



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:32 AM UTC

PDB ID : 4CX7 / pdb_00004cx7
Title : Structure of human iNOS heme domain in complex with (R)-6-(3-AMINO-2-(5-(2-(6-AMINO-4-METHYLPYRIDIN-2-YL)ETHYL)PYRIDIN-3-YL)PROPYL)-4-METHYLPYRIDIN-2-AMINE
Authors : Li, H.; Poulos, T.L.
Deposited on : 2014-04-03
Resolution : 3.16 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:

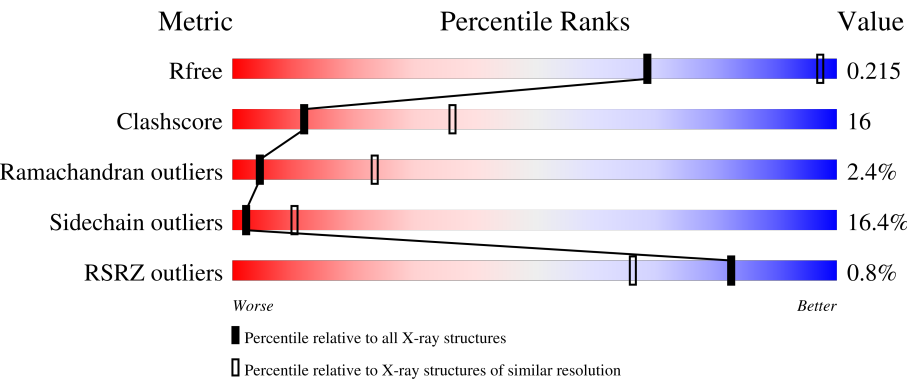
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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

The reported resolution of this entry is 3.16 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	431	
1	B	431	
1	C	431	
1	D	431	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13889 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 NITRIC OXIDE SYNTHASE, INDUCIBLE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	1
			3367	2155	589	602	21			
1	B	414	Total	C	N	O	S	0	0	1
			3367	2155	589	602	21			
1	C	414	Total	C	N	O	S	0	0	1
			3367	2155	589	602	21			
1	D	414	Total	C	N	O	S	0	0	1
			3367	2155	589	602	21			

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



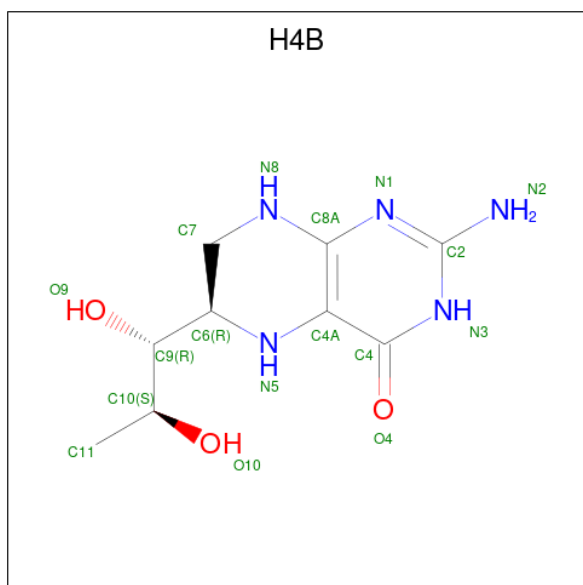
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		
2	B	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		

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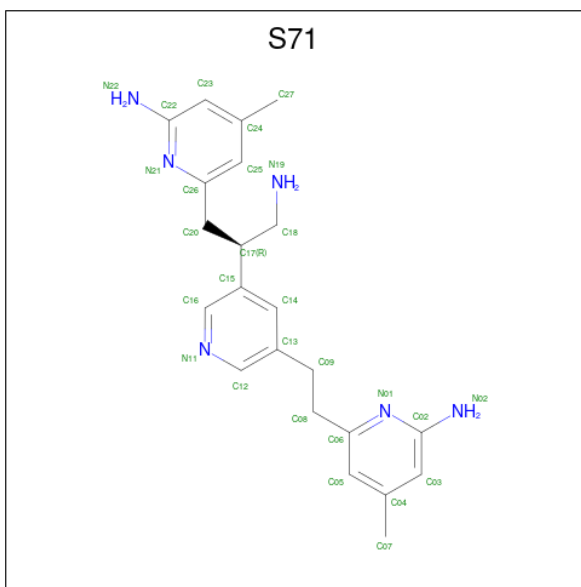
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula: $C_9H_{15}N_5O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		
3	C	1	Total	C	N	O	0	0
			17	9	5	3		
3	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is (R)-6-(3-amino-2-(5-(2-(6-amino-4-methylpyridin-2-yl)ethyl)pyridin-3-yl)propyl)-4-methylpyridin-2-amine (CCD ID: S71) (formula: $C_{22}H_{28}N_6$).



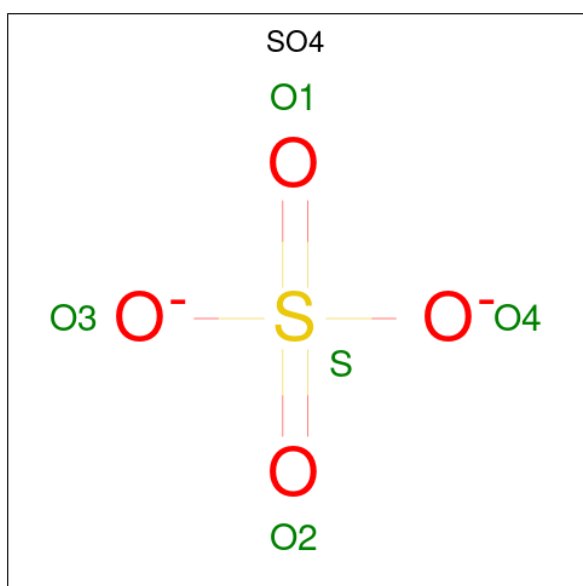
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			28	22	6		
4	B	1	Total	C	N	0	0
			28	22	6		
4	C	1	Total	C	N	0	0
			28	22	6		
4	D	1	Total	C	N	0	0
			28	22	6		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0

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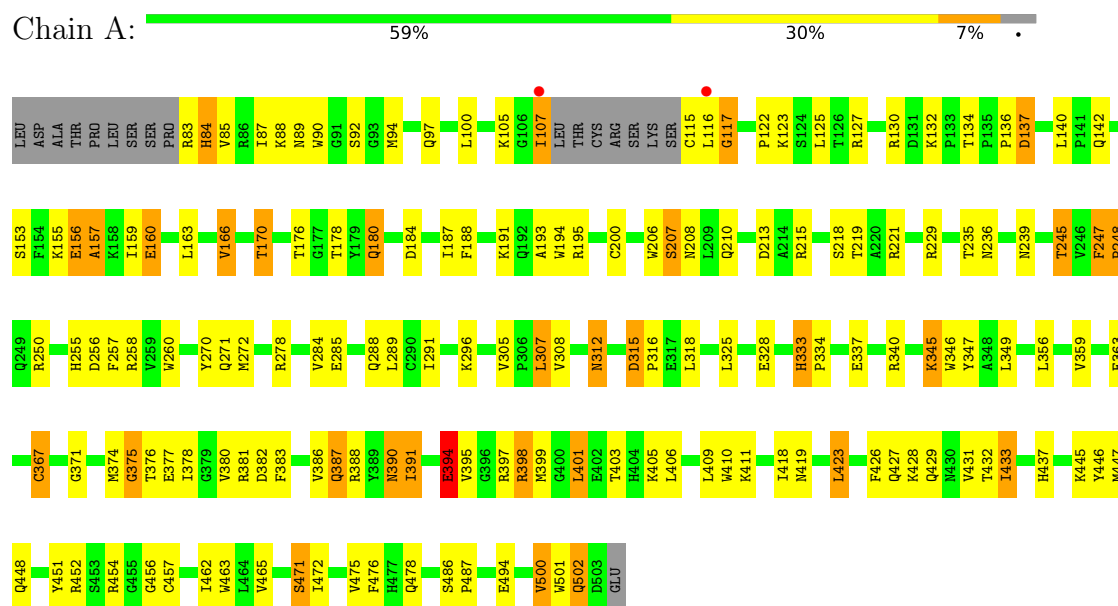
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	O	S	0	0
			5	4	1		

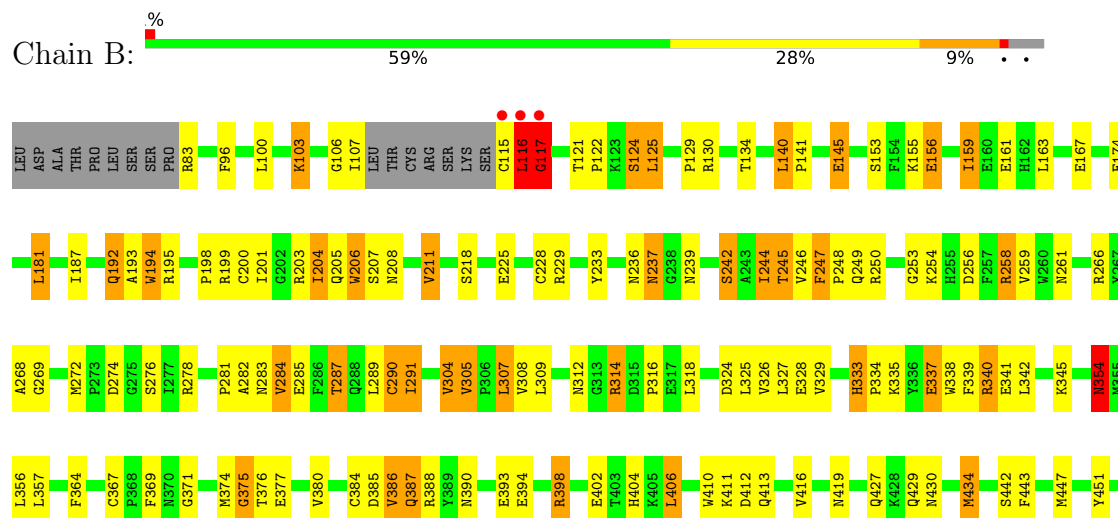
3 Residue-property plots

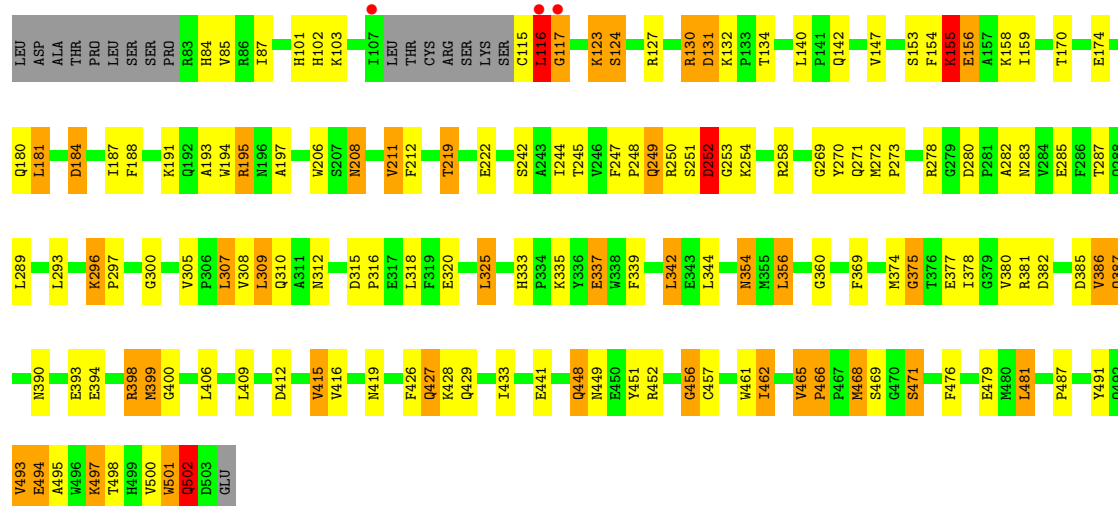
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: NITRIC OXIDE SYNTHASE, INDUCIBLE



• Molecule 1: NITRIC OXIDE SYNTHASE, INDUCIBLE





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	189.22Å 189.22Å 232.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	146.83 – 3.16 146.83 – 3.16	Depositor EDS
% Data completeness (in resolution range)	99.5 (146.83-3.16) 99.7 (146.83-3.16)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.174 , 0.216 0.174 , 0.215	Depositor DCC
R_{free} test set	3678 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	81.0	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13889	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: S71, SO4, GOL, H4B, 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	0.97	1/3465 (0.0%)	1.30	24/4703 (0.5%)
1	B	0.95	3/3465 (0.1%)	1.28	18/4703 (0.4%)
1	C	0.84	2/3465 (0.1%)	1.22	20/4703 (0.4%)
1	D	0.96	1/3465 (0.0%)	1.28	24/4703 (0.5%)
All	All	0.93	7/13860 (0.1%)	1.27	86/18812 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	2
1	D	0	1
All	All	0	5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	502	GLN	C-N	-7.07	1.23	1.33
1	C	502	GLN	C-N	-6.76	1.23	1.33
1	A	502	GLN	C-N	-6.65	1.24	1.33
1	B	502	GLN	C-N	-6.49	1.24	1.33
1	B	117	GLY	N-CA	6.02	1.54	1.45
1	C	85	VAL	N-CA	5.59	1.53	1.46
1	B	198	PRO	N-CA	-5.53	1.41	1.47

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	465	VAL	CA-C-N	13.95	129.84	119.66
1	D	465	VAL	C-N-CA	13.95	129.84	119.66
1	C	272	MET	CA-C-N	8.78	130.82	119.84
1	C	272	MET	C-N-CA	8.78	130.82	119.84
1	C	161	GLU	N-CA-C	-8.64	101.34	112.23
1	C	218	SER	N-CA-C	8.33	124.12	114.62
1	B	254	LYS	N-CA-C	-7.42	104.37	113.50
1	C	397	ARG	N-CA-C	-7.42	102.21	111.11
1	A	247	PHE	CA-C-N	7.41	129.10	119.84
1	A	247	PHE	C-N-CA	7.41	129.10	119.84
1	D	399	MET	N-CA-C	-7.38	104.28	113.20
1	B	430	ASN	N-CA-C	7.33	121.64	111.74
1	A	457	CYS	CA-C-N	7.12	127.38	119.90
1	A	457	CYS	C-N-CA	7.12	127.38	119.90
1	A	500	VAL	N-CA-CB	6.97	118.32	110.72
1	B	247	PHE	CA-C-N	6.86	128.42	119.84
1	B	247	PHE	C-N-CA	6.86	128.42	119.84
1	D	325	LEU	N-CA-C	-6.82	106.16	114.75
1	A	390	ASN	N-CA-C	6.80	120.62	111.24
1	D	466	PRO	N-CA-C	6.49	116.70	110.47
1	C	159	ILE	N-CA-C	6.42	117.17	110.62
1	D	219	THR	CB-CA-C	-6.39	99.39	110.45
1	D	211	VAL	N-CA-C	6.32	116.73	107.37
1	A	305	VAL	CA-C-N	-6.29	114.29	120.52
1	A	305	VAL	C-N-CA	-6.29	114.29	120.52
1	D	419	ASN	N-CA-C	6.29	119.11	111.82
1	B	121	THR	CB-CA-C	6.14	120.72	111.14
1	D	253	GLY	N-CA-C	-6.14	106.23	115.32
1	B	246	VAL	N-CA-C	6.14	116.46	107.37
1	A	359	VAL	CB-CA-C	-6.08	102.13	110.77
1	A	325	LEU	CA-C-N	-6.02	115.97	122.59
1	A	325	LEU	C-N-CA	-6.02	115.97	122.59
1	A	333	HIS	CA-C-N	-5.95	114.10	120.47
1	A	333	HIS	C-N-CA	-5.95	114.10	120.47
1	D	491	TYR	N-CA-C	-5.92	101.75	110.52
1	A	218	SER	N-CA-C	5.80	120.89	113.18
1	B	305	VAL	N-CA-CB	-5.79	103.10	111.21
1	B	483	TYR	N-CA-C	5.78	117.63	108.79
1	B	304	VAL	N-CA-CB	5.77	116.82	110.53
1	A	349	LEU	N-CA-C	5.77	119.08	108.69
1	C	430	ASN	N-CA-C	5.75	123.05	110.80
1	A	208	ASN	CB-CA-C	5.74	119.38	111.23
1	D	197	ALA	CA-C-N	-5.71	113.98	120.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	197	ALA	C-N-CA	-5.71	113.98	120.89
1	D	184	ASP	N-CA-C	5.67	117.32	111.03
1	D	250	ARG	N-CA-C	-5.64	102.17	110.52
1	D	457	CYS	CA-C-N	5.63	125.39	119.76
1	D	457	CYS	C-N-CA	5.63	125.39	119.76
1	B	194	TRP	N-CA-C	-5.63	105.06	111.14
1	C	84	HIS	N-CA-C	-5.61	99.76	108.90
1	D	180	GLN	CA-C-N	-5.56	113.92	122.87
1	D	180	GLN	C-N-CA	-5.56	113.92	122.87
1	D	493	VAL	CB-CA-C	-5.51	104.08	110.91
1	A	397	ARG	N-CA-C	-5.50	104.51	111.11
1	A	500	VAL	CB-CA-C	-5.46	104.14	110.91
1	C	85	VAL	N-CA-C	5.38	115.85	107.99
1	A	207	SER	N-CA-C	-5.37	106.70	113.20
1	C	321	ILE	CA-C-N	-5.37	114.85	120.38
1	C	321	ILE	C-N-CA	-5.37	114.85	120.38
1	C	268	ALA	CA-C-N	5.35	125.29	121.65
1	C	268	ALA	C-N-CA	5.35	125.29	121.65
1	C	179	TYR	N-CA-C	5.33	117.17	109.07
1	C	322	PRO	CA-C-N	5.33	126.50	119.84
1	C	322	PRO	C-N-CA	5.33	126.50	119.84
1	C	231	VAL	N-CA-C	5.32	115.53	110.42
1	B	333	HIS	N-CA-C	-5.30	103.39	110.07
1	C	253	GLY	N-CA-C	-5.26	107.25	114.67
1	B	386	VAL	CB-CA-C	-5.25	105.05	112.14
1	C	185	GLU	N-CA-C	-5.25	105.98	112.38
1	B	116	LEU	CA-CB-CG	5.22	134.56	116.30
1	B	272	MET	CA-C-N	5.20	126.34	119.84
1	B	272	MET	C-N-CA	5.20	126.34	119.84
1	A	394	GLU	N-CA-C	5.19	116.62	111.07
1	A	367	CYS	CA-C-N	-5.17	114.40	119.99
1	A	367	CYS	C-N-CA	-5.17	114.40	119.99
1	D	495	ALA	N-CA-C	5.17	116.91	111.28
1	D	325	LEU	CA-C-O	5.15	124.35	118.47
1	D	466	PRO	O-C-N	5.14	123.67	121.31
1	B	116	LEU	CA-C-N	5.12	131.45	121.41
1	B	116	LEU	C-N-CA	5.12	131.45	121.41
1	B	284	VAL	CB-CA-C	-5.11	105.33	111.88
1	A	315	ASP	CA-C-N	-5.10	115.32	120.31
1	A	315	ASP	C-N-CA	-5.10	115.32	120.31
1	D	456	GLY	N-CA-C	5.05	117.94	110.42
1	D	219	THR	N-CA-CB	5.03	118.26	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	304	VAL	N-CA-CB	5.03	117.49	111.31

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	284	VAL	Peptide
1	B	207	SER	Peptide
1	C	160	GLU	Peptide
1	C	284	VAL	Peptide
1	D	251	SER	Peptide

5.2 Too-close contacts [i](#)

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	3367	0	3268	102	0
1	B	3367	0	3268	103	0
1	C	3367	0	3268	135	0
1	D	3367	0	3268	98	0
2	A	43	0	30	2	0
2	B	43	0	30	5	0
2	C	43	0	30	3	0
2	D	43	0	30	2	0
3	A	17	0	15	1	0
3	B	17	0	15	0	0
3	C	17	0	15	0	0
3	D	17	0	15	0	0
4	A	28	0	28	2	0
4	B	28	0	28	1	0
4	C	28	0	28	0	0
4	D	28	0	28	1	0
5	A	6	0	8	2	0
5	B	6	0	8	1	0
5	C	6	0	8	1	0
5	D	6	0	8	1	0
6	A	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	10	0	0	0	0
6	C	10	0	0	0	0
6	D	10	0	0	0	0
All	All	13889	0	13396	430	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 16.

All (430) 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:B:387:GLN:H	1:B:387:GLN:HE21	1.05	1.02
1:C:140:LEU:HD21	1:C:170:THR:HG22	1.42	1.00
1:C:130:ARG:HH21	1:C:134:THR:HG23	1.25	1.00
1:C:278:ARG:HG3	1:C:278:ARG:HH11	1.29	0.98
1:B:283:ASN:O	1:B:287:THR:HG23	1.66	0.95
1:C:387:GLN:H	1:C:387:GLN:HE21	1.01	0.93
1:C:130:ARG:HG2	1:C:130:ARG:HH11	1.33	0.92
1:C:130:ARG:NH2	1:C:134:THR:HG23	1.84	0.92
1:A:387:GLN:H	1:A:387:GLN:HE21	0.94	0.91
1:D:448:GLN:NE2	1:D:452:ARG:HH12	1.69	0.90
1:B:181:LEU:HD23	1:B:181:LEU:H	1.38	0.87
1:D:269:GLY:H	1:D:287:THR:HG21	1.39	0.87
1:D:181:LEU:HD23	1:D:181:LEU:H	1.39	0.86
1:A:387:GLN:H	1:A:387:GLN:NE2	1.74	0.85
1:C:236:ASN:HB3	1:C:239:ASN:O	1.75	0.85
1:C:311:ALA:HB3	1:C:314:ARG:HH12	1.40	0.85
1:C:387:GLN:H	1:C:387:GLN:NE2	1.74	0.85
1:B:269:GLY:H	1:B:287:THR:HG21	1.39	0.85
1:A:387:GLN:HE21	1:A:387:GLN:N	1.74	0.83
1:A:247:PHE:HB3	1:A:248:PRO:HD2	1.62	0.82
1:B:181:LEU:HD23	1:B:181:LEU:N	1.94	0.81
1:C:182:THR:O	1:C:184:ASP:N	2.13	0.80
1:C:278:ARG:HH11	1:C:278:ARG:CG	1.96	0.78
1:A:160:GLU:CD	1:A:160:GLU:H	1.91	0.78
1:C:221:ARG:HB2	1:C:221:ARG:CZ	2.14	0.77
1:C:459:ALA:HB1	1:C:464:LEU:CD1	2.14	0.77
1:B:387:GLN:H	1:B:387:GLN:NE2	1.84	0.76
1:C:201:ILE:HG13	1:C:201:ILE:O	1.85	0.75
1:C:130:ARG:HH11	1:C:130:ARG:CG	1.99	0.75
1:C:387:GLN:HE21	1:C:387:GLN:N	1.83	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:PHE:CD2	2:B:550:HEM:HAC	2.23	0.73
1:C:278:ARG:HG3	1:C:278:ARG:NH1	1.96	0.73
1:A:100:LEU:HD22	1:A:454:ARG:HD2	1.71	0.73
1:C:130:ARG:HH21	1:C:134:THR:CG2	1.99	0.72
1:A:84:HIS:HB2	1:A:97:GLN:NE2	2.04	0.72
1:C:322:PRO:HD2	1:C:325:LEU:HD12	1.71	0.72
1:D:181:LEU:HD23	1:D:181:LEU:N	2.05	0.72
1:C:459:ALA:HB1	1:C:464:LEU:HD11	1.70	0.72
1:A:270:TYR:HB2	1:A:272:MET:CE	2.20	0.72
1:C:173:ILE:O	1:C:177:GLY:HA2	1.90	0.72
1:D:448:GLN:HE22	1:D:452:ARG:HH12	1.36	0.72
1:C:266:ARG:HH22	5:C:880:GOL:H2	1.55	0.71
1:D:116:LEU:HD13	1:D:123:LYS:HE3	1.73	0.71
1:A:213:ASP:OD1	1:A:215:ARG:HG3	1.91	0.71
1:D:252:ASP:HB3	1:D:254:LYS:H	1.56	0.70
1:C:182:THR:C	1:C:184:ASP:H	1.99	0.70
1:D:181:LEU:N	1:D:181:LEU:CD2	2.54	0.70
1:A:257:PHE:CE1	1:A:312:ASN:HB3	2.27	0.70
1:B:145:GLU:OE1	1:B:145:GLU:HA	1.91	0.69
1:B:187:ILE:HG12	1:B:211:VAL:HG21	1.74	0.69
1:B:129:PRO:HA	1:B:250:ARG:NH2	2.07	0.69
1:C:130:ARG:HG2	1:C:130:ARG:NH1	2.08	0.69
1:B:247:PHE:HB3	1:B:248:PRO:HD2	1.76	0.68
1:C:429:GLN:O	1:C:431:VAL:HG23	1.93	0.68
1:C:247:PHE:HB3	1:C:248:PRO:HD2	1.75	0.68
1:D:115:CYS:O	1:D:117:GLY:N	2.26	0.68
1:D:116:LEU:CD1	1:D:123:LYS:HE3	2.23	0.68
1:C:129:PRO:HA	1:C:250:ARG:HH22	1.59	0.68
1:D:181:LEU:H	1:D:181:LEU:CD2	2.07	0.67
1:B:266:ARG:NH2	1:B:388:ARG:NH2	2.42	0.67
1:A:122:PRO:HD2	1:A:125:LEU:HD12	1.76	0.67
1:B:181:LEU:N	1:B:181:LEU:CD2	2.58	0.67
1:B:380:VAL:HG11	1:B:467:PRO:HB2	1.75	0.67
1:B:398:ARG:CG	1:B:398:ARG:HH11	2.07	0.67
1:A:394:GLU:OE2	1:A:398:ARG:NH1	2.27	0.67
1:D:356:LEU:C	1:D:356:LEU:HD23	2.19	0.67
1:C:437:HIS:HB2	1:D:406:LEU:HD11	1.77	0.67
1:A:260:TRP:CZ2	1:A:316:PRO:HG3	2.30	0.66
1:C:484:VAL:HG12	1:C:488:PHE:CE2	2.31	0.66
1:D:412:ASP:O	1:D:416:VAL:HG23	1.96	0.66
1:B:115:CYS:O	1:B:117:GLY:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:HIS:ND1	1:B:334:PRO:HD2	2.10	0.65
1:D:116:LEU:HD13	1:D:123:LYS:CE	2.26	0.65
1:C:129:PRO:HA	1:C:250:ARG:NH2	2.11	0.64
1:A:378:ILE:HA	1:A:382:ASP:HB2	1.77	0.64
1:B:307:LEU:HB3	1:B:309:LEU:HD13	1.79	0.64
1:A:180:GLN:HA	1:A:180:GLN:NE2	2.11	0.64
1:A:451:TYR:CE1	1:A:456:GLY:HA2	2.32	0.64
1:B:380:VAL:O	1:B:384:CYS:HB2	1.97	0.64
1:D:155:LYS:HG3	1:D:156:GLU:OE2	1.98	0.64
1:A:250:ARG:NH2	1:A:256:ASP:OD2	2.31	0.63
1:B:107:ILE:HD12	1:B:124:SER:O	1.98	0.63
1:B:451:TYR:CE1	1:B:456:GLY:HA2	2.33	0.63
1:A:140:LEU:HD21	1:A:170:THR:HG23	1.80	0.63
1:B:281:PRO:O	1:B:284:VAL:HG23	1.99	0.63
1:A:127:ARG:NH1	1:A:363:GLU:OE2	2.32	0.62
1:A:115:CYS:O	1:A:117:GLY:N	2.25	0.62
1:D:448:GLN:NE2	1:D:452:ARG:NH1	2.45	0.62
1:B:129:PRO:HA	1:B:250:ARG:HH22	1.62	0.62
1:C:327:LEU:HD12	1:C:328:GLU:H	1.64	0.61
1:D:283:ASN:O	1:D:287:THR:HG23	2.00	0.61
1:C:244:ILE:HD11	1:C:367:CYS:HB2	1.82	0.61
1:B:357:LEU:HB3	1:B:364:PHE:HB2	1.83	0.61
1:C:140:LEU:CD2	1:C:170:THR:HG22	2.25	0.61
1:D:369:PHE:CD1	2:D:550:HEM:HAC	2.36	0.61
1:B:253:GLY:HA2	1:B:256:ASP:OD1	2.01	0.60
4:A:800:S71:H25	5:A:880:GOL:H11	1.84	0.60
1:C:263:GLN:HB3	1:C:351:ALA:O	2.00	0.60
1:A:328:GLU:CD	1:A:345:LYS:HE2	2.26	0.60
1:A:328:GLU:OE1	1:A:345:LYS:HE2	2.00	0.60
1:D:116:LEU:HD13	1:D:123:LYS:HZ1	1.66	0.60
1:A:270:TYR:HB2	1:A:272:MET:HE1	1.82	0.60
1:A:395:VAL:O	1:A:399:MET:HG3	2.02	0.60
1:C:184:ASP:HA	1:C:187:ILE:HD12	1.83	0.60
1:C:193:ALA:HB2	1:C:487:PRO:HB2	1.83	0.60
1:D:308:VAL:HG22	1:D:318:LEU:HD22	1.84	0.59
1:D:427:GLN:C	1:D:429:GLN:H	2.10	0.59
1:C:420:ILE:HG13	1:D:409:LEU:HD12	1.84	0.59
1:C:257:PHE:CE2	1:C:312:ASN:HB3	2.38	0.59
1:A:377:GLU:O	1:A:381:ARG:HB2	2.02	0.59
1:D:244:ILE:HD12	1:D:369:PHE:HB3	1.84	0.59
1:B:100:LEU:HB3	1:B:456:GLY:HA3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:GLU:O	1:B:340:ARG:HG3	2.03	0.59
1:A:308:VAL:HG22	1:A:318:LEU:HD22	1.85	0.58
1:C:498:THR:O	1:C:499:HIS:C	2.46	0.58
1:B:494:GLU:OE2	1:B:497:LYS:HE2	2.04	0.58
1:C:381:ARG:NH1	1:C:381:ARG:HG3	2.19	0.58
1:A:100:LEU:HB3	1:A:456:GLY:HA3	1.84	0.58
1:A:346:TRP:CD1	1:A:347:TYR:H	2.22	0.58
1:C:171:LYS:O	1:C:174:GLU:HB3	2.02	0.58
1:A:84:HIS:HB2	1:A:97:GLN:HE21	1.67	0.57
1:C:187:ILE:HA	1:C:211:VAL:HG21	1.85	0.57
1:D:354:ASN:C	1:D:354:ASN:HD22	2.12	0.57
1:D:387:GLN:NE2	1:D:387:GLN:H	2.01	0.57
1:A:156:GLU:O	1:A:157:ALA:CB	2.52	0.57
1:A:308:VAL:HG22	1:A:318:LEU:CD2	2.34	0.57
1:C:150:TYR:CE2	1:C:185:GLU:HA	2.39	0.57
1:C:309:LEU:O	1:C:316:PRO:HA	2.04	0.57
1:C:324:ASP:OD1	1:C:324:ASP:N	2.37	0.57
1:D:374:MET:O	1:D:375:GLY:C	2.47	0.57
1:C:484:VAL:HG12	1:C:488:PHE:CZ	2.40	0.57
1:A:100:LEU:CD2	1:A:454:ARG:HD2	2.35	0.56
1:A:155:LYS:HG3	1:A:156:GLU:H	1.69	0.56
1:C:220:ALA:O	1:C:223:MET:HB2	2.04	0.56
1:B:369:PHE:CD2	2:B:550:HEM:CAC	2.88	0.56
1:D:101:HIS:C	1:D:103:LYS:H	2.14	0.56
1:C:437:HIS:CB	1:D:406:LEU:HD11	2.36	0.56
1:A:383:PHE:HB3	1:A:391:ILE:HD13	1.88	0.56
1:C:327:LEU:HD12	1:C:328:GLU:N	2.21	0.56
1:C:119:ILE:HA	1:D:479:GLU:HG2	1.88	0.56
1:C:182:THR:C	1:C:184:ASP:N	2.58	0.56
1:C:333:HIS:NE2	1:C:417:GLU:OE1	2.37	0.56
1:A:356:LEU:HD23	1:A:356:LEU:C	2.31	0.56
1:D:252:ASP:HB3	1:D:254:LYS:N	2.21	0.56
1:A:193:ALA:HB2	1:A:487:PRO:HB2	1.87	0.56
1:B:205:GLN:O	1:B:208:ASN:HB3	2.06	0.55
1:A:247:PHE:HB3	1:A:248:PRO:CD	2.34	0.55
1:B:116:LEU:HD12	1:B:124:SER:OG	2.06	0.55
1:C:444:MET:HE1	1:C:478:GLN:OE1	2.07	0.55
1:C:380:VAL:O	1:C:384:CYS:HB2	2.07	0.55
1:D:195:ARG:HD2	1:D:206:TRP:CE2	2.42	0.55
1:C:307:LEU:HB3	1:C:309:LEU:HD21	1.89	0.55
1:C:326:VAL:O	1:C:326:VAL:CG1	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:TRP:CZ2	1:A:411:LYS:HG3	2.42	0.54
1:A:229:ARG:HB3	1:A:229:ARG:NH1	2.22	0.54
1:B:194:TRP:CE3	1:B:206:TRP:HA	2.43	0.54
1:A:398:ARG:HH11	1:A:398:ARG:CG	2.21	0.54
1:B:140:LEU:N	1:B:141:PRO:HD2	2.21	0.54
1:C:380:VAL:HG21	1:C:468:MET:HB3	1.90	0.54
1:B:282:ALA:HB1	5:B:880:GOL:H2	1.90	0.54
1:D:87:ILE:HG21	1:D:481:LEU:HD13	1.90	0.54
1:B:327:LEU:HD12	1:B:328:GLU:N	2.23	0.54
1:C:314:ARG:HB2	1:C:314:ARG:NH1	2.23	0.54
1:C:417:GLU:HA	1:C:420:ILE:HD12	1.89	0.54
1:B:274:ASP:OD1	1:B:276:SER:OG	2.26	0.54
1:C:437:HIS:HB2	1:D:406:LEU:CD1	2.37	0.54
1:B:333:HIS:CE1	1:B:335:LYS:HB2	2.43	0.53
1:C:381:ARG:HG3	1:C:381:ARG:HH11	1.72	0.53
1:B:390:ASN:C	1:B:390:ASN:HD22	2.15	0.53
1:C:461:TRP:CE3	1:D:462:ILE:HD13	2.44	0.53
1:A:388:ARG:HG3	1:A:388:ARG:HH11	1.73	0.53
1:C:378:ILE:HA	1:C:382:ASP:HB2	1.90	0.53
1:B:398:ARG:HH11	1:B:398:ARG:HG2	1.72	0.53
1:A:463:TRP:HA	3:A:600:H4B:N1	2.23	0.53
1:B:259:VAL:HG12	1:B:261:ASN:HB2	1.90	0.53
1:B:314:ARG:HG2	1:B:502:GLN:HE22	1.74	0.53
1:A:215:ARG:O	1:A:248:PRO:HG3	2.08	0.53
1:D:208:ASN:C	1:D:208:ASN:HD22	2.17	0.53
1:A:255:HIS:HB3	1:A:312:ASN:HB2	1.91	0.52
1:A:388:ARG:HG3	1:A:388:ARG:NH1	2.24	0.52
1:A:245:THR:O	1:A:367:CYS:HA	2.09	0.52
1:D:194:TRP:CE3	1:D:206:TRP:HA	2.44	0.52
1:C:255:HIS:HB3	1:C:312:ASN:HB2	1.91	0.52
1:D:426:PHE:CG	1:D:433:ILE:HD12	2.44	0.52
1:C:126:THR:HA	1:C:491:TYR:O	2.10	0.52
1:C:221:ARG:CZ	1:C:221:ARG:CB	2.86	0.52
1:C:412:ASP:O	1:C:415:VAL:HG12	2.10	0.52
1:C:461:TRP:CZ3	1:D:462:ILE:HG23	2.44	0.52
1:B:195:ARG:HD2	1:B:206:TRP:CE2	2.45	0.52
1:C:314:ARG:HB2	1:C:314:ARG:HH11	1.75	0.52
1:D:354:ASN:C	1:D:354:ASN:ND2	2.65	0.52
1:C:233:TYR:CE1	1:C:241:ARG:CZ	2.93	0.52
1:B:387:GLN:HE21	1:B:387:GLN:N	1.90	0.52
1:C:156:GLU:N	1:C:156:GLU:CD	2.68	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:PHE:CD2	2:C:550:HEM:HAC	2.45	0.52
1:A:236:ASN:HB3	1:A:239:ASN:O	2.10	0.51
1:B:269:GLY:N	1:B:287:THR:HG21	2.18	0.51
1:C:87:ILE:HD12	1:C:479:GLU:HB3	1.91	0.51
1:B:200:CYS:HB2	2:B:550:HEM:ND	2.24	0.51
1:C:311:ALA:HB3	1:C:314:ARG:NH1	2.18	0.51
1:A:472:ILE:HG22	1:A:472:ILE:O	2.11	0.51
1:C:145:GLU:HA	1:C:145:GLU:OE1	2.11	0.51
1:C:472:ILE:HG22	1:C:472:ILE:O	2.11	0.51
1:C:115:CYS:O	1:C:117:GLY:N	2.44	0.51
1:C:305:VAL:HG22	1:C:306:PRO:HD2	1.92	0.51
1:D:116:LEU:HD13	1:D:123:LYS:NZ	2.26	0.51
1:B:247:PHE:CB	1:B:248:PRO:HD2	2.37	0.51
1:B:380:VAL:HG23	1:B:419:ASN:HD21	1.77	0.50
1:A:92:SER:OG	1:A:94:MET:HB3	2.12	0.50
1:B:122:PRO:HG2	1:B:125:LEU:HD22	1.93	0.50
1:B:266:ARG:HH22	1:B:388:ARG:NH2	2.08	0.50
1:D:289:LEU:HD23	1:D:293:LEU:HD12	1.94	0.50
1:B:390:ASN:C	1:B:390:ASN:ND2	2.68	0.50
1:A:380:VAL:HG23	1:A:419:ASN:HD21	1.75	0.50
1:D:206:TRP:C	1:D:208:ASN:H	2.18	0.50
1:D:289:LEU:HD21	1:D:293:LEU:HD11	1.93	0.50
1:A:88:LYS:HD3	1:A:90:TRP:CE2	2.47	0.50
1:A:229:ARG:HB3	1:A:229:ARG:HH11	1.77	0.50
1:C:225:GLU:O	1:C:229:ARG:HG3	2.11	0.50
1:D:377:GLU:O	1:D:381:ARG:HB2	2.12	0.50
1:A:462:ILE:HG23	1:B:461:TRP:CZ3	2.47	0.50
1:A:429:GLN:O	1:A:431:VAL:HG23	2.12	0.50
1:B:309:LEU:O	1:B:316:PRO:HA	2.12	0.49
1:A:180:GLN:NE2	1:A:180:GLN:CA	2.72	0.49
1:C:247:PHE:HB3	1:C:248:PRO:CD	2.40	0.49
1:A:89:ASN:HB2	1:A:478:GLN:OE1	2.12	0.49
1:A:380:VAL:CG2	1:A:419:ASN:HD21	2.26	0.49
1:B:356:LEU:C	1:B:356:LEU:HD23	2.37	0.49
1:C:156:GLU:CD	1:C:156:GLU:H	2.19	0.49
1:D:342:LEU:HB3	1:D:344:LEU:HG	1.94	0.49
1:B:385:ASP:HB3	1:B:387:GLN:NE2	2.28	0.49
1:A:195:ARG:HD2	1:A:206:TRP:CE2	2.47	0.49
1:B:244:ILE:HD12	1:B:369:PHE:HB3	1.94	0.49
4:D:800:S71:H271	5:D:880:GOL:H31	1.93	0.49
1:A:180:GLN:CA	1:A:180:GLN:HE21	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:TYR:CE1	1:C:154:PHE:HE2	2.30	0.49
1:B:308:VAL:HG22	1:B:318:LEU:CD2	2.43	0.49
1:B:204:ILE:HG21	1:B:442:SER:OG	2.13	0.49
1:C:277:ILE:HG21	1:C:281:PRO:HB3	1.93	0.49
1:A:210:GLN:HA	1:A:210:GLN:NE2	2.28	0.48
1:B:304:VAL:HG21	1:B:326:VAL:HG11	1.94	0.48
1:B:338:TRP:O	1:B:341:GLU:HB2	2.13	0.48
1:D:154:PHE:CD2	1:D:158:LYS:HD2	2.47	0.48
1:A:333:HIS:CE1	1:A:334:PRO:HD2	2.48	0.48
1:A:156:GLU:O	1:A:157:ALA:HB3	2.13	0.48
1:A:471:SER:HB3	1:B:467:PRO:HB3	1.94	0.48
1:C:369:PHE:CD2	2:C:550:HEM:CAC	2.97	0.48
1:C:399:MET:O	1:C:401:LEU:HD23	2.14	0.48
2:B:550:HEM:O1A	4:B:800:S71:N19	2.47	0.48
1:A:187:ILE:HG22	1:A:191:LYS:HD2	1.95	0.48
1:A:184:ASP:HA	1:A:187:ILE:HD12	1.96	0.48
1:C:223:MET:HG2	1:C:247:PHE:CZ	2.49	0.48
1:C:245:THR:O	1:C:367:CYS:HA	2.13	0.47
1:A:195:ARG:HD2	1:A:206:TRP:CZ2	2.48	0.47
1:D:123:LYS:HE2	1:D:124:SER:H	1.78	0.47
1:C:191:LYS:HE2	1:C:207:SER:O	2.14	0.47
1:A:315:ASP:OD2	1:A:501:TRP:HE3	1.96	0.47
1:A:471:SER:HA	1:A:476:PHE:CG	2.49	0.47
1:B:159:ILE:H	1:B:159:ILE:HG12	1.44	0.47
1:B:308:VAL:HG22	1:B:318:LEU:HD22	1.95	0.47
1:C:326:VAL:O	1:C:326:VAL:HG12	2.14	0.47
1:C:244:ILE:HG13	1:C:368:PRO:O	2.14	0.47
1:A:388:ARG:HA	1:A:388:ARG:HD2	1.70	0.47
1:B:205:GLN:HG3	2:B:550:HEM:CBB	2.44	0.47
1:D:296:LYS:HE3	1:D:297:PRO:O	2.14	0.47
1:B:156:GLU:CD	1:B:156:GLU:H	2.23	0.47
1:B:187:ILE:HG12	1:B:211:VAL:CG2	2.42	0.47
1:D:212:PHE:HB2	1:D:245:THR:HA	1.96	0.47
1:C:307:LEU:O	1:C:318:LEU:HA	2.15	0.46
1:D:85:VAL:HG11	1:D:481:LEU:HD21	1.98	0.46
1:C:154:PHE:O	1:C:155:LYS:C	2.58	0.46
1:D:465:VAL:HA	1:D:466:PRO:HD3	1.76	0.46
1:A:194:TRP:CZ3	1:A:206:TRP:HA	2.50	0.46
1:C:249:GLN:H	1:C:249:GLN:HG2	1.59	0.46
1:C:161:GLU:O	1:C:165:ARG:N	2.47	0.46
1:A:374:MET:O	1:A:375:GLY:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:LEU:HD12	1:A:433:ILE:CG2	2.46	0.46
1:B:333:HIS:CG	1:B:334:PRO:HD2	2.50	0.46
1:C:314:ARG:HH11	1:C:314:ARG:CB	2.28	0.46
1:B:472:ILE:O	1:B:472:ILE:HG22	2.14	0.46
1:C:472:ILE:HD11	1:D:415:VAL:HG21	1.98	0.46
1:C:145:GLU:O	1:C:148:ASN:HB2	2.16	0.46
1:C:186:LEU:O	1:C:187:ILE:C	2.59	0.46
1:C:281:PRO:HD2	1:C:388:ARG:HA	1.98	0.46
1:D:272:MET:HB3	1:D:273:PRO:CD	2.47	0.45
1:C:380:VAL:N	1:C:419:ASN:HD21	2.15	0.45
1:B:193:ALA:HB2	1:B:487:PRO:HB2	1.97	0.45
1:C:135:PRO:O	1:C:136:PRO:C	2.57	0.45
1:A:229:ARG:HH11	1:A:229:ARG:CB	2.30	0.45
1:A:260:TRP:CE2	1:A:316:PRO:HG3	2.51	0.45
1:C:173:ILE:O	1:C:177:GLY:CA	2.61	0.45
1:B:337:GLU:O	1:B:339:PHE:N	2.49	0.45
1:C:448:GLN:HE21	1:C:448:GLN:HB3	1.37	0.45
1:D:427:GLN:C	1:D:429:GLN:N	2.74	0.45
1:C:380:VAL:HG11	1:C:467:PRO:HB2	1.99	0.45
1:C:101:HIS:NE2	1:C:102:HIS:HD2	2.15	0.45
1:D:387:GLN:H	1:D:387:GLN:CD	2.25	0.45
1:B:242:SER:HB3	1:B:371:GLY:HA2	1.98	0.45
1:A:401:LEU:O	1:A:403:THR:HG23	2.17	0.44
1:B:199:ARG:HD3	1:B:463:TRP:CD2	2.52	0.44
1:C:224:PHE:CD1	1:C:319:PHE:HB2	2.52	0.44
1:C:313:GLY:O	1:C:314:ARG:O	2.35	0.44
1:D:385:ASP:HB3	1:D:387:GLN:OE1	2.17	0.44
1:D:493:VAL:O	1:D:494:GLU:C	2.59	0.44
1:B:486:SER:HA	1:B:487:PRO:C	2.41	0.44
1:C:283:ASN:OD1	1:C:286:PHE:HB3	2.18	0.44
1:D:356:LEU:C	1:D:356:LEU:CD2	2.87	0.44
1:B:233:TYR:O	1:B:236:ASN:HB2	2.17	0.44
1:A:235:THR:O	1:A:236:ASN:C	2.60	0.44
1:B:374:MET:O	1:B:375:GLY:C	2.60	0.44
1:C:469:SER:H	1:D:469:SER:H	1.66	0.44
1:D:170:THR:O	1:D:174:GLU:HG2	2.17	0.44
1:A:84:HIS:N	1:A:84:HIS:ND1	2.66	0.44
1:A:465:VAL:HG22	1:A:475:VAL:HG23	2.00	0.44
1:D:156:GLU:CD	1:D:156:GLU:H	2.25	0.44
1:A:115:CYS:C	1:A:117:GLY:N	2.76	0.44
1:C:130:ARG:HD3	1:C:132:LYS:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:TRP:CE3	1:A:206:TRP:HA	2.53	0.44
1:D:115:CYS:C	1:D:117:GLY:N	2.76	0.44
1:B:192:GLN:HA	1:B:192:GLN:NE2	2.32	0.44
1:B:244:ILE:HD11	1:B:367:CYS:HB2	1.99	0.44
1:C:140:LEU:HD21	1:C:170:THR:CG2	2.30	0.44
1:D:378:ILE:HA	1:D:382:ASP:HB2	1.99	0.44
1:A:374:MET:HE3	1:A:376:THR:OG1	2.17	0.43
1:B:388:ARG:HA	1:B:388:ARG:HD2	1.81	0.43
1:C:163:LEU:HA	1:C:166:VAL:HG12	1.99	0.43
1:B:245:THR:O	1:B:367:CYS:HA	2.18	0.43
1:C:402:GLU:OE2	1:C:405:LYS:HD3	2.19	0.43
1:D:247:PHE:HB3	1:D:248:PRO:HD2	2.00	0.43
1:B:266:ARG:NH2	1:B:388:ARG:HH22	2.16	0.43
1:D:315:ASP:H	1:D:502:GLN:NE2	2.17	0.43
1:B:290:CYS:O	1:B:291:ILE:C	2.62	0.43
1:C:195:ARG:HD2	1:C:206:TRP:CE2	2.53	0.43
1:A:423:LEU:HD12	1:A:433:ILE:HG21	1.99	0.43
1:B:237:ASN:HD22	1:B:237:ASN:HA	1.60	0.43
1:B:354:ASN:N	1:B:354:ASN:HD22	2.15	0.43
1:A:127:ARG:HB2	1:A:356:LEU:HD13	2.00	0.43
1:A:163:LEU:O	1:A:166:VAL:HG12	2.18	0.43
1:D:307:LEU:HB3	1:D:309:LEU:HD13	2.01	0.43
1:D:494:GLU:HG3	1:D:497:LYS:HE3	2.00	0.43
1:A:176:THR:OG1	1:A:178:THR:O	2.36	0.43
1:C:335:LYS:HB3	1:C:335:LYS:HE3	1.61	0.43
1:B:228:CYS:O	1:B:229:ARG:C	2.62	0.43
1:B:329:VAL:HA	1:B:429:GLN:OE1	2.19	0.43
1:D:188:PHE:CD1	1:D:188:PHE:C	2.97	0.43
1:C:433:ILE:HD13	1:C:434:MET:H	1.84	0.43
1:D:270:TYR:HE2	1:D:300:GLY:H	1.65	0.43
1:D:398:ARG:C	1:D:400:GLY:H	2.26	0.43
1:A:437:HIS:CB	1:B:406:LEU:HD22	2.49	0.43
1:C:359:VAL:O	1:C:360:GLY:C	2.62	0.43
1:D:451:TYR:CE1	1:D:456:GLY:HA2	2.53	0.43
1:C:485:LEU:O	1:C:488:PHE:HB2	2.18	0.42
1:D:316:PRO:HD2	1:D:501:TRP:HZ3	1.84	0.42
1:A:446:TYR:O	1:A:447:MET:C	2.62	0.42
1:C:412:ASP:OD2	1:D:469:SER:HB2	2.19	0.42
1:B:194:TRP:CZ3	1:B:206:TRP:HA	2.54	0.42
1:C:465:VAL:HA	1:C:466:PRO:HD3	1.84	0.42
1:D:142:GLN:HE21	1:D:142:GLN:HB3	1.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:CYS:HB2	2:A:550:HEM:ND	2.35	0.42
1:C:85:VAL:HG11	1:C:481:LEU:HD11	2.02	0.42
1:C:221:ARG:CB	1:C:221:ARG:NH1	2.83	0.42
1:D:333:HIS:CE1	1:D:335:LYS:HB2	2.54	0.42
1:A:160:GLU:CD	1:A:160:GLU:N	2.65	0.42
1:B:256:ASP:HB3	1:B:258:ARG:HD3	2.01	0.42
1:C:307:LEU:HB3	1:C:309:LEU:CD2	2.50	0.42
1:C:194:TRP:O	1:C:203:ARG:HD3	2.19	0.42
1:D:206:TRP:C	1:D:208:ASN:N	2.78	0.42
1:A:398:ARG:HH11	1:A:398:ARG:HG3	1.83	0.42
1:B:239:ASN:OD1	1:B:239:ASN:C	2.62	0.42
1:D:194:TRP:CZ3	1:D:206:TRP:HA	2.54	0.42
1:C:431:VAL:O	1:C:432:THR:C	2.63	0.41
1:D:448:GLN:HE22	1:D:452:ARG:NH1	2.07	0.41
1:A:142:GLN:HE21	1:A:142:GLN:HB3	1.52	0.41
1:A:272:MET:HE3	1:A:278:ARG:HB3	2.01	0.41
1:B:410:TRP:CG	1:B:411:LYS:N	2.88	0.41
1:D:123:LYS:HE2	1:D:123:LYS:N	2.34	0.41
1:D:187:ILE:CG2	1:D:191:LYS:HE2	2.50	0.41
1:D:471:SER:HA	1:D:476:PHE:CG	2.54	0.41
1:A:307:LEU:O	1:A:318:LEU:HA	2.19	0.41
1:B:100:LEU:CB	1:B:456:GLY:HA3	2.49	0.41
1:A:187:ILE:O	1:A:188:PHE:C	2.62	0.41
1:C:87:ILE:HD13	1:C:87:ILE:HA	1.53	0.41
1:D:85:VAL:CG1	1:D:481:LEU:HD21	2.50	0.41
1:D:337:GLU:O	1:D:339:PHE:N	2.53	0.41
1:C:199:ARG:HG2	1:C:463:TRP:CG	2.55	0.41
1:D:386:VAL:HG23	1:D:387:GLN:NE2	2.34	0.41
1:C:249:GLN:HB2	1:C:250:ARG:H	1.62	0.41
1:D:130:ARG:O	1:D:131:ASP:HB3	2.20	0.41
1:A:406:LEU:HD12	1:A:406:LEU:HA	1.92	0.41
1:B:268:ALA:HA	1:B:287:THR:HG21	2.02	0.41
1:C:346:TRP:CD1	1:C:378:ILE:HG12	2.55	0.41
1:D:369:PHE:CG	2:D:550:HEM:HAC	2.55	0.41
1:A:371:GLY:CA	2:A:550:HEM:HAB	2.50	0.41
1:B:259:VAL:CG1	1:B:261:ASN:HB2	2.50	0.41
1:D:280:ASP:OD1	1:D:280:ASP:C	2.64	0.41
1:D:426:PHE:CD2	1:D:433:ILE:HD12	2.55	0.41
1:A:107:ILE:H	1:A:107:ILE:HG13	1.70	0.41
1:A:163:LEU:HD23	1:A:163:LEU:HA	1.83	0.41
1:A:409:LEU:HD23	1:A:409:LEU:HA	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ILE:O	1:B:204:ILE:HG13	2.18	0.41
1:B:434:MET:HE2	1:B:434:MET:HB2	1.78	0.41
1:B:442:SER:O	1:B:443:PHE:C	2.64	0.41
2:C:550:HEM:HBC2	2:C:550:HEM:CMC	2.51	0.41
1:D:193:ALA:HB2	1:D:487:PRO:HB2	2.01	0.41
1:D:296:LYS:HG2	1:D:297:PRO:HD2	2.03	0.41
1:D:399:MET:HE2	1:D:399:MET:HB3	1.99	0.41
1:D:466:PRO:C	1:D:468:MET:H	2.29	0.41
1:B:447:MET:HE2	1:B:451:TYR:HE2	1.85	0.41
1:C:83:ARG:HH11	1:C:83:ARG:HB2	1.85	0.41
1:C:413:GLN:HE21	1:C:413:GLN:HB2	1.42	0.41
1:D:116:LEU:HD11	1:D:123:LYS:HE3	2.01	0.41
1:D:155:LYS:H	1:D:155:LYS:HG2	1.57	0.41
1:A:431:VAL:O	1:A:432:THR:C	2.63	0.40
1:C:270:TYR:HB2	1:C:272:MET:CE	2.52	0.40
1:C:277:ILE:HD13	1:C:284:VAL:HG21	2.03	0.40
1:C:446:TYR:CZ	1:C:450:GLU:HG3	2.56	0.40
1:D:315:ASP:OD1	1:D:502:GLN:HG3	2.21	0.40
1:B:115:CYS:C	1:B:117:GLY:N	2.79	0.40
1:B:201:ILE:HG13	1:B:443:PHE:HB2	2.02	0.40
4:A:800:S71:H25	5:A:880:GOL:C1	2.50	0.40
1:B:96:PHE:CD2	1:B:451:TYR:CG	3.10	0.40
1:B:374:MET:HE3	1:B:376:THR:OG1	2.21	0.40
1:C:281:PRO:O	1:C:284:VAL:HG23	2.22	0.40
1:A:105:LYS:NZ	1:A:486:SER:HB2	2.36	0.40
1:A:426:PHE:CG	1:A:433:ILE:HG13	2.57	0.40
1:B:103:LYS:HD3	1:B:103:LYS:HA	1.63	0.40
1:B:266:ARG:HG2	1:B:283:ASN:ND2	2.36	0.40
1:B:412:ASP:O	1:B:416:VAL:HG23	2.21	0.40
1:D:337:GLU:C	1:D:339:PHE:N	2.76	0.40
1:D:461:TRP:CE2	1:D:465:VAL:HG21	2.57	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	410/431 (95%)	368 (90%)	32 (8%)	10 (2%)	4	23
1	B	410/431 (95%)	367 (90%)	35 (8%)	8 (2%)	6	27
1	C	410/431 (95%)	351 (86%)	47 (12%)	12 (3%)	3	20
1	D	410/431 (95%)	351 (86%)	49 (12%)	10 (2%)	4	23
All	All	1640/1724 (95%)	1437 (88%)	163 (10%)	40 (2%)	4	23

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	LEU
1	A	156	GLU
1	A	157	ALA
1	A	285	GLU
1	A	312	ASN
1	B	116	LEU
1	C	116	LEU
1	C	217	CYS
1	C	249	GLN
1	C	285	GLU
1	C	312	ASN
1	D	116	LEU
1	D	249	GLN
1	D	252	ASP
1	D	375	GLY
1	A	117	GLY
1	A	137	ASP
1	A	375	GLY
1	B	106	GLY
1	B	203	ARG
1	B	206	TRP
1	B	314	ARG
1	C	117	GLY
1	C	155	LYS
1	C	183	GLY
1	C	314	ARG
1	C	430	ASN
1	D	117	GLY
1	D	131	ASP
1	D	282	ALA

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Mol	Chain	Res	Type
1	B	354	ASN
1	C	499	HIS
1	D	360	GLY
1	B	375	GLY
1	D	155	LYS
1	A	136	PRO
1	B	117	GLY
1	D	501	TRP
1	C	360	GLY
1	A	248	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	359/376 (96%)	309 (86%)	50 (14%)	3	15
1	B	359/376 (96%)	295 (82%)	64 (18%)	2	8
1	C	359/376 (96%)	301 (84%)	58 (16%)	2	11
1	D	359/376 (96%)	296 (82%)	63 (18%)	2	9
All	All	1436/1504 (96%)	1201 (84%)	235 (16%)	2	10

All (235) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ARG
1	A	84	HIS
1	A	85	VAL
1	A	87	ILE
1	A	107	ILE
1	A	123	LYS
1	A	130	ARG
1	A	132	LYS
1	A	134	THR
1	A	137	ASP
1	A	153	SER

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Mol	Chain	Res	Type
1	A	159	ILE
1	A	160	GLU
1	A	166	VAL
1	A	170	THR
1	A	180	GLN
1	A	207	SER
1	A	219	THR
1	A	221	ARG
1	A	245	THR
1	A	258	ARG
1	A	271	GLN
1	A	288	GLN
1	A	289	LEU
1	A	291	ILE
1	A	296	LYS
1	A	307	LEU
1	A	337	GLU
1	A	340	ARG
1	A	345	LYS
1	A	386	VAL
1	A	387	GLN
1	A	390	ASN
1	A	391	ILE
1	A	394	GLU
1	A	398	ARG
1	A	401	LEU
1	A	405	LYS
1	A	418	ILE
1	A	423	LEU
1	A	427	GLN
1	A	428	LYS
1	A	433	ILE
1	A	445	LYS
1	A	448	GLN
1	A	452	ARG
1	A	471	SER
1	A	494	GLU
1	A	500	VAL
1	A	502	GLN
1	B	83	ARG
1	B	103	LYS
1	B	124	SER

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Mol	Chain	Res	Type
1	B	125	LEU
1	B	130	ARG
1	B	134	THR
1	B	140	LEU
1	B	145	GLU
1	B	153	SER
1	B	155	LYS
1	B	156	GLU
1	B	159	ILE
1	B	161	GLU
1	B	163	LEU
1	B	167	GLU
1	B	174	GLU
1	B	181	LEU
1	B	192	GLN
1	B	204	ILE
1	B	211	VAL
1	B	218	SER
1	B	225	GLU
1	B	237	ASN
1	B	242	SER
1	B	244	ILE
1	B	245	THR
1	B	249	GLN
1	B	258	ARG
1	B	278	ARG
1	B	285	GLU
1	B	287	THR
1	B	289	LEU
1	B	290	CYS
1	B	291	ILE
1	B	305	VAL
1	B	307	LEU
1	B	312	ASN
1	B	324	ASP
1	B	325	LEU
1	B	337	GLU
1	B	340	ARG
1	B	342	LEU
1	B	345	LYS
1	B	354	ASN
1	B	377	GLU

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Mol	Chain	Res	Type
1	B	386	VAL
1	B	387	GLN
1	B	393	GLU
1	B	394	GLU
1	B	398	ARG
1	B	402	GLU
1	B	404	HIS
1	B	406	LEU
1	B	413	GLN
1	B	427	GLN
1	B	434	MET
1	B	468	MET
1	B	480	MET
1	B	481	LEU
1	B	482	ASN
1	B	494	GLU
1	B	497	LYS
1	B	500	VAL
1	B	502	GLN
1	C	83	ARG
1	C	84	HIS
1	C	85	VAL
1	C	87	ILE
1	C	103	LYS
1	C	120	MET
1	C	121	THR
1	C	123	LYS
1	C	124	SER
1	C	125	LEU
1	C	130	ARG
1	C	134	THR
1	C	154	PHE
1	C	155	LYS
1	C	156	GLU
1	C	159	ILE
1	C	175	THR
1	C	201	ILE
1	C	219	THR
1	C	221	ARG
1	C	229	ARG
1	C	242	SER
1	C	249	GLN

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Mol	Chain	Res	Type
1	C	252	ASP
1	C	254	LYS
1	C	271	GLN
1	C	278	ARG
1	C	289	LEU
1	C	305	VAL
1	C	307	LEU
1	C	318	LEU
1	C	320	GLU
1	C	324	ASP
1	C	326	VAL
1	C	335	LYS
1	C	340	ARG
1	C	349	LEU
1	C	386	VAL
1	C	387	GLN
1	C	394	GLU
1	C	398	ARG
1	C	403	THR
1	C	405	LYS
1	C	413	GLN
1	C	423	LEU
1	C	427	GLN
1	C	428	LYS
1	C	433	ILE
1	C	434	MET
1	C	445	LYS
1	C	448	GLN
1	C	452	ARG
1	C	471	SER
1	C	475	VAL
1	C	492	GLN
1	C	494	GLU
1	C	497	LYS
1	C	500	VAL
1	D	84	HIS
1	D	102	HIS
1	D	116	LEU
1	D	123	LYS
1	D	124	SER
1	D	127	ARG
1	D	130	ARG

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Mol	Chain	Res	Type
1	D	132	LYS
1	D	134	THR
1	D	140	LEU
1	D	147	VAL
1	D	153	SER
1	D	155	LYS
1	D	156	GLU
1	D	159	ILE
1	D	181	LEU
1	D	184	ASP
1	D	195	ARG
1	D	208	ASN
1	D	211	VAL
1	D	219	THR
1	D	222	GLU
1	D	242	SER
1	D	249	GLN
1	D	252	ASP
1	D	258	ARG
1	D	271	GLN
1	D	278	ARG
1	D	285	GLU
1	D	296	LYS
1	D	305	VAL
1	D	307	LEU
1	D	309	LEU
1	D	310	GLN
1	D	312	ASN
1	D	320	GLU
1	D	325	LEU
1	D	337	GLU
1	D	342	LEU
1	D	354	ASN
1	D	356	LEU
1	D	380	VAL
1	D	386	VAL
1	D	387	GLN
1	D	390	ASN
1	D	393	GLU
1	D	394	GLU
1	D	398	ARG
1	D	415	VAL

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Mol	Chain	Res	Type
1	D	427	GLN
1	D	428	LYS
1	D	441	GLU
1	D	448	GLN
1	D	449	ASN
1	D	462	ILE
1	D	468	MET
1	D	471	SER
1	D	481	LEU
1	D	494	GLU
1	D	497	LYS
1	D	498	THR
1	D	500	VAL
1	D	502	GLN

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	97	GLN
1	A	142	GLN
1	A	180	GLN
1	A	192	GLN
1	A	205	GLN
1	A	210	GLN
1	A	226	HIS
1	A	237	ASN
1	A	271	GLN
1	A	387	GLN
1	A	390	ASN
1	A	413	GLN
1	A	482	ASN
1	A	502	GLN
1	B	192	GLN
1	B	208	ASN
1	B	226	HIS
1	B	237	ASN
1	B	271	GLN
1	B	354	ASN
1	B	387	GLN
1	B	390	ASN
1	B	413	GLN
1	B	419	ASN

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Mol	Chain	Res	Type
1	B	424	HIS
1	B	427	GLN
1	B	492	GLN
1	C	97	GLN
1	C	102	HIS
1	C	148	ASN
1	C	162	HIS
1	C	180	GLN
1	C	205	GLN
1	C	210	GLN
1	C	237	ASN
1	C	239	ASN
1	C	271	GLN
1	C	310	GLN
1	C	387	GLN
1	C	390	ASN
1	C	413	GLN
1	C	419	ASN
1	C	448	GLN
1	D	142	GLN
1	D	192	GLN
1	D	205	GLN
1	D	208	ASN
1	D	237	ASN
1	D	249	GLN
1	D	271	GLN
1	D	354	ASN
1	D	387	GLN
1	D	390	ASN
1	D	413	GLN
1	D	448	GLN
1	D	449	ASN
1	D	482	ASN
1	D	502	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

25 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
6	SO4	D	920	-	4,4,4	0.55	0	6,6,6	0.48	0
3	H4B	A	600	-	17,18,18	1.01	1 (5%)	14,26,26	1.59	3 (21%)
6	SO4	B	910	-	4,4,4	0.50	0	6,6,6	0.48	0
5	GOL	B	880	-	5,5,5	0.51	0	5,5,5	0.28	0
2	HEM	B	550	1	50,50,50	1.57	10 (20%)	67,82,82	2.09	25 (37%)
6	SO4	C	910	-	4,4,4	0.51	0	6,6,6	0.28	0
2	HEM	C	550	1	50,50,50	1.52	5 (10%)	67,82,82	1.65	13 (19%)
6	SO4	B	920	-	4,4,4	0.51	0	6,6,6	0.62	0
2	HEM	D	550	1	50,50,50	1.65	9 (18%)	67,82,82	2.00	17 (25%)
6	SO4	C	920	-	4,4,4	0.48	0	6,6,6	0.16	0
4	S71	A	800	-	29,30,30	0.64	0	34,41,41	2.12	13 (38%)
6	SO4	D	910	-	4,4,4	0.50	0	6,6,6	0.22	0
5	GOL	D	880	-	5,5,5	0.39	0	5,5,5	0.36	0
6	SO4	A	910	-	4,4,4	0.67	0	6,6,6	0.38	0
2	HEM	A	550	1	50,50,50	1.54	10 (20%)	67,82,82	1.84	20 (29%)
3	H4B	C	600	-	17,18,18	0.68	1 (5%)	14,26,26	1.78	5 (35%)
6	SO4	A	930	-	4,4,4	0.55	0	6,6,6	1.00	0
6	SO4	A	920	-	4,4,4	0.48	0	6,6,6	0.39	0
4	S71	B	800	-	29,30,30	0.99	1 (3%)	34,41,41	2.52	16 (47%)
3	H4B	B	600	-	17,18,18	0.84	1 (5%)	14,26,26	2.09	7 (50%)
3	H4B	D	600	-	17,18,18	0.95	0	14,26,26	1.87	5 (35%)
4	S71	C	800	-	29,30,30	0.91	1 (3%)	34,41,41	2.11	13 (38%)
4	S71	D	800	-	29,30,30	0.83	0	34,41,41	2.24	15 (44%)
5	GOL	C	880	-	5,5,5	0.45	0	5,5,5	0.32	0
5	GOL	A	880	-	5,5,5	0.38	0	5,5,5	1.21	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
2	HEM	A	550	1	-	4/14/54/54	-
3	H4B	D	600	-	-	2/8/17/17	0/2/2/2
5	GOL	B	880	-	-	4/4/4/4	-
2	HEM	B	550	1	-	6/14/54/54	-
2	HEM	C	550	1	-	2/14/54/54	-
3	H4B	C	600	-	-	0/8/17/17	0/2/2/2
2	HEM	D	550	1	-	11/14/54/54	-
5	GOL	D	880	-	-	2/4/4/4	-
4	S71	C	800	-	-	0/15/15/15	0/3/3/3
5	GOL	A	880	-	-	1/4/4/4	-
4	S71	D	800	-	-	3/15/15/15	0/3/3/3
4	S71	B	800	-	-	2/15/15/15	0/3/3/3
4	S71	A	800	-	-	2/15/15/15	0/3/3/3
5	GOL	C	880	-	-	1/4/4/4	-
3	H4B	B	600	-	-	0/8/17/17	0/2/2/2
3	H4B	A	600	-	-	0/8/17/17	0/2/2/2

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	550	HEM	FE-NB	5.71	2.12	1.94
2	C	550	HEM	FE-NB	4.83	2.09	1.94
2	A	550	HEM	FE-NB	4.66	2.09	1.94
2	B	550	HEM	FE-NB	4.37	2.08	1.94
2	B	550	HEM	C1B-NB	-4.14	1.33	1.40
2	C	550	HEM	C1B-NB	-4.08	1.33	1.40
2	C	550	HEM	FE-NC	4.06	2.08	1.95
2	D	550	HEM	FE-NC	3.69	2.07	1.95
2	A	550	HEM	C1B-NB	-3.68	1.33	1.40
2	D	550	HEM	C1B-NB	-3.68	1.33	1.40
2	B	550	HEM	FE-NC	3.55	2.06	1.95
2	D	550	HEM	C4D-ND	-3.40	1.34	1.40
2	A	550	HEM	FE-NC	3.07	2.05	1.95
2	B	550	HEM	C4D-ND	-2.97	1.35	1.40
2	A	550	HEM	C1C-C2C	-2.89	1.39	1.45
2	D	550	HEM	C4B-NB	-2.77	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	550	HEM	C4D-C3D	2.70	1.49	1.45
4	B	800	S71	C22-N21	2.69	1.41	1.35
2	C	550	HEM	C4B-NB	-2.66	1.33	1.38
2	B	550	HEM	C4B-NB	-2.52	1.33	1.38
2	A	550	HEM	C3B-C4B	2.50	1.49	1.44
2	B	550	HEM	C3C-C4C	-2.48	1.41	1.46
2	D	550	HEM	C1C-C2C	-2.46	1.40	1.45
2	A	550	HEM	C4C-NC	-2.45	1.35	1.39
2	C	550	HEM	C4D-ND	-2.40	1.36	1.40
2	A	550	HEM	C4D-C3D	2.37	1.49	1.45
3	B	600	H4B	O4-C4	2.33	1.28	1.23
2	A	550	HEM	C4B-NB	-2.28	1.34	1.38
2	B	550	HEM	C4D-C3D	2.23	1.48	1.45
2	A	550	HEM	C1D-ND	-2.20	1.34	1.38
2	A	550	HEM	C4D-ND	-2.14	1.36	1.40
2	B	550	HEM	C4C-NC	-2.14	1.35	1.39
2	B	550	HEM	C3B-C4B	2.11	1.49	1.44
2	D	550	HEM	C1C-NC	-2.11	1.35	1.39
4	C	800	S71	C16-C15	2.11	1.42	1.39
3	A	600	H4B	C7-C6	2.11	1.54	1.52
3	C	600	H4B	O4-C4	2.06	1.27	1.23
2	D	550	HEM	O2A-CGA	-2.00	1.24	1.30
2	B	550	HEM	C1C-C2C	-2.00	1.41	1.45

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	800	S71	C20-C26-N21	6.52	124.56	116.57
4	C	800	S71	C02-N01-C06	5.50	122.18	118.07
4	A	800	S71	C20-C26-N21	5.41	123.20	116.57
2	D	550	HEM	CHD-C1D-ND	5.28	130.10	124.42
2	B	550	HEM	C4B-C3B-C2B	-4.94	102.74	107.28
4	D	800	S71	C02-N01-C06	4.90	121.73	118.07
2	B	550	HEM	CHC-C4B-NB	4.72	129.51	124.42
2	B	550	HEM	CHD-C1D-C2D	-4.68	117.64	125.03
2	B	550	HEM	O2D-CGD-CBD	4.55	128.37	114.00
2	D	550	HEM	C4B-C3B-C2B	-4.44	103.20	107.28
4	D	800	S71	C22-N21-C26	4.43	121.38	118.07
2	D	550	HEM	O2D-CGD-CBD	4.22	127.32	114.00
2	C	550	HEM	C1B-NB-C4B	4.22	110.20	105.21
4	B	800	S71	C02-N01-C06	4.19	121.20	118.07
4	B	800	S71	N22-C22-N21	4.18	123.31	116.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	550	HEM	CHD-C1D-C2D	-4.18	118.43	125.03
2	B	550	HEM	CHD-C1D-ND	4.16	128.91	124.42
2	A	550	HEM	CHC-C4B-NB	4.11	128.84	124.42
2	C	550	HEM	CHA-C4D-ND	4.08	129.42	124.37
2	A	550	HEM	CBD-CAD-C3D	-4.06	101.30	112.53
2	C	550	HEM	CHC-C4B-NB	3.98	128.70	124.42
4	A	800	S71	C12-N11-C16	3.90	122.81	117.51
2	A	550	HEM	C4B-C3B-C2B	-3.90	103.70	107.28
4	B	800	S71	C23-C22-N22	-3.89	113.42	121.81
4	D	800	S71	N02-C02-N01	3.87	122.81	116.59
2	A	550	HEM	C1B-NB-C4B	3.85	109.77	105.21
2	D	550	HEM	CMB-C2B-C1B	3.82	131.01	125.03
4	B	800	S71	N02-C02-N01	3.80	122.69	116.59
2	B	550	HEM	C1B-NB-C4B	3.79	109.69	105.21
2	D	550	HEM	CHC-C4B-NB	3.77	128.47	124.42
4	A	800	S71	C02-N01-C06	3.69	120.83	118.07
4	B	800	S71	C12-N11-C16	3.65	122.47	117.51
2	B	550	HEM	C3B-C2B-C1B	3.64	109.15	106.41
2	B	550	HEM	CBA-CAA-C2A	-3.62	102.53	112.53
4	C	800	S71	C20-C26-N21	3.60	120.97	116.57
3	C	600	H4B	C2-N1-C8A	3.57	119.66	113.36
4	B	800	S71	C25-C26-N21	-3.53	118.71	122.73
2	D	550	HEM	CMB-C2B-C3B	-3.47	120.04	128.43
3	D	600	H4B	C2-N1-C8A	3.45	119.45	113.36
2	D	550	HEM	O2D-CGD-O1D	-3.44	114.47	123.33
4	C	800	S71	N02-C02-N01	3.40	122.06	116.59
2	A	550	HEM	CHA-C4D-ND	3.38	128.55	124.37
2	D	550	HEM	C3B-C2B-C1B	3.37	108.94	106.41
2	D	550	HEM	C4C-CHD-C1D	-3.37	118.86	126.02
2	C	550	HEM	CHD-C1D-ND	3.36	128.03	124.42
4	D	800	S71	C20-C26-N21	3.35	120.67	116.57
3	A	600	H4B	O4-C4-C4A	-3.32	119.25	127.26
4	A	800	S71	C27-C24-C25	-3.24	116.53	120.92
4	D	800	S71	C25-C26-N21	-3.22	119.06	122.73
4	B	800	S71	C14-C13-C12	3.22	119.88	116.90
2	D	550	HEM	CAD-C3D-C4D	3.19	130.26	124.70
4	C	800	S71	N22-C22-N21	3.19	121.71	116.59
4	C	800	S71	C14-C13-C12	3.11	119.78	116.90
2	A	550	HEM	CAD-CBD-CGD	3.10	121.89	113.67
2	C	550	HEM	CHA-C4D-C3D	-3.08	119.55	125.23
3	B	600	H4B	C2-N1-C8A	3.08	118.79	113.36
2	B	550	HEM	C2D-C1D-ND	3.04	113.42	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	800	S71	C14-C13-C12	3.02	119.70	116.90
3	B	600	H4B	O4-C4-C4A	-2.99	120.06	127.26
2	B	550	HEM	O2D-CGD-O1D	-2.96	115.72	123.33
2	A	550	HEM	O2D-CGD-CBD	2.94	123.30	114.00
2	B	550	HEM	CAD-CBD-CGD	2.91	121.37	113.67
2	A	550	HEM	CHD-C1D-ND	2.89	127.54	124.42
2	B	550	HEM	CAD-C3D-C4D	2.89	129.73	124.70
4	A	800	S71	C20-C26-C25	-2.89	115.12	121.06
4	D	800	S71	C09-C13-C14	-2.89	115.69	120.54
2	C	550	HEM	CBD-CAD-C3D	-2.87	104.59	112.53
2	A	550	HEM	CHC-C1C-NC	2.84	127.55	124.45
2	A	550	HEM	C3B-C2B-C1B	2.83	108.53	106.41
4	A	800	S71	C15-C16-N11	-2.82	119.65	124.05
3	C	600	H4B	C4-C4A-N5	2.80	123.90	116.27
2	A	550	HEM	CHA-C4D-C3D	-2.79	120.09	125.23
4	D	800	S71	C15-C16-N11	-2.78	119.70	124.05
3	B	600	H4B	O9-C9-C6	2.78	115.95	109.28
2	C	550	HEM	C3B-C4B-NB	-2.76	107.49	109.47
4	B	800	S71	C03-C04-C05	2.68	121.09	118.11
4	B	800	S71	C20-C17-C15	-2.67	106.73	111.79
4	A	800	S71	N02-C02-N01	2.67	120.88	116.59
3	D	600	H4B	C2-N3-C4	-2.66	120.28	125.11
4	C	800	S71	C09-C13-C14	-2.66	116.08	120.54
3	B	600	H4B	N2-C2-N3	2.64	122.33	116.76
2	A	550	HEM	CHD-C1D-C2D	-2.64	120.87	125.03
2	D	550	HEM	C1B-NB-C4B	2.63	108.32	105.21
2	C	550	HEM	O2D-CGD-CBD	2.63	122.32	114.00
2	C	550	HEM	C1A-CHA-C4D	-2.63	120.06	126.25
4	D	800	S71	C20-C17-C15	-2.60	106.86	111.79
4	B	800	S71	C08-C09-C13	-2.59	104.42	113.23
4	A	800	S71	C13-C12-N11	-2.58	118.81	123.75
3	C	600	H4B	O4-C4-C4A	-2.58	121.03	127.26
4	C	800	S71	C05-C06-N01	-2.57	119.80	122.73
2	B	550	HEM	O2A-CGA-CBA	2.57	122.11	114.00
2	A	550	HEM	O2D-CGD-O1D	-2.54	116.80	123.33
2	D	550	HEM	CAD-CBD-CGD	2.53	120.38	113.67
2	A	550	HEM	C4C-CHD-C1D	-2.51	120.68	126.02
4	B	800	S71	C13-C12-N11	-2.51	118.95	123.75
4	D	800	S71	C14-C13-C12	2.50	119.22	116.90
4	A	800	S71	C27-C24-C23	2.50	124.30	120.92
4	C	800	S71	C12-N11-C16	2.50	120.90	117.51
3	A	600	H4B	C2-N3-C4	-2.50	120.58	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	550	HEM	CBD-CAD-C3D	-2.46	105.73	112.53
4	B	800	S71	C25-C24-C23	2.45	120.84	118.11
2	D	550	HEM	CHA-C4D-ND	2.43	127.37	124.37
3	B	600	H4B	C2-N3-C4	-2.41	120.73	125.11
4	D	800	S71	N22-C22-N21	2.40	120.45	116.59
2	B	550	HEM	C4C-CHD-C1D	-2.40	120.91	126.02
2	A	550	HEM	C1A-CHA-C4D	-2.39	120.63	126.25
3	D	600	H4B	C4-C4A-N5	2.34	122.66	116.27
2	B	550	HEM	O2A-CGA-O1A	-2.34	117.31	123.33
2	C	550	HEM	CAD-CBD-CGD	2.34	119.88	113.67
4	D	800	S71	C12-N11-C16	2.34	120.69	117.51
3	B	600	H4B	O10-C10-C9	-2.34	105.91	109.77
4	D	800	S71	C14-C15-C17	-2.33	115.11	120.88
2	C	550	HEM	C4C-CHD-C1D	-2.33	121.07	126.02
2	A	550	HEM	O2A-CGA-O1A	-2.31	117.39	123.33
2	A	550	HEM	C4A-CHB-C1B	-2.31	120.82	126.25
2	B	550	HEM	O1D-CGD-CBD	-2.31	115.78	123.09
3	D	600	H4B	O9-C9-C6	2.31	114.80	109.28
3	A	600	H4B	C4A-C4-N3	2.30	118.45	112.13
3	C	600	H4B	C4A-C4-N3	2.28	118.39	112.13
2	B	550	HEM	CHC-C4B-C3B	-2.27	120.54	125.07
4	C	800	S71	C15-C16-N11	-2.26	120.52	124.05
2	A	550	HEM	CHB-C1B-NB	2.24	127.14	124.37
2	B	550	HEM	C1D-C2D-C3D	-2.23	104.63	106.98
4	C	800	S71	C22-N21-C26	2.22	119.73	118.07
4	C	800	S71	C14-C15-C17	-2.21	115.40	120.88
2	C	550	HEM	CHD-C1D-C2D	-2.21	121.54	125.03
4	C	800	S71	C08-C06-N01	2.20	119.40	116.06
3	B	600	H4B	N2-C2-N1	-2.19	115.39	119.67
4	A	800	S71	C09-C13-C14	-2.18	116.88	120.54
4	D	800	S71	C07-C04-C03	-2.16	117.99	120.92
4	A	800	S71	N22-C22-N21	2.14	120.02	116.59
2	B	550	HEM	C1A-CHA-C4D	-2.13	121.24	126.25
4	D	800	S71	C08-C09-C13	-2.13	106.00	113.23
4	B	800	S71	C20-C26-C25	-2.11	116.71	121.06
4	B	800	S71	C07-C04-C03	-2.11	118.07	120.92
2	A	550	HEM	CAD-C3D-C4D	2.11	128.37	124.70
2	B	550	HEM	CAD-C3D-C2D	-2.10	123.93	127.87
2	D	550	HEM	CHA-C4D-C3D	-2.10	121.35	125.23
4	C	800	S71	C23-C22-N22	-2.08	117.32	121.81
2	B	550	HEM	CMA-C3A-C4A	2.08	128.58	125.42
2	D	550	HEM	CHC-C4B-C3B	-2.06	120.96	125.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	600	H4B	C4A-C4-N3	2.06	117.79	112.13
4	B	800	S71	C08-C06-N01	2.04	119.16	116.06
3	C	600	H4B	N2-C2-N3	2.04	121.06	116.76
2	B	550	HEM	CMC-C2C-C1C	2.03	128.31	124.73
2	A	550	HEM	C4C-NC-C1C	2.03	109.13	105.82
2	B	550	HEM	CBC-CAC-C3C	-2.03	117.39	127.53
4	A	800	S71	C14-C15-C17	-2.03	115.86	120.88
4	D	800	S71	C18-C17-C15	-2.02	106.89	110.97
2	B	550	HEM	CMB-C2B-C3B	-2.02	123.55	128.43
2	D	550	HEM	C1A-CHA-C4D	-2.02	121.50	126.25
2	C	550	HEM	O2A-CGA-CBA	2.01	120.36	114.00

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	550	HEM	C2B-C3B-CAB-CBB
2	C	550	HEM	C2B-C3B-CAB-CBB
2	D	550	HEM	C2B-C3B-CAB-CBB
4	A	800	S71	C18-C17-C20-C26
4	A	800	S71	C15-C17-C18-N19
4	B	800	S71	C15-C17-C18-N19
4	D	800	S71	C18-C17-C20-C26
5	B	880	GOL	O1-C1-C2-C3
2	D	550	HEM	C3D-CAD-CBD-CGD
5	B	880	GOL	C1-C2-C3-O3
5	C	880	GOL	O1-C1-C2-C3
5	D	880	GOL	O1-C1-C2-C3
5	B	880	GOL	O1-C1-C2-O2
2	D	550	HEM	C4D-C3D-CAD-CBD
2	A	550	HEM	C4B-C3B-CAB-CBB
2	D	550	HEM	C4B-C3B-CAB-CBB
5	B	880	GOL	O2-C2-C3-O3
2	D	550	HEM	C2D-C3D-CAD-CBD
4	B	800	S71	C20-C17-C18-N19
5	A	880	GOL	O2-C2-C3-O3
2	A	550	HEM	C2C-C3C-CAC-CBC
2	B	550	HEM	C2B-C3B-CAB-CBB
2	C	550	HEM	C4B-C3B-CAB-CBB
4	D	800	S71	C16-C15-C17-C18
4	D	800	S71	C14-C15-C17-C18
2	B	550	HEM	C4D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
2	A	550	HEM	C4C-C3C-CAC-CBC
2	D	550	HEM	C4C-C3C-CAC-CBC
2	B	550	HEM	C3D-CAD-CBD-CGD
2	B	550	HEM	CAD-CBD-CGD-O2D
2	D	550	HEM	CAD-CBD-CGD-O2D
2	B	550	HEM	CAD-CBD-CGD-O1D
2	D	550	HEM	CAD-CBD-CGD-O1D
3	D	600	H4B	C7-C6-C9-O9
2	D	550	HEM	CAA-CBA-CGA-O2A
2	D	550	HEM	C2C-C3C-CAC-CBC
2	B	550	HEM	C4B-C3B-CAB-CBB
2	D	550	HEM	CAA-CBA-CGA-O1A
3	D	600	H4B	N5-C6-C9-O9
5	D	880	GOL	O1-C1-C2-O2

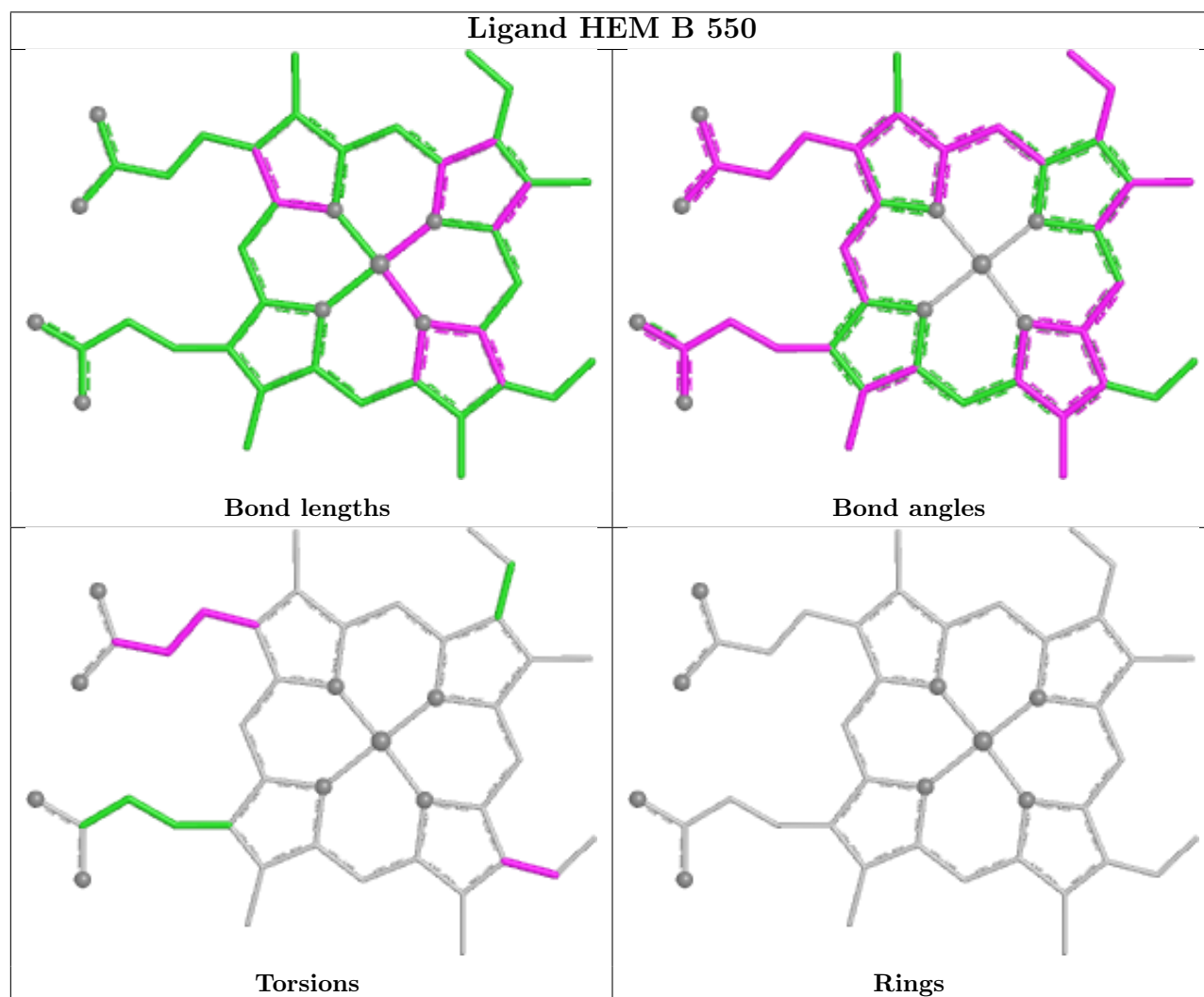
There are no ring outliers.

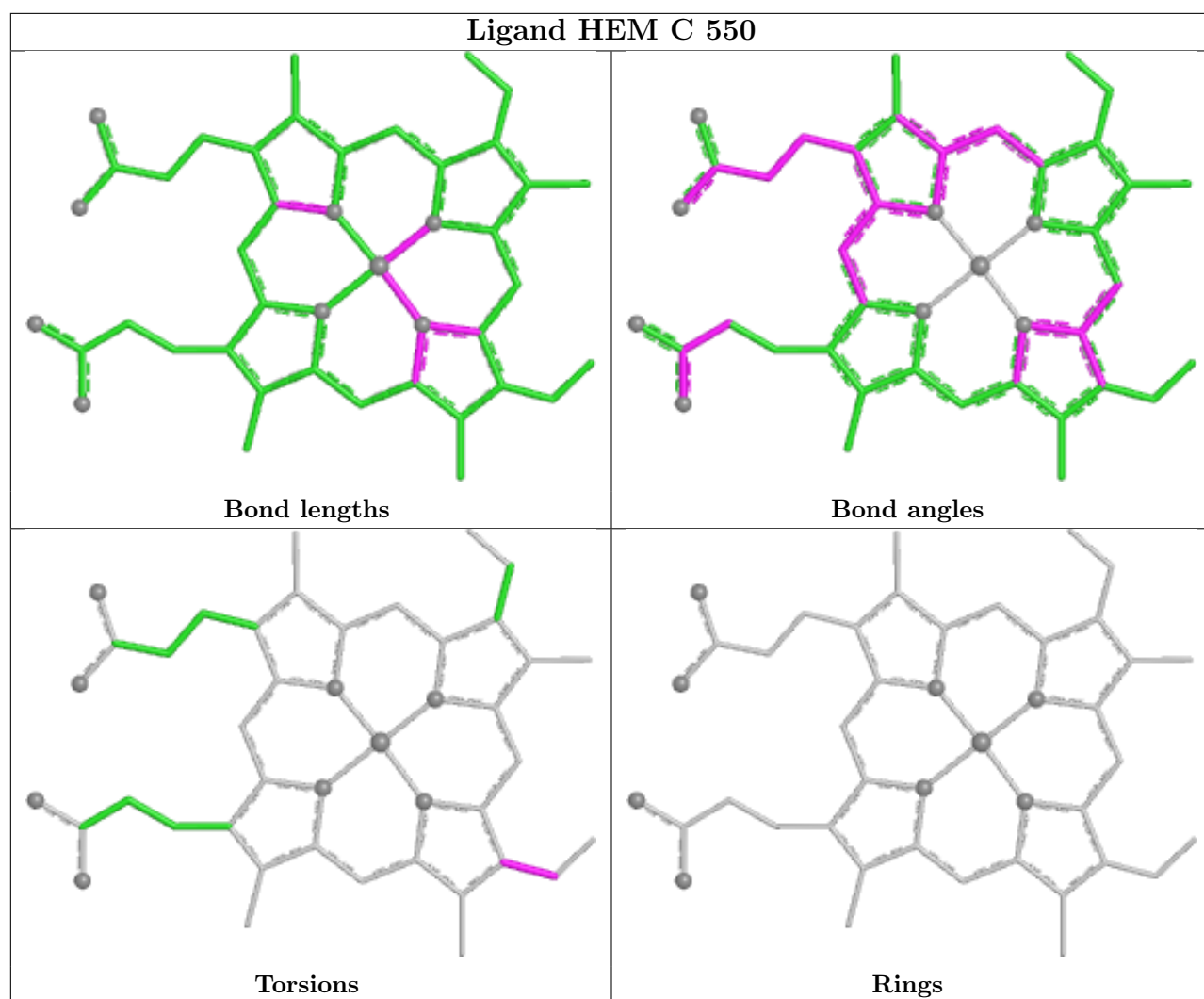
12 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	H4B	1	0
5	B	880	GOL	1	0
2	B	550	HEM	5	0
2	C	550	HEM	3	0
2	D	550	HEM	2	0
4	A	800	S71	2	0
5	D	880	GOL	1	0
2	A	550	HEM	2	0
4	B	800	S71	1	0
4	D	800	S71	1	0
5	C	880	GOL	1	0
5	A	880	GOL	2	0

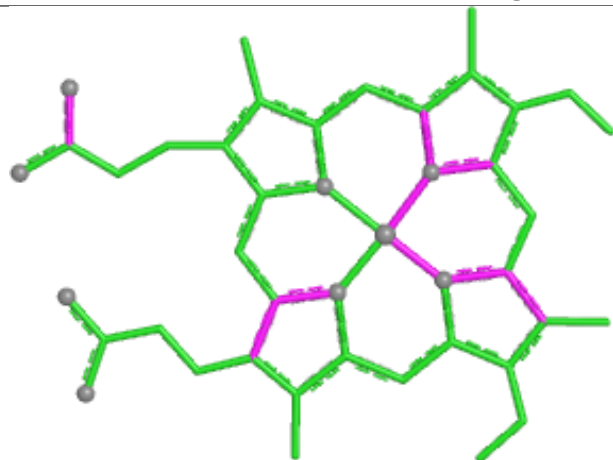
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

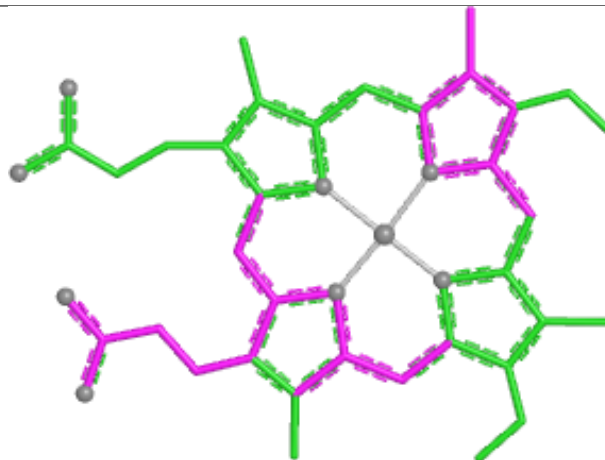




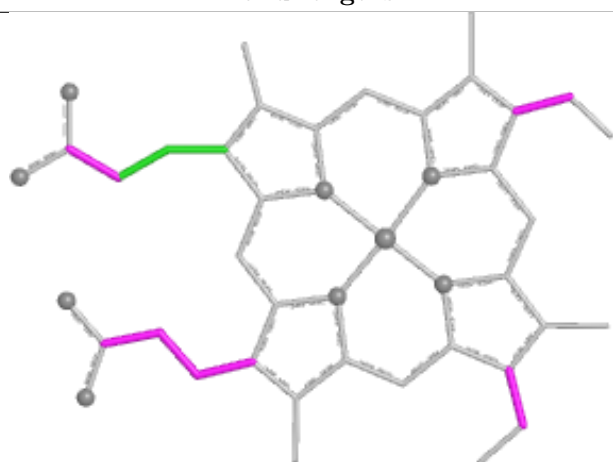
Ligand HEM D 550



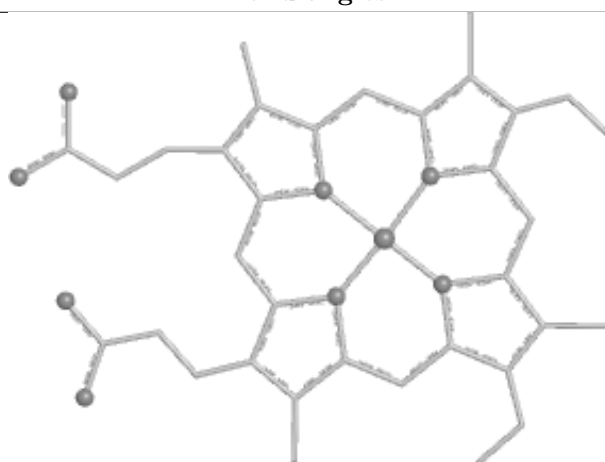
Bond lengths



Bond angles

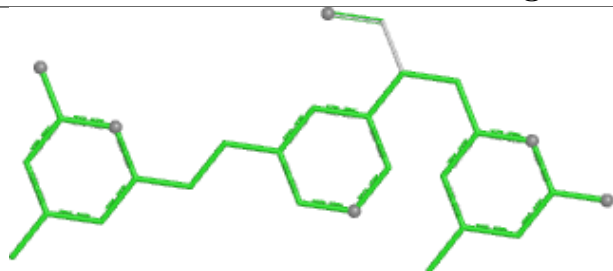


Torsions



Rings

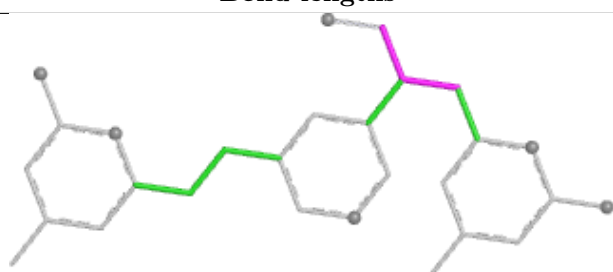
Ligand S71 A 800



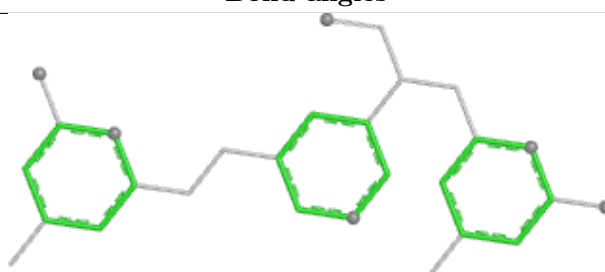
Bond lengths



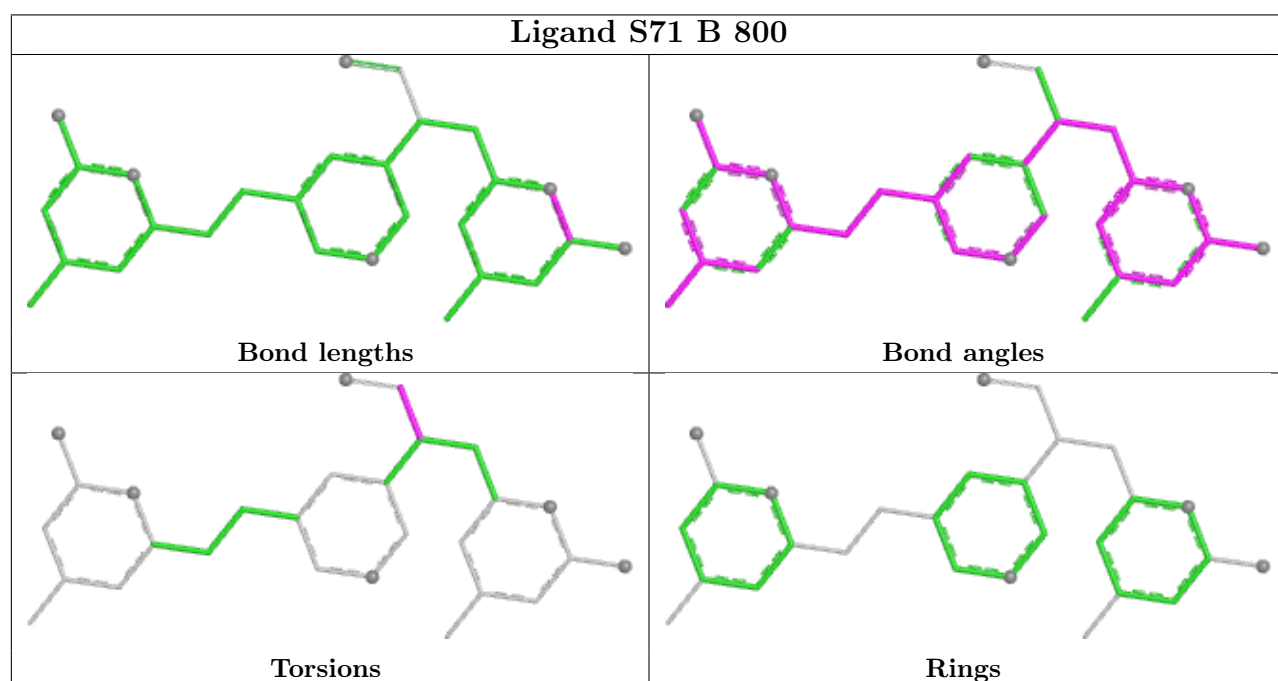
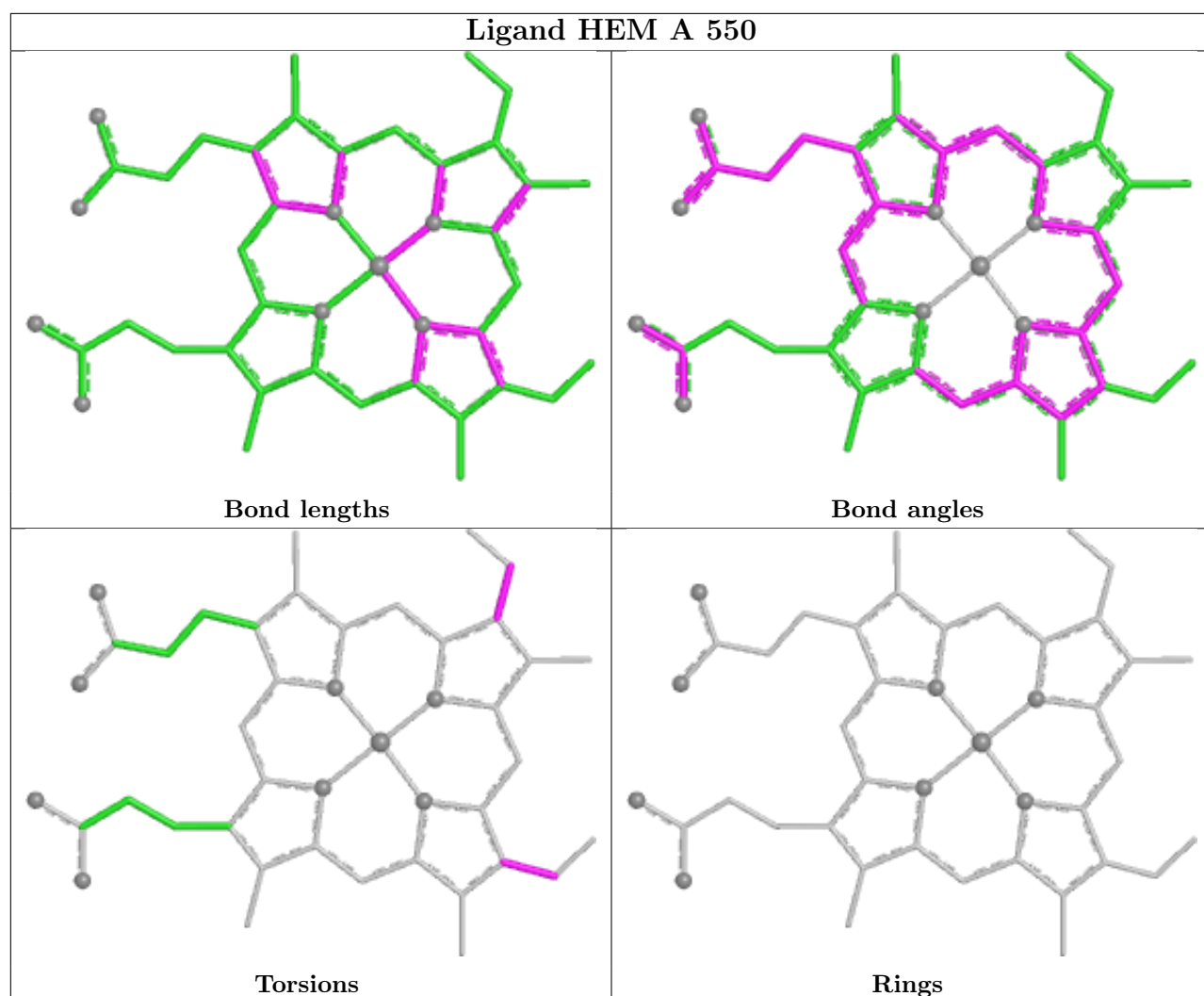
Bond angles

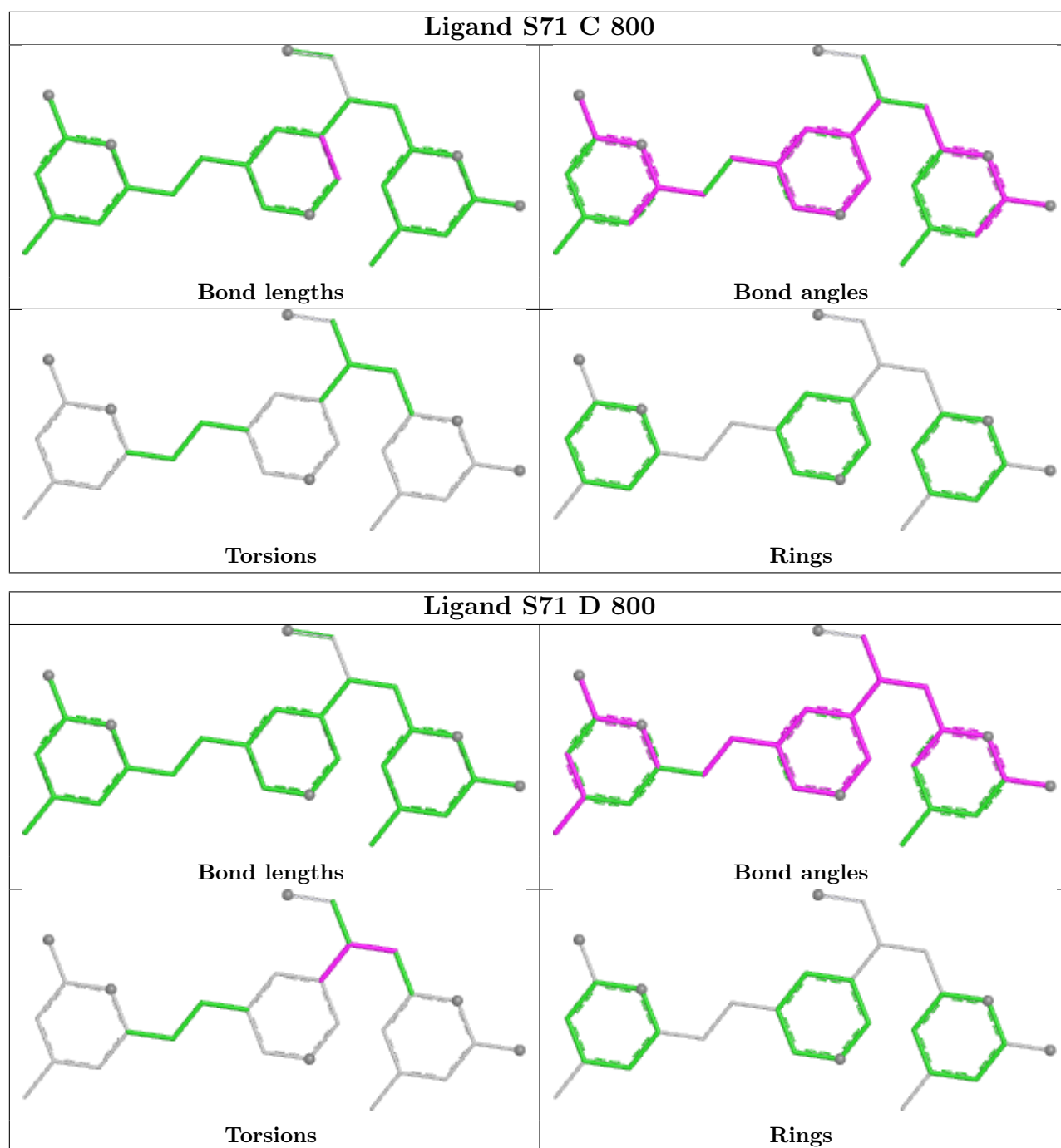


Torsions



Rings





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	414/431 (96%)	-0.83	2 (0%) 87 75	43, 65, 113, 147	0
1	B	414/431 (96%)	-0.83	3 (0%) 84 69	45, 67, 98, 131	0
1	C	414/431 (96%)	-0.48	5 (1%) 76 57	51, 97, 145, 175	0
1	D	414/431 (96%)	-0.84	3 (0%) 84 69	45, 69, 103, 132	0
All	All	1656/1724 (96%)	-0.74	13 (0%) 82 66	43, 72, 126, 175	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	116	LEU	4.5
1	D	116	LEU	3.9
1	A	107	ILE	3.6
1	C	116	LEU	3.6
1	D	107	ILE	3.2
1	B	116	LEU	3.1
1	B	117	GLY	2.9
1	D	117	GLY	2.6
1	B	115	CYS	2.5
1	C	117	GLY	2.5
1	C	107	ILE	2.4
1	C	105	LYS	2.3
1	C	155	LYS	2.1

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

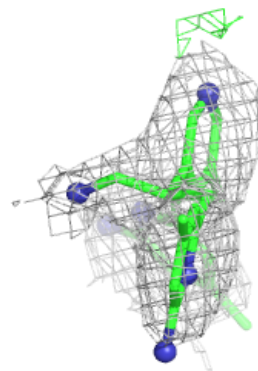
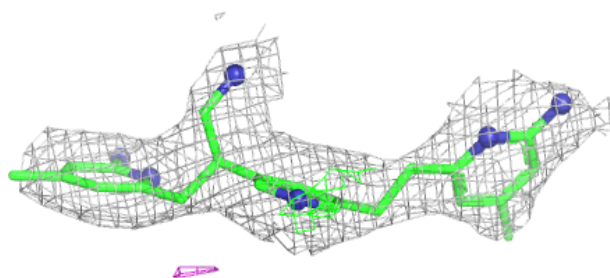
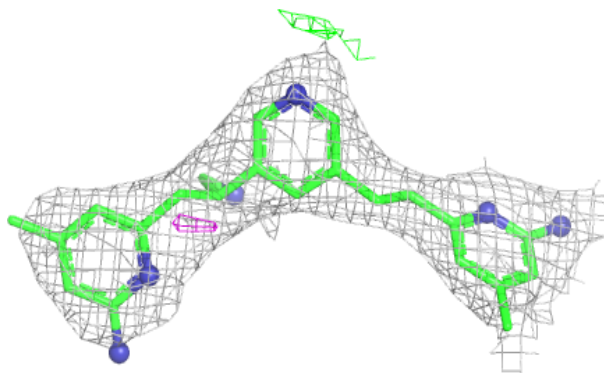
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	SO4	C	920	5/5	0.77	0.09	155,161,183,196	0
6	SO4	C	910	5/5	0.84	0.21	121,143,163,168	0
6	SO4	B	910	5/5	0.84	0.12	117,120,140,148	0
6	SO4	D	910	5/5	0.85	0.16	114,119,142,142	0
6	SO4	B	920	5/5	0.86	0.16	105,129,142,162	0
6	SO4	D	920	5/5	0.90	0.14	120,123,135,138	0
5	GOL	B	880	6/6	0.91	0.25	56,76,89,97	0
6	SO4	A	920	5/5	0.92	0.09	98,127,139,151	0
5	GOL	D	880	6/6	0.93	0.13	64,79,84,85	0
6	SO4	A	910	5/5	0.94	0.15	82,88,99,100	0
5	GOL	A	880	6/6	0.94	0.14	60,67,84,85	0
6	SO4	A	930	5/5	0.95	0.11	75,82,87,97	0
4	S71	C	800	28/28	0.97	0.10	66,74,82,91	0
5	GOL	C	880	6/6	0.97	0.12	70,79,84,86	0
3	H4B	C	600	17/17	0.98	0.05	58,64,73,77	0
4	S71	D	800	28/28	0.98	0.08	47,68,78,80	0
3	H4B	D	600	17/17	0.98	0.06	62,67,72,72	0
4	S71	A	800	28/28	0.98	0.07	48,58,67,69	0
4	S71	B	800	28/28	0.98	0.08	47,56,69,71	0
2	HEM	B	550	43/43	0.99	0.06	46,58,67,87	0
2	HEM	C	550	43/43	0.99	0.06	68,84,102,110	0
2	HEM	D	550	43/43	0.99	0.06	51,57,78,85	0
3	H4B	A	600	17/17	0.99	0.04	44,48,51,52	0
3	H4B	B	600	17/17	0.99	0.04	43,49,53,55	0
2	HEM	A	550	43/43	0.99	0.05	47,53,67,79	0

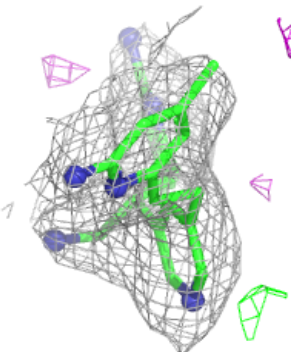
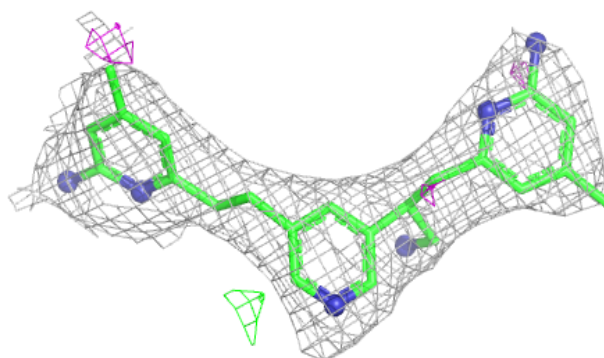
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around S71 C 800:

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

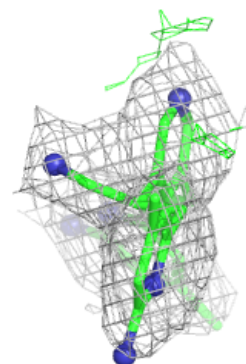
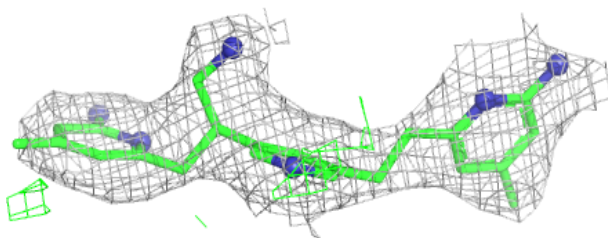
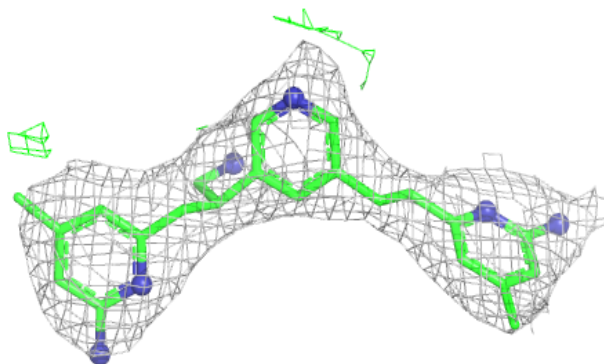
**Electron density around S71 D 800:**

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

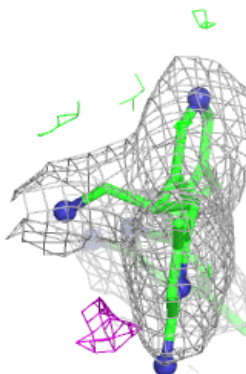
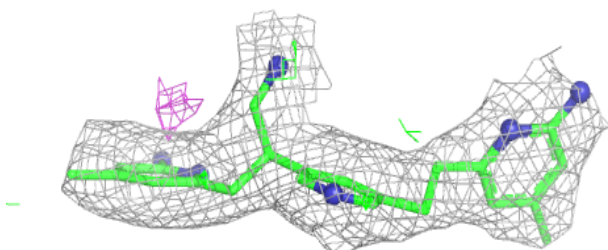
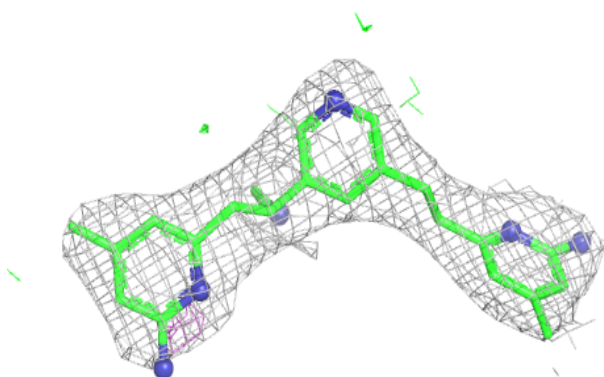


Electron density around S71 A 800:

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

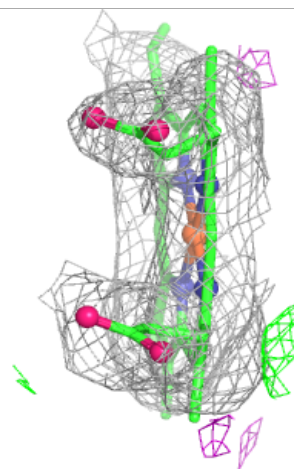
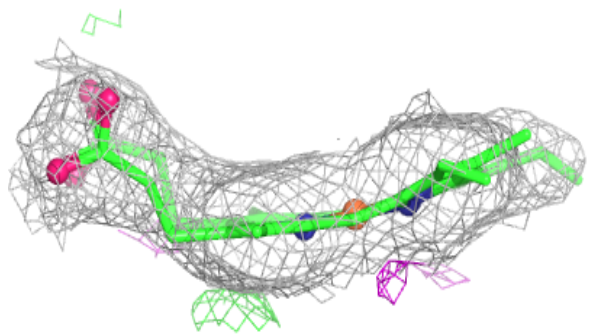
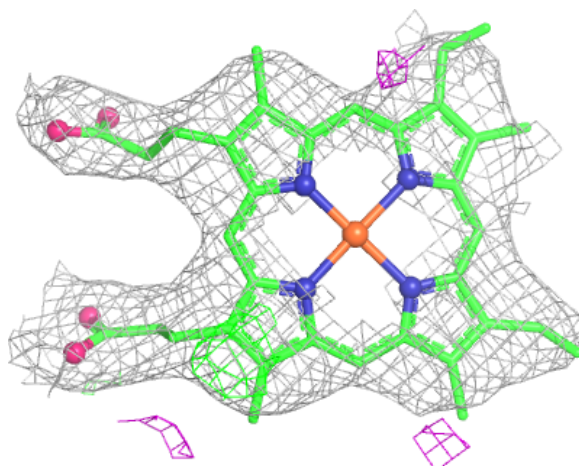
**Electron density around S71 B 800:**

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



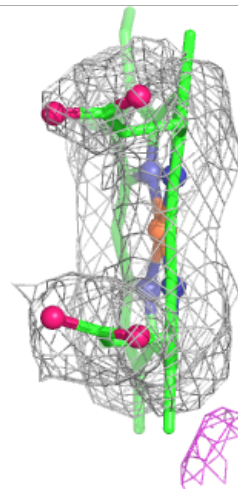
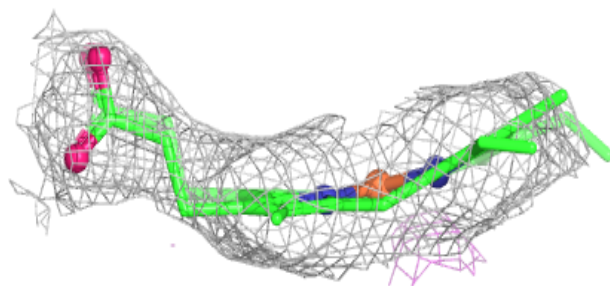
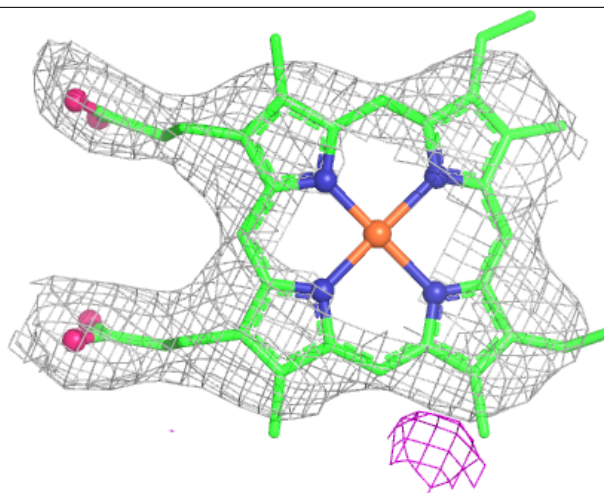
Electron density around HEM B 550:

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



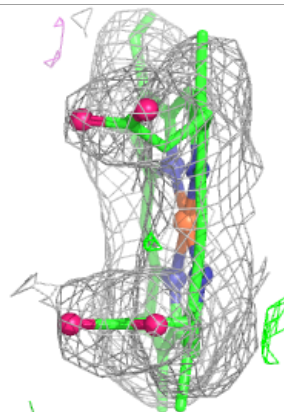
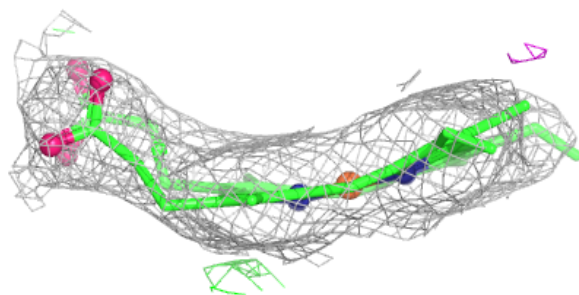
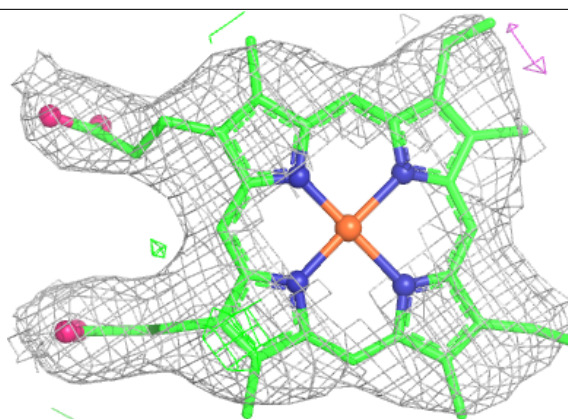
Electron density around HEM C 550:

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



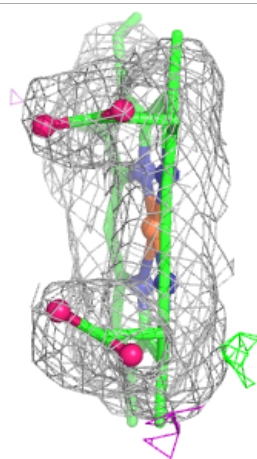
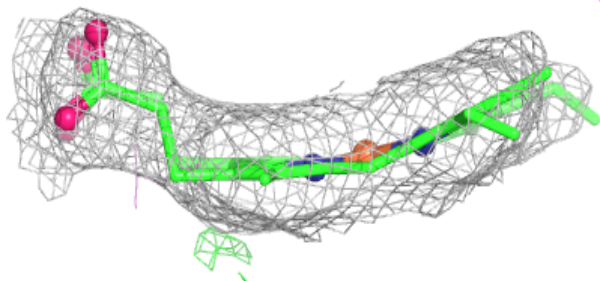
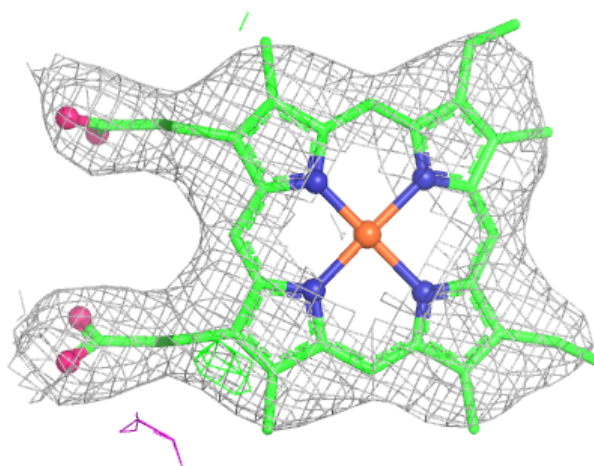
Electron density around HEM D 550:

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



Electron density around HEM A 550:

$2mF_o-DF_c$ (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.