



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:32 AM UTC

PDB ID : 5QJ2 / pdb_00005qj2
Title : CRYSTAL STRUCTURE OF MYELOPEROXIDASE SUBFORM C (MPO)
COMPLEX WITH COMPOUND-20 AKA 7-((3-(1-METHYL-1H-PYRAZOL-
3- YL)BENZYL)OXY)- 1H-[1,2,3]TRIAZOLO[4,5-B]PYRIDIN-5-AMINE
Authors : Khan, J.A.
Deposited on : 2018-09-26
Resolution : 2.82 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

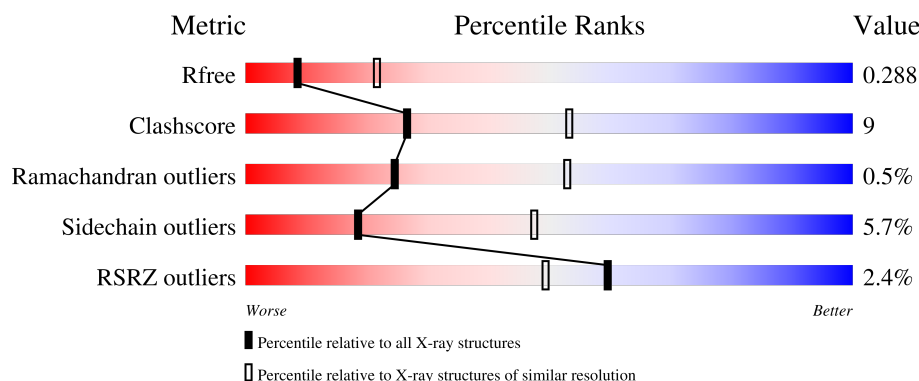
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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.



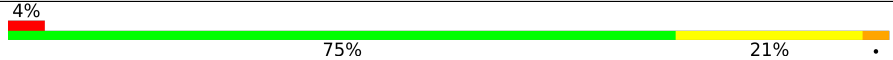
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	105	70%27%..
1	D	105	2% 77%20%..
1	F	105	2% 78%16%..
1	H	105	% 76%20%..

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Mol	Chain	Length	Quality of chain
2	B	467	
2	E	467	
2	G	467	
2	I	467	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	BMA	G	609	-	-	X	-
8	JXS	G	612	-	X	-	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 18513 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 Myeloperoxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	103	Total	C	N	O	S	3	0	0
			812	515	144	148	5			
1	D	103	Total	C	N	O	S	4	0	0
			825	522	145	153	5			
1	F	103	Total	C	N	O	S	0	0	0
			813	516	144	148	5			
1	H	103	Total	C	N	O	S	3	0	0
			821	520	144	152	5			

- Molecule 2 is a protein called Myeloperoxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	465	Total	C	N	O	S	24	0	0
			3617	2289	648	653	27			
2	E	465	Total	C	N	O	S	19	0	0
			3619	2296	645	651	27			
2	G	465	Total	C	N	O	S	12	0	0
			3608	2290	642	650	26			
2	I	465	Total	C	N	O	S	28	0	0
			3605	2283	645	650	27			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	112	ALA	GLY	conflict	UNP P05164
E	112	ALA	GLY	conflict	UNP P05164
G	112	ALA	GLY	conflict	UNP P05164
I	112	ALA	GLY	conflict	UNP P05164

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



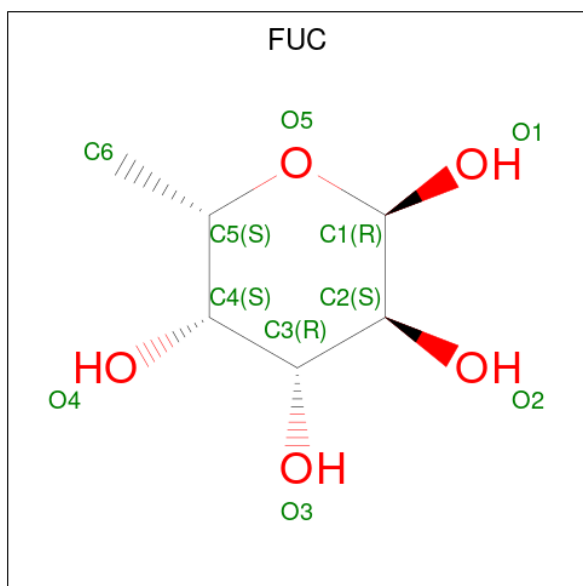
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	I	1	Total	C	N	O	0	0
			14	8	1	5		
3	I	1	Total	C	N	O	0	0
			14	8	1	5		
3	I	1	Total	C	N	O	0	0
			14	8	1	5		
3	I	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is alpha-L-fucopyranose (CCD ID: FUC) (formula: $C_6H_{12}O_5$).



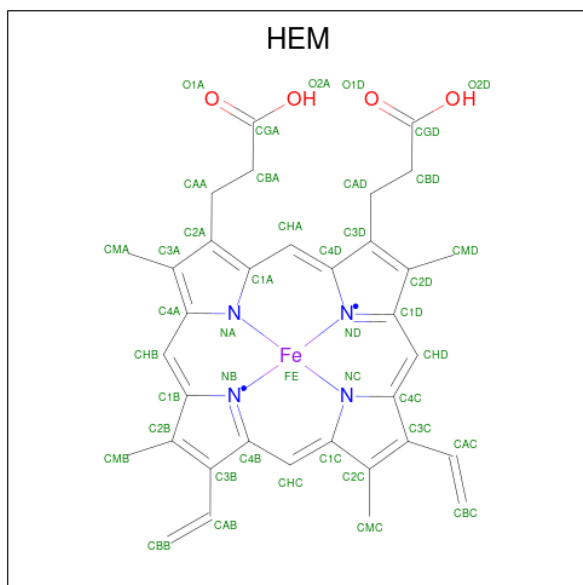
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			10	6	4		
4	E	1	Total	C	O	0	0
			10	6	4		
4	G	1	Total	C	O	0	0
			10	6	4		

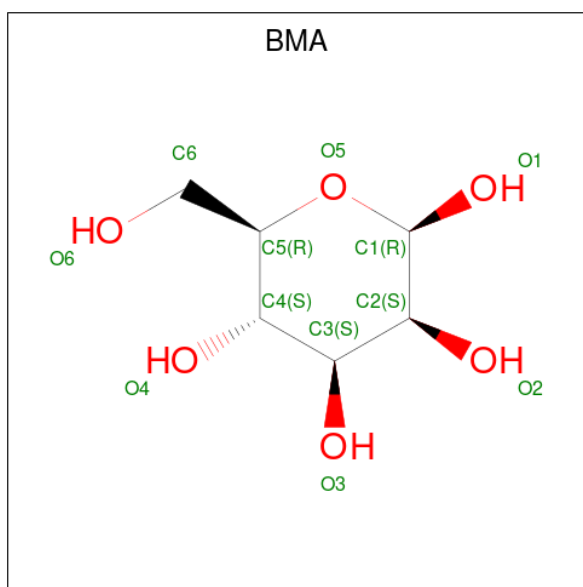
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	I	1	Total	C	O	0	0
			10	6	4		

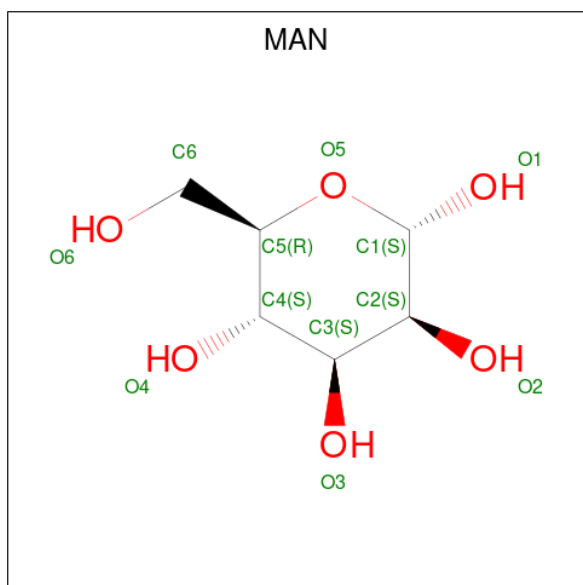
- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).





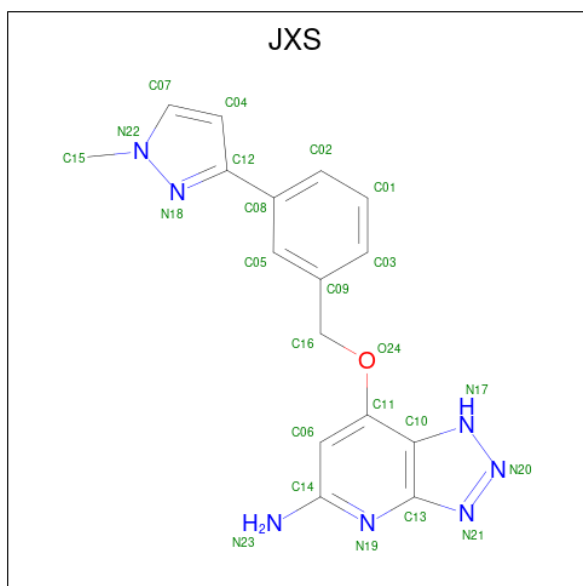
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			11	6	5		
6	E	1	Total	C	O	0	0
			11	6	5		
6	G	1	Total	C	O	0	0
			11	6	5		
6	I	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is alpha-D-mannopyranose (CCD ID: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			11	6	5		
7	B	1	Total	C	O	0	0
			11	6	5		
7	E	1	Total	C	O	0	0
			11	6	5		
7	E	1	Total	C	O	0	0
			11	6	5		
7	G	1	Total	C	O	0	0
			11	6	5		
7	G	1	Total	C	O	0	0
			11	6	5		
7	I	1	Total	C	O	0	0
			11	6	5		
7	I	1	Total	C	O	0	0
			11	6	5		

- Molecule 8 is 7-{[3-(1-methyl-1H-pyrazol-3-yl)phenyl]methoxy}-1H-[1,2,3]triazolo[4,5-b]pyridin-5-amine (CCD ID: JXS) (formula: C₁₆H₁₅N₇O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			24	16	7	1		
8	E	1	Total	C	N	O	0	0
			24	16	7	1		
8	G	1	Total	C	N	O	0	0
			24	16	7	1		

- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Ca 1 1	0	0
9	E	1	Total Ca 1 1	0	0
9	G	1	Total Ca 1 1	0	0
9	I	1	Total Ca 1 1	0	0

- Molecule 10 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Cl 1 1	0	0
10	G	1	Total Cl 1 1	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	2	Total O 2 2	0	0
11	B	11	Total O 11 11	0	0
11	D	2	Total O 2 2	0	0
11	E	10	Total O 10 10	0	0
11	F	4	Total O 4 4	0	0
11	G	21	Total O 21 21	0	0
11	H	4	Total O 4 4	0	0
11	I	9	Total O 9 9	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: Myeloperoxidase

Chain A: 



- Molecule 1: Myeloperoxidase

Chain D: 



- Molecule 1: Myeloperoxidase

Chain F: 



- Molecule 1: Myeloperoxidase

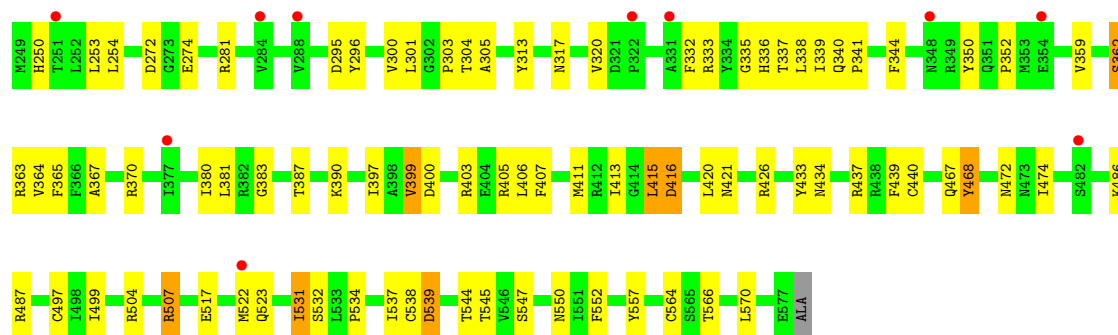
Chain H: 



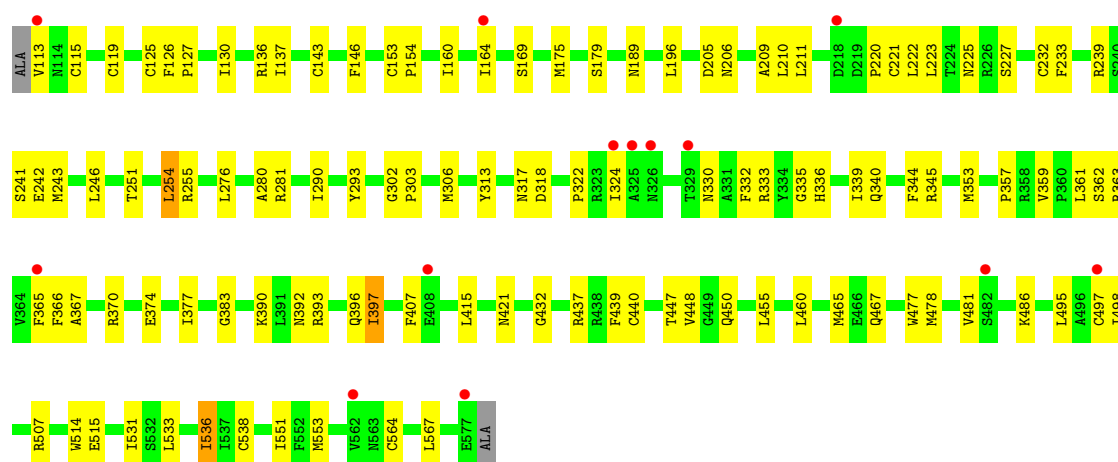
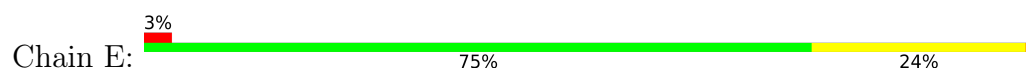
- Molecule 2: Myeloperoxidase

Chain B: 

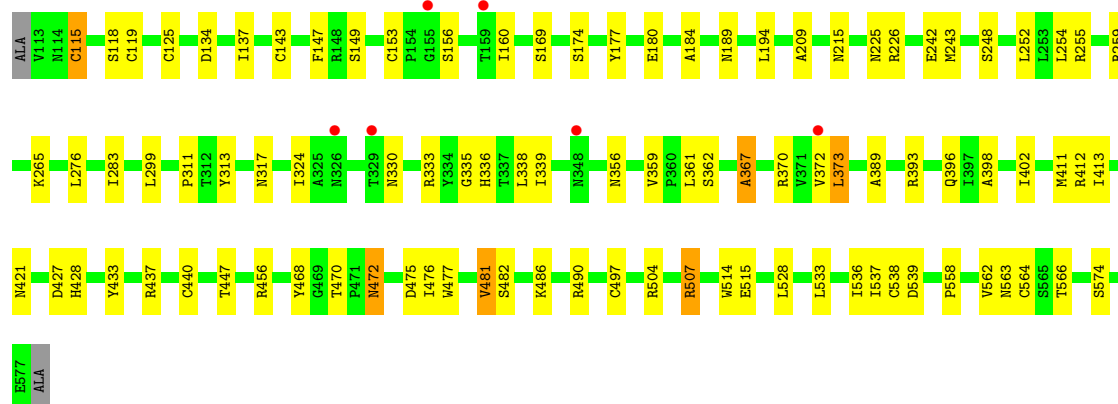
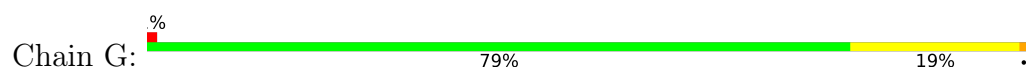




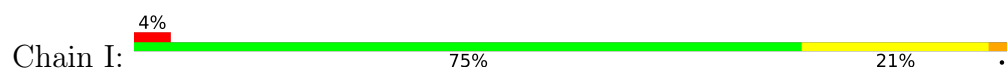
• Molecule 2: Myeloperoxidase

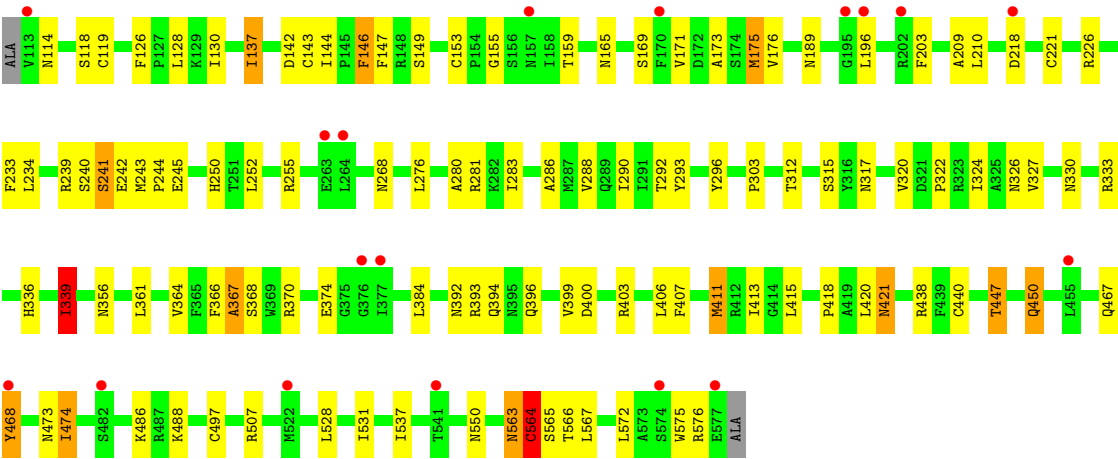


• Molecule 2: Myeloperoxidase



• Molecule 2: Myeloperoxidase





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	143.82Å 150.95Å 233.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	116.55 – 2.82 116.55 – 2.82	Depositor EDS
% Data completeness (in resolution range)	99.7 (116.55-2.82) 99.7 (116.55-2.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.82Å)	Xtriage
Refinement program	BUSTER 2.9.6	Depositor
R, R_{free}	0.206 , 0.272 0.218 , 0.288	Depositor DCC
R_{free} test set	3114 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	58.1	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 71.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.056 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	18513	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, CL, HEM, BMA, MAN, JXS, CA, NAG

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	0.80	0/837	1.38	6/1143 (0.5%)
1	D	0.81	0/850	1.38	9/1159 (0.8%)
1	F	0.83	0/838	1.40	11/1144 (1.0%)
1	H	0.84	0/846	1.39	9/1154 (0.8%)
2	B	0.86	0/3703	1.39	26/5043 (0.5%)
2	E	0.85	0/3704	1.36	21/5043 (0.4%)
2	G	0.90	0/3693	1.38	20/5030 (0.4%)
2	I	0.86	0/3690	1.42	33/5026 (0.7%)
All	All	0.86	0/18161	1.39	135/24742 (0.5%)

There are no bond length outliers.

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	43	LEU	N-CA-C	8.30	120.10	109.72
2	B	177	TYR	N-CA-C	7.14	120.11	111.40
2	I	550	ASN	CA-CB-CG	6.96	119.56	112.60
2	B	550	ASN	CA-CB-CG	6.93	119.53	112.60
2	I	147	PHE	CA-CB-CG	6.67	120.47	113.80
2	G	118	SER	N-CA-C	6.62	118.55	110.41
1	D	96	ASP	N-CA-C	-6.49	105.00	113.17
1	A	20	PRO	N-CA-C	6.46	122.31	113.98
2	E	205	ASP	CA-CB-CG	6.41	119.01	112.60
2	I	447	THR	CA-C-N	6.41	129.56	120.53
2	I	447	THR	C-N-CA	6.41	129.56	120.53
2	E	293	TYR	N-CA-C	6.39	118.33	111.36
1	H	96	ASP	N-CA-C	-6.35	105.53	113.28
1	H	29	PHE	CA-CB-CG	6.30	120.11	113.80
2	E	189	ASN	CA-CB-CG	6.27	118.87	112.60
2	G	177	TYR	N-CA-C	6.21	120.98	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	20	PRO	N-CA-C	6.20	121.63	114.20
2	B	407	PHE	CA-C-N	6.19	128.57	120.28
2	B	407	PHE	C-N-CA	6.19	128.57	120.28
2	G	156	SER	N-CA-C	6.18	119.32	110.24
1	H	15	ASN	N-CA-C	-6.18	104.47	111.14
2	B	397	ILE	N-CA-C	6.17	116.35	110.74
2	B	365	PHE	CA-CB-CG	6.15	119.95	113.80
2	G	472	ASN	CA-CB-CG	6.15	118.75	112.60
1	H	98	ASP	N-CA-C	6.10	119.43	109.06
2	B	399	VAL	N-CA-C	6.05	117.38	109.58
2	I	468	TYR	N-CA-C	6.05	117.74	111.03
2	B	468	TYR	N-CA-C	6.04	119.83	112.23
1	D	5	ASP	CA-CB-CG	6.03	118.63	112.60
2	E	392	ASN	CA-CB-CG	6.03	118.63	112.60
2	I	564	CYS	N-CA-C	6.03	118.63	111.33
1	D	12	GLY	CA-C-N	6.01	129.38	120.90
1	D	12	GLY	C-N-CA	6.01	129.38	120.90
2	B	426	ARG	CA-C-N	5.99	128.30	120.28
2	B	426	ARG	C-N-CA	5.99	128.30	120.28
2	I	218	ASP	CA-CB-CG	5.97	118.57	112.60
2	I	146	PHE	CA-CB-CG	5.94	119.74	113.80
2	G	558	PRO	CA-C-N	5.93	128.48	120.65
2	G	558	PRO	C-N-CA	5.93	128.48	120.65
1	D	96	ASP	CA-CB-CG	5.92	118.52	112.60
2	I	326	ASN	CA-C-N	5.84	128.13	120.60
2	I	326	ASN	C-N-CA	5.84	128.13	120.60
2	E	130	ILE	N-CA-C	5.81	114.35	107.73
2	G	226	ARG	CA-C-N	5.80	127.98	120.44
2	G	226	ARG	C-N-CA	5.80	127.98	120.44
2	E	437	ARG	CA-C-N	5.78	127.96	120.44
2	E	437	ARG	C-N-CA	5.78	127.96	120.44
2	G	215	ASN	CA-CB-CG	5.74	118.34	112.60
1	F	37	TYR	CA-C-N	5.73	127.89	120.44
1	F	37	TYR	C-N-CA	5.73	127.89	120.44
1	H	5	ASP	CA-CB-CG	5.73	118.33	112.60
2	E	432	GLY	CA-C-N	5.69	128.70	120.79
2	E	432	GLY	C-N-CA	5.69	128.70	120.79
2	I	203	PHE	N-CA-C	5.69	118.50	110.14
1	F	98	ASP	CA-C-N	5.64	129.97	121.40
1	F	98	ASP	C-N-CA	5.64	129.97	121.40
2	G	482	SER	CA-C-N	5.63	128.68	120.51
2	G	482	SER	C-N-CA	5.63	128.68	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	32	TRP	N-CA-C	-5.63	106.40	113.72
2	B	522	MET	CA-C-N	5.61	128.06	120.65
2	B	522	MET	C-N-CA	5.61	128.06	120.65
1	F	98	ASP	N-CA-C	5.61	117.92	109.23
2	E	377	ILE	CA-C-N	5.60	127.73	120.44
2	E	377	ILE	C-N-CA	5.60	127.73	120.44
2	G	367	ALA	CA-C-N	5.59	128.33	120.28
2	G	367	ALA	C-N-CA	5.59	128.33	120.28
2	I	438	ARG	CA-C-N	5.58	128.03	120.38
2	I	438	ARG	C-N-CA	5.58	128.03	120.38
2	I	374	GLU	N-CA-C	5.57	120.29	112.72
2	G	180	GLU	CA-C-N	5.57	127.05	120.09
2	G	180	GLU	C-N-CA	5.57	127.05	120.09
1	A	98	ASP	N-CA-C	5.56	118.51	109.06
1	D	61	ALA	CA-C-N	5.55	128.03	120.54
1	D	61	ALA	C-N-CA	5.55	128.03	120.54
2	G	427	ASP	CA-CB-CG	5.53	118.13	112.60
2	I	420	LEU	CA-C-N	5.53	128.01	120.54
2	I	420	LEU	C-N-CA	5.53	128.01	120.54
2	I	293	TYR	N-CA-C	5.50	117.36	111.36
2	B	539	ASP	CA-CB-CG	5.48	118.08	112.60
2	B	421	ASN	CA-CB-CG	5.48	118.08	112.60
2	I	421	ASN	CA-CB-CG	5.44	118.04	112.60
2	B	272	ASP	CA-C-N	5.42	126.00	119.98
2	B	272	ASP	C-N-CA	5.42	126.00	119.98
2	I	407	PHE	CA-C-N	5.37	127.42	120.44
2	I	407	PHE	C-N-CA	5.37	127.42	120.44
1	A	37	TYR	CA-C-N	5.37	128.88	120.82
1	A	37	TYR	C-N-CA	5.37	128.88	120.82
2	E	154	PRO	N-CA-C	5.34	119.25	111.03
1	D	20	PRO	N-CA-C	5.30	120.98	114.35
2	I	565	SER	CA-C-N	5.29	127.81	120.29
2	I	565	SER	C-N-CA	5.29	127.81	120.29
2	G	373	LEU	N-CA-C	5.29	118.55	112.57
2	E	281	ARG	CA-C-N	5.28	127.36	120.28
2	E	281	ARG	C-N-CA	5.28	127.36	120.28
1	H	65	SER	CA-C-N	5.28	127.35	120.28
1	H	65	SER	C-N-CA	5.28	127.35	120.28
2	I	137	ILE	N-CA-C	5.27	114.85	107.37
1	H	86	PHE	CA-C-N	5.27	127.29	120.44
1	H	86	PHE	C-N-CA	5.27	127.29	120.44
1	F	96	ASP	N-CA-C	-5.23	106.74	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	114	ASN	CA-C-N	5.22	127.80	120.28
2	B	114	ASN	C-N-CA	5.22	127.80	120.28
2	I	474	ILE	N-CA-CB	5.21	116.60	110.82
2	E	227	SER	CA-C-N	5.19	127.76	120.28
2	E	227	SER	C-N-CA	5.19	127.76	120.28
2	I	281	ARG	CA-C-N	5.18	127.65	120.29
2	I	281	ARG	C-N-CA	5.18	127.65	120.29
2	B	187	LEU	N-CA-C	-5.18	108.72	114.62
1	A	88	GLN	N-CA-C	5.16	116.90	111.28
2	G	421	ASN	CA-CB-CG	5.16	117.76	112.60
2	I	142	ASP	CA-CB-CG	5.14	117.74	112.60
2	B	504	ARG	CA-C-N	5.14	127.17	120.28
2	B	504	ARG	C-N-CA	5.14	127.17	120.28
2	B	274	GLU	CA-C-N	5.14	127.17	120.28
2	B	274	GLU	C-N-CA	5.14	127.17	120.28
2	I	330	ASN	N-CA-C	-5.14	107.56	113.88
2	G	481	VAL	CA-C-N	5.14	127.43	120.44
2	G	481	VAL	C-N-CA	5.14	127.43	120.44
2	E	374	GLU	N-CA-C	5.14	119.11	111.87
2	B	247	THR	CA-C-N	5.13	127.47	120.54
2	B	247	THR	C-N-CA	5.13	127.47	120.54
2	I	327	VAL	N-CA-C	5.13	115.74	110.36
2	I	392	ASN	CA-CB-CG	5.11	117.71	112.60
1	F	88	GLN	N-CA-C	5.10	116.84	111.28
2	E	280	ALA	CA-C-N	5.06	127.06	120.28
2	E	280	ALA	C-N-CA	5.06	127.06	120.28
2	I	563	ASN	CA-C-N	5.06	127.31	120.38
2	I	563	ASN	C-N-CA	5.06	127.31	120.38
2	B	416	ASP	CA-CB-CG	5.03	117.63	112.60
2	E	536	ILE	CA-C-N	5.03	126.89	120.56
2	E	536	ILE	C-N-CA	5.03	126.89	120.56
1	A	54	ASN	CA-CB-CG	5.02	117.62	112.60
1	F	5	ASP	CA-CB-CG	5.02	117.62	112.60
1	F	96	ASP	CA-CB-CG	5.02	117.62	112.60
2	I	339	ILE	N-CA-C	5.01	115.69	108.93

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	812	0	764	21	0
1	D	825	0	780	13	0
1	F	813	0	766	12	0
1	H	821	0	774	14	0
2	B	3617	0	3529	72	0
2	E	3619	0	3555	71	0
2	G	3608	0	3526	57	0
2	I	3605	0	3513	62	0
3	B	98	0	91	18	0
3	E	56	0	52	8	0
3	G	84	0	78	17	0
3	I	70	0	65	10	0
4	B	10	0	10	1	0
4	E	10	0	10	0	0
4	G	10	0	10	0	0
4	I	10	0	10	1	0
5	B	43	0	30	12	0
5	E	43	0	30	8	0
5	G	43	0	30	11	0
5	I	43	0	30	9	0
6	B	11	0	10	3	0
6	E	11	0	10	5	0
6	G	11	0	10	8	0
6	I	11	0	10	2	0
7	B	22	0	20	0	0
7	E	22	0	20	4	0
7	G	22	0	20	5	0
7	I	22	0	20	1	0
8	B	24	0	0	0	0
8	E	24	0	0	0	0
8	G	24	0	0	0	0
9	B	1	0	0	0	0
9	E	1	0	0	0	0
9	G	1	0	0	0	0
9	I	1	0	0	0	0
10	B	1	0	0	0	0
10	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	2	0	0	0	0
11	B	11	0	0	0	0
11	D	2	0	0	1	0
11	E	10	0	0	0	0
11	F	4	0	0	0	0
11	G	21	0	0	2	0
11	H	4	0	0	0	0
11	I	9	0	0	0	0
All	All	18513	0	17773	318	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 9.

All (318) 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)
2:G:317:ASN:HD21	3:G:604:NAG:C1	1.35	1.37
2:E:115:CYS:SG	2:E:125:CYS:SG	1.35	1.28
2:E:115:CYS:CB	2:E:125:CYS:SG	2.25	1.23
1:A:94:ASP:OD2	5:B:608:HEM:HMD1	1.41	1.17
1:F:94:ASP:OD2	5:G:607:HEM:HMD1	1.46	1.15
2:I:173:ALA:HA	2:I:175:MET:HE1	1.33	1.09
2:E:335:GLY:HA3	5:E:609:HEM:HBC2	1.31	1.09
2:B:225:ASN:HD21	3:B:602:NAG:C1	1.66	1.07
2:G:317:ASN:ND2	3:G:604:NAG:C1	2.16	1.07
2:I:317:ASN:HD21	3:I:608:NAG:C1	1.69	1.05
2:I:173:ALA:HA	2:I:175:MET:CE	1.88	1.01
2:G:242:GLU:OE2	5:G:607:HEM:HMB3	1.61	1.01
6:G:609:BMA:H62	7:G:611:MAN:H2	1.44	0.98
2:G:119:CYS:HG	2:G:143:CYS:HG	1.12	0.97
2:G:440:CYS:HG	2:G:497:CYS:HG	1.09	0.94
2:G:538:CYS:HG	2:G:564:CYS:HG	0.96	0.93
2:G:243:MET:SD	5:G:607:HEM:HBB1	2.10	0.91
2:G:311:PRO:O	2:G:507:ARG:NH2	2.02	0.91
2:B:440:CYS:HG	2:B:497:CYS:HG	1.19	0.90
2:E:242:GLU:OE2	5:E:609:HEM:HMB1	1.72	0.90
1:F:94:ASP:OD2	5:G:607:HEM:CMD	2.20	0.88
2:B:243:MET:SD	5:B:608:HEM:HBB1	2.14	0.87
2:E:119:CYS:HG	2:E:143:CYS:HG	1.13	0.87
1:A:94:ASP:OD2	5:B:608:HEM:CMD	2.26	0.82
6:E:601:BMA:H3	7:E:602:MAN:H2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:ASP:OD2	5:E:609:HEM:HMD1	1.82	0.80
2:E:333:ARG:HH21	5:E:609:HEM:HAD1	1.47	0.80
2:E:242:GLU:OE2	5:E:609:HEM:CMB	2.31	0.79
2:E:221:CYS:HG	2:E:232:CYS:HG	0.88	0.78
6:G:609:BMA:H62	7:G:611:MAN:C2	2.13	0.78
2:B:153:CYS:HG	2:E:153:CYS:HG	1.28	0.78
2:B:243:MET:CE	5:B:608:HEM:HBB1	2.15	0.77
2:I:173:ALA:CA	2:I:175:MET:CE	2.62	0.77
2:G:115:CYS:HG	2:G:125:CYS:HG	0.79	0.76
2:E:317:ASN:HD21	3:E:607:NAG:C1	1.97	0.76
2:I:175:MET:CE	2:I:176:VAL:HG23	2.17	0.75
2:E:344:PHE:O	2:E:383:GLY:HA3	1.87	0.73
2:G:225:ASN:HD21	3:G:602:NAG:C1	2.02	0.73
2:B:127:PRO:HB2	2:B:143:CYS:SG	2.28	0.73
6:E:601:BMA:H3	7:E:602:MAN:C1	2.19	0.72
2:I:242:GLU:OE2	5:I:610:HEM:HMB1	1.89	0.72
3:B:609:NAG:H4	6:B:610:BMA:C1	2.21	0.71
2:I:175:MET:HE3	2:I:176:VAL:HG23	1.73	0.70
1:A:91:GLN:HE22	5:B:608:HEM:HBB2	1.57	0.69
2:B:243:MET:HE3	5:B:608:HEM:HBB1	1.75	0.69
2:I:173:ALA:CA	2:I:175:MET:HE1	2.18	0.69
3:G:604:NAG:O4	3:I:601:NAG:C1	2.41	0.69
6:E:601:BMA:H3	7:E:602:MAN:C2	2.23	0.68
3:G:602:NAG:H4	3:G:603:NAG:C1	2.23	0.68
2:G:153:CYS:HG	2:I:153:CYS:HG	1.38	0.68
2:G:242:GLU:CD	5:G:607:HEM:HMB3	2.18	0.68
2:I:173:ALA:CA	2:I:175:MET:HE2	2.24	0.68
3:B:604:NAG:O4	3:B:605:NAG:C1	2.42	0.68
2:G:242:GLU:OE2	5:G:607:HEM:CMB	2.40	0.67
2:B:242:GLU:OE2	5:B:608:HEM:CMB	2.43	0.67
2:E:221:CYS:CB	2:E:232:CYS:HG	2.08	0.66
2:E:115:CYS:CB	2:E:125:CYS:HG	1.90	0.66
2:I:209:ALA:HB3	2:I:255:ARG:HG2	1.78	0.66
2:E:225:ASN:HD21	3:E:605:NAG:C1	2.08	0.66
2:E:393:ARG:HB2	2:E:396:GLN:HB2	1.78	0.66
2:I:317:ASN:ND2	3:I:608:NAG:C1	2.52	0.65
2:G:137:ILE:HG12	2:G:413:ILE:HD11	1.79	0.65
2:B:313:TYR:HD1	2:B:507:ARG:HD3	1.62	0.65
3:G:604:NAG:C4	3:I:601:NAG:C1	2.74	0.65
2:B:119:CYS:HG	2:B:143:CYS:HG	0.72	0.64
2:E:333:ARG:NH2	5:E:609:HEM:HAD1	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:317:ASN:HD21	3:B:604:NAG:C1	2.10	0.64
2:E:336:HIS:HA	2:E:339:ILE:HD12	1.80	0.64
2:I:173:ALA:C	2:I:175:MET:HE2	2.23	0.64
3:G:608:NAG:C1	3:I:608:NAG:O4	2.47	0.62
3:B:604:NAG:O6	4:B:606:FUC:C1	2.47	0.62
2:G:242:GLU:OE1	5:G:607:HEM:HBB2	2.00	0.62
1:A:33:LEU:HD21	3:B:609:NAG:H81	1.81	0.62
2:B:211:LEU:HD11	2:B:250:HIS:HB3	1.81	0.62
2:I:243:MET:SD	5:I:610:HEM:HAB	2.41	0.61
2:I:336:HIS:HA	2:I:339:ILE:HD12	1.82	0.61
2:B:313:TYR:CD1	2:B:507:ARG:HD3	2.36	0.61
2:G:252:LEU:HD11	2:G:537:ILE:HA	1.81	0.61
2:E:115:CYS:HB3	2:E:125:CYS:SG	2.36	0.60
2:G:243:MET:CG	5:G:607:HEM:HBB1	2.31	0.60
2:G:259:ARG:HD2	2:G:539:ASP:HB3	1.83	0.60
6:G:609:BMA:C6	7:G:611:MAN:H2	2.27	0.60
1:F:10:ILE:HG21	2:G:184:ALA:HB2	1.84	0.59
6:G:609:BMA:H2	7:G:610:MAN:H5	1.84	0.59
2:B:242:GLU:OE2	5:B:608:HEM:HMB1	2.03	0.58
2:G:477:TRP:O	2:G:481:VAL:HG22	2.03	0.58
2:I:119:CYS:SG	2:I:143:CYS:CB	2.90	0.58
3:G:608:NAG:H4	6:G:609:BMA:C1	2.34	0.58
1:H:69:VAL:HG11	2:I:418:PRO:HG2	1.85	0.58
3:E:605:NAG:H4	3:E:606:NAG:C1	2.33	0.58
2:I:233:PHE:CE2	2:I:368:SER:HB2	2.40	0.57
2:E:115:CYS:CA	2:E:125:CYS:SG	2.92	0.57
2:I:242:GLU:OE2	5:I:610:HEM:CMB	2.52	0.57
2:I:440:CYS:HG	2:I:497:CYS:CB	2.18	0.57
3:G:608:NAG:C1	3:I:608:NAG:C4	2.82	0.57
1:H:63:ALA:O	1:H:67:GLU:HG2	2.04	0.57
2:E:538:CYS:HG	2:E:564:CYS:HG	1.48	0.56
1:F:100:THR:HG21	2:G:428:HIS:CE1	2.40	0.56
1:F:16:ASN:O	1:F:20:PRO:HA	2.05	0.56
2:I:189:ASN:HD21	3:I:605:NAG:H2	1.69	0.56
2:E:533:LEU:HA	2:E:536:ILE:HD12	1.87	0.56
2:B:468:TYR:CD2	2:B:474:ILE:HG12	2.40	0.56
2:G:209:ALA:HB3	2:G:255:ARG:HG2	1.86	0.56
2:G:335:GLY:HA2	2:G:338:LEU:HD12	1.87	0.56
1:D:35:ALA:HB3	2:E:160:ILE:CG2	2.36	0.56
2:G:115:CYS:CB	2:G:125:CYS:HG	2.17	0.56
1:F:35:ALA:HB3	2:G:160:ILE:HG21	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ILE:HD11	2:B:467:GLN:HG3	1.88	0.55
2:I:126:PHE:O	2:I:146:PHE:HB3	2.06	0.55
2:B:320:VAL:HG22	3:B:604:NAG:H62	1.88	0.55
2:G:265:LYS:HD3	2:G:276:LEU:HD11	1.88	0.55
3:B:602:NAG:O4	3:B:603:NAG:H2	2.07	0.55
2:E:335:GLY:CA	5:E:609:HEM:HBC2	2.20	0.55
2:G:189:ASN:HD21	3:G:601:NAG:H2	1.72	0.54
1:F:60:LEU:O	1:F:64:VAL:HG23	2.07	0.54
2:E:313:TYR:HD1	2:E:507:ARG:HD3	1.71	0.54
2:G:367:ALA:HB1	2:G:370:ARG:HG3	1.88	0.54
3:G:604:NAG:H4	3:I:601:NAG:C1	2.38	0.54
1:H:29:PHE:CE1	2:I:165:ASN:HB2	2.43	0.54
2:G:412:ARG:HG3	2:G:413:ILE:HG22	1.90	0.54
2:E:447:THR:HG23	2:E:450:GLN:H	1.72	0.54
2:G:333:ARG:HH21	5:G:607:HEM:HAD1	1.71	0.54
2:I:243:MET:SD	5:I:610:HEM:CAB	2.96	0.53
1:D:59:ALA:HB2	2:E:467:GLN:O	2.08	0.53
1:H:22:LEU:HB3	2:I:322:PRO:HD2	1.90	0.53
2:I:252:LEU:HD11	2:I:537:ILE:HA	1.90	0.53
1:A:86:PHE:HA	2:B:552:PHE:HD1	1.74	0.53
2:B:333:ARG:HG2	5:B:608:HEM:C2D	2.43	0.53
2:G:169:SER:HB2	2:G:324:ILE:HG12	1.91	0.53
2:I:241:SER:O	2:I:366:PHE:HA	2.09	0.53
2:B:128:LEU:HB2	2:B:144:ILE:HB	1.91	0.53
2:E:455:LEU:HD13	2:E:460:LEU:HD23	1.89	0.53
2:E:317:ASN:ND2	3:E:607:NAG:C1	2.71	0.52
2:B:341:PRO:HD3	2:B:399:VAL:HG11	1.91	0.52
1:A:84:LEU:HD11	2:B:340:GLN:HB2	1.91	0.52
2:B:242:GLU:OE2	5:B:608:HEM:HMB2	2.08	0.52
1:D:16:ASN:O	1:D:20:PRO:HA	2.09	0.52
1:A:99:PHE:O	1:A:101:PRO:HD3	2.09	0.52
2:G:225:ASN:ND2	3:G:602:NAG:C1	2.70	0.52
2:B:177:TYR:OH	2:B:281:ARG:HA	2.09	0.52
2:B:440:CYS:HG	2:B:497:CYS:CB	2.22	0.52
2:B:189:ASN:HD21	3:B:601:NAG:C1	2.23	0.52
2:G:336:HIS:HA	2:G:339:ILE:HD12	1.91	0.52
6:E:601:BMA:C3	7:E:602:MAN:H2	2.39	0.51
5:I:610:HEM:HMC2	5:I:610:HEM:HBC2	1.91	0.51
2:E:220:PRO:HA	2:E:223:LEU:HD12	1.92	0.51
2:B:221:CYS:HG	2:B:232:CYS:HG	0.59	0.51
3:I:606:NAG:H4	3:I:607:NAG:C1	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:ASN:ND2	3:B:602:NAG:C1	2.52	0.51
2:B:433:TYR:CZ	2:B:437:ARG:HD3	2.45	0.51
1:D:94:ASP:OD2	2:E:332:PHE:HD2	1.94	0.51
2:G:313:TYR:CD1	2:G:507:ARG:HD3	2.45	0.51
2:I:169:SER:HB2	2:I:324:ILE:HG12	1.92	0.51
2:I:268:ASN:HD21	2:I:576:ARG:HA	1.74	0.51
1:D:25:SER:HB3	2:E:179:SER:HB3	1.92	0.51
2:G:189:ASN:HB3	11:G:702:HOH:O	2.10	0.51
2:G:283:ILE:HG23	2:G:528:LEU:HD21	1.91	0.51
1:A:29:PHE:CE1	2:B:165:ASN:HB2	2.46	0.51
2:B:337:THR:O	2:B:390:LYS:HD3	2.11	0.51
1:F:84:LEU:HD13	2:G:389:ALA:HA	1.93	0.51
2:I:221:CYS:SG	2:I:366:PHE:O	2.65	0.51
6:I:602:BMA:H62	7:I:604:MAN:C1	2.42	0.50
2:B:532:SER:HB2	2:B:534:PRO:HD2	1.92	0.50
2:G:514:TRP:CE2	2:G:515:GLU:HG3	2.46	0.50
2:I:175:MET:HE2	2:I:176:VAL:HG23	1.90	0.50
2:B:381:LEU:HD13	2:B:537:ILE:HG12	1.93	0.50
3:B:609:NAG:C4	6:B:610:BMA:C1	2.90	0.50
2:I:393:ARG:HB2	2:I:396:GLN:HB2	1.93	0.50
1:H:44:PRO:HD2	1:H:47:TRP:HB2	1.93	0.49
2:I:320:VAL:HG22	4:I:609:FUC:H61	1.92	0.49
2:B:538:CYS:HG	2:B:564:CYS:HG	1.58	0.49
1:F:13:MET:HE1	1:F:21:THR:HG22	1.94	0.49
2:G:134:ASP:HB3	2:G:137:ILE:O	2.12	0.49
2:G:440:CYS:HG	2:G:497:CYS:CB	2.23	0.49
2:I:173:ALA:HA	2:I:175:MET:HE2	1.79	0.49
2:B:544:THR:HA	2:B:564:CYS:SG	2.52	0.49
2:E:221:CYS:SG	2:E:366:PHE:O	2.70	0.49
2:B:344:PHE:CD1	2:B:387:THR:HG21	2.47	0.49
2:E:440:CYS:HG	2:E:497:CYS:HG	1.53	0.49
2:E:363:ARG:O	2:E:370:ARG:NH1	2.46	0.49
2:G:440:CYS:SG	2:G:497:CYS:HB3	2.53	0.49
2:G:398:ALA:HB1	2:G:402:ILE:HD11	1.94	0.49
1:A:18:ARG:HB3	1:D:36:GLU:OE2	2.13	0.49
2:I:175:MET:HB2	2:I:250:HIS:HE1	1.77	0.49
1:D:22:LEU:HB3	2:E:322:PRO:HD2	1.94	0.48
1:H:94:ASP:OD2	5:I:610:HEM:CMD	2.61	0.48
1:A:41:PHE:HA	2:B:160:ILE:HG23	1.93	0.48
2:B:119:CYS:SG	2:G:456:ARG:HD3	2.54	0.48
1:D:35:ALA:HB3	2:E:160:ILE:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:125:CYS:C	2:E:127:PRO:HD3	2.39	0.48
2:E:333:ARG:HH11	2:E:421:ASN:HD22	1.61	0.48
2:G:225:ASN:HD21	3:G:602:NAG:C2	2.27	0.48
3:G:608:NAG:H61	6:G:609:BMA:C1	2.43	0.48
1:D:81:GLU:O	2:E:553:MET:HA	2.15	0.47
2:E:317:ASN:ND2	3:E:607:NAG:O5	2.46	0.47
6:G:609:BMA:H62	7:G:611:MAN:C1	2.45	0.47
2:E:126:PHE:O	2:E:146:PHE:HB3	2.14	0.47
2:G:563:ASN:HB3	11:G:709:HOH:O	2.13	0.47
5:G:607:HEM:CMB	5:G:607:HEM:CBB	2.91	0.47
2:E:330:ASN:HA	2:E:333:ARG:HD2	1.96	0.47
2:B:153:CYS:SG	2:B:156:SER:HB2	2.55	0.47
2:I:333:ARG:HH11	2:I:421:ASN:HD22	1.62	0.47
2:B:335:GLY:HA2	2:B:338:LEU:HD12	1.97	0.46
2:E:448:VAL:HB	2:E:465:MET:HG3	1.96	0.46
2:I:280:ALA:HA	2:I:283:ILE:HD12	1.97	0.46
1:A:13:MET:HE1	1:A:27:ARG:HH21	1.80	0.46
2:E:209:ALA:O	2:E:255:ARG:NE	2.46	0.46
1:A:98:ASP:HA	2:B:165:ASN:OD1	2.15	0.46
1:H:61:ALA:HB3	2:I:128:LEU:HD23	1.98	0.46
3:B:604:NAG:C4	3:B:605:NAG:C1	2.93	0.46
2:G:313:TYR:HD1	2:G:507:ARG:HD3	1.81	0.46
1:A:44:PRO:HD3	2:B:148:ARG:NH1	2.30	0.46
2:G:468:TYR:HE1	2:G:475:ASP:OD2	1.98	0.46
2:I:144:ILE:HG23	2:I:415:LEU:HD23	1.97	0.46
2:E:440:CYS:HG	2:E:497:CYS:CB	2.29	0.45
2:G:533:LEU:HA	2:G:536:ILE:HD12	1.98	0.45
2:I:292:THR:HA	2:I:296:TYR:HB3	1.98	0.45
5:G:607:HEM:HMC1	5:G:607:HEM:HBC2	1.97	0.45
3:B:605:NAG:H2	2:E:439:PHE:HA	1.98	0.45
2:E:335:GLY:HA3	5:E:609:HEM:CBC	2.23	0.45
2:I:137:ILE:HG12	2:I:413:ILE:HD11	1.98	0.45
2:E:440:CYS:HG	2:E:497:CYS:HB3	1.81	0.45
2:I:244:PRO:HD3	2:I:364:VAL:O	2.15	0.45
2:I:447:THR:HG22	2:I:450:GLN:HE21	1.81	0.45
2:E:211:LEU:HD23	2:E:254:LEU:HD13	1.99	0.45
2:B:440:CYS:SG	2:B:497:CYS:HB3	2.56	0.45
2:G:317:ASN:ND2	3:G:604:NAG:O5	2.48	0.45
1:D:84:LEU:HD11	2:E:340:GLN:HG3	1.99	0.45
2:E:365:PHE:HB3	2:E:407:PHE:HD1	1.81	0.45
2:I:564:CYS:HA	2:I:567:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLU:HG2	1:A:51:VAL:HG11	1.98	0.45
2:E:169:SER:HB2	2:E:324:ILE:HG12	1.99	0.45
2:E:440:CYS:SG	2:E:497:CYS:SG	3.05	0.45
2:I:175:MET:HE3	2:I:176:VAL:CG2	2.43	0.45
2:I:303:PRO:HD3	2:I:488:LYS:HB2	1.98	0.45
2:E:210:LEU:HD23	2:E:251:THR:HG21	1.98	0.45
2:G:372:VAL:HG12	2:G:373:LEU:HG	1.97	0.44
2:B:137:ILE:HG12	2:B:413:ILE:HD11	1.98	0.44
3:B:602:NAG:H4	3:B:603:NAG:C1	2.47	0.44
1:D:91:GLN:HG2	2:E:246:LEU:HD13	1.98	0.44
2:I:406:LEU:HD21	5:I:610:HEM:HMA1	2.00	0.44
2:I:245:GLU:HB3	2:I:384:LEU:HD11	1.98	0.44
1:A:86:PHE:HA	2:B:552:PHE:CD1	2.52	0.44
2:B:243:MET:HE3	5:B:608:HEM:CBB	2.43	0.44
2:B:363:ARG:O	2:B:370:ARG:NH1	2.51	0.44
2:B:406:LEU:HD23	2:B:415:LEU:HB2	1.99	0.44
2:E:225:ASN:HD21	3:E:605:NAG:H2	1.82	0.44
2:E:333:ARG:HH11	2:E:421:ASN:ND2	2.15	0.44
2:E:367:ALA:HB1	2:E:370:ARG:HG3	1.99	0.44
2:B:158:ILE:HG21	2:E:164:ILE:HG12	2.00	0.44
2:B:296:TYR:CE2	2:B:300:VAL:HG21	2.52	0.44
2:E:533:LEU:HB3	2:E:551:ILE:HG21	1.99	0.44
2:B:434:ASN:HB2	2:B:472:ASN:HA	1.99	0.44
2:B:362:SER:HB3	2:B:405:ARG:HB3	1.99	0.44
2:I:286:ALA:O	2:I:290:ILE:HG13	2.17	0.44
2:I:468:TYR:CD2	2:I:474:ILE:HG12	2.52	0.44
2:B:332:PHE:HD1	2:B:499:ILE:HG12	1.83	0.43
2:E:233:PHE:H	2:E:241:SER:HG	1.65	0.43
2:I:440:CYS:HG	2:I:497:CYS:HB3	1.81	0.43
1:F:100:THR:HG21	2:G:428:HIS:HE1	1.84	0.43
2:I:130:ILE:HG13	2:I:137:ILE:HG21	2.01	0.43
1:A:19:SER:HA	11:D:202:HOH:O	2.18	0.43
2:B:545:THR:HG23	3:B:607:NAG:H82	2.00	0.43
2:E:225:ASN:HD21	3:E:605:NAG:C2	2.31	0.43
2:E:302:GLY:O	2:E:306:MET:HB2	2.18	0.43
2:G:470:THR:HG23	2:G:472:ASN:HB2	2.00	0.43
2:B:332:PHE:O	5:B:608:HEM:HAC	2.18	0.43
2:G:490:ARG:HA	2:G:490:ARG:HD3	1.81	0.43
3:B:605:NAG:O4	6:E:601:BMA:C1	2.67	0.43
2:E:390:LYS:NZ	2:E:396:GLN:O	2.51	0.43
2:G:440:CYS:SG	2:G:497:CYS:CB	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ILE:CD1	2:B:467:GLN:HG3	2.48	0.43
1:A:92:LEU:HD21	2:B:253:LEU:HD11	2.01	0.43
2:B:303:PRO:HD2	2:B:487:ARG:O	2.19	0.42
2:B:416:ASP:O	2:B:420:LEU:HG	2.19	0.42
1:H:87:MET:SD	1:H:87:MET:C	3.02	0.42
3:B:602:NAG:C4	3:B:603:NAG:H2	2.49	0.42
2:I:366:PHE:O	2:I:368:SER:N	2.52	0.42
2:B:336:HIS:HA	2:B:339:ILE:HD12	2.01	0.42
2:B:317:ASN:ND2	3:B:604:NAG:C1	2.81	0.42
1:F:103:PRO:HD2	2:G:147:PHE:HB3	2.02	0.42
1:H:37:TYR:HB3	1:H:43:LEU:O	2.20	0.42
1:A:64:VAL:HG11	2:B:468:TYR:OH	2.20	0.42
1:H:31:ARG:CZ	1:H:35:ALA:HB2	2.49	0.42
2:I:119:CYS:SG	2:I:143:CYS:HB3	2.59	0.42
2:I:400:ASP:HA	2:I:403:ARG:HB3	2.01	0.42
2:I:563:ASN:O	2:I:566:THR:OG1	2.32	0.42
2:G:393:ARG:HB2	2:G:396:GLN:HB2	2.02	0.42
2:B:192:ASN:HD21	2:B:196:LEU:HD12	1.84	0.42
2:B:531:ILE:HG22	2:B:570:LEU:HB2	2.02	0.42
2:E:397:ILE:HD13	2:E:478:MET:HE1	2.01	0.42
1:H:96:ASP:HB2	2:I:175:MET:SD	2.59	0.42
2:B:301:LEU:HB3	2:B:305:ALA:HB3	2.01	0.42
2:B:400:ASP:HA	2:B:403:ARG:HB3	2.02	0.42
2:E:136:ARG:HG2	2:E:137:ILE:HG13	2.02	0.42
2:E:514:TRP:CE2	2:E:515:GLU:HG3	2.55	0.42
1:H:67:GLU:HG3	2:I:467:GLN:NE2	2.35	0.42
2:E:317:ASN:HD21	3:E:607:NAG:C2	2.31	0.41
2:E:477:TRP:O	2:E:481:VAL:HG22	2.20	0.41
2:B:219:ASP:HB3	2:B:222:LEU:HD12	2.02	0.41
2:I:411:MET:SD	2:I:415:LEU:HD11	2.60	0.41
1:A:40:GLY:HA2	1:D:20:PRO:HD2	2.02	0.41
2:B:344:PHE:O	2:B:383:GLY:HA3	2.20	0.41
2:I:528:LEU:HG	2:I:575:TRP:HH2	1.85	0.41
2:I:333:ARG:HG2	5:I:610:HEM:C1D	2.55	0.41
2:B:350:TYR:HE2	2:B:545:THR:HB	1.86	0.41
1:F:22:LEU:HD11	1:H:34:PRO:HG3	2.02	0.41
2:G:433:TYR:CZ	2:G:437:ARG:HD3	2.55	0.41
3:G:602:NAG:H4	3:G:603:NAG:O5	2.20	0.41
1:H:94:ASP:OD1	5:I:610:HEM:HMD3	2.21	0.41
2:I:367:ALA:HB1	2:I:370:ARG:HG3	2.03	0.41
2:B:545:THR:HG21	2:B:557:TYR:HE1	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:601:NAG:O4	6:I:602:BMA:C1	2.69	0.40
2:B:192:ASN:HD22	2:B:194:LEU:H	1.69	0.40
2:E:290:ILE:HB	2:E:531:ILE:HD11	2.03	0.40
2:B:439:PHE:O	6:B:610:BMA:O5	2.39	0.40
2:E:241:SER:O	2:E:366:PHE:HA	2.22	0.40
3:G:608:NAG:H4	6:G:609:BMA:O5	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	101/105 (96%)	94 (93%)	7 (7%)	0	100	100
1	D	101/105 (96%)	93 (92%)	7 (7%)	1 (1%)	12	36
1	F	101/105 (96%)	94 (93%)	7 (7%)	0	100	100
1	H	101/105 (96%)	94 (93%)	7 (7%)	0	100	100
2	B	463/467 (99%)	428 (92%)	33 (7%)	2 (0%)	30	58
2	E	463/467 (99%)	433 (94%)	27 (6%)	3 (1%)	21	48
2	G	463/467 (99%)	426 (92%)	36 (8%)	1 (0%)	43	71
2	I	463/467 (99%)	428 (92%)	31 (7%)	4 (1%)	14	38
All	All	2256/2288 (99%)	2090 (93%)	155 (7%)	11 (0%)	24	53

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	367	ALA
1	D	74	ASP
2	I	155	GLY
2	I	572	LEU

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Mol	Chain	Res	Type
2	B	352	PRO
2	B	367	ALA
2	E	397	ILE
2	I	394	GLN
2	E	357	PRO
2	G	476	ILE
2	E	303	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	85/90 (94%)	79 (93%)	6 (7%)	13	38
1	D	88/90 (98%)	83 (94%)	5 (6%)	18	47
1	F	85/90 (94%)	80 (94%)	5 (6%)	18	46
1	H	87/90 (97%)	85 (98%)	2 (2%)	44	76
2	B	386/411 (94%)	364 (94%)	22 (6%)	18	47
2	E	387/411 (94%)	367 (95%)	20 (5%)	21	51
2	G	382/411 (93%)	362 (95%)	20 (5%)	21	51
2	I	382/411 (93%)	354 (93%)	28 (7%)	13	36
All	All	1882/2004 (94%)	1774 (94%)	108 (6%)	18	47

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	CYS
1	A	10	ILE
1	A	22	LEU
1	A	43	LEU
1	A	73	THR
1	A	84	LEU
2	B	164	ILE
2	B	175	MET

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Mol	Chain	Res	Type
2	B	187	LEU
2	B	196	LEU
2	B	217	HIS
2	B	254	LEU
2	B	295	ASP
2	B	304	THR
2	B	359	VAL
2	B	362	SER
2	B	364	VAL
2	B	380	ILE
2	B	411	MET
2	B	415	LEU
2	B	486	LYS
2	B	507	ARG
2	B	517	GLU
2	B	523	GLN
2	B	531	ILE
2	B	539	ASP
2	B	547	SER
2	B	566	THR
1	D	1	CYS
1	D	42	SER
1	D	54	ASN
1	D	68	ILE
1	D	70	ARG
2	E	113	VAL
2	E	175	MET
2	E	196	LEU
2	E	206	ASN
2	E	222	LEU
2	E	239	ARG
2	E	243	MET
2	E	254	LEU
2	E	276	LEU
2	E	318	ASP
2	E	345	ARG
2	E	353	MET
2	E	359	VAL
2	E	361	LEU
2	E	362	SER
2	E	415	LEU
2	E	486	LYS

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Mol	Chain	Res	Type
2	E	495	LEU
2	E	498	ILE
2	E	567	LEU
1	F	14	CYS
1	F	64	VAL
1	F	73	THR
1	F	84	LEU
1	F	88	GLN
2	G	115	CYS
2	G	149	SER
2	G	174	SER
2	G	194	LEU
2	G	248	SER
2	G	254	LEU
2	G	299	LEU
2	G	330	ASN
2	G	356	ASN
2	G	359	VAL
2	G	361	LEU
2	G	362	SER
2	G	411	MET
2	G	447	THR
2	G	486	LYS
2	G	504	ARG
2	G	507	ARG
2	G	562	VAL
2	G	566	THR
2	G	574	SER
1	H	73	THR
1	H	74	ASP
2	I	114	ASN
2	I	118	SER
2	I	149	SER
2	I	159	THR
2	I	171	VAL
2	I	175	MET
2	I	196	LEU
2	I	210	LEU
2	I	226	ARG
2	I	234	LEU
2	I	239	ARG
2	I	240	SER

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Mol	Chain	Res	Type
2	I	241	SER
2	I	276	LEU
2	I	288	VAL
2	I	312	THR
2	I	315	SER
2	I	339	ILE
2	I	356	ASN
2	I	361	LEU
2	I	399	VAL
2	I	411	MET
2	I	450	GLN
2	I	473	ASN
2	I	486	LYS
2	I	507	ARG
2	I	531	ILE
2	I	564	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
2	B	121	GLN
2	B	139	ASN
2	B	189	ASN
2	B	192	ASN
2	B	225	ASN
2	B	409	GLN
2	B	549	ASN
1	D	54	ASN
1	D	88	GLN
1	D	91	GLN
2	E	114	ASN
2	E	121	GLN
2	E	189	ASN
2	E	392	ASN
2	E	434	ASN
2	E	540	ASN
2	E	563	ASN
2	E	571	ASN
1	F	54	ASN
1	F	88	GLN
1	F	91	GLN

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Mol	Chain	Res	Type
2	G	317	ASN
2	G	396	GLN
2	G	549	ASN
1	H	75	GLN
2	I	189	ASN
2	I	250	HIS
2	I	317	ASN
2	I	450	GLN
2	I	467	GLN
2	I	540	ASN
2	I	549	ASN
2	I	555	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 51 ligands modelled in this entry, 6 are monoatomic - leaving 45 for Mogul analysis.

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	$\# Z > 2$
7	MAN	E	603	-	11,11,12	1.27	1 (9%)	15,15,17	3.23	6 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	I	606	-	14,14,15	1.50	3 (21%)	17,19,21	2.08	5 (29%)
3	NAG	B	603	-	14,14,15	1.80	5 (35%)	17,19,21	2.29	8 (47%)
3	NAG	G	606	-	14,14,15	1.59	2 (14%)	17,19,21	1.70	6 (35%)
4	FUC	G	605	-	10,10,11	1.46	1 (10%)	14,14,16	2.26	5 (35%)
3	NAG	B	605	-	14,14,15	0.88	0	17,19,21	2.14	6 (35%)
3	NAG	B	609	-	14,14,15	1.02	1 (7%)	17,19,21	2.90	8 (47%)
3	NAG	E	606	-	14,14,15	1.41	3 (21%)	17,19,21	1.81	5 (29%)
7	MAN	G	610	-	11,11,12	1.07	1 (9%)	15,15,17	2.07	3 (20%)
3	NAG	G	601	-	14,14,15	2.03	6 (42%)	17,19,21	2.13	6 (35%)
5	HEM	E	609	2	50,50,50	1.33	7 (14%)	67,82,82	1.45	13 (19%)
6	BMA	I	602	-	11,11,12	1.36	2 (18%)	15,15,17	2.32	7 (46%)
7	MAN	E	602	-	11,11,12	1.32	2 (18%)	15,15,17	1.78	4 (26%)
4	FUC	I	609	-	10,10,11	1.60	3 (30%)	14,14,16	2.37	5 (35%)
3	NAG	I	608	-	14,14,15	1.49	2 (14%)	17,19,21	4.17	10 (58%)
8	JXS	G	612	-	27,27,27	5.12	19 (70%)	33,38,38	2.49	13 (39%)
4	FUC	E	608	-	10,10,11	2.01	3 (30%)	14,14,16	2.53	7 (50%)
6	BMA	G	609	-	11,11,12	1.22	1 (9%)	15,15,17	2.93	5 (33%)
3	NAG	G	602	-	14,14,15	1.67	2 (14%)	17,19,21	2.44	5 (29%)
7	MAN	B	611	-	11,11,12	1.04	0	15,15,17	1.15	1 (6%)
3	NAG	B	604	-	14,14,15	1.08	0	17,19,21	2.37	7 (41%)
8	JXS	B	613	-	27,27,27	5.03	19 (70%)	33,38,38	2.35	9 (27%)
3	NAG	E	604	-	14,14,15	1.65	3 (21%)	17,19,21	2.24	7 (41%)
3	NAG	B	607	-	14,14,15	1.50	2 (14%)	17,19,21	1.63	3 (17%)
3	NAG	E	607	-	14,14,15	1.10	2 (14%)	17,19,21	2.62	6 (35%)
3	NAG	B	602	-	14,14,15	1.33	2 (14%)	17,19,21	2.59	6 (35%)
3	NAG	G	603	-	14,14,15	1.16	1 (7%)	17,19,21	1.89	5 (29%)
3	NAG	I	601	-	14,14,15	1.43	2 (14%)	17,19,21	2.64	8 (47%)
7	MAN	B	612	-	11,11,12	1.79	5 (45%)	15,15,17	1.95	5 (33%)
6	BMA	B	610	-	11,11,12	1.16	1 (9%)	15,15,17	2.19	6 (40%)
6	BMA	E	601	-	11,11,12	1.35	1 (9%)	15,15,17	2.46	5 (33%)
5	HEM	B	608	2	50,50,50	1.64	13 (26%)	67,82,82	1.66	18 (26%)
3	NAG	I	605	-	14,14,15	1.41	2 (14%)	17,19,21	1.44	3 (17%)
5	HEM	G	607	2	50,50,50	1.38	8 (16%)	67,82,82	1.75	16 (23%)
3	NAG	B	601	-	14,14,15	1.89	4 (28%)	17,19,21	2.37	7 (41%)
7	MAN	I	603	-	11,11,12	1.34	0	15,15,17	1.67	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	G	611	-	11,11,12	1.26	2 (18%)	15,15,17	1.62	4 (26%)
7	MAN	I	604	-	11,11,12	1.44	2 (18%)	15,15,17	1.58	3 (20%)
8	JXS	E	610	-	27,27,27	4.99	18 (66%)	33,38,38	2.41	9 (27%)
3	NAG	E	605	-	14,14,15	1.18	1 (7%)	17,19,21	1.64	3 (17%)
5	HEM	I	610	2	50,50,50	1.53	9 (18%)	67,82,82	1.71	14 (20%)
3	NAG	G	608	-	14,14,15	1.09	1 (7%)	17,19,21	2.24	7 (41%)
4	FUC	B	606	-	10,10,11	1.98	3 (30%)	14,14,16	2.37	5 (35%)
3	NAG	G	604	-	14,14,15	1.37	2 (14%)	17,19,21	3.87	9 (52%)
3	NAG	I	607	-	14,14,15	1.17	1 (7%)	17,19,21	2.20	5 (29%)

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
7	MAN	E	603	-	-	2/2/19/22	0/1/1/1
3	NAG	I	606	-	-	2/6/23/26	0/1/1/1
3	NAG	B	603	-	-	0/6/23/26	0/1/1/1
3	NAG	G	606	-	-	0/6/23/26	0/1/1/1
4	FUC	G	605	-	-	-	0/1/1/1
3	NAG	B	605	-	-	2/6/23/26	0/1/1/1
3	NAG	B	609	-	-	3/6/23/26	0/1/1/1
3	NAG	E	606	-	-	2/6/23/26	0/1/1/1
7	MAN	G	610	-	-	2/2/19/22	1/1/1/1
3	NAG	G	601	-	-	2/6/23/26	0/1/1/1
5	HEM	E	609	2	-	7/14/54/54	-
6	BMA	I	602	-	-	2/2/19/22	0/1/1/1
7	MAN	E	602	-	-	1/2/19/22	0/1/1/1
4	FUC	I	609	-	-	-	0/1/1/1
3	NAG	I	608	-	-	0/6/23/26	0/1/1/1
8	JXS	G	612	-	-	0/9/9/9	0/4/4/4
6	BMA	G	609	-	-	1/2/19/22	0/1/1/1
7	MAN	B	611	-	-	2/2/19/22	0/1/1/1
3	NAG	G	602	-	-	0/6/23/26	0/1/1/1
4	FUC	E	608	-	-	-	0/1/1/1
3	NAG	B	604	-	-	3/6/23/26	0/1/1/1
8	JXS	B	613	-	-	0/9/9/9	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	604	-	-	0/6/23/26	0/1/1/1
3	NAG	B	607	-	-	2/6/23/26	0/1/1/1
3	NAG	E	607	-	-	0/6/23/26	0/1/1/1
3	NAG	B	602	-	-	2/6/23/26	0/1/1/1
3	NAG	G	603	-	-	1/6/23/26	0/1/1/1
3	NAG	I	601	-	-	2/6/23/26	0/1/1/1
7	MAN	B	612	-	-	2/2/19/22	0/1/1/1
6	BMA	B	610	-	-	2/2/19/22	0/1/1/1
6	BMA	E	601	-	-	2/2/19/22	0/1/1/1
5	HEM	B	608	2	-	6/14/54/54	-
3	NAG	I	605	-	-	2/6/23/26	0/1/1/1
5	HEM	G	607	2	-	6/14/54/54	-
3	NAG	B	601	-	-	1/6/23/26	0/1/1/1
7	MAN	I	603	-	-	2/2/19/22	0/1/1/1
7	MAN	G	611	-	-	2/2/19/22	0/1/1/1
7	MAN	I	604	-	-	2/2/19/22	1/1/1/1
8	JXS	E	610	-	-	0/9/9/9	0/4/4/4
3	NAG	E	605	-	-	3/6/23/26	0/1/1/1
5	HEM	I	610	2	-	3/14/54/54	-
3	NAG	G	608	-	-	2/6/23/26	0/1/1/1
4	FUC	B	606	-	-	-	0/1/1/1
3	NAG	G	604	-	-	0/6/23/26	0/1/1/1
3	NAG	I	607	-	-	1/6/23/26	0/1/1/1

All (168) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	610	JXS	C13-N19	13.18	1.52	1.34
8	B	613	JXS	C13-N19	13.14	1.52	1.34
8	G	612	JXS	C13-N19	13.08	1.52	1.34
8	B	613	JXS	C02-C08	9.33	1.53	1.39
8	G	612	JXS	C02-C08	9.17	1.53	1.39
8	E	610	JXS	C02-C08	9.17	1.53	1.39
8	G	612	JXS	C10-C11	9.15	1.54	1.40
8	G	612	JXS	C05-C09	8.68	1.54	1.39
8	E	610	JXS	C05-C09	8.40	1.53	1.39
8	B	613	JXS	C05-C09	8.31	1.53	1.39
8	B	613	JXS	C10-C11	7.95	1.52	1.40
8	E	610	JXS	C10-C11	7.30	1.51	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	610	JXS	C01-C02	7.12	1.51	1.38
8	B	613	JXS	C01-C02	6.89	1.50	1.38
8	G	612	JXS	C01-C02	6.77	1.50	1.38
8	G	612	JXS	C03-C09	6.63	1.52	1.38
8	B	613	JXS	C03-C09	6.59	1.51	1.38
8	E	610	JXS	C03-C09	6.59	1.51	1.38
8	B	613	JXS	C01-C03	6.03	1.49	1.38
8	E	610	JXS	C01-C03	6.01	1.49	1.38
8	G	612	JXS	C01-C03	5.89	1.49	1.38
8	B	613	JXS	C05-C08	5.84	1.48	1.39
8	G	612	JXS	C05-C08	5.81	1.48	1.39
8	E	610	JXS	C05-C08	5.27	1.47	1.39
8	G	612	JXS	C14-N19	4.96	1.47	1.35
8	E	610	JXS	C14-N19	4.94	1.47	1.35
5	I	610	HEM	C1D-C2D	4.86	1.54	1.44
4	E	608	FUC	O5-C5	4.84	1.53	1.43
8	B	613	JXS	C14-N19	4.82	1.46	1.35
8	B	613	JXS	C06-C11	4.57	1.46	1.38
8	G	612	JXS	C10-N17	4.51	1.39	1.36
3	B	601	NAG	C4-C5	4.44	1.62	1.53
8	E	610	JXS	C06-C11	4.39	1.46	1.38
5	I	610	HEM	C1B-NB	-4.21	1.33	1.40
3	G	604	NAG	O5-C1	-4.17	1.36	1.43
4	B	606	FUC	C2-C3	4.13	1.58	1.52
3	I	601	NAG	C4-C5	4.13	1.61	1.53
5	G	607	HEM	C4D-ND	-4.12	1.33	1.40
8	G	612	JXS	C06-C11	4.06	1.45	1.38
8	B	613	JXS	C07-N22	3.98	1.38	1.34
5	B	608	HEM	C1B-NB	-3.96	1.33	1.40
8	G	612	JXS	C07-N22	3.94	1.38	1.34
5	E	609	HEM	C1B-NB	-3.77	1.33	1.40
8	E	610	JXS	N22-N18	3.52	1.41	1.36
8	E	610	JXS	C07-N22	3.51	1.38	1.34
3	G	606	NAG	C1-C2	3.51	1.57	1.52
3	G	601	NAG	C2-N2	3.48	1.52	1.46
3	G	602	NAG	O5-C1	-3.43	1.37	1.43
5	G	607	HEM	C3D-C2D	-3.27	1.29	1.36
7	E	603	MAN	O2-C2	3.21	1.50	1.43
3	G	601	NAG	C4-C5	3.20	1.59	1.53
5	B	608	HEM	C4D-ND	-3.18	1.34	1.40
8	B	613	JXS	N22-N18	3.18	1.40	1.36
8	G	612	JXS	N22-N18	3.17	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	610	JXS	C15-N22	-3.16	1.42	1.46
3	E	605	NAG	C1-C2	3.16	1.56	1.52
8	B	613	JXS	C10-N17	3.15	1.38	1.36
5	B	608	HEM	C1C-C2C	-3.14	1.39	1.45
3	I	608	NAG	O5-C5	-3.13	1.37	1.43
8	E	610	JXS	C06-C14	3.11	1.44	1.40
8	B	613	JXS	C15-N22	-3.09	1.42	1.46
3	G	602	NAG	C4-C5	3.09	1.59	1.53
3	B	603	NAG	C1-C2	3.07	1.56	1.52
8	G	612	JXS	N21-N20	3.04	1.38	1.31
5	B	608	HEM	C4B-NB	-3.03	1.32	1.38
8	B	613	JXS	C06-C14	3.03	1.44	1.40
8	E	610	JXS	C08-C12	3.03	1.52	1.47
3	G	601	NAG	C4-C3	3.00	1.60	1.52
5	I	610	HEM	C4C-NC	-2.98	1.34	1.39
8	G	612	JXS	C06-C14	2.97	1.44	1.40
3	E	604	NAG	C3-C2	2.93	1.58	1.52
4	G	605	FUC	C1-C2	2.91	1.59	1.52
8	E	610	JXS	C10-N17	2.90	1.38	1.36
8	E	610	JXS	N21-N20	2.89	1.38	1.31
6	B	610	BMA	C4-C5	2.89	1.59	1.53
3	B	607	NAG	C1-C2	2.89	1.56	1.52
3	E	607	NAG	C4-C5	2.88	1.59	1.53
3	I	605	NAG	C1-C2	2.86	1.56	1.52
3	E	604	NAG	O5-C5	2.86	1.49	1.43
5	B	608	HEM	CMD-C2D	-2.85	1.44	1.50
5	B	608	HEM	C1C-NC	-2.82	1.34	1.39
4	B	606	FUC	O5-C5	2.81	1.49	1.43
6	E	601	BMA	C4-C3	2.81	1.59	1.52
8	G	612	JXS	C08-C12	2.81	1.51	1.47
3	B	602	NAG	C4-C3	2.78	1.59	1.52
6	I	602	BMA	C4-C5	2.78	1.58	1.53
5	I	610	HEM	C1C-C2C	-2.77	1.39	1.45
3	I	606	NAG	C1-C2	2.77	1.56	1.52
6	G	609	BMA	O2-C2	2.76	1.49	1.43
8	E	610	JXS	C14-N23	2.74	1.42	1.35
8	B	613	JXS	C08-C12	2.73	1.51	1.47
3	G	601	NAG	C3-C2	2.72	1.58	1.52
5	B	608	HEM	C3B-C2B	-2.72	1.31	1.37
3	I	606	NAG	C4-C5	2.72	1.58	1.53
3	E	606	NAG	C4-C3	2.71	1.59	1.52
8	B	613	JXS	N21-N20	2.70	1.37	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	607	HEM	C4B-NB	-2.66	1.33	1.38
5	E	609	HEM	C1D-C2D	2.63	1.49	1.44
7	G	611	MAN	C4-C3	2.60	1.59	1.52
5	G	607	HEM	C3B-C2B	-2.60	1.31	1.37
4	B	606	FUC	O4-C4	2.59	1.49	1.43
8	G	612	JXS	C14-N23	2.59	1.42	1.35
3	B	601	NAG	C1-C2	2.58	1.55	1.52
5	B	608	HEM	CHB-C4A	-2.56	1.33	1.39
4	I	609	FUC	O4-C4	2.55	1.49	1.43
5	B	608	HEM	C1B-C2B	-2.55	1.39	1.44
7	E	602	MAN	C1-C2	2.54	1.58	1.52
3	B	603	NAG	C2-N2	2.53	1.50	1.46
7	B	612	MAN	C2-C3	2.53	1.56	1.52
3	B	602	NAG	C4-C5	2.53	1.58	1.53
3	B	603	NAG	C4-C3	2.53	1.58	1.52
5	E	609	HEM	C2A-C3A	-2.50	1.32	1.38
6	I	602	BMA	C4-C3	2.49	1.58	1.52
5	B	608	HEM	C3D-C2D	-2.48	1.31	1.36
8	G	612	JXS	C15-N22	-2.47	1.43	1.46
3	B	601	NAG	O5-C5	2.47	1.48	1.43
7	I	604	MAN	O5-C1	2.45	1.47	1.43
4	E	608	FUC	C2-C3	2.43	1.56	1.52
3	I	608	NAG	O3-C3	2.43	1.49	1.43
5	I	610	HEM	C4B-NB	-2.42	1.34	1.38
3	B	607	NAG	C4-C5	2.41	1.58	1.53
3	B	603	NAG	C3-C2	2.41	1.57	1.52
4	E	608	FUC	C1-C2	2.40	1.57	1.52
3	G	608	NAG	C3-C2	2.40	1.57	1.52
5	B	608	HEM	O2A-CGA	2.39	1.38	1.30
8	G	612	JXS	O24-C11	2.39	1.42	1.37
3	G	601	NAG	C1-C2	2.36	1.55	1.52
5	I	610	HEM	CHA-C1A	-2.35	1.34	1.39
8	B	613	JXS	C14-N23	2.35	1.41	1.35
8	B	613	JXS	O24-C11	2.34	1.42	1.37
7	E	602	MAN	O5-C5	2.33	1.48	1.43
5	E	609	HEM	C4B-NB	-2.33	1.34	1.38
7	B	612	MAN	O2-C2	2.32	1.48	1.43
5	B	608	HEM	C4C-NC	-2.30	1.35	1.39
4	I	609	FUC	C1-C2	2.30	1.57	1.52
5	E	609	HEM	C3B-C2B	-2.27	1.32	1.37
3	E	604	NAG	C4-C5	2.27	1.57	1.53
5	E	609	HEM	C1C-C2C	-2.26	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	609	HEM	C4D-ND	-2.25	1.36	1.40
3	G	606	NAG	C3-C2	2.25	1.57	1.52
3	E	607	NAG	C4-C3	2.25	1.58	1.52
3	B	601	NAG	O4-C4	2.23	1.48	1.43
7	B	612	MAN	O5-C5	2.22	1.47	1.43
3	I	605	NAG	C4-C3	2.22	1.58	1.52
3	E	606	NAG	C7-N2	2.22	1.41	1.34
5	B	608	HEM	CHA-C1A	-2.22	1.34	1.39
5	G	607	HEM	C2A-C3A	-2.21	1.33	1.38
3	I	607	NAG	C4-C3	2.21	1.58	1.52
3	B	609	NAG	O6-C6	2.20	1.51	1.42
7	G	610	MAN	C2-C3	2.17	1.55	1.52
4	I	609	FUC	O5-C1	2.16	1.47	1.43
5	I	610	HEM	C1B-C2B	-2.16	1.40	1.44
5	G	607	HEM	C1B-NB	-2.15	1.36	1.40
5	I	610	HEM	CHB-C4A	-2.12	1.34	1.39
3	I	601	NAG	C3-C2	2.12	1.57	1.52
7	B	612	MAN	O5-C1	2.11	1.47	1.43
7	G	611	MAN	O2-C2	2.09	1.47	1.43
3	I	606	NAG	C4-C3	2.08	1.57	1.52
7	B	612	MAN	C4-C3	2.07	1.57	1.52
3	G	601	NAG	C7-N2	2.07	1.41	1.34
3	G	603	NAG	C4-C3	2.06	1.57	1.52
3	B	603	NAG	C4-C5	2.05	1.57	1.53
3	E	606	NAG	C4-C5	2.04	1.57	1.53
7	I	604	MAN	C1-C2	2.03	1.57	1.52
5	G	607	HEM	FE-ND	2.01	2.01	1.94
5	I	610	HEM	C3B-C2B	-2.01	1.33	1.37
5	G	607	HEM	C1D-C2D	2.01	1.48	1.44
3	G	604	NAG	C4-C5	2.01	1.57	1.53

All (300) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	604	NAG	C1-C2-N2	-12.53	90.70	110.43
3	I	608	NAG	C1-O5-C5	-12.43	95.52	112.19
7	E	603	MAN	C1-O5-C5	9.25	124.58	112.19
3	B	609	NAG	C1-O5-C5	7.59	122.36	112.19
3	G	602	NAG	C1-O5-C5	-7.49	102.14	112.19
8	G	612	JXS	C07-N22-N18	-7.20	107.92	112.01
8	B	613	JXS	C07-N22-N18	-6.97	108.06	112.01
8	E	610	JXS	C07-N22-N18	-6.92	108.08	112.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	NAG	C1-O5-C5	-6.89	102.95	112.19
3	E	607	NAG	C1-O5-C5	-6.85	103.01	112.19
6	G	609	BMA	C1-C2-C3	-6.69	99.91	109.64
6	G	609	BMA	O5-C5-C6	-6.57	94.87	107.66
6	E	601	BMA	C1-O5-C5	-6.38	103.64	112.19
3	E	604	NAG	C1-O5-C5	6.14	120.42	112.19
3	I	608	NAG	O4-C4-C3	-6.13	95.92	110.38
7	G	610	MAN	C1-O5-C5	6.07	120.32	112.19
3	I	607	NAG	O5-C1-C2	-5.91	102.14	111.29
8	E	610	JXS	C15-N22-N18	5.88	125.55	119.57
8	B	613	JXS	C15-N22-N18	5.75	125.41	119.57
3	B	601	NAG	C1-C2-N2	5.75	119.49	110.43
5	I	610	HEM	CMD-C2D-C1D	5.69	133.92	125.03
8	G	612	JXS	C15-N22-N18	5.47	125.13	119.57
3	I	606	NAG	C4-C3-C2	5.42	118.96	111.02
3	I	601	NAG	C1-C2-N2	-5.38	101.96	110.43
8	G	612	JXS	C10-C13-N19	-5.25	119.60	124.22
8	E	610	JXS	C10-C13-N19	-5.16	119.68	124.22
4	I	609	FUC	C1-C2-C3	5.15	117.15	109.64
3	E	607	NAG	C3-C4-C5	5.10	119.48	110.23
7	E	603	MAN	O2-C2-C3	5.05	120.61	110.15
3	G	608	NAG	O5-C1-C2	-5.04	103.49	111.29
4	E	608	FUC	O5-C5-C4	4.94	118.45	109.55
8	B	613	JXS	C10-C13-N19	-4.90	119.91	124.22
4	E	608	FUC	C1-C2-C3	4.88	116.75	109.64
5	G	607	HEM	CMD-C2D-C1D	4.82	132.56	125.03
3	B	604	NAG	C3-C4-C5	4.81	118.96	110.23
3	B	602	NAG	C4-C3-C2	4.77	118.00	111.02
3	I	608	NAG	O4-C4-C5	-4.76	97.60	109.32
3	I	607	NAG	C1-C2-N2	4.72	117.87	110.43
4	B	606	FUC	C1-O5-C5	4.44	123.43	112.97
3	B	603	NAG	C1-C2-N2	4.41	117.39	110.43
3	I	608	NAG	C6-C5-C4	4.36	123.73	113.02
3	I	601	NAG	C8-C7-N2	-4.36	108.89	116.12
6	B	610	BMA	O3-C3-C2	-4.34	101.20	110.05
7	I	603	MAN	C1-O5-C5	4.32	117.98	112.19
3	B	603	NAG	C4-C3-C2	4.27	117.28	111.02
3	I	601	NAG	C2-N2-C7	4.24	128.59	122.90
6	B	610	BMA	O4-C4-C3	-4.24	100.39	110.38
3	B	609	NAG	C1-C2-N2	-4.22	103.78	110.43
3	I	608	NAG	C3-C4-C5	4.21	117.86	110.23
8	E	610	JXS	C08-C12-N18	4.19	126.00	120.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	605	NAG	C1-O5-C5	-4.18	106.58	112.19
5	E	609	HEM	CBA-CAA-C2A	-4.18	100.97	112.53
3	B	607	NAG	C1-C2-N2	4.18	117.02	110.43
3	B	604	NAG	C2-N2-C7	4.18	128.50	122.90
4	B	606	FUC	O2-C2-C3	4.15	118.74	110.15
3	B	605	NAG	O5-C5-C6	4.14	115.72	107.66
5	I	610	HEM	CBA-CAA-C2A	-4.13	101.12	112.53
3	G	604	NAG	C8-C7-N2	-4.11	109.31	116.12
3	I	601	NAG	O3-C3-C2	4.09	117.89	109.40
3	G	603	NAG	C4-C3-C2	4.06	116.97	111.02
6	I	602	BMA	C1-C2-C3	-4.05	103.75	109.64
4	I	609	FUC	C1-O5-C5	4.02	122.45	112.97
6	E	601	BMA	C2-C3-C4	4.01	117.92	110.86
4	I	609	FUC	O3-C3-C2	-4.00	101.89	110.05
4	G	605	FUC	O5-C5-C4	3.98	116.72	109.55
3	B	605	NAG	O4-C4-C5	-3.95	99.58	109.32
3	G	603	NAG	O5-C1-C2	-3.95	105.18	111.29
5	I	610	HEM	C2B-C1B-NB	3.94	114.37	109.84
3	G	604	NAG	C3-C4-C5	3.94	117.37	110.23
7	B	612	MAN	C1-O5-C5	3.90	117.41	112.19
5	G	607	HEM	CBB-CAB-C3B	-3.88	108.13	127.53
3	G	604	NAG	C1-O5-C5	-3.85	107.03	112.19
3	G	601	NAG	C2-N2-C7	3.83	128.03	122.90
4	B	606	FUC	O3-C3-C4	-3.81	101.40	110.38
3	B	609	NAG	C8-C7-N2	-3.80	109.82	116.12
5	G	607	HEM	CBA-CAA-C2A	-3.72	102.25	112.53
8	G	612	JXS	C12-N18-N22	3.71	108.10	104.26
5	I	610	HEM	CHA-C4D-C3D	-3.71	118.39	125.23
6	G	609	BMA	O3-C3-C2	-3.70	102.50	110.05
5	B	608	HEM	C2B-C1B-NB	3.68	114.07	109.84
7	G	611	MAN	O2-C2-C3	3.68	117.77	110.15
3	E	607	NAG	O5-C1-C2	-3.67	105.61	111.29
3	E	605	NAG	O5-C1-C2	-3.64	105.66	111.29
5	B	608	HEM	CBB-CAB-C3B	-3.64	109.33	127.53
3	G	601	NAG	C1-C2-N2	3.62	116.14	110.43
3	G	606	NAG	C2-N2-C7	3.61	127.74	122.90
3	G	604	NAG	O5-C1-C2	3.58	116.83	111.29
3	B	604	NAG	O4-C4-C5	-3.56	100.56	109.32
4	G	605	FUC	O4-C4-C5	3.55	117.58	109.74
3	B	609	NAG	O4-C4-C5	-3.50	100.69	109.32
8	B	613	JXS	C08-C12-N18	3.50	125.10	120.49
3	G	608	NAG	O3-C3-C2	3.49	116.66	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	607	HEM	CHC-C4B-NB	3.47	128.16	124.42
8	B	613	JXS	C12-N18-N22	3.46	107.84	104.26
3	G	601	NAG	O5-C1-C2	-3.46	105.94	111.29
7	B	612	MAN	O2-C2-C3	3.46	117.31	110.15
7	I	604	MAN	O5-C5-C6	3.44	114.36	107.66
3	G	602	NAG	C3-C4-C5	3.42	116.44	110.23
3	B	601	NAG	O4-C4-C5	3.40	117.70	109.32
5	I	610	HEM	C4A-NA-C1A	-3.38	100.31	105.82
5	B	608	HEM	CBA-CAA-C2A	-3.38	103.20	112.53
6	I	602	BMA	C6-C5-C4	3.36	121.28	113.02
7	E	602	MAN	C1-C2-C3	3.35	114.53	109.64
5	B	608	HEM	C3A-C4A-NA	3.34	115.49	110.14
8	E	610	JXS	C12-N18-N22	3.32	107.70	104.26
3	E	606	NAG	O3-C3-C4	3.32	118.20	110.38
3	E	606	NAG	O5-C1-C2	-3.29	106.19	111.29
3	I	608	NAG	O6-C6-C5	-3.28	100.15	111.33
3	B	604	NAG	C1-C2-N2	-3.28	105.27	110.43
4	B	606	FUC	C1-C2-C3	3.25	114.37	109.64
3	B	601	NAG	C1-O5-C5	3.22	116.50	112.19
3	G	604	NAG	O7-C7-C8	3.22	127.78	122.05
3	E	605	NAG	C3-C4-C5	3.21	116.06	110.23
7	E	602	MAN	C1-O5-C5	3.21	116.48	112.19
3	G	608	NAG	C1-O5-C5	-3.20	107.90	112.19
4	G	605	FUC	C1-C2-C3	3.19	114.28	109.64
4	E	608	FUC	O4-C4-C3	-3.19	102.87	110.38
3	I	608	NAG	C1-C2-N2	-3.16	105.45	110.43
8	B	613	JXS	C11-C10-N17	3.15	131.95	128.66
3	B	609	NAG	O3-C3-C4	3.14	117.79	110.38
6	I	602	BMA	C2-C3-C4	3.13	116.36	110.86
3	B	603	NAG	C1-O5-C5	3.13	116.38	112.19
5	G	607	HEM	CHA-C4D-C3D	-3.12	119.48	125.23
7	E	602	MAN	O5-C1-C2	3.11	118.20	110.79
8	G	612	JXS	C11-C10-N17	3.11	131.90	128.66
3	B	605	NAG	O3-C3-C4	3.11	117.70	110.38
5	B	608	HEM	C4A-NA-C1A	-3.10	100.76	105.82
3	B	603	NAG	C2-N2-C7	3.10	127.06	122.90
3	G	602	NAG	C6-C5-C4	3.09	120.60	113.02
8	E	610	JXS	N23-C14-N19	3.08	121.54	116.59
3	B	601	NAG	O5-C5-C4	3.07	118.30	110.83
5	B	608	HEM	CMD-C2D-C1D	3.07	129.83	125.03
3	B	603	NAG	O5-C1-C2	-3.07	106.54	111.29
3	B	602	NAG	O3-C3-C4	3.07	117.60	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	605	FUC	O4-C4-C3	-3.06	103.17	110.38
5	I	610	HEM	CHA-C4D-ND	3.06	128.15	124.37
4	E	608	FUC	O5-C1-C2	3.05	118.07	110.79
7	E	603	MAN	O5-C5-C6	3.05	113.59	107.66
4	E	608	FUC	C1-O5-C5	3.04	120.14	112.97
5	E	609	HEM	CHC-C4B-NB	3.04	127.69	124.42
6	B	610	BMA	O5-C5-C6	-3.03	101.77	107.66
3	G	601	NAG	C4-C3-C2	3.02	115.45	111.02
3	E	604	NAG	C2-N2-C7	3.01	126.94	122.90
5	E	609	HEM	CMD-C2D-C1D	3.01	129.74	125.03
3	G	608	NAG	C2-N2-C7	3.00	126.93	122.90
4	G	605	FUC	O3-C3-C4	-3.00	103.30	110.38
3	B	601	NAG	O5-C1-C2	-3.00	106.65	111.29
6	E	601	BMA	O5-C1-C2	-3.00	103.64	110.79
3	B	601	NAG	C3-C4-C5	3.00	115.67	110.23
3	B	604	NAG	C8-C7-N2	-3.00	111.15	116.12
3	B	602	NAG	C6-C5-C4	2.97	120.32	113.02
5	B	608	HEM	CHA-C4D-C3D	-2.96	119.78	125.23
4	B	606	FUC	C6-C5-C4	-2.95	107.69	113.08
3	I	606	NAG	O5-C1-C2	2.93	115.82	111.29
5	G	607	HEM	C4A-NA-C1A	-2.92	101.06	105.82
5	E	609	HEM	C4A-NA-C1A	-2.92	101.07	105.82
5	G	607	HEM	CMB-C2B-C1B	2.90	129.57	125.03
5	I	610	HEM	CHB-C1B-C2B	-2.90	118.72	126.95
5	B	608	HEM	O2A-CGA-CBA	2.89	123.13	114.00
6	I	602	BMA	O3-C3-C4	2.88	117.17	110.38
4	I	609	FUC	C2-C3-C4	2.88	115.92	110.86
3	B	609	NAG	C3-C4-C5	2.87	115.43	110.23
3	G	603	NAG	C3-C4-C5	2.86	115.42	110.23
7	B	612	MAN	O5-C5-C6	2.84	113.19	107.66
3	G	602	NAG	O4-C4-C3	-2.81	103.74	110.38
3	I	606	NAG	C3-C4-C5	2.81	115.32	110.23
8	G	612	JXS	C02-C08-C12	-2.80	117.74	120.87
8	G	612	JXS	C08-C12-N18	2.78	124.15	120.49
3	G	606	NAG	C1-O5-C5	2.76	115.88	112.19
3	I	605	NAG	C1-C2-N2	2.76	114.78	110.43
3	I	605	NAG	O5-C1-C2	-2.75	107.04	111.29
7	G	610	MAN	O2-C2-C3	2.75	115.84	110.15
3	G	604	NAG	O4-C4-C3	-2.74	103.92	110.38
5	B	608	HEM	O1A-CGA-CBA	-2.73	114.43	123.09
3	G	602	NAG	C4-C3-C2	2.73	115.02	111.02
5	I	610	HEM	C3A-C4A-NA	2.73	114.52	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	612	JXS	C16-O24-C11	2.73	123.16	117.76
6	G	609	BMA	C6-C5-C4	2.72	119.70	113.02
5	I	610	HEM	CBD-CAD-C3D	-2.72	105.02	112.53
7	B	611	MAN	O4-C4-C5	2.71	116.00	109.32
3	I	601	NAG	C1-O5-C5	-2.70	108.57	112.19
7	G	611	MAN	C1-C2-C3	-2.70	105.72	109.64
8	G	612	JXS	O24-C11-C10	2.70	118.62	114.77
6	B	610	BMA	C3-C4-C5	2.69	115.11	110.23
7	E	603	MAN	O5-C1-C2	2.69	117.20	110.79
3	E	606	NAG	C1-O5-C5	2.68	115.78	112.19
3	E	606	NAG	O3-C3-C2	2.68	114.96	109.40
6	E	601	BMA	C6-C5-C4	2.67	119.58	113.02
5	B	608	HEM	CHA-C4D-ND	2.66	127.66	124.37
3	I	608	NAG	O5-C1-C2	-2.66	107.18	111.29
6	I	602	BMA	O5-C1-C2	-2.61	104.55	110.79
3	G	601	NAG	C6-C5-C4	2.61	119.44	113.02
3	E	607	NAG	O4-C4-C5	-2.61	102.90	109.32
5	G	607	HEM	CHB-C1B-NB	2.60	127.58	124.37
8	E	610	JXS	C11-C10-N17	2.60	131.37	128.66
3	G	604	NAG	O3-C3-C4	2.59	116.49	110.38
3	E	607	NAG	O4-C4-C3	-2.59	104.27	110.38
3	B	603	NAG	O5-C5-C6	2.58	112.69	107.66
3	G	606	NAG	O5-C5-C4	2.58	117.09	110.83
3	E	604	NAG	O5-C5-C4	2.57	117.07	110.83
7	G	610	MAN	O4-C4-C5	2.56	115.62	109.32
8	G	612	JXS	C04-C12-N18	-2.53	108.36	110.87
5	I	610	HEM	C3B-C2B-C1B	-2.53	104.52	106.41
8	E	610	JXS	C04-C12-N18	-2.52	108.37	110.87
3	B	605	NAG	O4-C4-C3	-2.52	104.44	110.38
3	G	608	NAG	O5-C5-C6	2.51	112.56	107.66
3	I	608	NAG	O3-C3-C2	2.51	114.61	109.40
6	B	610	BMA	O3-C3-C4	2.51	116.28	110.38
5	E	609	HEM	CBD-CAD-C3D	-2.50	105.61	112.53
5	B	608	HEM	C4A-C3A-C2A	-2.50	103.95	106.82
5	B	608	HEM	CHB-C1B-C2B	-2.50	119.83	126.95
7	E	603	MAN	O4-C4-C3	-2.50	104.48	110.38
3	I	606	NAG	O7-C7-N2	2.49	126.39	121.98
5	G	607	HEM	CHB-C1B-C2B	-2.48	119.91	126.95
8	B	613	JXS	C16-O24-C11	2.47	122.65	117.76
5	G	607	HEM	CBD-CAD-C3D	-2.47	105.71	112.53
3	B	607	NAG	C1-O5-C5	2.47	115.49	112.19
3	G	606	NAG	C3-C4-C5	2.45	114.67	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	601	NAG	C1-O5-C5	-2.45	108.91	112.19
3	B	601	NAG	C8-C7-N2	-2.44	112.07	116.12
5	E	609	HEM	C3B-C4B-NB	2.43	111.22	109.47
3	G	603	NAG	O5-C5-C4	2.43	116.74	110.83
7	E	602	MAN	O5-C5-C4	2.43	116.73	110.83
7	B	612	MAN	C2-C3-C4	2.42	115.12	110.86
3	I	608	NAG	O3-C3-C4	2.42	116.08	110.38
6	I	602	BMA	C1-O5-C5	-2.41	108.95	112.19
3	B	602	NAG	C8-C7-N2	-2.41	112.12	116.12
3	I	607	NAG	C2-N2-C7	-2.41	119.67	122.90
3	I	606	NAG	C8-C7-N2	-2.40	112.13	116.12
8	G	612	JXS	N23-C14-N19	2.40	120.45	116.59
6	I	602	BMA	O4-C4-C3	-2.39	104.74	110.38
5	B	608	HEM	CHB-C4A-C3A	-2.39	120.49	127.43
5	G	607	HEM	CAA-C2A-C1A	2.39	129.60	124.94
3	I	601	NAG	O7-C7-C8	2.39	126.30	122.05
3	B	604	NAG	C1-O5-C5	-2.38	108.99	112.19
5	G	607	HEM	O2D-CGD-CBD	2.37	121.49	114.00
3	B	607	NAG	O5-C5-C4	2.36	116.56	110.83
7	E	603	MAN	C2-C3-C4	2.35	114.99	110.86
3	G	606	NAG	C4-C3-C2	2.35	114.46	111.02
3	B	605	NAG	O3-C3-C2	2.34	114.27	109.40
3	E	604	NAG	O4-C4-C5	2.34	115.08	109.32
8	G	612	JXS	C07-C04-C12	2.33	107.60	105.29
7	I	603	MAN	O5-C1-C2	2.33	116.34	110.79
8	G	612	JXS	C08-C05-C09	-2.32	117.88	120.86
5	G	607	HEM	C2B-C1B-NB	2.32	112.51	109.84
3	B	602	NAG	C2-N2-C7	2.31	126.00	122.90
3	B	604	NAG	O7-C7-N2	2.30	126.05	121.98
3	B	603	NAG	C3-C4-C5	2.30	114.41	110.23
3	G	606	NAG	C8-C7-N2	-2.29	112.32	116.12
3	B	609	NAG	O5-C5-C6	2.29	112.11	107.66
3	I	601	NAG	O4-C4-C3	-2.28	105.01	110.38
3	E	604	NAG	C4-C3-C2	2.28	114.35	111.02
3	I	607	NAG	C4-C3-C2	2.27	114.34	111.02
3	G	608	NAG	C8-C7-N2	-2.26	112.37	116.12
3	B	603	NAG	O5-C5-C4	2.25	116.31	110.83
3	E	606	NAG	C2-N2-C7	2.25	125.92	122.90
7	B	612	MAN	O3-C3-C2	2.24	114.62	110.05
8	E	610	JXS	C07-C04-C12	2.24	107.50	105.29
3	G	603	NAG	C1-O5-C5	2.24	115.19	112.19
8	B	613	JXS	C04-C12-N18	-2.24	108.65	110.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	609	NAG	O7-C7-N2	2.24	125.94	121.98
4	E	608	FUC	C2-C3-C4	2.24	114.79	110.86
5	E	609	HEM	CHA-C4D-C3D	-2.23	121.12	125.23
5	I	610	HEM	C1D-C2D-C3D	-2.22	104.65	106.98
6	E	601	BMA	O5-C5-C6	2.21	111.97	107.66
8	B	613	JXS	N23-C14-N19	2.20	120.13	116.59
6	G	609	BMA	O2-C2-C3	2.20	114.70	110.15
3	G	604	NAG	O6-C6-C5	-2.19	103.88	111.33
5	B	608	HEM	CBD-CAD-C3D	-2.18	106.51	112.53
3	I	601	NAG	O4-C4-C5	2.17	114.67	109.32
7	G	611	MAN	O4-C4-C5	-2.17	103.99	109.32
5	I	610	HEM	CHC-C4B-NB	2.17	126.75	124.42
5	E	609	HEM	O2D-CGD-CBD	2.15	120.80	114.00
3	E	607	NAG	O3-C3-C2	-2.15	104.94	109.40
3	E	605	NAG	O5-C5-C6	2.14	111.83	107.66
5	E	609	HEM	CHC-C4B-C3B	-2.14	120.81	125.07
5	G	607	HEM	C3D-C4D-ND	2.12	112.50	110.17
3	E	604	NAG	C8-C7-N2	-2.12	112.60	116.12
5	B	608	HEM	O2D-CGD-CBD	2.11	120.68	114.00
5	I	610	HEM	C3D-C4D-ND	2.11	112.49	110.17
5	B	608	HEM	CHC-C4B-NB	2.11	126.69	124.42
7	I	604	MAN	O6-C6-C5	2.11	118.50	111.33
5	E	609	HEM	C2A-C1A-NA	2.10	112.48	110.15
4	E	608	FUC	O5-C5-C6	2.10	111.95	107.40
5	G	607	HEM	CHC-C1C-NC	-2.09	122.18	124.45
4	I	609	FUC	O2-C2-C1	2.08	113.99	109.22
7	G	611	MAN	O3-C3-C4	2.06	115.24	110.38
3	E	604	NAG	C3-C4-C5	2.06	113.97	110.23
3	I	607	NAG	C3-C4-C5	2.05	113.96	110.23
5	I	610	HEM	CHB-C1B-NB	2.05	126.90	124.37
5	B	608	HEM	C3C-C2C-C1C	-2.05	105.11	107.05
3	G	608	NAG	O7-C7-N2	2.05	125.60	121.98
6	B	610	BMA	C6-C5-C4	2.05	118.05	113.02
5	G	607	HEM	O2A-CGA-CBA	2.04	120.44	114.00
5	E	609	HEM	C2B-C1B-NB	2.04	112.18	109.84
7	I	604	MAN	C1-C2-C3	-2.03	106.69	109.64
5	B	608	HEM	CMB-C2B-C1B	2.03	128.20	125.03
3	I	605	NAG	C3-C4-C5	2.01	113.87	110.23
5	E	609	HEM	C4B-C3B-C2B	-2.01	105.44	107.28
5	E	609	HEM	C3D-C4D-ND	2.00	112.37	110.17

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	608	HEM	C2B-C3B-CAB-CBB
5	B	608	HEM	C4B-C3B-CAB-CBB
6	I	602	BMA	C4-C5-C6-O6
6	B	610	BMA	C4-C5-C6-O6
3	G	608	NAG	O5-C5-C6-O6
3	B	604	NAG	C4-C5-C6-O6
6	B	610	BMA	O5-C5-C6-O6
3	B	604	NAG	O5-C5-C6-O6
6	E	601	BMA	O5-C5-C6-O6
3	G	608	NAG	C4-C5-C6-O6
3	I	601	NAG	C4-C5-C6-O6
3	I	606	NAG	C4-C5-C6-O6
7	B	611	MAN	C4-C5-C6-O6
3	B	602	NAG	C4-C5-C6-O6
3	I	606	NAG	O5-C5-C6-O6
3	I	605	NAG	O5-C5-C6-O6
3	E	605	NAG	O5-C5-C6-O6
6	I	602	BMA	O5-C5-C6-O6
7	B	612	MAN	O5-C5-C6-O6
7	G	610	MAN	O5-C5-C6-O6
6	E	601	BMA	C4-C5-C6-O6
7	I	604	MAN	O5-C5-C6-O6
3	E	606	NAG	C4-C5-C6-O6
7	I	603	MAN	C4-C5-C6-O6
7	I	603	MAN	O5-C5-C6-O6
3	B	609	NAG	C4-C5-C6-O6
7	I	604	MAN	C4-C5-C6-O6
3	E	605	NAG	C4-C5-C6-O6
3	I	601	NAG	O5-C5-C6-O6
7	B	611	MAN	O5-C5-C6-O6
3	B	609	NAG	O5-C5-C6-O6
7	E	603	MAN	O5-C5-C6-O6
3	I	605	NAG	C4-C5-C6-O6
7	B	612	MAN	C4-C5-C6-O6
7	G	610	MAN	C4-C5-C6-O6
3	G	601	NAG	C4-C5-C6-O6
3	E	606	NAG	O5-C5-C6-O6
3	B	605	NAG	C4-C5-C6-O6
3	B	607	NAG	O5-C5-C6-O6
7	G	611	MAN	C4-C5-C6-O6
3	G	603	NAG	C4-C5-C6-O6
3	B	601	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	I	607	NAG	C4-C5-C6-O6
3	B	602	NAG	O5-C5-C6-O6
7	G	611	MAN	O5-C5-C6-O6
6	G	609	BMA	O5-C5-C6-O6
3	B	607	NAG	C4-C5-C6-O6
5	E	609	HEM	C2B-C3B-CAB-CBB
5	E	609	HEM	C2C-C3C-CAC-CBC
5	G	607	HEM	C2B-C3B-CAB-CBB
3	G	601	NAG	O5-C5-C6-O6
7	E	603	MAN	C4-C5-C6-O6
7	E	602	MAN	O5-C5-C6-O6
5	I	610	HEM	CAD-CBD-CGD-O1D
5	E	609	HEM	CAD-CBD-CGD-O2D
5	E	609	HEM	CAD-CBD-CGD-O1D
3	B	604	NAG	C1-C2-N2-C7
3	B	605	NAG	C1-C2-N2-C7
3	B	609	NAG	C1-C2-N2-C7
3	E	605	NAG	C1-C2-N2-C7
5	E	609	HEM	CAA-CBA-CGA-O2A
5	G	607	HEM	CAD-CBD-CGD-O2D
5	B	608	HEM	CAD-CBD-CGD-O2D
5	G	607	HEM	CAA-CBA-CGA-O2A
5	I	610	HEM	CAD-CBD-CGD-O2D
5	G	607	HEM	CAA-CBA-CGA-O1A
5	B	608	HEM	CAD-CBD-CGD-O1D
5	B	608	HEM	CAA-CBA-CGA-O2A
5	E	609	HEM	C4B-C3B-CAB-CBB
5	G	607	HEM	C4B-C3B-CAB-CBB
5	E	609	HEM	CAA-CBA-CGA-O1A
5	B	608	HEM	CAA-CBA-CGA-O1A
5	G	607	HEM	CAD-CBD-CGD-O1D
5	I	610	HEM	CAA-CBA-CGA-O2A

All (2) ring outliers are listed below:

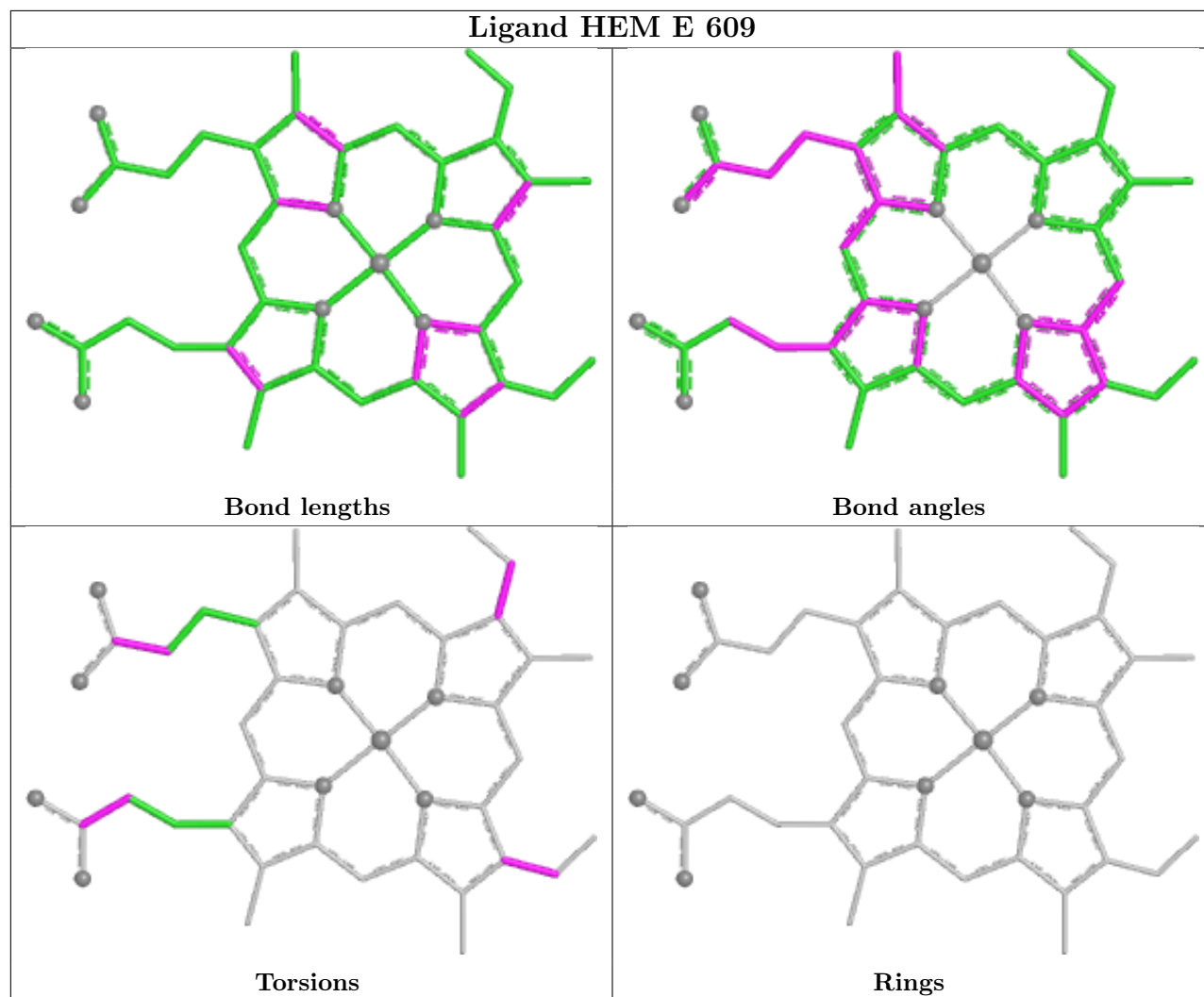
Mol	Chain	Res	Type	Atoms
7	G	610	MAN	C1-C2-C3-C4-C5-O5
7	I	604	MAN	C1-C2-C3-C4-C5-O5

34 monomers are involved in 100 short contacts:

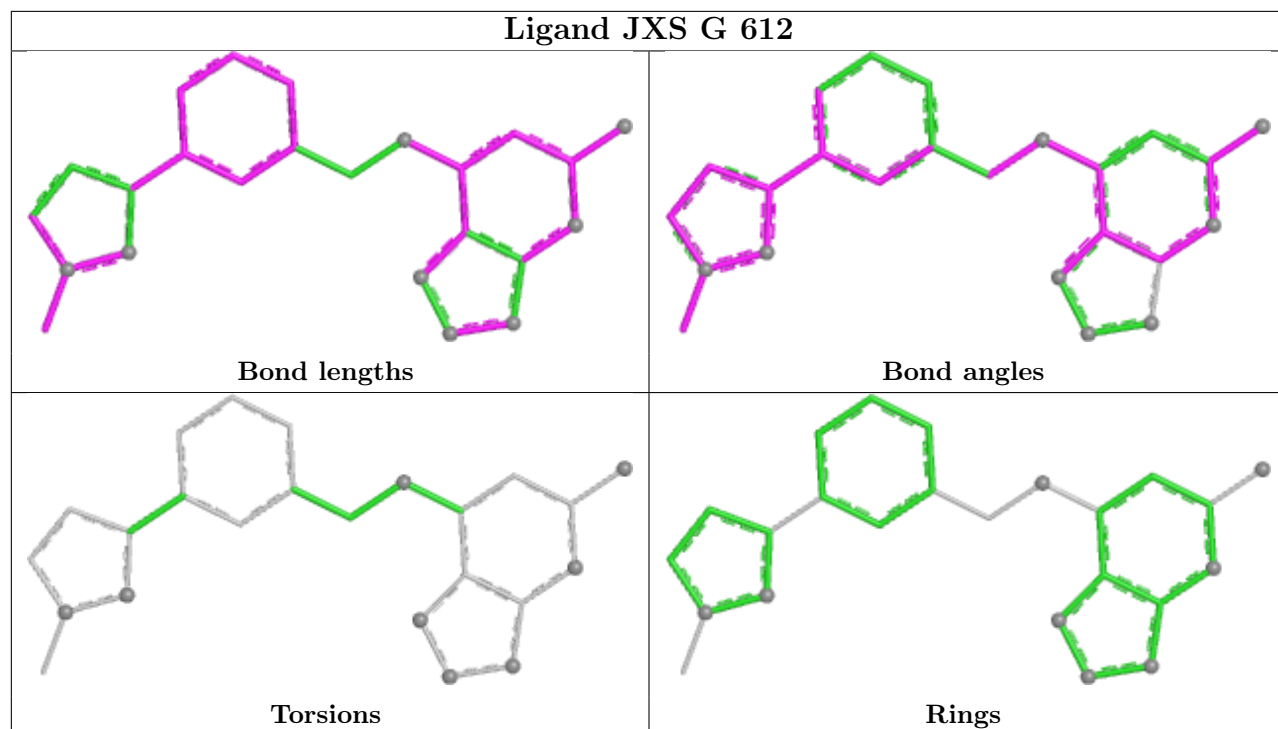
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	606	NAG	1	0
3	B	603	NAG	3	0
3	B	605	NAG	4	0
3	B	609	NAG	3	0
3	E	606	NAG	1	0
7	G	610	MAN	1	0
3	G	601	NAG	1	0
5	E	609	HEM	8	0
6	I	602	BMA	2	0
7	E	602	MAN	4	0
4	I	609	FUC	1	0
3	I	608	NAG	4	0
6	G	609	BMA	8	0
3	G	602	NAG	5	0
3	B	604	NAG	6	0
3	B	607	NAG	1	0
3	E	607	NAG	4	0
3	B	602	NAG	5	0
3	G	603	NAG	2	0
3	I	601	NAG	4	0
6	B	610	BMA	3	0
6	E	601	BMA	5	0
5	B	608	HEM	12	0
3	I	605	NAG	1	0
5	G	607	HEM	11	0
3	B	601	NAG	1	0
7	G	611	MAN	4	0
7	I	604	MAN	1	0
3	E	605	NAG	4	0
5	I	610	HEM	9	0
3	G	608	NAG	5	0
4	B	606	FUC	1	0
3	G	604	NAG	6	0
3	I	607	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

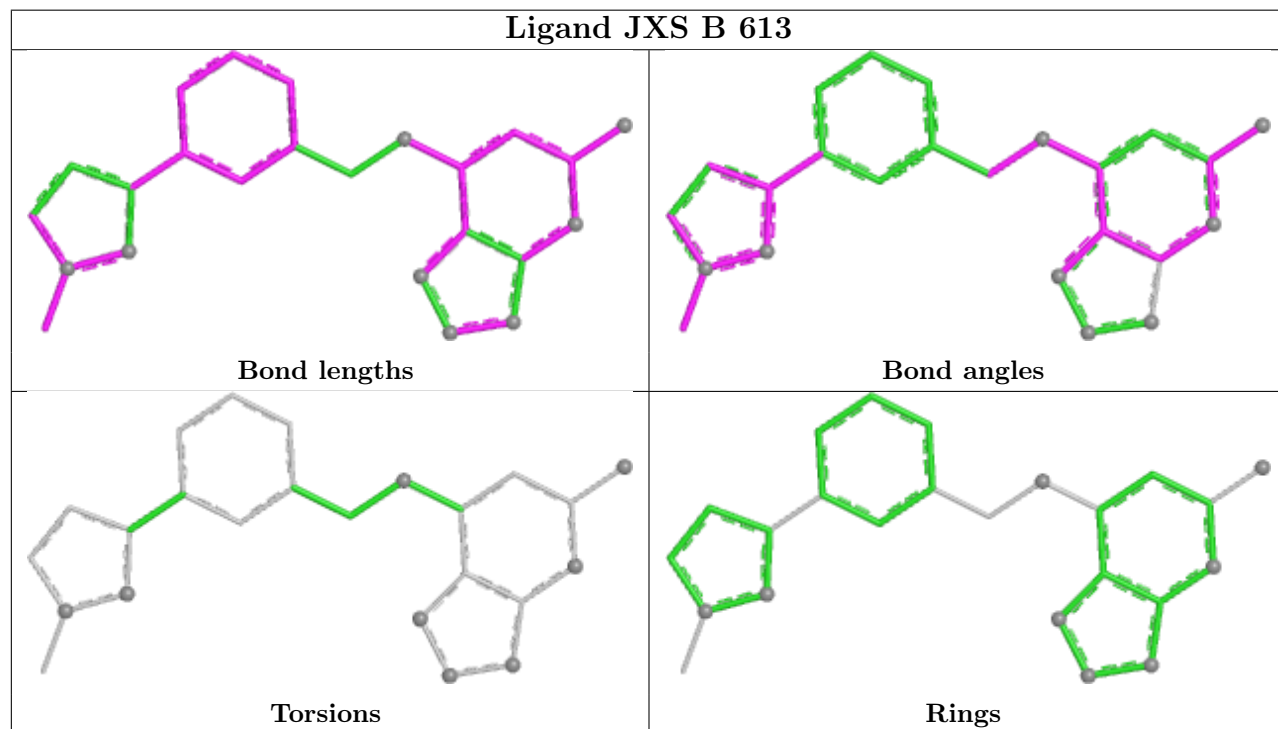
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

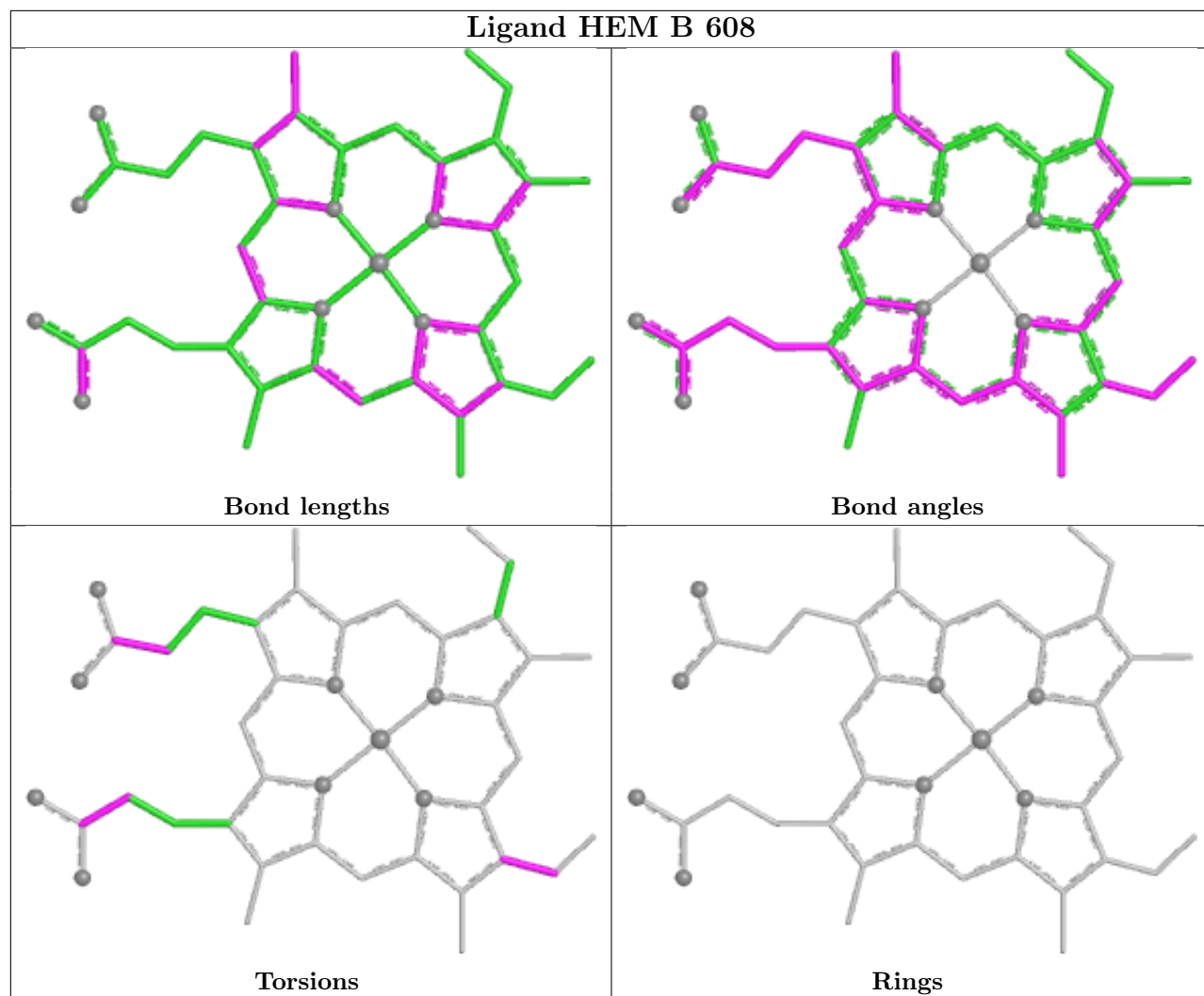


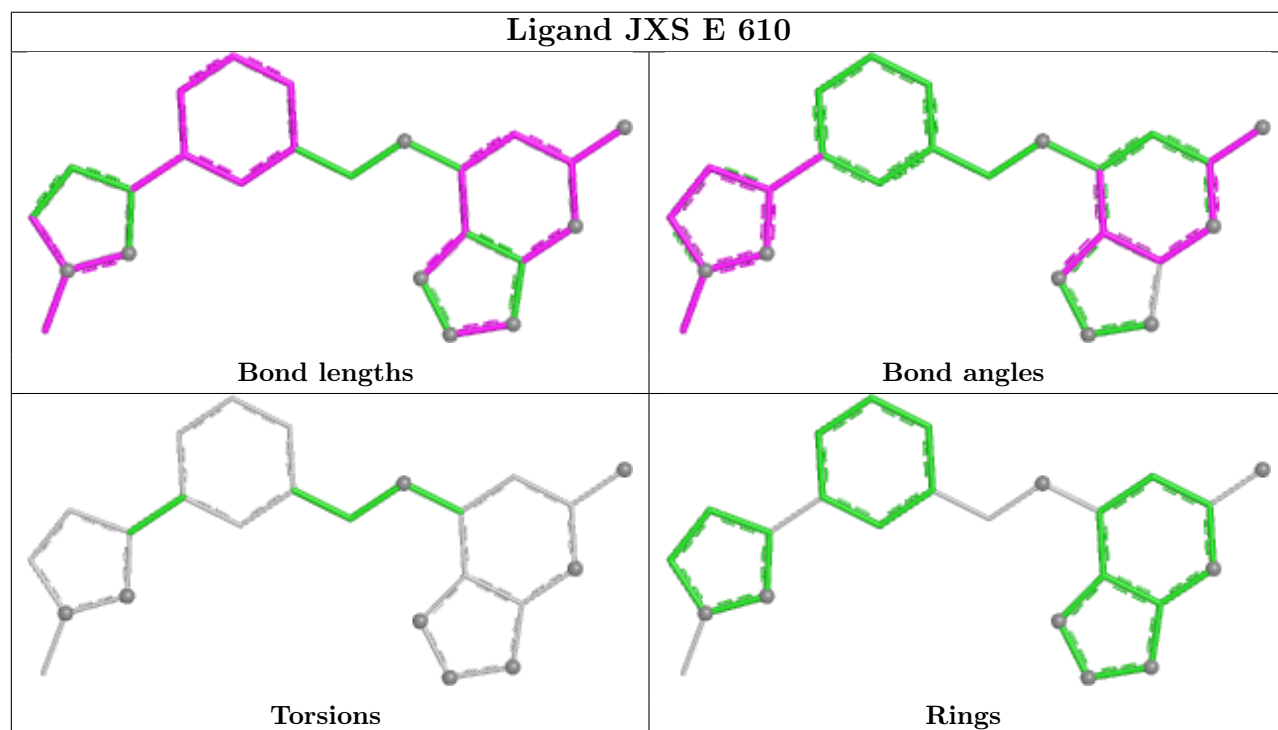
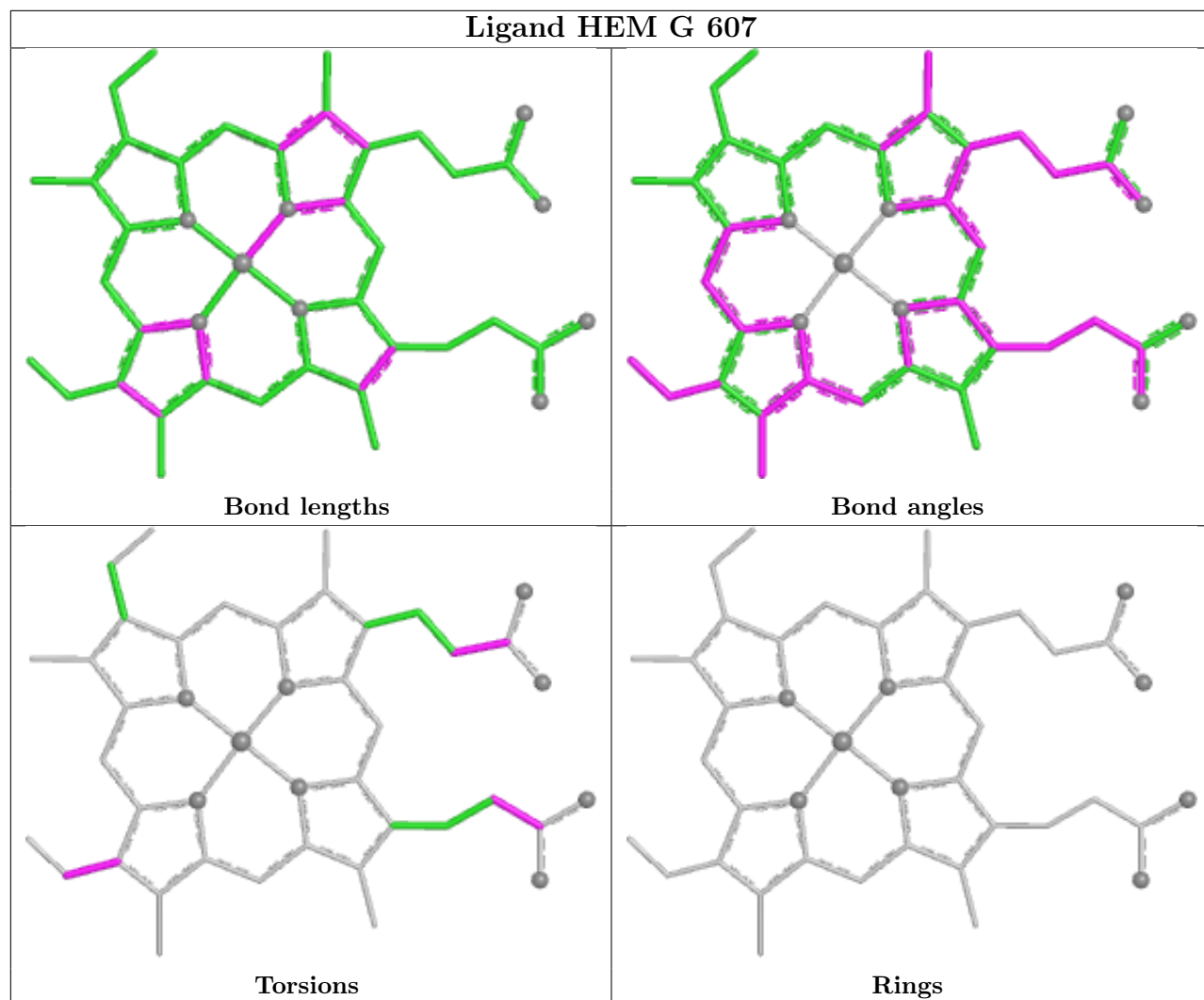
Ligand JXS G 612

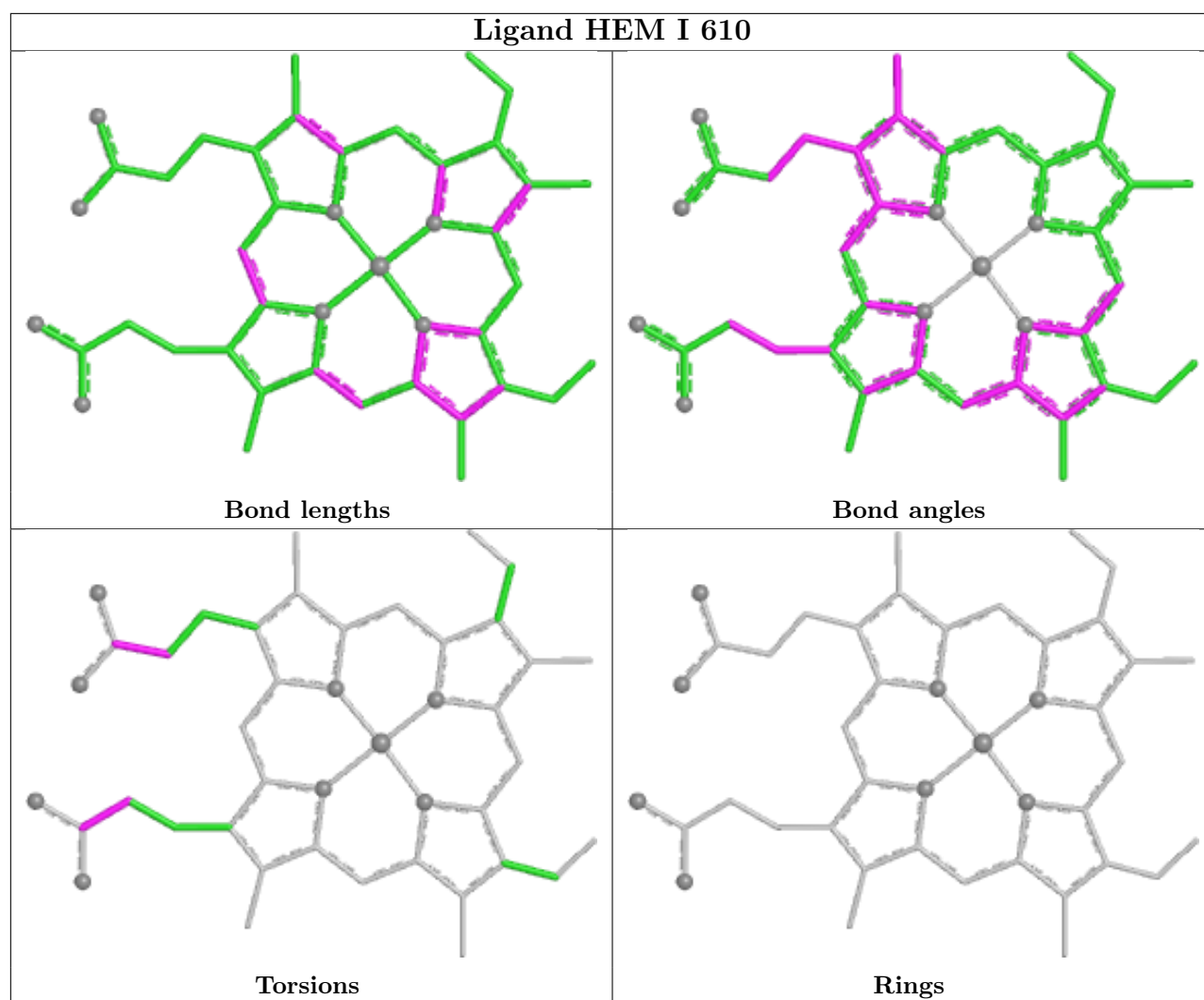


Ligand JXS B 613









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	103/105 (98%)	0.11	0 100 100	29, 51, 77, 85	1 (0%)
1	D	103/105 (98%)	0.31	2 (1%) 66 57	38, 54, 74, 90	2 (1%)
1	F	103/105 (98%)	0.34	2 (1%) 66 57	35, 52, 70, 86	0
1	H	103/105 (98%)	0.17	1 (0%) 79 72	29, 52, 80, 95	1 (0%)
2	B	465/467 (99%)	0.43	13 (2%) 55 44	27, 58, 86, 112	7 (1%)
2	E	465/467 (99%)	0.43	13 (2%) 55 44	32, 58, 79, 90	6 (1%)
2	G	465/467 (99%)	0.26	6 (1%) 75 66	26, 54, 75, 94	7 (1%)
2	I	465/467 (99%)	0.53	18 (3%) 43 34	29, 62, 94, 111	10 (2%)
All	All	2272/2288 (99%)	0.38	55 (2%) 59 49	26, 56, 84, 112	34 (1%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	482	SER	7.0
2	I	482	SER	3.4
2	I	522	MET	3.2
2	B	348	ASN	3.0
2	B	248	SER	2.9
2	B	354	GLU	2.8
2	G	329	THR	2.8
2	B	113	VAL	2.8
2	B	288	VAL	2.8
2	I	577	GLU	2.8
2	B	331	ALA	2.8
2	G	159	THR	2.7
2	G	155	GLY	2.7
2	E	325	ALA	2.7
2	I	202	ARG	2.6
2	I	170	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	377	ILE	2.5
1	H	1	CYS	2.5
2	I	218	ASP	2.5
2	I	468	TYR	2.5
2	I	377	ILE	2.5
1	F	29	PHE	2.5
2	E	497	CYS	2.5
2	G	326	ASN	2.5
2	E	482	SER	2.4
2	E	365	PHE	2.4
2	B	251	THR	2.4
2	I	264	LEU	2.4
2	I	455	LEU	2.4
2	G	372	VAL	2.4
1	D	29	PHE	2.4
2	E	562	VAL	2.3
2	I	113	VAL	2.3
2	E	326	ASN	2.3
2	E	577	GLU	2.3
2	B	284	VAL	2.3
2	E	164	ILE	2.2
2	I	195	GLY	2.2
1	D	32	TRP	2.2
2	B	115	CYS	2.2
2	B	322	PRO	2.2
2	I	263	GLU	2.2
2	B	522	MET	2.2
2	E	113	VAL	2.1
2	I	574	SER	2.1
2	E	408	GLU	2.1
1	F	30	VAL	2.1
2	I	157	ASN	2.1
2	I	196	LEU	2.1
2	E	218	ASP	2.1
2	G	348	ASN	2.0
2	I	376	GLY	2.0
2	E	324	ILE	2.0
2	E	329	THR	2.0
2	I	541	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	B	603	14/15	0.30	0.18	120,124,126,126	0
3	NAG	G	603	14/15	0.51	0.16	112,115,118,118	0
3	NAG	B	607	14/15	0.53	0.18	114,117,120,120	0
3	NAG	G	606	14/15	0.53	0.17	117,121,123,123	0
3	NAG	E	606	14/15	0.74	0.12	81,85,88,88	0
7	MAN	I	603	11/12	0.75	0.16	85,88,90,90	0
3	NAG	I	605	14/15	0.77	0.13	90,94,96,96	0
7	MAN	E	602	11/12	0.78	0.13	70,72,74,76	0
3	NAG	B	601	14/15	0.78	0.14	73,77,79,79	0
7	MAN	G	610	11/12	0.80	0.13	76,78,80,82	0
3	NAG	E	604	14/15	0.80	0.13	77,81,83,83	0
3	NAG	I	607	14/15	0.81	0.12	91,95,97,97	0
3	NAG	B	602	14/15	0.83	0.14	96,100,102,103	0
3	NAG	I	606	14/15	0.83	0.13	80,84,86,86	0
3	NAG	G	602	14/15	0.84	0.14	74,78,80,80	0
3	NAG	E	605	14/15	0.84	0.14	87,90,93,93	0
7	MAN	B	611	11/12	0.84	0.11	54,57,59,60	0
8	JXS	B	613	24/24	0.85	0.15	70,76,84,85	0
3	NAG	G	601	14/15	0.86	0.11	61,64,67,67	0
7	MAN	I	604	11/12	0.87	0.12	46,48,51,51	0
6	BMA	G	609	11/12	0.87	0.13	45,47,49,49	0
8	JXS	E	610	24/24	0.87	0.14	66,70,72,74	0
7	MAN	B	612	11/12	0.88	0.11	51,54,56,56	0
7	MAN	G	611	11/12	0.88	0.09	37,39,41,41	0
4	FUC	B	606	10/11	0.88	0.12	47,48,49,49	0
3	NAG	I	608	14/15	0.89	0.11	46,49,52,52	0
4	FUC	I	609	10/11	0.90	0.11	53,53,54,55	0

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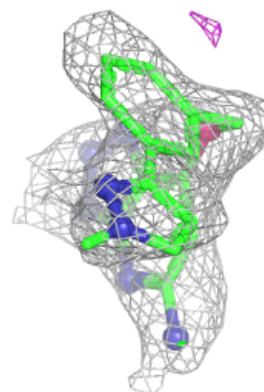
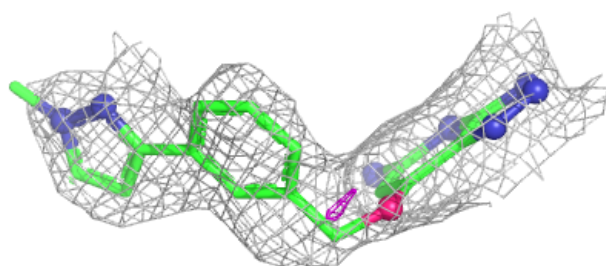
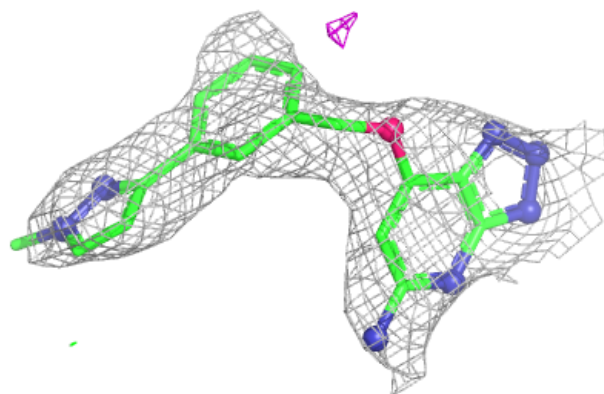
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	BMA	E	601	11/12	0.90	0.17	63,65,67,68	0
3	NAG	E	607	14/15	0.90	0.10	58,62,64,64	0
8	JXS	G	612	24/24	0.90	0.11	46,54,64,68	0
3	NAG	B	609	14/15	0.91	0.09	40,44,47,47	0
6	BMA	I	602	11/12	0.91	0.14	62,65,66,67	0
6	BMA	B	610	11/12	0.91	0.12	52,54,55,57	0
3	NAG	B	604	14/15	0.91	0.11	48,52,54,55	0
3	NAG	G	604	14/15	0.92	0.09	40,44,46,47	0
7	MAN	E	603	11/12	0.93	0.08	36,39,41,41	0
4	FUC	E	608	10/11	0.93	0.10	49,49,51,51	0
5	HEM	B	608	43/43	0.94	0.11	49,50,54,56	0
3	NAG	G	608	14/15	0.94	0.10	51,54,57,57	0
3	NAG	B	605	14/15	0.95	0.07	35,38,41,42	0
3	NAG	I	601	14/15	0.95	0.08	30,35,37,38	0
5	HEM	E	609	43/43	0.95	0.11	59,60,64,67	0
5	HEM	G	607	43/43	0.95	0.10	44,45,49,50	0
5	HEM	I	610	43/43	0.95	0.10	45,46,49,55	0
10	CL	G	614	1/1	0.95	0.12	50,50,50,50	0
4	FUC	G	605	10/11	0.96	0.09	41,41,42,42	0
10	CL	B	615	1/1	0.97	0.27	62,62,62,62	0
9	CA	E	611	1/1	0.97	0.04	44,44,44,44	0
9	CA	I	611	1/1	0.99	0.07	51,51,51,51	0
9	CA	B	614	1/1	0.99	0.05	43,43,43,43	0
9	CA	G	613	1/1	0.99	0.03	40,40,40,40	0

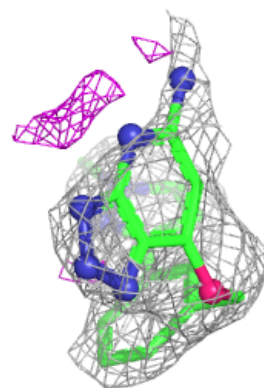
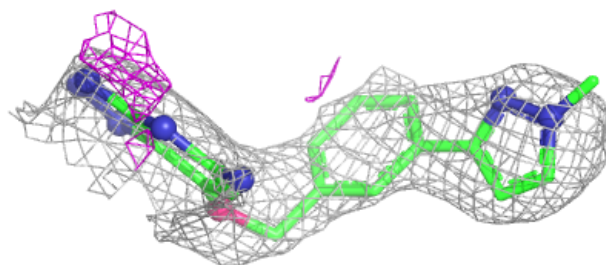
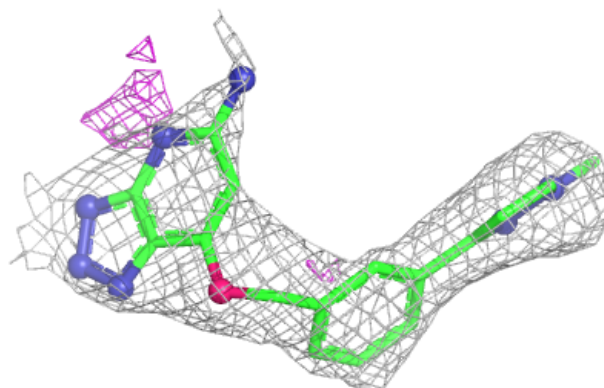
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JXS B 613:

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

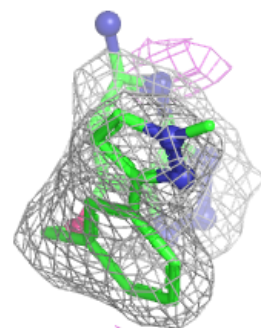
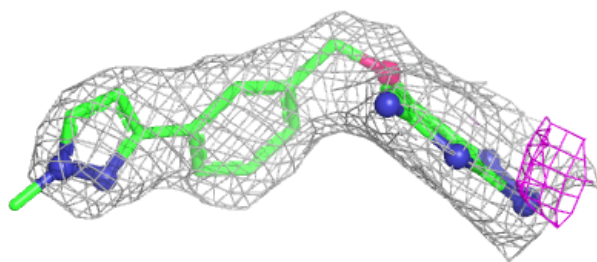
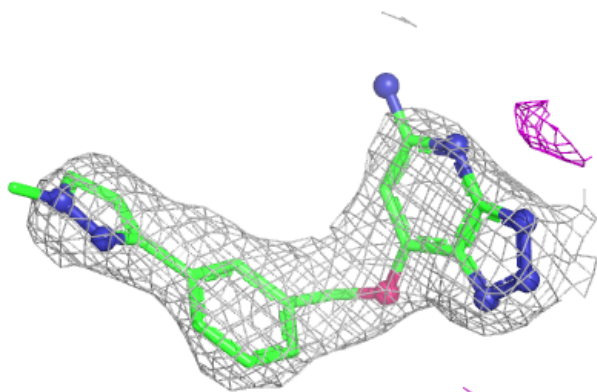
**Electron density around JXS E 610:**

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



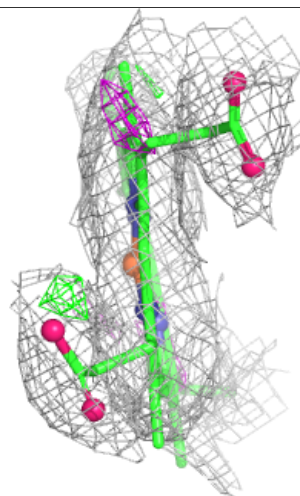
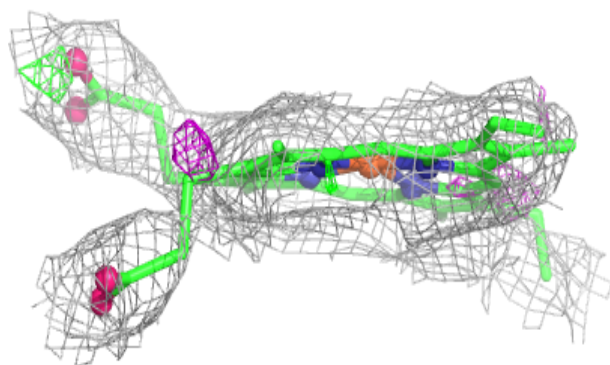
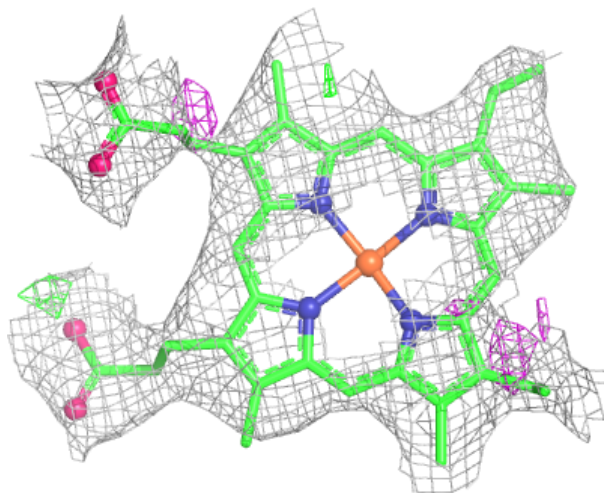
Electron density around JXS G 612:

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



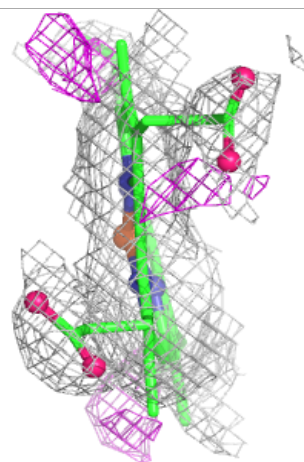
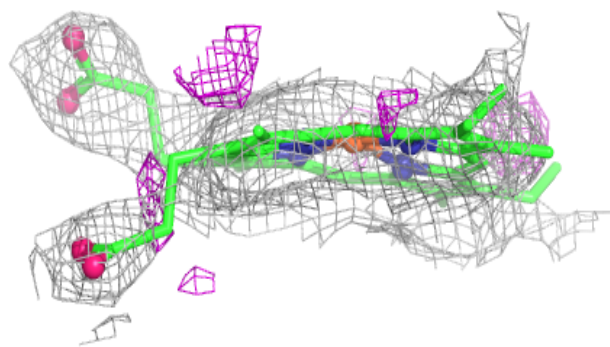
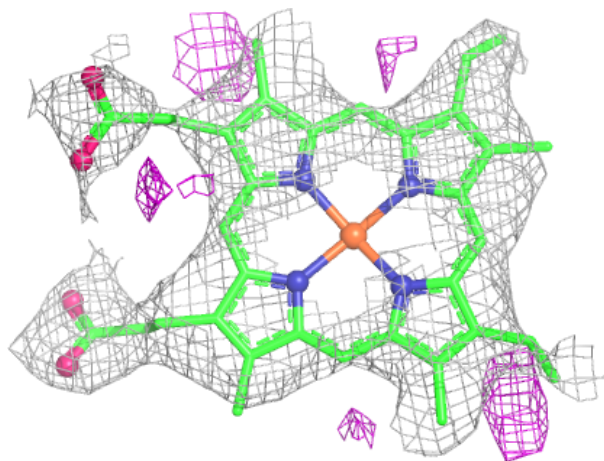
Electron density around HEM B 608:

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



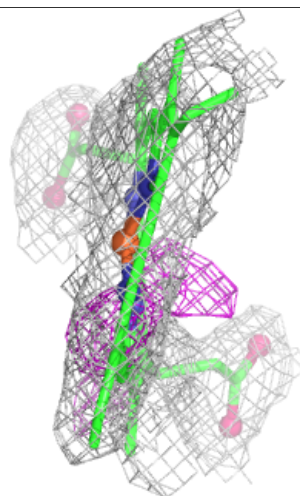
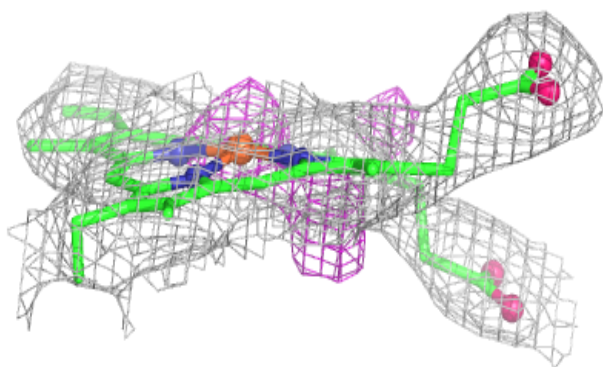
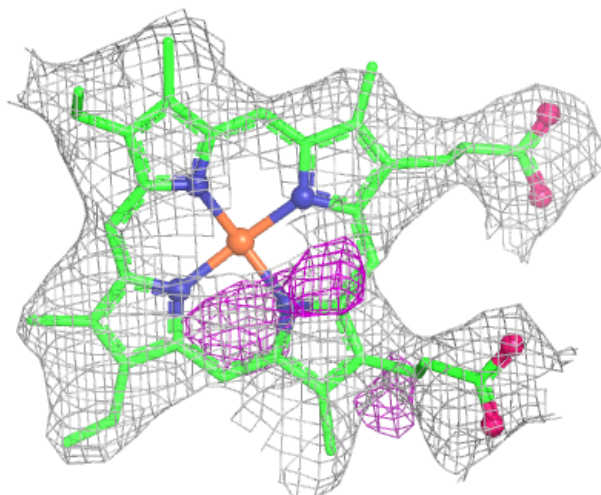
Electron density around HEM E 609:

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



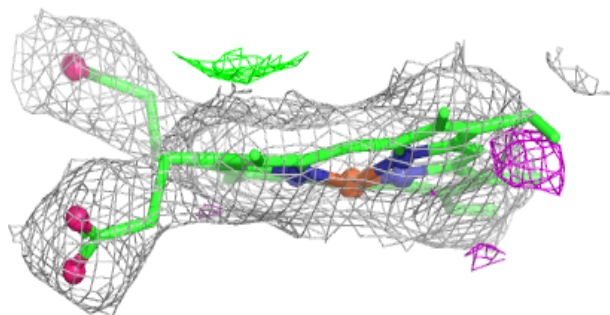
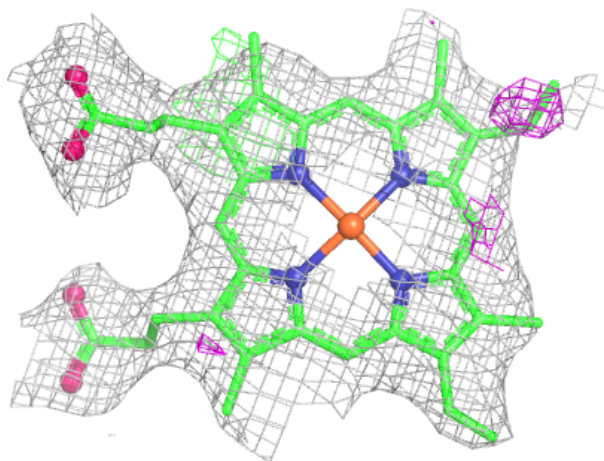
Electron density around HEM G 607:

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



Electron density around HEM I 610:

$2mF_o-DF_c$ (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.