



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:15 AM UTC

PDB ID : 2FDW / pdb_00002fdw
Title : Crystal Structure Of Human Microsomal P450 2A6 with the inhibitor (5-(Pyridin-3-yl)furan-2-yl)methanamine bound
Authors : Yano, J.K.; Stout, C.D.; Johnson, E.F.
Deposited on : 2005-12-14
Resolution : 2.05 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

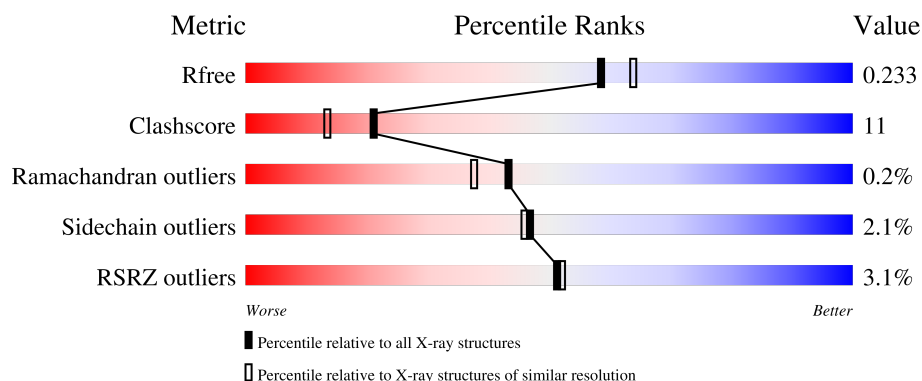
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	% 79% 17% ..
1	B	476	8% 66% 30% ..
1	C	476	% 76% 20% ..
1	D	476	3% 76% 20% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16056 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
1	A	465	Total	C	N	O	S	0	0	0
			3760	2414	650	678	18			
1	B	465	Total	C	N	O	S	0	0	0
			3767	2418	653	678	18			
1	C	464	Total	C	N	O	S	0	0	0
			3751	2408	648	677	18			
1	D	464	Total	C	N	O	S	0	0	0
			3751	2408	648	677	18			

There are 40 discrepancies between the modelled and reference sequences:

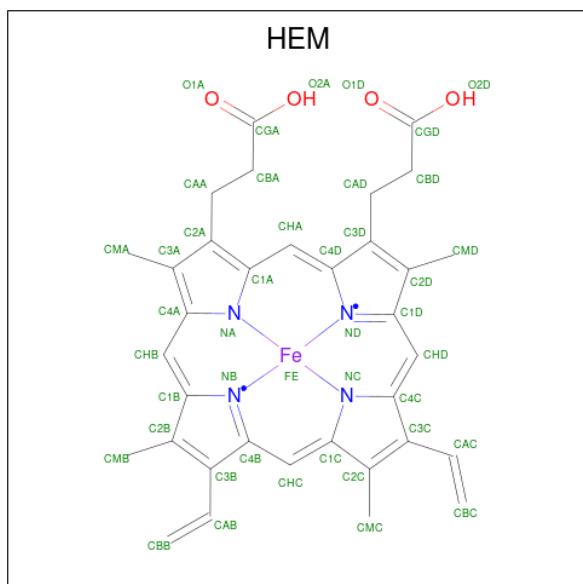
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	cloning artifact	UNP P11509
A	24	ALA	-	cloning artifact	UNP P11509
A	25	LYS	-	cloning artifact	UNP P11509
A	26	LYS	-	cloning artifact	UNP P11509
A	27	THR	-	cloning artifact	UNP P11509
A	28	SER	-	cloning artifact	UNP P11509
A	495	HIS	-	expression 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	495	HIS	-	expression tag	UNP P11509
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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	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: $C_{34}H_{32}FeN_4O_4$).



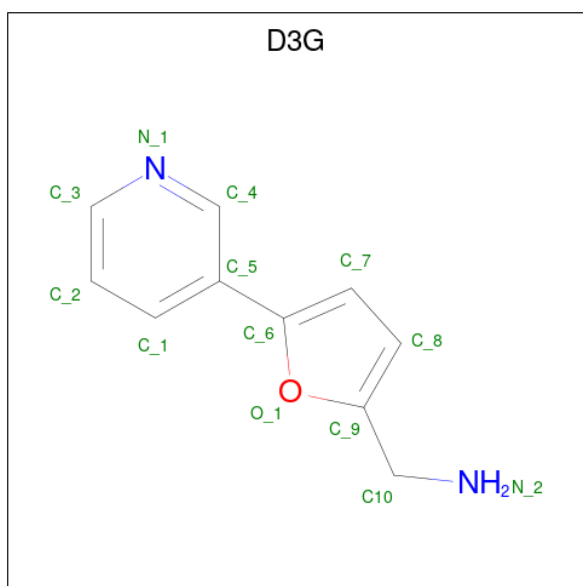
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	

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

- Molecule 3 is (5-(PYRIDIN-3-YL)FURAN-2-YL)METHANAMINE (CCD ID: D3G) (formula: C₁₀H₁₀N₂O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			13	10	2	1		
3	B	1	Total	C	N	O	0	0
			13	10	2	1		
3	C	1	Total	C	N	O	0	0
			13	10	2	1		
3	D	1	Total	C	N	O	0	0
			13	10	2	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	230	Total	O	0	0
			230	230		
4	B	120	Total	O	0	0
			120	120		

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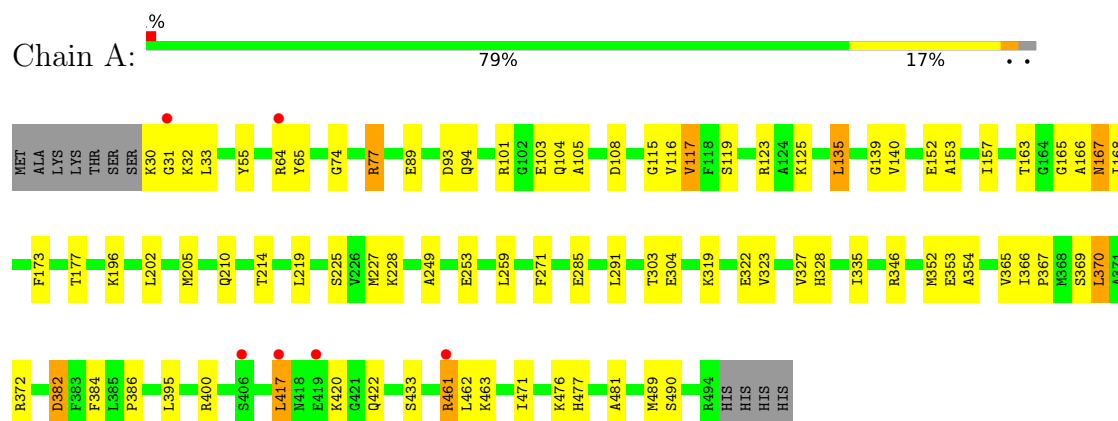
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	234	Total 234	O 234	0	0
4	D	219	Total 219	O 219	0	0

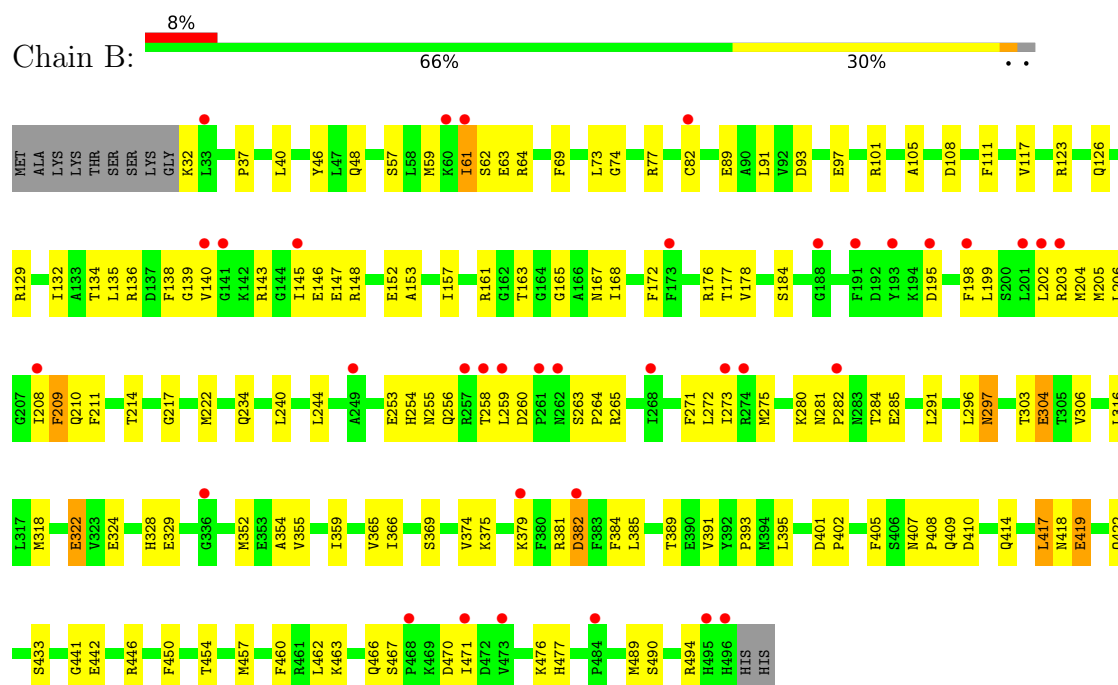
3 Residue-property plots [i](#)

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.

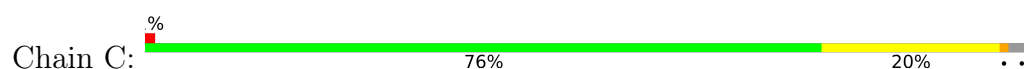
• Molecule 1: Cytochrome P450 2A6

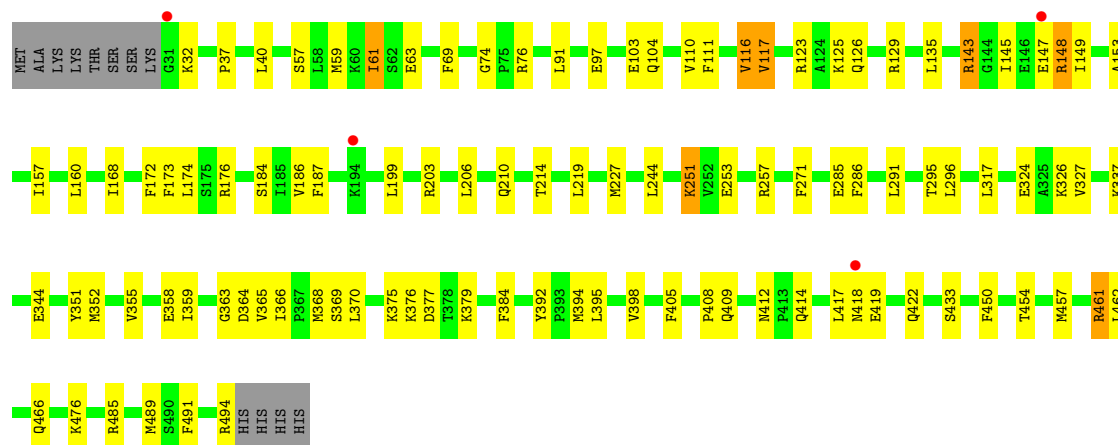


• Molecule 1: Cytochrome P450 2A6

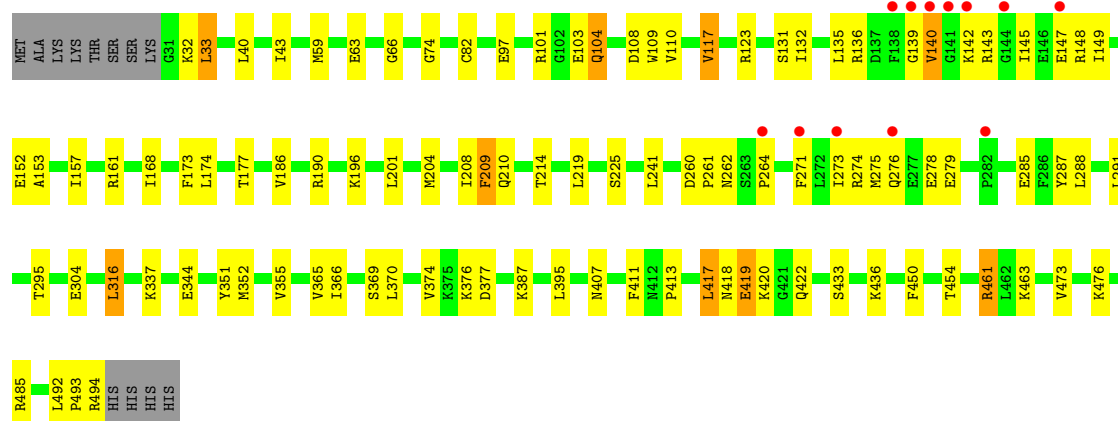
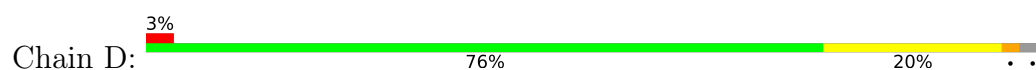


• Molecule 1: Cytochrome P450 2A6





• Molecule 1: Cytochrome P450 2A6



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.75Å 157.56Å 103.79Å 90.00° 91.88° 90.00°	Depositor
Resolution (Å)	34.59 – 2.05 34.59 – 2.05	Depositor EDS
% Data completeness (in resolution range)	93.9 (34.59-2.05) 93.9 (34.59-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.205 , 0.241 0.199 , 0.233	Depositor DCC
R_{free} test set	7563 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16056	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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: D3G, 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	0.40	0/3851	0.92	17/5186 (0.3%)
1	B	0.36	0/3860	0.89	8/5200 (0.2%)
1	C	0.41	0/3842	0.94	15/5175 (0.3%)
1	D	0.40	0/3842	0.91	15/5175 (0.3%)
All	All	0.39	0/15395	0.91	55/20736 (0.3%)

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	461	ARG	N-CA-C	-7.46	98.17	110.17
1	A	104	GLN	N-CA-C	-6.99	95.56	107.23
1	B	365	VAL	N-CA-C	6.88	118.46	110.62
1	A	365	VAL	N-CA-C	6.65	118.20	110.62
1	C	117	VAL	N-CA-C	6.50	116.66	110.42
1	C	219	LEU	N-CA-C	-6.43	104.35	111.36
1	A	461	ARG	N-CA-C	-6.40	99.29	109.59
1	B	366	ILE	CA-C-N	6.36	126.57	119.32
1	B	366	ILE	C-N-CA	6.36	126.57	119.32
1	B	494	ARG	N-CA-C	-6.33	103.91	112.26
1	A	173	PHE	N-CA-C	-6.21	104.59	111.36
1	B	304	GLU	N-CA-C	6.12	117.95	111.28
1	D	461	ARG	N-CA-C	-6.06	100.32	109.95
1	C	116	VAL	N-CA-C	6.05	116.23	110.42
1	C	370	LEU	N-CA-C	-6.00	99.42	109.07
1	D	370	LEU	N-CA-C	-5.99	99.43	109.07
1	D	219	LEU	N-CA-C	-5.94	104.93	111.82
1	A	117	VAL	N-CA-C	5.77	115.84	110.42
1	D	366	ILE	CA-C-N	5.77	125.63	119.28
1	D	366	ILE	C-N-CA	5.77	125.63	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	GLY	N-CA-C	-5.75	100.61	112.34
1	A	304	GLU	N-CA-C	5.72	117.51	111.28
1	D	436	LYS	N-CA-C	5.69	119.49	112.54
1	C	168	ILE	N-CA-C	5.66	117.07	108.80
1	C	173	PHE	N-CA-C	-5.66	105.19	111.36
1	A	227	MET	N-CA-C	5.66	117.45	111.28
1	D	173	PHE	N-CA-C	-5.55	105.23	111.28
1	A	219	LEU	N-CA-C	-5.54	105.33	111.36
1	C	104	GLN	N-CA-C	-5.53	98.00	107.23
1	D	365	VAL	N-CA-C	5.52	116.92	110.62
1	D	104	GLN	N-CA-C	-5.50	96.83	107.44
1	D	66	GLY	CA-C-N	5.47	125.14	119.56
1	D	66	GLY	C-N-CA	5.47	125.14	119.56
1	A	105	ALA	N-CA-C	5.46	117.66	111.11
1	A	370	LEU	N-CA-C	-5.44	100.31	109.07
1	C	366	ILE	CA-C-N	5.42	125.50	119.32
1	C	366	ILE	C-N-CA	5.42	125.50	119.32
1	C	365	VAL	N-CA-C	5.39	116.77	110.62
1	A	366	ILE	CA-C-N	5.38	125.46	119.32
1	A	366	ILE	C-N-CA	5.38	125.46	119.32
1	A	335	ILE	N-CA-C	5.34	116.40	111.81
1	A	116	VAL	N-CA-C	5.33	116.81	111.00
1	D	117	VAL	N-CA-C	5.30	115.44	110.30
1	A	139	GLY	N-CA-C	5.26	120.95	114.69
1	C	91	LEU	N-CA-C	5.24	117.74	111.71
1	C	74	GLY	N-CA-C	-5.22	101.69	112.34
1	B	441	GLY	N-CA-C	-5.20	106.56	115.61
1	C	398	VAL	N-CA-C	-5.20	105.78	110.82
1	B	105	ALA	N-CA-C	5.17	117.31	111.11
1	D	407	ASN	CA-C-N	5.14	124.94	119.28
1	D	407	ASN	C-N-CA	5.14	124.94	119.28
1	A	259	LEU	N-CA-C	5.14	117.76	110.10
1	B	139	GLY	N-CA-C	5.13	120.83	114.37
1	C	227	MET	N-CA-C	5.10	117.57	111.71
1	D	74	GLY	N-CA-C	-5.05	102.04	112.34

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	3760	0	3747	58	0
1	B	3767	0	3745	124	0
1	C	3751	0	3734	73	0
1	D	3751	0	3734	84	0
2	A	43	0	30	3	0
2	B	43	0	30	2	0
2	C	43	0	30	2	0
2	D	43	0	30	3	0
3	A	13	0	9	0	0
3	B	13	0	9	1	0
3	C	13	0	9	1	0
3	D	13	0	9	0	0
4	A	230	0	0	9	0
4	B	120	0	0	7	0
4	C	234	0	0	4	0
4	D	219	0	0	5	0
All	All	16056	0	15116	334	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 11.

All (334) 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:392:TYR:HB3	1:C:394:MET:HE3	1.43	0.98
1:C:32:LYS:HB3	1:C:384:PHE:HB3	1.41	0.97
1:B:135:LEU:HG	1:B:140:VAL:HG21	1.48	0.94
1:B:208:ILE:HD11	1:B:240:LEU:HB2	1.47	0.94
1:D:135:LEU:HG	1:D:140:VAL:HG21	1.51	0.92
1:C:125:LYS:HE2	1:C:129:ARG:NH2	1.87	0.88
1:B:352:MET:HE3	1:B:454:THR:HG22	1.57	0.86
1:B:318:MET:HE1	1:B:489:MET:HB2	1.58	0.84
1:A:249:ALA:O	1:A:253:GLU:HG3	1.80	0.82
1:A:30:LYS:HG3	1:A:32:LYS:H	1.46	0.81
1:A:77:ARG:HG2	1:A:77:ARG:HH11	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:ARG:HH12	1:B:389:THR:HG23	1.47	0.80
1:A:33:LEU:HD21	1:A:386:PRO:HD2	1.67	0.76
1:D:463:LYS:HD3	1:D:492:LEU:HD11	1.65	0.76
1:C:199:LEU:HG	1:C:203:ARG:NH1	2.03	0.73
1:A:354:ALA:HB2	1:A:417:LEU:HD13	1.72	0.72
1:A:163:THR:HG21	1:A:168:ILE:HD13	1.72	0.70
1:D:316:LEU:HD13	1:D:473:VAL:HG21	1.73	0.70
1:C:143:ARG:NH1	1:C:147:GLU:HG2	2.06	0.70
1:B:148:ARG:HD3	1:B:184:SER:HB3	1.74	0.69
1:C:352:MET:HE3	1:C:454:THR:HG22	1.72	0.69
1:D:110:VAL:HG21	1:D:241:LEU:HB3	1.75	0.69
1:D:271:PHE:CG	1:D:291:LEU:HD13	2.29	0.68
1:C:123:ARG:HA	1:C:285:GLU:HG3	1.74	0.68
1:C:392:TYR:HB3	1:C:394:MET:CE	2.21	0.68
1:B:172:PHE:CE1	1:B:199:LEU:HD13	2.30	0.67
1:B:210:GLN:O	1:B:214:THR:HG23	1.93	0.67
1:C:125:LYS:HE2	1:C:129:ARG:HH21	1.59	0.66
1:B:77:ARG:NH1	1:B:389:THR:HG23	2.10	0.66
1:C:257:ARG:HH11	1:C:257:ARG:HG2	1.61	0.66
1:C:61:ILE:HD11	1:C:69:PHE:CD1	2.31	0.66
1:B:40:LEU:HD21	1:D:43:ILE:HD13	1.78	0.65
1:C:418:ASN:HB3	1:C:422:GLN:H	1.62	0.65
1:D:316:LEU:CD1	1:D:473:VAL:HG21	2.27	0.65
1:D:418:ASN:ND2	1:D:422:GLN:HB2	2.11	0.65
1:B:258:THR:HG23	1:B:265:ARG:HH12	1.61	0.64
1:C:405:PHE:O	1:C:408:PRO:HD3	1.97	0.64
1:B:199:LEU:HG	1:B:203:ARG:NH1	2.13	0.64
1:C:466:GLN:HG2	4:C:645:HOH:O	1.97	0.64
1:D:264:PRO:HG3	1:D:273:ILE:HD12	1.80	0.64
1:D:419:GLU:H	1:D:419:GLU:CD	2.06	0.64
1:B:163:THR:HG21	1:B:168:ILE:HD13	1.80	0.63
1:B:148:ARG:HD3	1:B:184:SER:CB	2.28	0.63
1:A:30:LYS:HG2	1:A:382:ASP:O	1.98	0.63
1:B:418:ASN:HD21	1:B:422:GLN:HB2	1.62	0.63
1:C:251:LYS:HZ2	1:C:251:LYS:HB3	1.64	0.63
1:D:461:ARG:HG3	1:D:492:LEU:HB2	1.80	0.63
1:D:148:ARG:HH21	1:D:190:ARG:HB3	1.62	0.63
1:D:186:VAL:HG11	1:D:295:THR:HG23	1.81	0.63
1:B:354:ALA:HB2	1:B:417:LEU:HD13	1.80	0.62
1:B:176:ARG:HG3	1:B:198:PHE:HE2	1.65	0.62
1:D:59:MET:O	1:D:63:GLU:HG3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:461:ARG:NH1	1:D:494:ARG:HA	2.13	0.62
1:B:77:ARG:HH12	1:B:389:THR:CG2	2.12	0.62
1:A:433:SER:HB3	2:A:500:HEM:HBA1	1.82	0.61
1:D:161:ARG:HG3	1:D:161:ARG:HH11	1.65	0.61
1:A:369:SER:HB2	1:A:395:LEU:HG	1.82	0.61
1:B:61:ILE:HD11	1:B:69:PHE:CD1	2.35	0.61
1:B:318:MET:HE3	1:B:489:MET:HE3	1.82	0.61
1:B:375:LYS:HE2	4:B:555:HOH:O	2.00	0.61
1:A:476:LYS:HE2	1:A:477:HIS:NE2	2.14	0.61
1:D:418:ASN:HD21	1:D:422:GLN:HB2	1.64	0.60
1:C:59:MET:O	1:C:63:GLU:HG3	1.99	0.60
1:D:344:GLU:HG3	4:D:600:HOH:O	2.01	0.60
1:B:254:HIS:O	1:B:258:THR:HG22	2.01	0.60
1:B:318:MET:HE3	1:B:462:LEU:HB3	1.83	0.60
1:B:57:SER:O	1:B:61:ILE:HG23	2.01	0.60
1:B:108:ASP:HB3	4:B:566:HOH:O	2.01	0.60
1:C:368:MET:HB3	1:C:394:MET:HE1	1.84	0.60
1:A:117:VAL:HG22	2:A:500:HEM:HAD1	1.84	0.60
1:D:59:MET:HE1	1:D:82:CYS:SG	2.42	0.60
1:A:166:ALA:HB1	1:B:167:ASN:ND2	2.17	0.59
1:A:89:GLU:O	1:A:93:ASP:HB2	2.03	0.59
1:D:352:MET:HE3	1:D:454:THR:HG22	1.83	0.59
1:D:271:PHE:CD2	1:D:291:LEU:HB2	2.37	0.59
1:C:32:LYS:HE2	1:C:384:PHE:HB2	1.85	0.59
1:C:462:LEU:HD22	1:C:489:MET:HE1	1.84	0.59
1:C:97:GLU:HG3	4:C:650:HOH:O	2.03	0.59
1:D:139:GLY:HA2	1:D:142:LYS:HG2	1.84	0.59
1:B:59:MET:HE1	1:B:82:CYS:SG	2.43	0.58
1:B:466:GLN:OE1	1:B:471:ILE:HA	2.03	0.58
1:B:206:LEU:HB3	4:B:596:HOH:O	2.03	0.58
1:C:172:PHE:O	1:C:176:ARG:HG3	2.03	0.58
1:C:61:ILE:HD11	1:C:69:PHE:CG	2.38	0.58
1:D:108:ASP:HB2	4:D:687:HOH:O	2.02	0.58
1:A:210:GLN:O	1:A:214:THR:HG23	2.04	0.58
1:B:148:ARG:HH11	1:B:184:SER:HB3	1.69	0.57
1:B:176:ARG:HG3	1:B:198:PHE:CE2	2.39	0.57
1:D:461:ARG:HH12	1:D:494:ARG:HA	1.69	0.57
1:B:476:LYS:HE3	1:B:477:HIS:CD2	2.39	0.57
1:B:418:ASN:ND2	1:B:422:GLN:HB2	2.18	0.57
1:C:344:GLU:HG3	4:C:591:HOH:O	2.05	0.57
1:D:271:PHE:CE2	1:D:291:LEU:HB2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:412:ASN:ND2	1:C:414:GLN:H	2.02	0.57
1:B:244:LEU:HB3	1:B:296:LEU:HD11	1.87	0.57
1:D:148:ARG:NH2	1:D:190:ARG:HD2	2.19	0.57
1:D:433:SER:HB3	2:D:500:HEM:HBA1	1.86	0.57
1:B:46:TYR:HA	1:B:222:MET:HE1	1.87	0.57
1:B:355:VAL:O	1:B:359:ILE:HG13	2.05	0.56
1:B:407:ASN:HB3	1:B:410:ASP:OD2	2.05	0.56
1:C:433:SER:HB3	2:C:500:HEM:HBA1	1.87	0.56
1:A:328:HIS:HE1	1:A:461:ARG:HD2	1.70	0.56
1:C:369:SER:HB2	1:C:395:LEU:HG	1.87	0.56
1:C:375:LYS:HE2	4:C:607:HOH:O	2.05	0.56
1:C:412:ASN:ND2	1:C:414:GLN:HB2	2.21	0.56
1:A:77:ARG:HG2	1:A:77:ARG:NH1	2.17	0.56
1:A:167:ASN:HB2	4:A:642:HOH:O	2.06	0.56
1:A:463:LYS:HB3	1:A:490:SER:OG	2.04	0.56
1:A:135:LEU:HG	1:A:140:VAL:HG21	1.87	0.55
1:D:271:PHE:CB	1:D:291:LEU:HD13	2.36	0.55
1:A:328:HIS:CE1	1:A:461:ARG:HD2	2.41	0.55
1:B:40:LEU:HD21	1:D:43:ILE:CD1	2.36	0.55
1:B:161:ARG:HG3	1:B:161:ARG:HH11	1.71	0.55
1:B:419:GLU:CD	1:B:419:GLU:H	2.15	0.55
1:B:264:PRO:HG3	1:B:273:ILE:CD1	2.37	0.54
1:B:73:LEU:HA	1:B:222:MET:HE3	1.89	0.54
1:B:381:ARG:O	1:B:382:ASP:HB2	2.06	0.54
1:D:186:VAL:CG1	1:D:295:THR:HG23	2.38	0.54
1:D:264:PRO:HG3	1:D:273:ILE:CD1	2.36	0.54
1:B:467:SER:HB3	1:B:470:ASP:OD2	2.08	0.54
1:D:117:VAL:HG22	2:D:500:HEM:HAD1	1.90	0.54
1:B:165:GLY:O	1:B:490:SER:HB2	2.07	0.54
1:B:322:GLU:H	1:B:322:GLU:CD	2.15	0.54
1:C:37:PRO:HD3	1:C:61:ILE:HD13	1.90	0.54
1:C:143:ARG:HH11	1:C:147:GLU:HG2	1.73	0.54
1:B:178:VAL:HG11	1:B:306:VAL:HB	1.90	0.53
1:B:433:SER:HB3	2:B:500:HEM:HBA1	1.90	0.53
1:B:77:ARG:HG2	1:B:77:ARG:HH11	1.74	0.53
1:B:260:ASP:HB3	1:B:263:SER:HB3	1.90	0.53
1:B:117:VAL:HG22	2:B:500:HEM:HAD1	1.90	0.53
1:D:139:GLY:HA2	1:D:142:LYS:CD	2.38	0.53
1:B:409:GLN:HA	1:B:409:GLN:NE2	2.23	0.53
1:C:326:LYS:HB2	1:C:351:TYR:CE2	2.44	0.53
1:B:463:LYS:HB3	1:B:490:SER:OG	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:450:PHE:O	1:D:454:THR:HG23	2.09	0.53
1:A:94:GLN:HG3	4:A:545:HOH:O	2.09	0.52
1:B:255:ASN:HA	1:B:265:ARG:HH22	1.75	0.52
1:B:369:SER:HB2	1:B:395:LEU:HG	1.91	0.52
1:D:473:VAL:HG22	1:D:473:VAL:O	2.09	0.52
1:B:37:PRO:HD3	1:B:61:ILE:HD13	1.91	0.52
1:A:33:LEU:HD13	1:A:77:ARG:HD2	1.91	0.52
1:B:123:ARG:HA	1:B:285:GLU:HG3	1.92	0.52
1:B:466:GLN:HG2	4:B:617:HOH:O	2.10	0.52
1:B:324:GLU:HG2	1:B:328:HIS:CD2	2.44	0.52
1:B:111:PHE:CZ	3:B:501:D3G:H_3	2.45	0.51
1:B:409:GLN:HA	1:B:409:GLN:HE21	1.75	0.51
1:D:139:GLY:HA2	1:D:142:LYS:CG	2.41	0.51
1:B:318:MET:CE	1:B:489:MET:HB2	2.37	0.51
1:A:462:LEU:HD22	1:A:489:MET:HE1	1.92	0.51
1:D:97:GLU:HG3	4:D:541:HOH:O	2.11	0.51
1:D:271:PHE:HB3	1:D:291:LEU:HD13	1.92	0.51
1:D:131:SER:O	1:D:135:LEU:HB2	2.11	0.51
1:D:123:ARG:HA	1:D:285:GLU:HG3	1.92	0.51
1:B:161:ARG:HG2	1:B:460:PHE:HZ	1.76	0.51
1:A:382:ASP:OD2	1:A:382:ASP:N	2.34	0.50
1:B:324:GLU:HG3	1:B:457:MET:CE	2.41	0.50
1:D:33:LEU:HD12	1:D:33:LEU:N	2.26	0.50
1:B:202:LEU:HD23	1:B:205:MET:CE	2.41	0.50
1:A:370:LEU:O	4:A:502:HOH:O	2.19	0.50
1:B:143:ARG:HD2	1:B:146:GLU:OE2	2.12	0.50
1:B:318:MET:CE	1:B:489:MET:HE3	2.41	0.50
1:D:161:ARG:HG3	1:D:161:ARG:NH1	2.27	0.50
1:A:101:ARG:NH1	4:A:502:HOH:O	2.44	0.50
1:B:258:THR:CG2	1:B:265:ARG:HH12	2.25	0.50
1:B:253:GLU:HA	1:B:256:GLN:HG2	1.93	0.50
1:C:57:SER:O	1:C:61:ILE:HG23	2.11	0.50
1:A:166:ALA:HB1	1:B:167:ASN:HD21	1.75	0.50
1:B:61:ILE:HD12	1:B:61:ILE:O	2.12	0.49
1:B:143:ARG:O	1:B:147:GLU:HG3	2.11	0.49
1:B:205:MET:HE1	1:B:303:THR:HG21	1.92	0.49
1:A:55:TYR:CZ	1:A:400:ARG:NH2	2.80	0.49
1:C:476:LYS:HB2	1:C:485:ARG:HA	1.93	0.49
1:D:101:ARG:CD	1:D:117:VAL:O	2.60	0.49
1:D:168:ILE:C	1:D:168:ILE:HD12	2.37	0.49
1:B:271:PHE:CG	1:B:291:LEU:HD13	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:MET:HE2	1:B:463:LYS:C	2.37	0.49
1:D:152:GLU:HG3	1:D:177:THR:HG23	1.94	0.49
1:C:117:VAL:HG22	2:C:500:HEM:HAD1	1.93	0.49
1:A:202:LEU:HD23	1:A:205:MET:CE	2.43	0.49
1:C:412:ASN:HD21	1:C:414:GLN:HB2	1.78	0.49
1:A:225:SER:HB2	1:D:225:SER:HB2	1.95	0.48
1:B:281:ASN:O	1:B:284:THR:HG22	2.12	0.48
1:D:33:LEU:H	1:D:33:LEU:CD1	2.26	0.48
1:A:322:GLU:HG2	1:A:323:VAL:N	2.27	0.48
1:D:139:GLY:HA2	1:D:142:LYS:HD2	1.95	0.48
1:A:346:ARG:HD2	1:A:353:GLU:OE2	2.13	0.48
1:C:61:ILE:HD12	1:C:61:ILE:O	2.13	0.48
1:C:418:ASN:OD1	1:C:419:GLU:N	2.45	0.48
1:A:461:ARG:HD3	4:A:574:HOH:O	2.13	0.48
1:C:271:PHE:CE2	1:C:291:LEU:HB2	2.48	0.48
1:B:354:ALA:CB	1:B:417:LEU:HD13	2.43	0.48
1:B:442:GLU:O	1:B:446:ARG:HG2	2.13	0.48
1:C:257:ARG:HG2	1:C:257:ARG:NH1	2.27	0.48
1:D:101:ARG:HD3	1:D:117:VAL:O	2.13	0.48
1:A:291:LEU:HD12	1:A:291:LEU:O	2.15	0.47
1:C:111:PHE:CZ	3:C:501:D3G:H_3	2.49	0.47
1:C:317:LEU:HD13	1:C:457:MET:CE	2.45	0.47
1:A:323:VAL:O	1:A:327:VAL:HG23	2.14	0.47
1:C:450:PHE:O	1:C:454:THR:HG23	2.13	0.47
1:B:89:GLU:CD	1:B:381:ARG:HH21	2.23	0.47
1:C:412:ASN:C	1:C:412:ASN:HD22	2.21	0.47
1:C:251:LYS:HB3	1:C:251:LYS:NZ	2.29	0.47
1:D:132:ILE:O	1:D:136:ARG:HG3	2.14	0.47
1:A:328:HIS:ND1	1:A:461:ARG:NH1	2.63	0.46
1:C:76:ARG:NH2	1:C:103:GLU:HG3	2.30	0.46
1:C:210:GLN:O	1:C:214:THR:HG23	2.16	0.46
1:A:420:LYS:HG2	1:A:422:GLN:CD	2.41	0.46
1:D:376:LYS:O	1:D:377:ASP:C	2.58	0.46
1:C:271:PHE:CG	1:C:291:LEU:HD13	2.50	0.46
1:D:143:ARG:O	1:D:147:GLU:HG2	2.16	0.46
1:B:209:PHE:CG	1:B:304:GLU:HG2	2.50	0.46
1:B:211:PHE:O	1:B:217:GLY:HA3	2.15	0.46
1:D:433:SER:CB	2:D:500:HEM:HBA1	2.45	0.46
1:C:244:LEU:HB3	1:C:296:LEU:HD11	1.97	0.46
1:A:123:ARG:HA	1:A:285:GLU:HG3	1.98	0.46
1:B:37:PRO:HB2	1:B:48:GLN:NE2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:374:VAL:HG12	1:D:376:LYS:O	2.16	0.46
1:B:259:LEU:HD12	1:B:260:ASP:H	1.81	0.46
1:A:103:GLU:HB2	1:A:108:ASP:OD2	2.16	0.45
1:B:101:ARG:HD2	1:B:117:VAL:O	2.16	0.45
1:B:126:GLN:HG2	4:B:541:HOH:O	2.16	0.45
1:B:272:LEU:O	1:B:275:MET:HB2	2.16	0.45
1:C:145:ILE:O	1:C:149:ILE:HG13	2.15	0.45
1:D:413:PRO:O	1:D:417:LEU:HD22	2.16	0.45
1:C:186:VAL:HG12	1:C:187:PHE:CD1	2.51	0.45
1:D:109:TRP:HE3	1:D:110:VAL:HG23	1.82	0.45
1:D:275:MET:HE3	1:D:287:TYR:HA	1.99	0.45
1:B:64:ARG:HB2	4:B:577:HOH:O	2.15	0.45
1:B:161:ARG:HG2	1:B:460:PHE:CZ	2.51	0.45
1:B:255:ASN:HA	1:B:265:ARG:NH2	2.31	0.45
1:D:276:GLN:O	1:D:279:GLU:HG3	2.16	0.45
1:D:476:LYS:HB2	1:D:485:ARG:HA	1.98	0.45
1:B:59:MET:O	1:B:63:GLU:HG3	2.15	0.45
1:D:196:LYS:HB2	4:D:646:HOH:O	2.17	0.45
1:B:89:GLU:O	1:B:93:ASP:HB2	2.16	0.45
1:D:208:ILE:HD13	1:D:241:LEU:CD2	2.47	0.45
1:A:372:ARG:CD	4:A:502:HOH:O	2.64	0.45
1:C:153:ALA:O	1:C:157:ILE:HG12	2.17	0.45
1:C:412:ASN:ND2	1:C:412:ASN:C	2.75	0.45
1:C:461:ARG:HG3	1:C:494:ARG:HG2	1.98	0.45
1:D:153:ALA:O	1:D:157:ILE:HG12	2.16	0.45
1:A:33:LEU:HD23	1:A:384:PHE:O	2.17	0.44
1:A:165:GLY:O	1:A:490:SER:HB2	2.18	0.44
1:B:62:SER:C	1:B:64:ARG:H	2.25	0.44
1:C:110:VAL:HG13	1:C:111:PHE:CD1	2.52	0.44
1:D:139:GLY:C	1:D:142:LYS:HG2	2.42	0.44
1:B:153:ALA:O	1:B:157:ILE:HG12	2.17	0.44
1:C:355:VAL:O	1:C:359:ILE:HG13	2.18	0.44
1:B:255:ASN:O	1:B:259:LEU:HB2	2.17	0.44
1:A:433:SER:CB	2:A:500:HEM:HBA1	2.48	0.44
1:C:271:PHE:CD2	1:C:291:LEU:HB2	2.51	0.44
1:D:274:ARG:O	1:D:278:GLU:HG2	2.18	0.44
1:D:351:TYR:O	1:D:355:VAL:HG23	2.18	0.44
1:D:145:ILE:O	1:D:149:ILE:HG13	2.18	0.44
1:A:271:PHE:CD2	1:A:291:LEU:HB2	2.53	0.43
1:D:369:SER:HB2	1:D:395:LEU:HG	2.00	0.43
1:B:405:PHE:O	1:B:408:PRO:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:LEU:HD13	1:C:491:PHE:CD2	2.53	0.43
1:B:132:ILE:O	1:B:136:ARG:HG3	2.18	0.43
1:D:201:LEU:HA	1:D:204:MET:HE3	2.00	0.43
1:D:275:MET:HE3	1:D:288:LEU:N	2.34	0.43
1:B:198:PHE:O	1:B:202:LEU:HG	2.19	0.43
1:B:384:PHE:C	1:B:385:LEU:HD12	2.44	0.43
1:B:275:MET:HE3	4:B:574:HOH:O	2.19	0.43
1:B:381:ARG:O	1:B:382:ASP:CB	2.66	0.43
1:D:210:GLN:O	1:D:214:THR:HG23	2.19	0.43
1:D:208:ILE:HD13	1:D:241:LEU:HG	1.99	0.43
1:B:74:GLY:H	1:B:222:MET:HE2	1.83	0.43
1:B:161:ARG:HG3	1:B:161:ARG:NH1	2.34	0.43
1:B:418:ASN:HB2	1:B:419:GLU:OE2	2.19	0.43
1:B:450:PHE:O	1:B:454:THR:HG23	2.19	0.42
1:B:91:LEU:HD12	1:B:91:LEU:N	2.34	0.42
1:D:32:LYS:HB2	4:D:592:HOH:O	2.19	0.42
1:D:103:GLU:CG	1:D:104:GLN:N	2.82	0.42
1:D:420:LYS:NZ	1:D:420:LYS:HB3	2.34	0.42
1:A:30:LYS:N	4:A:587:HOH:O	2.52	0.42
1:B:97:GLU:O	1:B:374:VAL:HA	2.19	0.42
1:B:280:LYS:O	1:B:282:PRO:HD3	2.20	0.42
1:A:367:PRO:HD2	1:A:481:ALA:HA	2.00	0.42
1:B:271:PHE:CE2	1:B:291:LEU:HB2	2.54	0.42
1:A:152:GLU:HG3	1:A:177:THR:HG23	2.01	0.42
1:C:126:GLN:HG3	1:C:286:PHE:CE2	2.54	0.42
1:C:143:ARG:HH11	1:C:147:GLU:CG	2.33	0.42
1:D:139:GLY:CA	1:D:142:LYS:HG2	2.47	0.42
1:D:209:PHE:CG	1:D:304:GLU:HG2	2.55	0.42
1:A:115:GLY:O	1:A:119:SER:HB3	2.19	0.42
1:A:64:ARG:HG3	1:A:65:TYR:CD2	2.54	0.42
1:B:199:LEU:HD21	1:B:203:ARG:NH2	2.34	0.42
1:B:271:PHE:CD2	1:B:291:LEU:HB2	2.55	0.42
1:B:401:ASP:HA	1:B:402:PRO:HD2	1.87	0.41
1:D:33:LEU:N	1:D:33:LEU:CD1	2.83	0.41
1:B:89:GLU:HA	1:B:93:ASP:OD2	2.21	0.41
1:B:258:THR:HG23	1:B:265:ARG:NH1	2.31	0.41
1:C:327:VAL:HG13	1:C:352:MET:HE2	2.03	0.41
1:A:327:VAL:HG13	1:A:352:MET:HE2	2.02	0.41
1:C:116:VAL:HG13	1:C:117:VAL:N	2.36	0.41
1:A:205:MET:HE1	1:A:303:THR:HG21	2.02	0.41
1:B:271:PHE:HB3	1:B:291:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:376:LYS:HA	1:D:387:LYS:CG	2.50	0.41
1:D:492:LEU:HA	1:D:493:PRO:HD3	1.98	0.41
1:A:153:ALA:O	1:A:157:ILE:HG12	2.20	0.41
1:A:372:ARG:HD3	4:A:502:HOH:O	2.21	0.41
1:B:134:THR:O	1:B:138:PHE:HD2	2.04	0.41
1:D:33:LEU:HD12	1:D:33:LEU:H	1.85	0.41
1:B:145:ILE:HD12	1:B:145:ILE:HA	1.95	0.41
1:C:251:LYS:NZ	1:C:251:LYS:CB	2.83	0.41
1:C:253:GLU:O	1:C:257:ARG:HG3	2.20	0.41
1:C:324:GLU:HG3	1:C:457:MET:CE	2.50	0.41
1:A:33:LEU:HD11	1:A:77:ARG:CZ	2.51	0.41
1:A:319:LYS:HD3	1:A:471:ILE:HB	2.04	0.41
1:B:381:ARG:O	1:B:381:ARG:HG3	2.21	0.41
1:C:206:LEU:O	1:C:210:GLN:HG3	2.21	0.41
1:C:358:GLU:HA	1:C:358:GLU:OE1	2.21	0.41
1:C:376:LYS:O	1:C:377:ASP:C	2.62	0.41
1:C:379:LYS:HE2	1:C:379:LYS:HB3	1.89	0.41
1:D:316:LEU:HG	1:D:411:PHE:CD1	2.56	0.41
1:B:199:LEU:HG	1:B:203:ARG:HH12	1.81	0.40
1:C:409:GLN:HA	1:C:409:GLN:NE2	2.36	0.40
1:D:260:ASP:O	1:D:262:ASN:N	2.54	0.40
1:D:337:LYS:HE2	1:D:494:ARG:NH1	2.36	0.40
1:D:374:VAL:CG1	1:D:376:LYS:O	2.69	0.40
1:A:30:LYS:HG3	1:A:31:GLY:N	2.35	0.40
1:B:391:VAL:O	1:B:393:PRO:HD3	2.21	0.40
1:B:101:ARG:CD	1:B:117:VAL:O	2.69	0.40
1:B:152:GLU:HG3	1:B:177:THR:HG23	2.03	0.40
1:B:204:MET:O	1:B:208:ILE:HG12	2.22	0.40
1:A:196:LYS:HG3	4:A:563:HOH:O	2.20	0.40
1:B:129:ARG:HG3	1:B:129:ARG:HH11	1.86	0.40
1:C:148:ARG:HD3	1:C:184:SER:OG	2.21	0.40
1:C:186:VAL:HG13	1:C:295:THR:HG23	2.04	0.40
1:C:326:LYS:HE2	1:C:326:LYS:HB3	1.93	0.40
1:A:420:LYS:HG3	1:A:420:LYS:O	2.21	0.40
1:B:297:ASN:HD22	1:B:297:ASN:HA	1.67	0.40
1:C:363:GLY:O	1:C:364:ASP:C	2.65	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	463/476 (97%)	450 (97%)	13 (3%)	0	100	100
1	B	463/476 (97%)	435 (94%)	26 (6%)	2 (0%)	30	22
1	C	462/476 (97%)	446 (96%)	16 (4%)	0	100	100
1	D	462/476 (97%)	443 (96%)	17 (4%)	2 (0%)	30	22
All	All	1850/1904 (97%)	1774 (96%)	72 (4%)	4 (0%)	43	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	140	VAL
1	B	195	ASP
1	B	382	ASP
1	D	261	PRO

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	412/422 (98%)	405 (98%)	7 (2%)	53	53
1	B	413/422 (98%)	401 (97%)	12 (3%)	37	33
1	C	411/422 (97%)	402 (98%)	9 (2%)	45	44
1	D	411/422 (97%)	404 (98%)	7 (2%)	53	53
All	All	1647/1688 (98%)	1612 (98%)	35 (2%)	47	46

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ARG
1	A	125	LYS
1	A	135	LEU
1	A	167	ASN
1	A	228	LYS
1	A	382	ASP
1	A	417	LEU
1	B	32	LYS
1	B	61	ILE
1	B	209	PHE
1	B	234	GLN
1	B	297	ASN
1	B	316	LEU
1	B	322	GLU
1	B	329	GLU
1	B	379	LYS
1	B	414	GLN
1	B	417	LEU
1	B	419	GLU
1	C	40	LEU
1	C	61	ILE
1	C	135	LEU
1	C	143	ARG
1	C	148	ARG
1	C	174	LEU
1	C	251	LYS
1	C	337	LYS
1	C	417	LEU
1	D	33	LEU
1	D	40	LEU
1	D	174	LEU
1	D	209	PHE
1	D	316	LEU
1	D	417	LEU
1	D	419	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	239	GLN

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Mol	Chain	Res	Type
1	A	297	ASN
1	A	338	ASN
1	A	466	GLN
1	B	50	ASN
1	B	56	ASN
1	B	72	HIS
1	B	150	GLN
1	B	167	ASN
1	B	297	ASN
1	B	409	GLN
1	B	414	GLN
1	B	477	HIS
1	C	53	GLN
1	C	56	ASN
1	C	229	HIS
1	C	236	GLN
1	C	239	GLN
1	C	242	GLN
1	C	297	ASN
1	C	328	HIS
1	C	340	GLN
1	C	409	GLN
1	C	412	ASN
1	C	414	GLN
1	C	422	GLN
1	D	53	GLN
1	D	56	ASN
1	D	229	HIS
1	D	236	GLN
1	D	242	GLN
1	D	256	GLN
1	D	276	GLN
1	D	297	ASN
1	D	407	ASN
1	D	409	GLN
1	D	466	GLN

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](#)

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
3	D3G	B	501	2	14,14,14	1.71	3 (21%)	17,18,18	0.44	0
2	HEM	C	500	1,3	50,50,50	2.35	23 (46%)	67,82,82	1.32	10 (14%)
2	HEM	B	500	1,3	50,50,50	2.37	25 (50%)	67,82,82	1.36	12 (17%)
3	D3G	C	501	2	14,14,14	1.69	2 (14%)	17,18,18	0.62	0
2	HEM	A	500	1,3	50,50,50	2.37	24 (48%)	67,82,82	1.34	11 (16%)
3	D3G	D	501	2	14,14,14	1.70	2 (14%)	17,18,18	0.45	0
2	HEM	D	500	1,3	50,50,50	2.37	23 (46%)	67,82,82	1.32	11 (16%)
3	D3G	A	501	2	14,14,14	1.74	3 (21%)	17,18,18	0.42	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	D3G	B	501	2	-	0/6/6/6	0/2/2/2
2	HEM	C	500	1,3	-	2/14/54/54	-
2	HEM	B	500	1,3	-	4/14/54/54	-
3	D3G	C	501	2	-	0/6/6/6	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	500	1,3	-	2/14/54/54	-
3	D3G	D	501	2	-	0/6/6/6	0/2/2/2
2	HEM	D	500	1,3	-	4/14/54/54	-
3	D3G	A	501	2	-	0/6/6/6	0/2/2/2

All (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C1D-ND	-4.70	1.29	1.38
2	B	500	HEM	C1D-ND	-4.51	1.30	1.38
2	B	500	HEM	FE-ND	4.29	2.08	1.94
2	A	500	HEM	FE-ND	4.26	2.08	1.94
2	D	500	HEM	C1B-NB	-4.23	1.32	1.40
2	D	500	HEM	CMA-C3A	4.12	1.59	1.50
2	C	500	HEM	FE-NA	4.10	2.08	1.95
2	B	500	HEM	C4A-NA	-4.05	1.32	1.39
2	D	500	HEM	C4A-NA	-4.01	1.32	1.39
2	C	500	HEM	CMA-C3A	3.99	1.59	1.50
2	C	500	HEM	C1D-ND	-3.99	1.31	1.38
2	D	500	HEM	FE-ND	3.95	2.07	1.94
2	A	500	HEM	CBB-CAB	3.92	1.49	1.30
2	C	500	HEM	FE-ND	3.91	2.06	1.94
2	A	500	HEM	FE-NB	3.91	2.06	1.94
2	D	500	HEM	FE-NB	3.90	2.06	1.94
2	A	500	HEM	C1B-NB	-3.90	1.33	1.40
2	D	500	HEM	C1C-NC	-3.89	1.32	1.39
2	C	500	HEM	C1C-NC	-3.88	1.32	1.39
2	D	500	HEM	FE-NA	3.86	2.07	1.95
2	D	500	HEM	C1D-ND	-3.83	1.31	1.38
2	C	500	HEM	C4A-NA	-3.82	1.32	1.39
2	D	500	HEM	C1C-C2C	-3.78	1.37	1.45
2	A	500	HEM	C4D-ND	-3.78	1.33	1.40
2	B	500	HEM	CBB-CAB	3.78	1.48	1.30
2	A	500	HEM	C4A-NA	-3.75	1.32	1.39
2	D	500	HEM	CBB-CAB	3.75	1.48	1.30
2	B	500	HEM	C1B-NB	-3.75	1.33	1.40
2	B	500	HEM	C1C-NC	-3.72	1.32	1.39
2	A	500	HEM	C1C-NC	-3.71	1.32	1.39
2	B	500	HEM	FE-NA	3.70	2.07	1.95
2	C	500	HEM	CAC-C3C	-3.68	1.37	1.47
2	D	500	HEM	CAC-C3C	-3.68	1.37	1.47
2	C	500	HEM	CBB-CAB	3.61	1.47	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	CAC-C3C	-3.58	1.37	1.47
2	B	500	HEM	C4D-ND	-3.56	1.34	1.40
2	A	500	HEM	CMA-C3A	3.51	1.58	1.50
2	B	500	HEM	FE-NB	3.46	2.05	1.94
2	A	500	HEM	CAC-C3C	-3.45	1.38	1.47
2	C	500	HEM	C1B-NB	-3.45	1.34	1.40
2	A	500	HEM	FE-NA	3.44	2.06	1.95
2	B	500	HEM	C1C-C2C	-3.43	1.38	1.45
2	B	500	HEM	C4B-NB	-3.40	1.32	1.38
2	C	500	HEM	FE-NB	3.38	2.05	1.94
2	C	500	HEM	C4D-ND	-3.36	1.34	1.40
3	A	501	D3G	C_4-C_5	3.35	1.44	1.39
2	C	500	HEM	C1C-C2C	-3.33	1.38	1.45
2	B	500	HEM	CMA-C3A	3.28	1.57	1.50
3	B	501	D3G	C_4-C_5	3.27	1.44	1.39
2	D	500	HEM	C4B-NB	-3.27	1.32	1.38
2	D	500	HEM	C4D-ND	-3.25	1.34	1.40
3	D	501	D3G	C_4-C_5	3.24	1.44	1.39
3	C	501	D3G	C_1-C_5	3.24	1.44	1.39
2	A	500	HEM	C4B-NB	-3.20	1.32	1.38
2	C	500	HEM	FE-NC	3.18	2.05	1.95
2	A	500	HEM	CMC-C2C	3.17	1.57	1.50
2	C	500	HEM	C3B-C2B	3.15	1.43	1.37
2	C	500	HEM	C4B-NB	-3.13	1.32	1.38
2	B	500	HEM	CMC-C2C	3.09	1.57	1.50
2	B	500	HEM	C3B-C2B	3.08	1.43	1.37
2	A	500	HEM	C1C-C2C	-3.05	1.39	1.45
2	A	500	HEM	FE-NC	3.01	2.05	1.95
3	B	501	D3G	C_1-C_5	3.01	1.44	1.39
3	A	501	D3G	C_1-C_5	2.99	1.43	1.39
2	C	500	HEM	CMC-C2C	2.97	1.56	1.50
3	D	501	D3G	C_1-C_5	2.95	1.43	1.39
2	D	500	HEM	FE-NC	2.91	2.04	1.95
2	B	500	HEM	FE-NC	2.88	2.04	1.95
3	C	501	D3G	C_4-C_5	2.85	1.43	1.39
2	A	500	HEM	C3B-C2B	2.71	1.42	1.37
2	D	500	HEM	CMC-C2C	2.70	1.56	1.50
2	C	500	HEM	C4D-C3D	-2.68	1.40	1.45
2	B	500	HEM	O2A-CGA	-2.67	1.22	1.30
2	D	500	HEM	C3B-C2B	2.60	1.42	1.37
2	A	500	HEM	C4D-C3D	-2.53	1.40	1.45
2	B	500	HEM	C4D-C3D	-2.50	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	CBC-CAC	2.50	1.42	1.30
2	C	500	HEM	CBC-CAC	2.48	1.42	1.30
2	A	500	HEM	CBD-CGD	2.45	1.56	1.50
2	A	500	HEM	CBC-CAC	2.44	1.42	1.30
2	B	500	HEM	C4C-NC	-2.43	1.35	1.39
2	C	500	HEM	C4C-NC	-2.38	1.35	1.39
2	A	500	HEM	O2A-CGA	-2.38	1.23	1.30
2	D	500	HEM	CBC-CAC	2.32	1.41	1.30
2	C	500	HEM	O2A-CGA	-2.32	1.23	1.30
2	D	500	HEM	O2A-CGA	-2.32	1.23	1.30
2	D	500	HEM	C4C-NC	-2.29	1.35	1.39
2	C	500	HEM	CMD-C2D	2.25	1.55	1.50
2	A	500	HEM	C4C-NC	-2.19	1.35	1.39
2	D	500	HEM	C4D-C3D	-2.18	1.41	1.45
2	A	500	HEM	C3C-C4C	-2.16	1.42	1.46
3	B	501	D3G	C_7-C_6	2.12	1.39	1.35
2	D	500	HEM	C3C-C4C	-2.11	1.42	1.46
3	A	501	D3G	C_7-C_6	2.10	1.39	1.35
2	D	500	HEM	CMD-C2D	2.10	1.55	1.50
2	A	500	HEM	O2D-CGD	-2.07	1.24	1.30
2	B	500	HEM	C3C-C4C	-2.07	1.42	1.46
2	B	500	HEM	C3C-C2C	2.06	1.41	1.37
2	C	500	HEM	CAD-C3D	2.05	1.56	1.51
2	B	500	HEM	CAD-C3D	2.04	1.56	1.51
2	D	500	HEM	CAD-C3D	2.03	1.56	1.51
2	B	500	HEM	CBD-CGD	2.03	1.55	1.50
2	A	500	HEM	CAD-C3D	2.02	1.56	1.51
2	B	500	HEM	O2D-CGD	-2.01	1.24	1.30
2	C	500	HEM	C1D-C2D	-2.00	1.40	1.44

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	HEM	CHD-C4C-NC	-2.97	121.22	124.45
2	B	500	HEM	C3B-C4B-NB	2.92	111.56	109.47
2	A	500	HEM	CHD-C4C-NC	-2.88	121.31	124.45
2	A	500	HEM	C4B-C3B-C2B	-2.86	104.65	107.28
2	B	500	HEM	CHD-C4C-NC	-2.84	121.36	124.45
2	B	500	HEM	C4B-C3B-C2B	-2.77	104.73	107.28
2	D	500	HEM	C4B-C3B-C2B	-2.76	104.75	107.28
2	A	500	HEM	C3B-C4B-NB	2.75	111.44	109.47
2	B	500	HEM	C3B-C2B-C1B	-2.74	104.35	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	500	HEM	C3B-C4B-NB	2.73	111.43	109.47
2	D	500	HEM	CHD-C4C-NC	-2.63	121.59	124.45
2	D	500	HEM	O2A-CGA-CBA	2.62	122.28	114.00
2	D	500	HEM	C1C-CHC-C4B	2.60	131.54	126.02
2	C	500	HEM	O2A-CGA-CBA	2.59	122.20	114.00
2	B	500	HEM	C1C-CHC-C4B	2.59	131.53	126.02
2	B	500	HEM	C4C-C3C-C2C	-2.58	104.58	106.81
2	A	500	HEM	C1C-CHC-C4B	2.56	131.46	126.02
2	C	500	HEM	C3B-C2B-C1B	-2.56	104.49	106.41
2	C	500	HEM	C1C-CHC-C4B	2.55	131.44	126.02
2	A	500	HEM	O2A-CGA-CBA	2.54	122.03	114.00
2	B	500	HEM	O2A-CGA-CBA	2.51	121.92	114.00
2	A	500	HEM	C4C-C3C-C2C	-2.49	104.66	106.81
2	C	500	HEM	C4B-C3B-C2B	-2.47	105.01	107.28
2	D	500	HEM	C4D-ND-C1D	2.45	108.10	105.21
2	C	500	HEM	C1B-NB-C4B	2.43	108.09	105.21
2	C	500	HEM	C3B-C4B-NB	2.41	111.20	109.47
2	B	500	HEM	C4D-ND-C1D	2.40	108.05	105.21
2	D	500	HEM	C4C-C3C-C2C	-2.38	104.75	106.81
2	A	500	HEM	C4D-ND-C1D	2.38	108.02	105.21
2	B	500	HEM	C1B-NB-C4B	2.36	108.00	105.21
2	D	500	HEM	C3B-C2B-C1B	-2.33	104.66	106.41
2	D	500	HEM	C1B-NB-C4B	2.33	107.96	105.21
2	C	500	HEM	C4D-ND-C1D	2.31	107.95	105.21
2	A	500	HEM	C4A-CHB-C1B	2.30	131.66	126.25
2	A	500	HEM	C1B-NB-C4B	2.30	107.93	105.21
2	C	500	HEM	C4C-C3C-C2C	-2.29	104.83	106.81
2	A	500	HEM	C4C-CHD-C1D	2.28	130.87	126.02
2	A	500	HEM	C3B-C2B-C1B	-2.26	104.71	106.41
2	D	500	HEM	C4A-CHB-C1B	2.25	131.54	126.25
2	C	500	HEM	C4C-CHD-C1D	2.23	130.77	126.02
2	B	500	HEM	C4A-CHB-C1B	2.18	131.36	126.25
2	B	500	HEM	C4C-CHD-C1D	2.10	130.49	126.02
2	B	500	HEM	CHC-C1C-NC	-2.03	122.24	124.45
2	D	500	HEM	C4C-CHD-C1D	2.01	130.28	126.02

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	500	HEM	C2C-C3C-CAC-CBC
2	B	500	HEM	C4C-C3C-CAC-CBC

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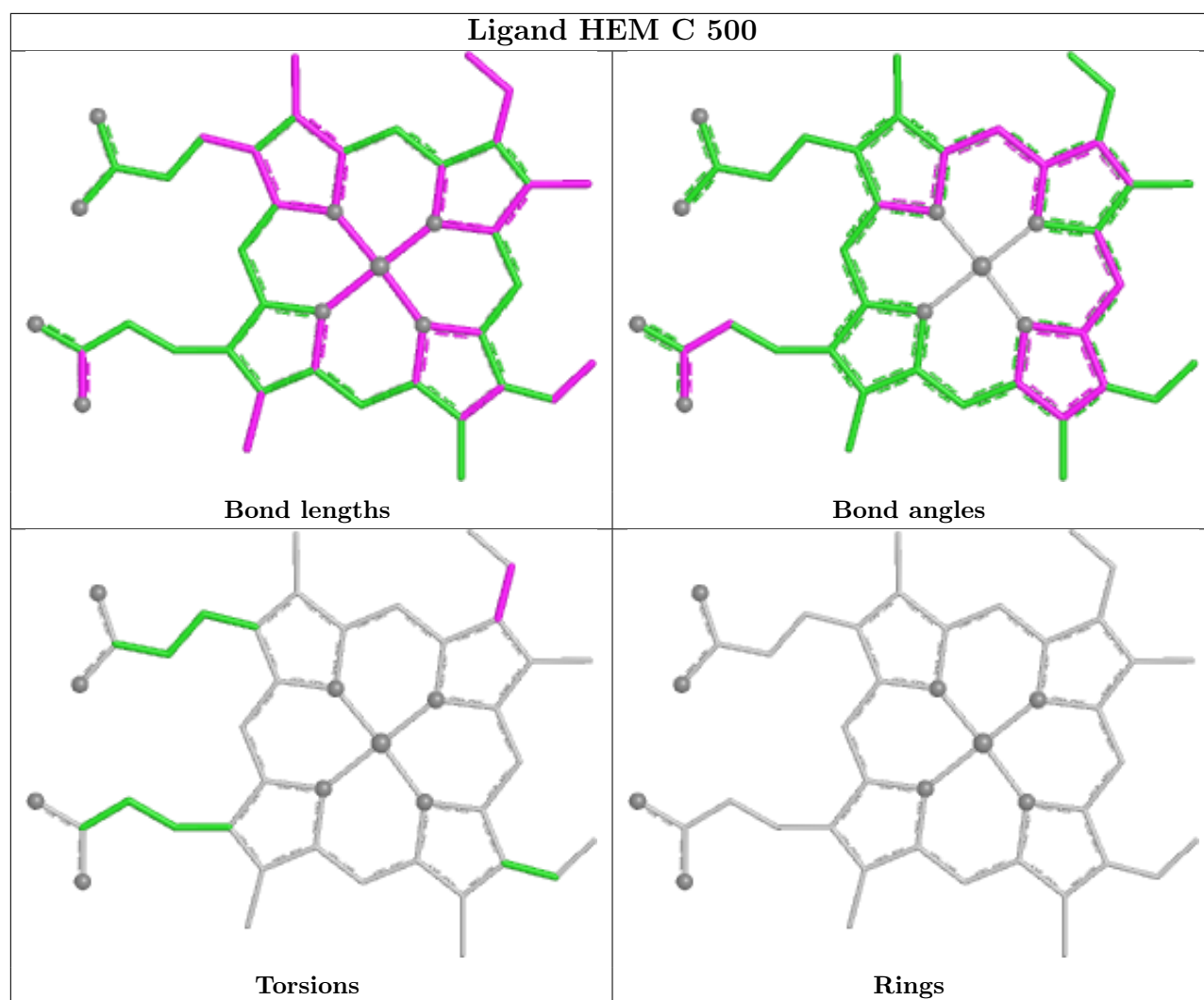
Mol	Chain	Res	Type	Atoms
2	C	500	HEM	C2C-C3C-CAC-CBC
2	D	500	HEM	C2C-C3C-CAC-CBC
2	D	500	HEM	C4C-C3C-CAC-CBC
2	C	500	HEM	C4C-C3C-CAC-CBC
2	A	500	HEM	C2C-C3C-CAC-CBC
2	A	500	HEM	C4C-C3C-CAC-CBC
2	B	500	HEM	CAA-CBA-CGA-O1A
2	B	500	HEM	CAA-CBA-CGA-O2A
2	D	500	HEM	CAD-CBD-CGD-O2D
2	D	500	HEM	CAD-CBD-CGD-O1D

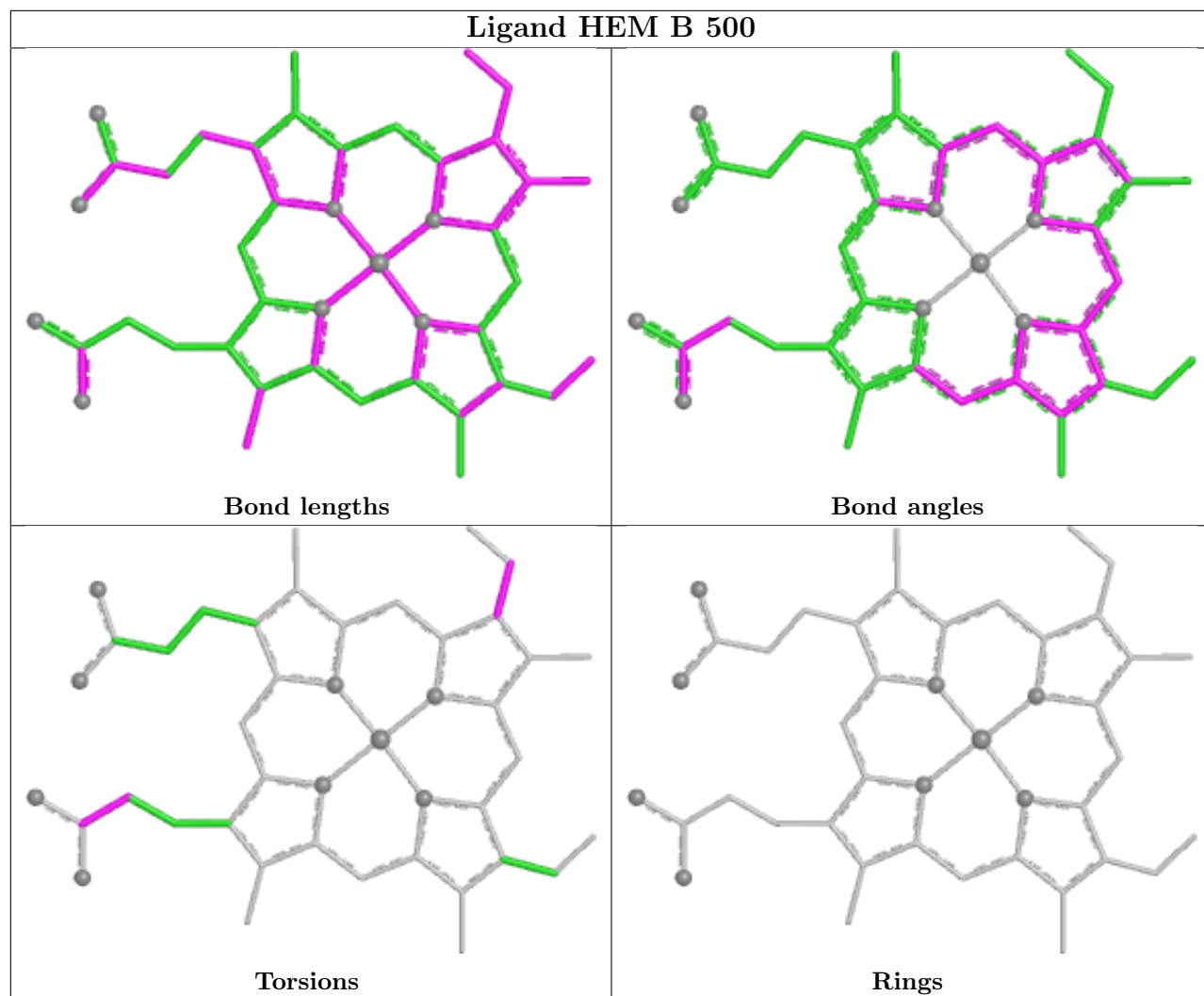
There are no ring outliers.

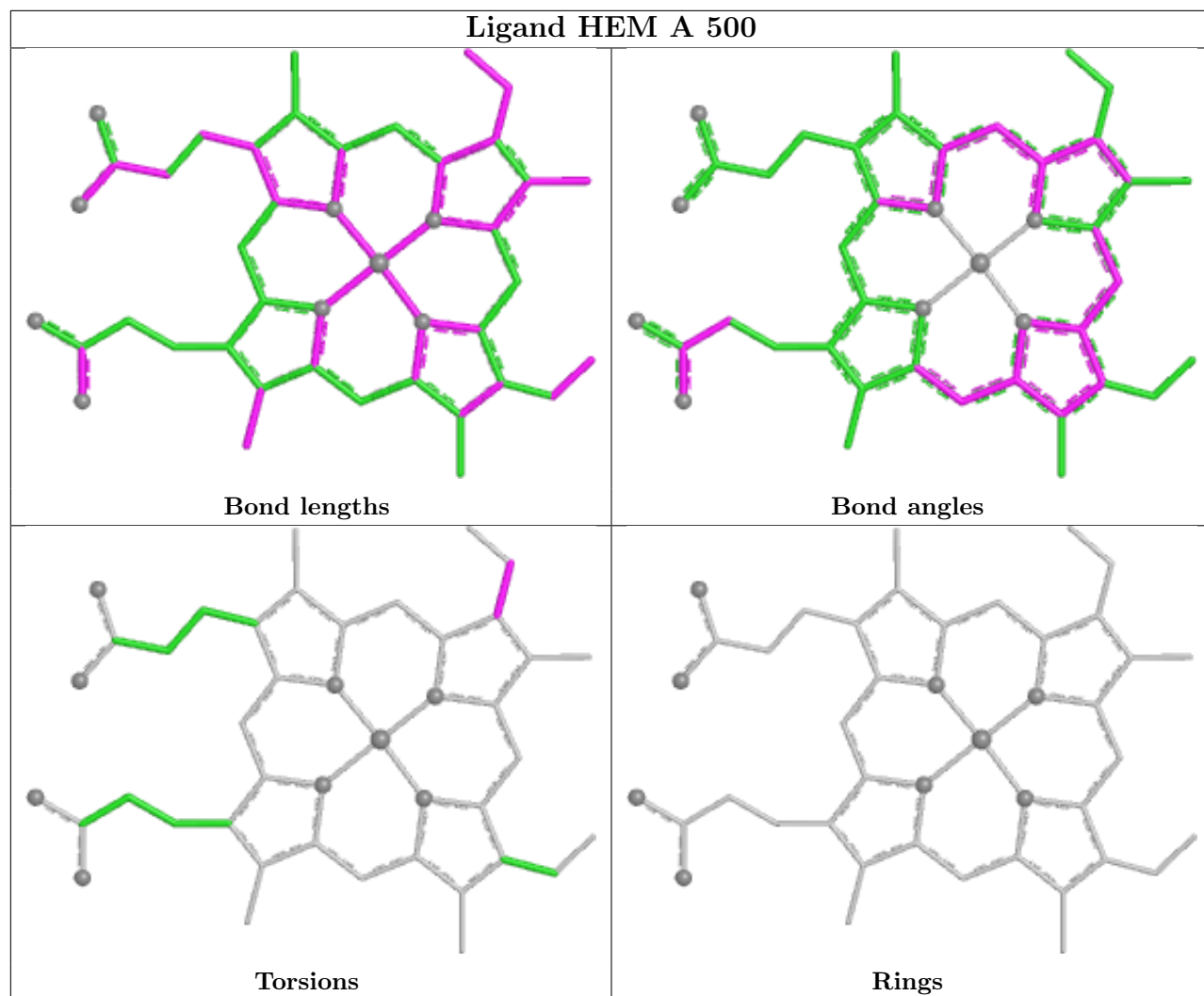
6 monomers are involved in 12 short contacts:

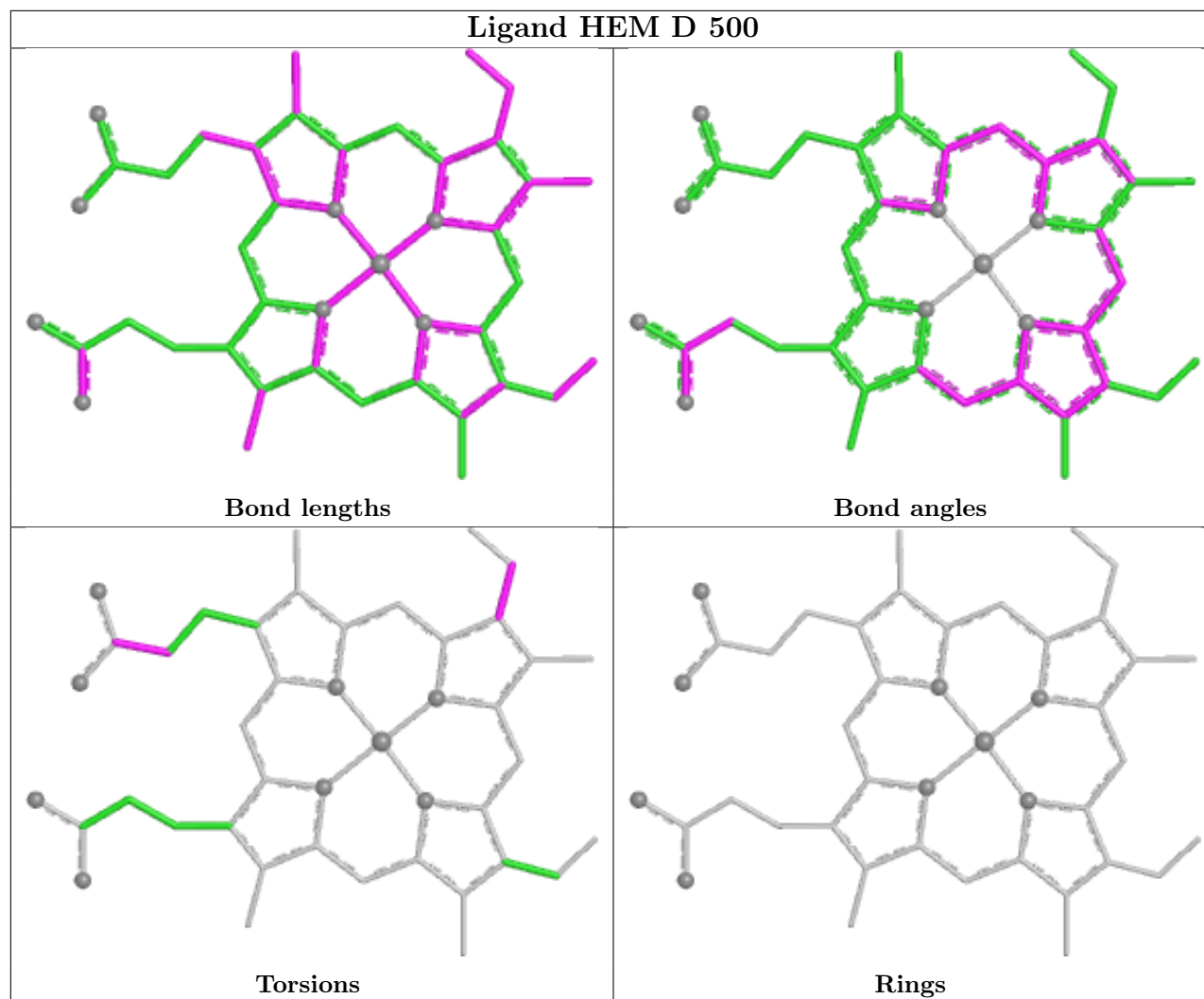
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	D3G	1	0
2	C	500	HEM	2	0
2	B	500	HEM	2	0
3	C	501	D3G	1	0
2	A	500	HEM	3	0
2	D	500	HEM	3	0

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	465/476 (97%)	0.06	6 (1%) 75 76	21, 33, 53, 73	0
1	B	465/476 (97%)	0.68	36 (7%) 19 20	25, 43, 65, 87	0
1	C	464/476 (97%)	-0.02	4 (0%) 81 83	21, 32, 52, 69	0
1	D	464/476 (97%)	0.14	12 (2%) 57 59	21, 33, 60, 76	0
All	All	1858/1904 (97%)	0.22	58 (3%) 51 52	21, 35, 58, 87	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	31	GLY	4.8
1	D	141	GLY	4.0
1	D	140	VAL	3.9
1	B	193	TYR	3.9
1	B	198	PHE	3.4
1	B	258	THR	3.3
1	D	139	GLY	3.3
1	B	273	ILE	3.2
1	B	61	ILE	3.0
1	A	31	GLY	3.0
1	A	419	GLU	3.0
1	B	471	ILE	3.0
1	D	138	PHE	2.9
1	B	473	VAL	2.8
1	B	259	LEU	2.7
1	B	496	HIS	2.7
1	B	468	PRO	2.7
1	C	147	GLU	2.7
1	B	140	VAL	2.7
1	D	273	ILE	2.7
1	B	203	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	142	LYS	2.6
1	B	173	PHE	2.6
1	B	195	ASP	2.6
1	B	262	ASN	2.5
1	B	188	GLY	2.5
1	D	264	PRO	2.4
1	B	261	PRO	2.4
1	B	33	LEU	2.4
1	C	418	ASN	2.3
1	B	257	ARG	2.3
1	D	282	PRO	2.3
1	A	461	ARG	2.3
1	B	495	HIS	2.3
1	A	417	LEU	2.2
1	B	268	ILE	2.2
1	B	336	GLY	2.2
1	D	144	GLY	2.2
1	B	208	ILE	2.2
1	B	249	ALA	2.2
1	A	64	ARG	2.1
1	D	271	PHE	2.1
1	B	202	LEU	2.1
1	C	194	LYS	2.1
1	B	82	CYS	2.1
1	B	282	PRO	2.1
1	B	145	ILE	2.1
1	D	147	GLU	2.1
1	B	141	GLY	2.1
1	B	379	LYS	2.1
1	B	191	PHE	2.1
1	A	406	SER	2.1
1	B	382	ASP	2.0
1	D	276	GLN	2.0
1	B	201	LEU	2.0
1	B	274	ARG	2.0
1	B	60	LYS	2.0
1	B	484	PRO	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

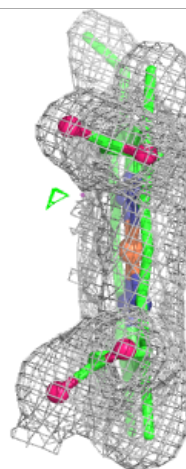
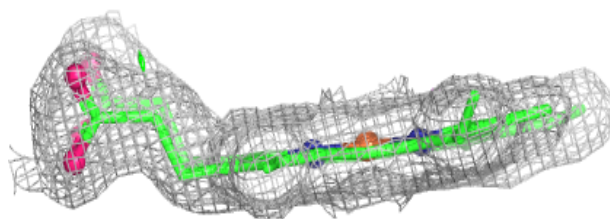
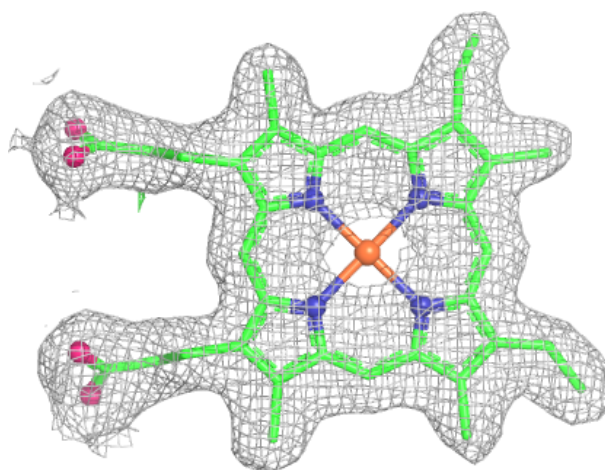
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	D3G	D	501	13/13	0.93	0.07	21,24,27,27	0
3	D3G	B	501	13/13	0.94	0.08	30,35,36,37	0
3	D3G	A	501	13/13	0.94	0.07	23,27,29,31	0
3	D3G	C	501	13/13	0.95	0.07	25,25,26,28	0
2	HEM	A	500	43/43	0.98	0.05	19,23,27,28	0
2	HEM	B	500	43/43	0.98	0.06	24,30,35,37	0
2	HEM	C	500	43/43	0.98	0.06	21,24,27,29	0
2	HEM	D	500	43/43	0.98	0.06	20,25,28,31	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.

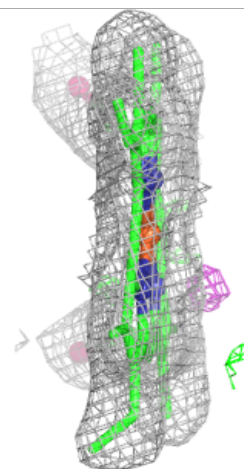
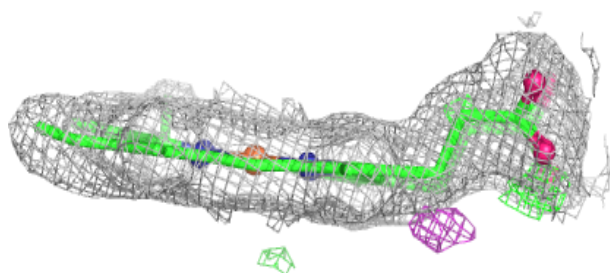
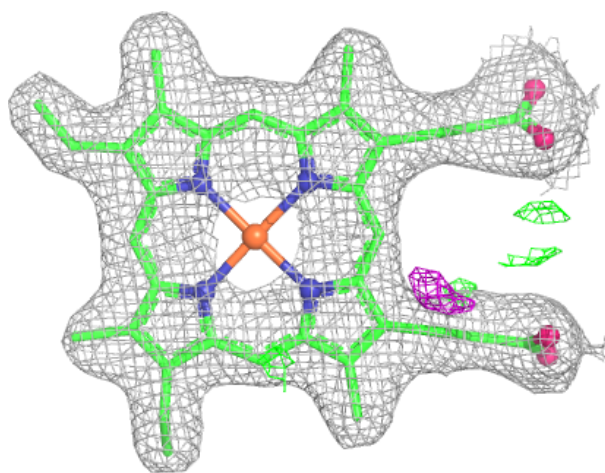
Electron density around HEM A 500:

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



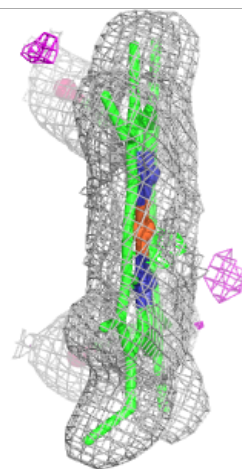
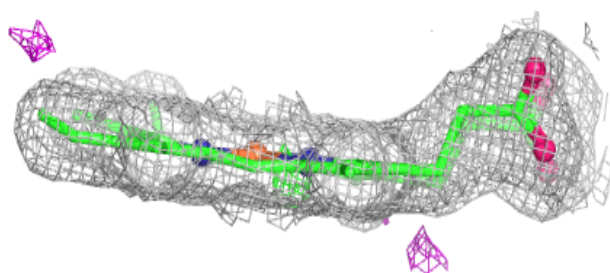
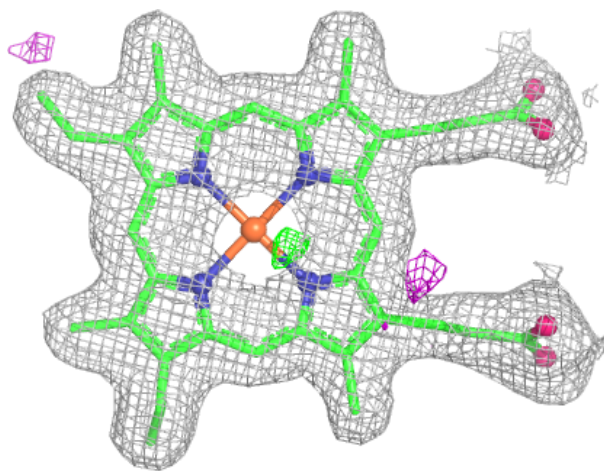
Electron density around HEM B 500:

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



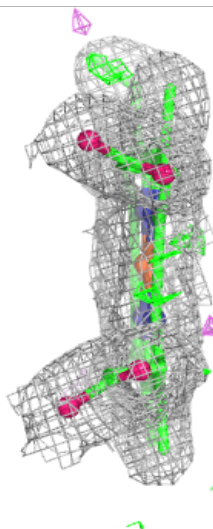
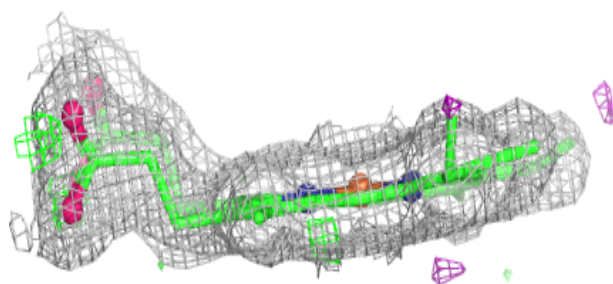
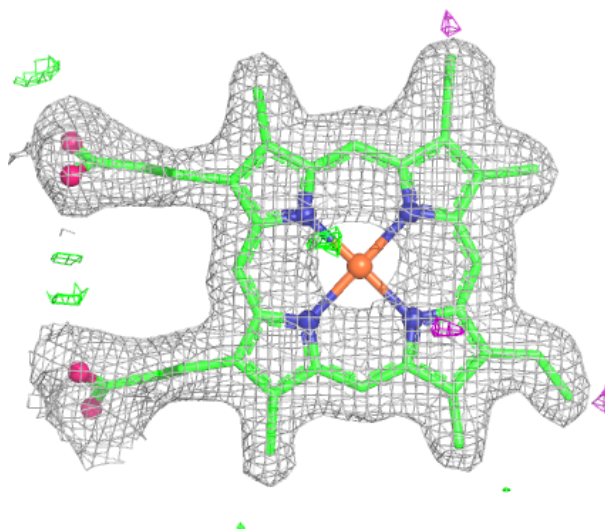
Electron density around HEM C 500:

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



Electron density around HEM 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.