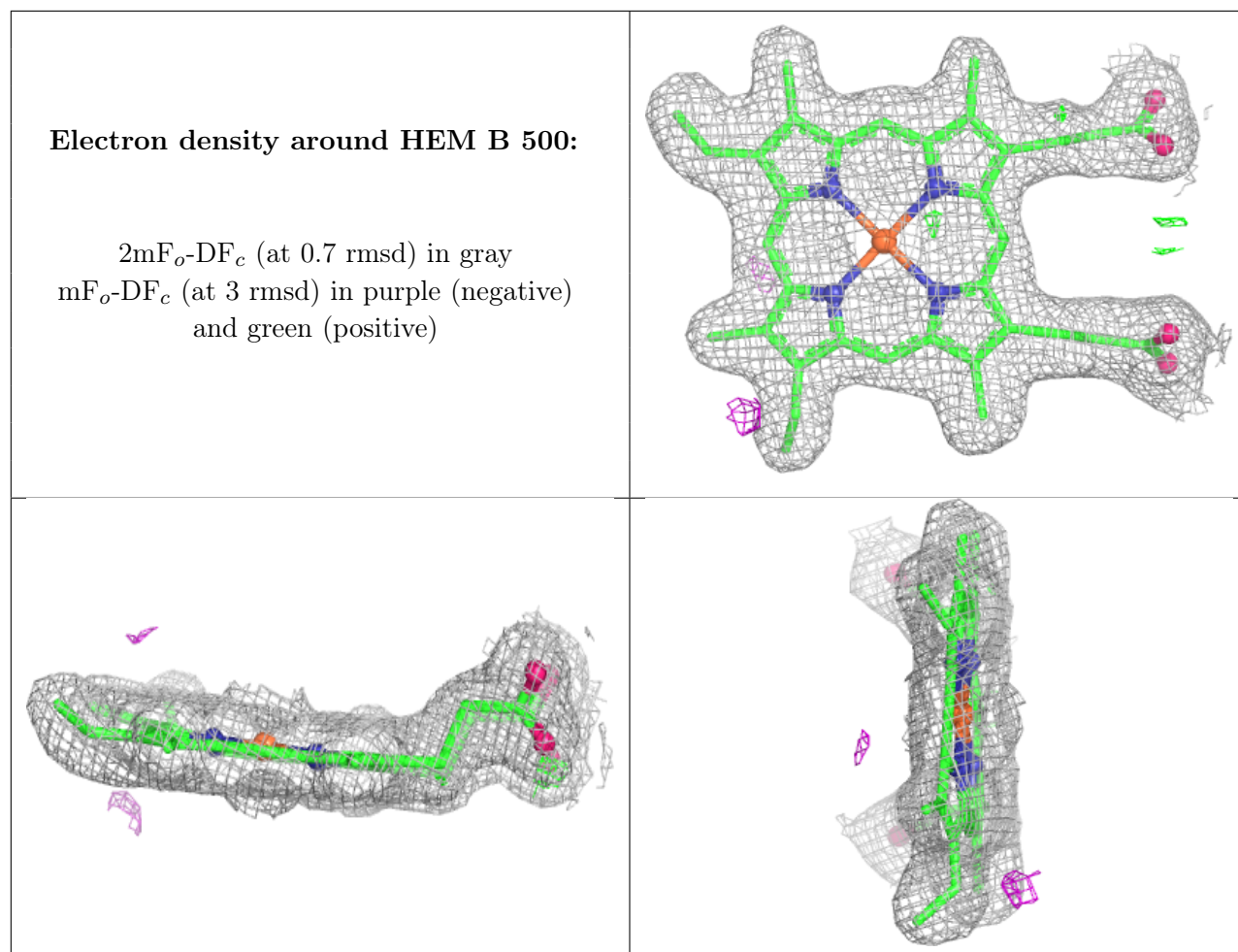




Electron density around HEM A 500:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.