



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 28, 2024 – 06:12 AM EDT

PDB ID : 5QJ2
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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

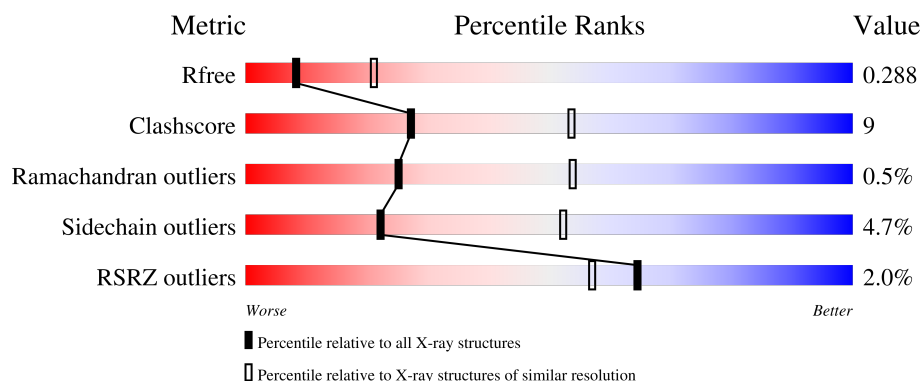
1 Overall quality at a glance

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.






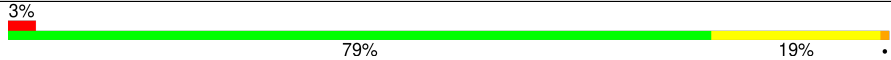
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	4293 (2.84-2.80)
Clashscore	180529	4801 (2.84-2.80)
Ramachandran outliers	177936	4739 (2.84-2.80)
Sidechain outliers	177891	4741 (2.84-2.80)
RSRZ outliers	164620	4295 (2.84-2.80)

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	
1	D	105	
1	F	105	
1	H	105	

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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	-

2 Entry composition

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 (three-letter code: NAG) (formula: C₈H₁₅NO₆).



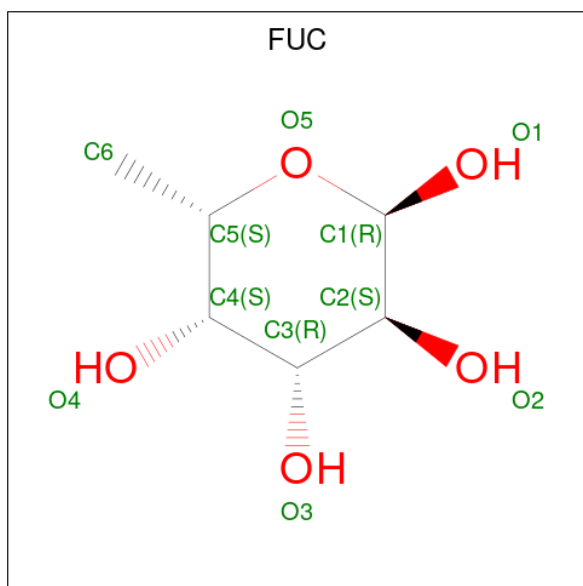
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	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 (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



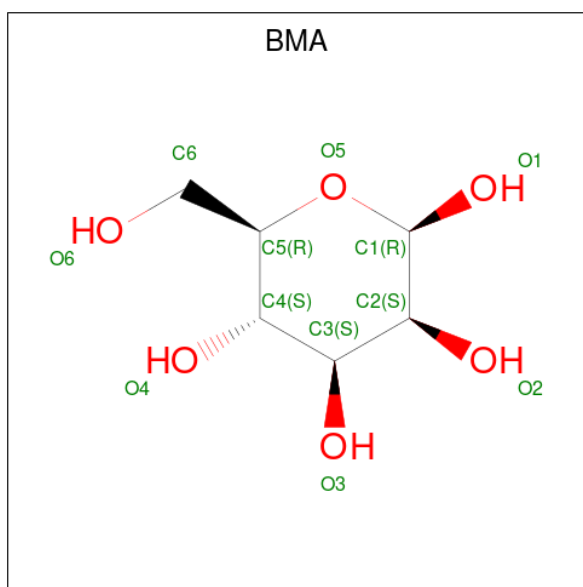
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			10	6	4		
4	E	1	Total	C	O	0	0
			10	6	4		
4	G	1	Total	C	O	0	0
			10	6	4		

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

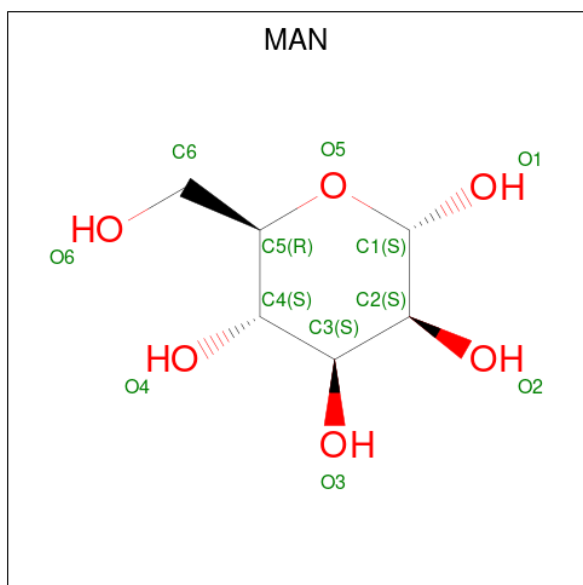
- # HEM

- Molecule 6 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



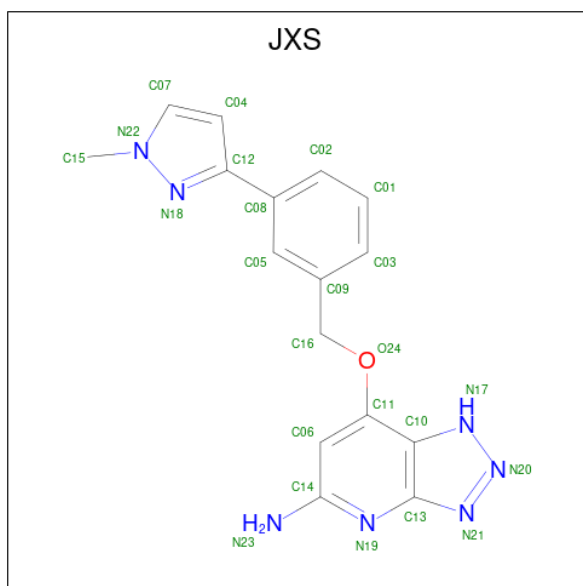
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			11	6	5		
6	E	1	Total	C	O	0	0
			11	6	5		
6	G	1	Total	C	O	0	0
			11	6	5		
6	I	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).



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

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



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

- Molecule 9 is CALCIUM ION (three-letter code: 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 (three-letter code: 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.

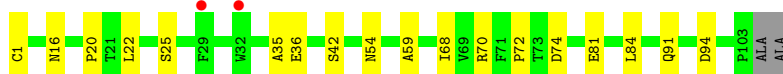
- Molecule 1: Myeloperoxidase

Chain A: 




- Molecule 1: Myeloperoxidase

Chain D: 




- Molecule 1: Myeloperoxidase

Chain F: 




- Molecule 1: Myeloperoxidase

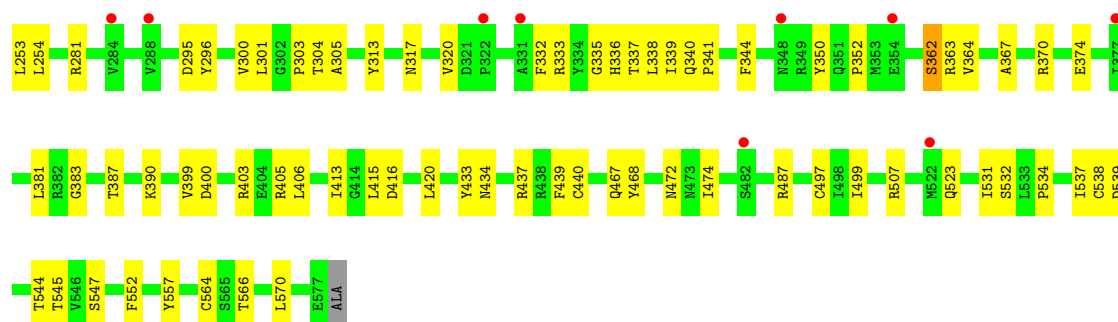
Chain H: 



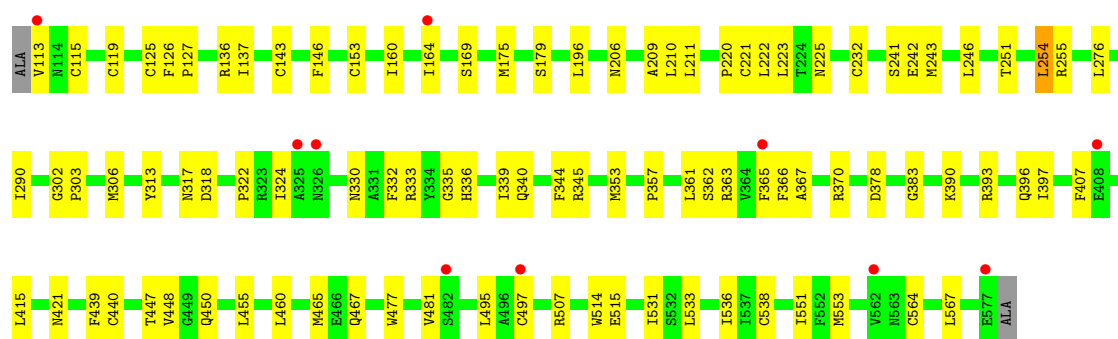
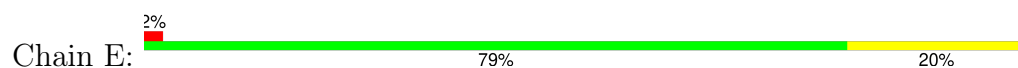
- Molecule 2: Myeloperoxidase

Chain B: 

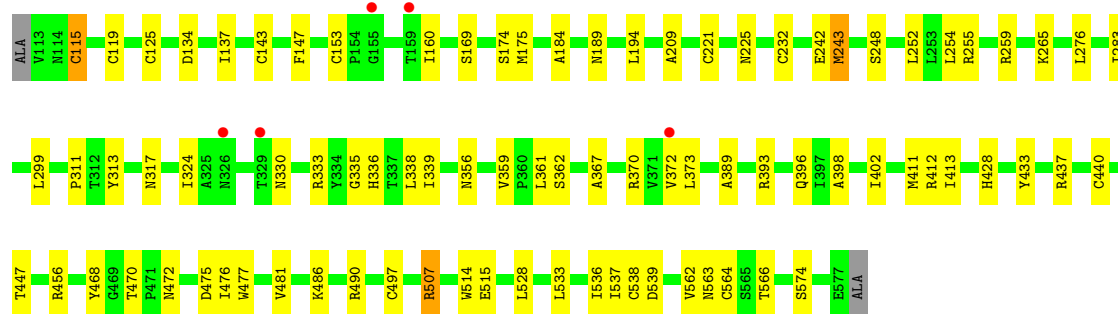
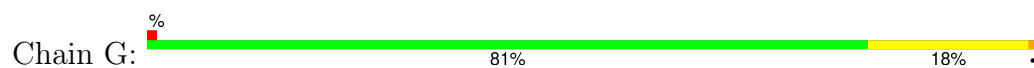




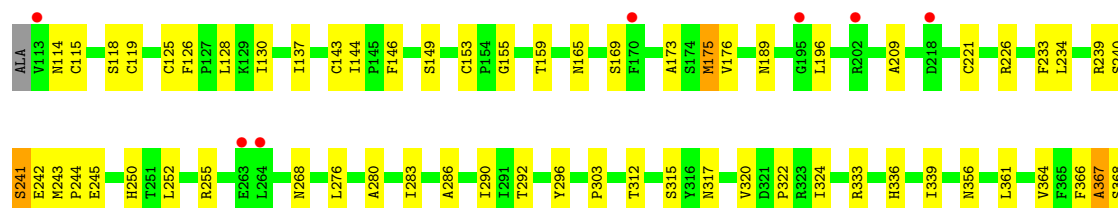
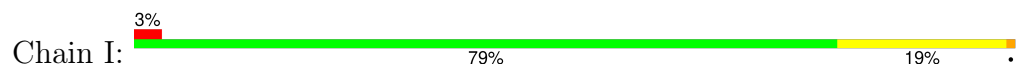
• Molecule 2: Myeloperoxidase

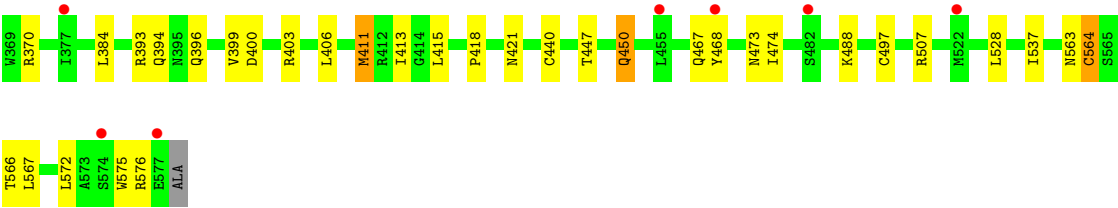


• Molecule 2: Myeloperoxidase



• 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	3100 reflections (5.07%)	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.47	0/837	0.75	0/1143
1	D	0.47	0/850	0.74	0/1159
1	F	0.49	0/838	0.75	0/1144
1	H	0.49	0/846	0.76	0/1154
2	B	0.50	0/3703	0.71	0/5043
2	E	0.49	0/3704	0.71	0/5043
2	G	0.52	0/3693	0.72	0/5030
2	I	0.50	0/3690	0.71	0/5026
All	All	0.50	0/18161	0.72	0/24742

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	812	0	764	20	0
1	D	825	0	780	13	0
1	F	813	0	766	11	0
1	H	821	0	774	13	0
2	B	3617	0	3529	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	3619	0	3555	69	0
2	G	3608	0	3526	56	0
2	I	3605	0	3513	61	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	10	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
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	309	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 (309) 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
2:I:173:ALA:HA	2:I:175:MET:HE1	1.18	1.17
1:F:94:ASP:OD2	5:G:607:HEM:HMD1	1.46	1.15
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
6:G:609:BMA:H62	7:G:611:MAN:H2	1.44	0.98
2:G:242:GLU:OE2	5:G:607:HEM:HMB1	1.65	0.96
2:G:119:CYS:HG	2:G:143:CYS:HG	1.14	0.95
2:G:440:CYS:HG	2:G:497:CYS:HG	1.09	0.94
2:G:221:CYS:HG	2:G:232:CYS:HG	1.19	0.91
2:G:243:MET:SD	5:G:607:HEM:HBB1	2.10	0.91
2:B:440:CYS:HG	2:B:497:CYS:HG	1.16	0.91
2:G:311:PRO:O	2:G:507:ARG:NH2	2.02	0.91
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:I:173:ALA:CA	2:I:175:MET:HE1	2.04	0.84
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
1:D:94:ASP:OD2	5:E:609:HEM:HMD1	1.82	0.80
2:B:153:CYS:HG	2:E:153:CYS:HG	1.29	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:119:CYS:HG	2:E:143:CYS:HG	0.79	0.79
2:E:221:CYS:HG	2:E:232:CYS:HG	0.88	0.78
2:G:538:CYS:HG	2:G:564:CYS:HG	0.79	0.78
6:G:609:BMA:H62	7:G:611:MAN:C2	2.13	0.78
2:B:243:MET:CE	5:B:608:HEM:HBB1	2.15	0.77
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:I:173:ALA:CA	2:I:175:MET:CE	2.62	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:I:115:CYS:HG	2:I:125:CYS:HG	0.75	0.72
3:B:609:NAG:H4	6:B:610:BMA:C1	2.21	0.71
2:I:175:MET:HE2	2:I:176:VAL:HG23	1.73	0.70
1:A:91:GLN:HE22	5:B:608:HEM:HBB2	1.57	0.69
2:G:242:GLU:OE2	5:G:607:HEM:CMB	2.40	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
3:B:604:NAG:O4	3:B:605:NAG:C1	2.42	0.68
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
5:G:607:HEM:CBB	5:G:607:HEM:HMB2	2.26	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:E:333:ARG:NH2	5:E:609:HEM:HAD1	2.12	0.64
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:G:115:CYS:CB	2:G:125:CYS:HG	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:F:35:ALA:HB3	2:G:160:ILE:HG21	1.87	0.55
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
2:E:538:CYS:HG	2:E:564:CYS:HG	1.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:440:CYS:HG	2:B:497:CYS:CB	2.21	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
5:G:607:HEM:HBC2	5:G:607:HEM:HMC2	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
2:I:175:MET:HE3	2:I:176:VAL:HG23	1.90	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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:173:ALA:CA	2:I:175:MET:HE2	2.39	0.50
2:G:514:TRP:CE2	2:G:515:GLU:HG3	2.46	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: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: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
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
2:I:221:CYS:SG	2:I:366:PHE:O	2.65	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
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:I:173:ALA:C	2:I:175:MET:HE2	2.36	0.46
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
5:G:607:HEM:HMB2	5:G:607:HEM:HBB2	1.97	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:440:CYS:HG	2:I:497:CYS:HB3	1.81	0.43
2:E:125:CYS:C	2:E:127:PRO:HD3	2.39	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
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
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
2:B:538:CYS:HG	2:B:564:CYS:HG	1.64	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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	101/105 (96%)	94 (93%)	7 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	101/105 (96%)	93 (92%)	7 (7%)	1 (1%)	13	37
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	59
2	E	463/467 (99%)	433 (94%)	27 (6%)	3 (1%)	22	49
2	G	463/467 (99%)	426 (92%)	36 (8%)	1 (0%)	44	71
2	I	463/467 (99%)	428 (92%)	31 (7%)	4 (1%)	14	39
All	All	2256/2288 (99%)	2090 (93%)	155 (7%)	11 (0%)	25	54

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
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%)	82 (96%)	3 (4%)	31	63
1	D	88/90 (98%)	82 (93%)	6 (7%)	13	36
1	F	85/90 (94%)	82 (96%)	3 (4%)	31	63
1	H	87/90 (97%)	83 (95%)	4 (5%)	23	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	386/411 (94%)	373 (97%)	13 (3%)	32	64
2	E	387/411 (94%)	370 (96%)	17 (4%)	24	55
2	G	382/411 (93%)	362 (95%)	20 (5%)	19	48
2	I	382/411 (93%)	360 (94%)	22 (6%)	17	43
All	All	1882/2004 (94%)	1794 (95%)	88 (5%)	22	52

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	CYS
1	A	73	THR
1	A	84	LEU
2	B	175	MET
2	B	196	LEU
2	B	217	HIS
2	B	254	LEU
2	B	295	ASP
2	B	304	THR
2	B	362	SER
2	B	364	VAL
2	B	374	GLU
2	B	523	GLN
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
1	D	72	PRO
2	E	113	VAL
2	E	175	MET
2	E	196	LEU
2	E	206	ASN
2	E	222	LEU
2	E	243	MET
2	E	254	LEU
2	E	276	LEU
2	E	318	ASP
2	E	345	ARG

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Mol	Chain	Res	Type
2	E	353	MET
2	E	361	LEU
2	E	362	SER
2	E	378	ASP
2	E	415	LEU
2	E	495	LEU
2	E	567	LEU
1	F	64	VAL
1	F	73	THR
1	F	84	LEU
2	G	115	CYS
2	G	174	SER
2	G	175	MET
2	G	194	LEU
2	G	243	MET
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	507	ARG
2	G	562	VAL
2	G	566	THR
2	G	574	SER
1	H	18	ARG
1	H	71	PHE
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	175	MET
2	I	196	LEU
2	I	226	ARG
2	I	234	LEU

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Mol	Chain	Res	Type
2	I	239	ARG
2	I	240	SER
2	I	241	SER
2	I	276	LEU
2	I	312	THR
2	I	315	SER
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	507	ARG
2	I	564	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	121	GLN
2	B	189	ASN
2	B	192	ASN
2	B	225	ASN
2	B	250	HIS
1	D	54	ASN
2	E	189	ASN
2	E	225	ASN
2	E	392	ASN
2	E	563	ASN
1	F	26	ASN
2	G	121	GLN
2	G	317	ASN
2	G	563	ASN
1	H	75	GLN
2	I	114	ASN
2	I	189	ASN
2	I	250	HIS
2	I	317	ASN
2	I	450	GLN
2	I	467	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 ⓘ

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$
4	FUC	G	605	-	10,10,11	1.46	1 (10%)	14,14,16	2.26	5 (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%)
8	JXS	E	610	-	23,27,27	5.03	16 (69%)	28,38,38	2.20	8 (28%)
7	MAN	I	604	-	11,11,12	1.44	2 (18%)	15,15,17	1.58	3 (20%)
3	NAG	E	604	-	14,14,15	1.65	3 (21%)	17,19,21	2.24	7 (41%)
4	FUC	E	608	-	10,10,11	2.01	3 (30%)	14,14,16	2.53	7 (50%)
3	NAG	I	607	-	14,14,15	1.17	1 (7%)	17,19,21	2.20	5 (29%)
3	NAG	G	606	-	14,14,15	1.59	2 (14%)	17,19,21	1.70	6 (35%)
7	MAN	E	602	-	11,11,12	1.32	2 (18%)	15,15,17	1.78	4 (26%)
7	MAN	E	603	-	11,11,12	1.27	1 (9%)	15,15,17	3.23	6 (40%)
3	NAG	B	604	-	14,14,15	1.08	0	17,19,21	2.37	7 (41%)
4	FUC	I	609	-	10,10,11	1.60	3 (30%)	14,14,16	2.37	5 (35%)
8	JXS	B	613	-	23,27,27	5.04	15 (65%)	28,38,38	2.08	8 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	JXS	G	612	-	23,27,27	5.11	15 (65%)	28,38,38	2.19	8 (28%)
7	MAN	B	612	-	11,11,12	1.79	5 (45%)	15,15,17	1.95	5 (33%)
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	G	601	-	14,14,15	2.03	6 (42%)	17,19,21	2.13	6 (35%)
3	NAG	I	606	-	14,14,15	1.50	3 (21%)	17,19,21	2.08	5 (29%)
7	MAN	G	610	-	11,11,12	1.07	1 (9%)	15,15,17	2.07	3 (20%)
5	HEM	G	607	2	42,50,50	1.50	7 (16%)	46,82,82	2.04	13 (28%)
3	NAG	B	603	-	14,14,15	1.80	5 (35%)	17,19,21	2.29	8 (47%)
7	MAN	I	603	-	11,11,12	1.34	0	15,15,17	1.67	2 (13%)
6	BMA	I	602	-	11,11,12	1.36	2 (18%)	15,15,17	2.32	7 (46%)
3	NAG	G	604	-	14,14,15	1.37	2 (14%)	17,19,21	3.87	9 (52%)
3	NAG	B	609	-	14,14,15	1.02	1 (7%)	17,19,21	2.90	8 (47%)
3	NAG	B	602	-	14,14,15	1.33	2 (14%)	17,19,21	2.59	6 (35%)
4	FUC	B	606	-	10,10,11	1.98	3 (30%)	14,14,16	2.37	5 (35%)
3	NAG	G	608	-	14,14,15	1.09	1 (7%)	17,19,21	2.24	7 (41%)
3	NAG	E	606	-	14,14,15	1.41	3 (21%)	17,19,21	1.81	5 (29%)
3	NAG	E	605	-	14,14,15	1.18	1 (7%)	17,19,21	1.64	3 (17%)
5	HEM	B	608	2	42,50,50	1.69	12 (28%)	46,82,82	1.95	15 (32%)
6	BMA	E	601	-	11,11,12	1.35	1 (9%)	15,15,17	2.46	5 (33%)
6	BMA	G	609	-	11,11,12	1.22	1 (9%)	15,15,17	2.93	5 (33%)
5	HEM	I	610	2	42,50,50	1.51	7 (16%)	46,82,82	2.11	16 (34%)
7	MAN	G	611	-	11,11,12	1.26	2 (18%)	15,15,17	1.62	4 (26%)
3	NAG	I	605	-	14,14,15	1.41	2 (14%)	17,19,21	1.44	3 (17%)
7	MAN	B	611	-	11,11,12	1.04	0	15,15,17	1.15	1 (6%)
3	NAG	I	608	-	14,14,15	1.49	2 (14%)	17,19,21	4.17	10 (58%)
6	BMA	B	610	-	11,11,12	1.16	1 (9%)	15,15,17	2.19	6 (40%)
3	NAG	B	605	-	14,14,15	0.88	0	17,19,21	2.14	6 (35%)
3	NAG	B	601	-	14,14,15	1.89	4 (28%)	17,19,21	2.37	7 (41%)
3	NAG	G	602	-	14,14,15	1.67	2 (14%)	17,19,21	2.44	5 (29%)
5	HEM	E	609	2	42,50,50	1.49	8 (19%)	46,82,82	1.76	11 (23%)

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
4	FUC	G	605	-	-	-	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
8	JXS	E	610	-	-	0/9/9/9	0/4/4/4
7	MAN	I	604	-	-	2/2/19/22	1/1/1/1
3	NAG	E	604	-	-	0/6/23/26	0/1/1/1
4	FUC	E	608	-	-	-	0/1/1/1
3	NAG	I	607	-	-	1/6/23/26	0/1/1/1
3	NAG	G	606	-	-	0/6/23/26	0/1/1/1
7	MAN	E	602	-	-	1/2/19/22	0/1/1/1
7	MAN	E	603	-	-	2/2/19/22	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
4	FUC	I	609	-	-	-	0/1/1/1
8	JXS	G	612	-	-	0/9/9/9	0/4/4/4
7	MAN	B	612	-	-	2/2/19/22	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	G	601	-	-	2/6/23/26	0/1/1/1
3	NAG	I	606	-	-	2/6/23/26	0/1/1/1
7	MAN	G	610	-	-	2/2/19/22	1/1/1/1
5	HEM	G	607	2	-	6/12/54/54	-
3	NAG	B	603	-	-	0/6/23/26	0/1/1/1
7	MAN	I	603	-	-	2/2/19/22	0/1/1/1
6	BMA	I	602	-	-	2/2/19/22	0/1/1/1
3	NAG	G	604	-	-	0/6/23/26	0/1/1/1
3	NAG	B	609	-	-	3/6/23/26	0/1/1/1
3	NAG	B	602	-	-	2/6/23/26	0/1/1/1
4	FUC	B	606	-	-	-	0/1/1/1
3	NAG	G	608	-	-	2/6/23/26	0/1/1/1
3	NAG	E	606	-	-	2/6/23/26	0/1/1/1
3	NAG	E	605	-	-	3/6/23/26	0/1/1/1
5	HEM	B	608	2	-	6/12/54/54	-
6	BMA	E	601	-	-	2/2/19/22	0/1/1/1
6	BMA	G	609	-	-	1/2/19/22	0/1/1/1
5	HEM	I	610	2	-	3/12/54/54	-
7	MAN	G	611	-	-	2/2/19/22	0/1/1/1
3	NAG	I	605	-	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	B	611	-	-	2/2/19/22	0/1/1/1
3	NAG	I	608	-	-	0/6/23/26	0/1/1/1
6	BMA	B	610	-	-	2/2/19/22	0/1/1/1
3	NAG	B	605	-	-	2/6/23/26	0/1/1/1
3	NAG	B	601	-	-	1/6/23/26	0/1/1/1
3	NAG	G	602	-	-	0/6/23/26	0/1/1/1
5	HEM	E	609	2	-	6/12/54/54	-

All (155) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	612	JXS	C14-N19	11.52	1.47	1.33
8	E	610	JXS	C14-N19	11.48	1.47	1.33
8	B	613	JXS	C14-N19	11.24	1.46	1.33
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	E	610	JXS	C13-N19	7.91	1.52	1.36
8	B	613	JXS	C13-N19	7.88	1.52	1.36
8	G	612	JXS	C13-N19	7.84	1.52	1.36
8	G	612	JXS	C11-C10	7.78	1.54	1.42
8	B	613	JXS	C02-C08	7.12	1.53	1.39
8	E	610	JXS	C01-C02	7.12	1.51	1.38
8	G	612	JXS	C02-C08	7.00	1.53	1.39
8	E	610	JXS	C02-C08	7.00	1.53	1.39
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	C11-C10	6.53	1.52	1.42
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	E	610	JXS	C15-N22	-5.90	1.42	1.47
8	G	612	JXS	C01-C03	5.89	1.49	1.38
8	E	610	JXS	C11-C10	5.87	1.51	1.42
8	B	613	JXS	C15-N22	-5.80	1.42	1.47
8	B	613	JXS	C05-C08	4.89	1.48	1.39
8	G	612	JXS	C15-N22	-4.87	1.43	1.47
8	G	612	JXS	C05-C08	4.86	1.48	1.39
5	I	610	HEM	C1D-C2D	4.86	1.54	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	608	FUC	O5-C5	4.84	1.53	1.43
3	B	601	NAG	C4-C5	4.44	1.62	1.53
8	E	610	JXS	C05-C08	4.39	1.47	1.39
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
5	B	608	HEM	C1B-NB	-3.96	1.33	1.40
5	E	609	HEM	C1B-NB	-3.77	1.33	1.40
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
3	E	605	NAG	C1-C2	3.16	1.56	1.52
3	I	608	NAG	O5-C5	-3.13	1.37	1.43
8	E	610	JXS	C06-C14	3.11	1.44	1.40
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	B	613	JXS	C06-C11	3.05	1.46	1.37
5	B	608	HEM	C4B-NB	-3.03	1.32	1.38
8	B	613	JXS	C06-C14	3.03	1.44	1.40
3	G	601	NAG	C4-C3	3.00	1.60	1.52
8	G	612	JXS	C06-C14	2.97	1.44	1.40
8	E	610	JXS	C06-C11	2.94	1.46	1.37
3	E	604	NAG	C3-C2	2.93	1.58	1.52
4	G	605	FUC	C1-C2	2.91	1.59	1.52
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
8	E	610	JXS	C13-N21	2.86	1.39	1.34
5	B	608	HEM	CMD-C2D	-2.85	1.44	1.50
8	B	613	JXS	C07-N22	2.83	1.38	1.35
8	G	612	JXS	C13-N21	2.82	1.39	1.34
4	B	606	FUC	O5-C5	2.81	1.49	1.43
6	E	601	BMA	C4-C3	2.81	1.59	1.52
5	E	609	HEM	CHB-C1B	2.81	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	612	JXS	C07-N22	2.79	1.38	1.35
3	B	602	NAG	C4-C3	2.78	1.59	1.52
6	I	602	BMA	C4-C5	2.78	1.58	1.53
3	I	606	NAG	C1-C2	2.77	1.56	1.52
6	G	609	BMA	O2-C2	2.76	1.49	1.43
5	B	608	HEM	C3C-C2C	-2.76	1.36	1.40
8	G	612	JXS	C06-C11	2.75	1.45	1.37
8	E	610	JXS	C14-N23	2.74	1.42	1.35
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
5	G	607	HEM	C4B-NB	-2.66	1.33	1.38
5	B	608	HEM	C4A-CHB	-2.63	1.33	1.41
5	E	609	HEM	C1D-C2D	2.63	1.49	1.44
8	B	613	JXS	C13-N21	2.61	1.38	1.34
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
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
6	I	602	BMA	C4-C3	2.49	1.58	1.52
5	B	608	HEM	C3D-C2D	-2.48	1.31	1.36
3	B	601	NAG	O5-C5	2.47	1.48	1.43
5	I	610	HEM	C1A-CHA	-2.46	1.34	1.41
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
5	B	608	HEM	C3C-C4C	2.37	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	601	NAG	C1-C2	2.36	1.55	1.52
5	B	608	HEM	C1A-CHA	-2.35	1.34	1.41
8	E	610	JXS	C07-N22	2.35	1.38	1.35
8	B	613	JXS	C14-N23	2.35	1.41	1.35
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	E	609	HEM	C3C-C4C	2.31	1.44	1.41
4	I	609	FUC	C1-C2	2.30	1.57	1.52
5	G	607	HEM	CHB-C1B	2.29	1.40	1.34
5	I	610	HEM	C4A-CHB	-2.28	1.34	1.41
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	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
3	I	607	NAG	C4-C3	2.21	1.58	1.52
5	E	609	HEM	C3C-C2C	-2.21	1.37	1.40
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
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
8	E	610	JXS	C08-C12	2.08	1.52	1.49
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	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 (287) 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
3	B	602	NAG	C1-O5-C5	-6.89	102.95	112.19
5	E	609	HEM	CBA-CAA-C2A	-6.88	100.97	112.54
3	E	607	NAG	C1-O5-C5	-6.85	103.01	112.19
5	I	610	HEM	CBA-CAA-C2A	-6.79	101.12	112.54
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
8	G	612	JXS	C07-N22-N18	-6.55	107.92	111.73
6	E	601	BMA	C1-O5-C5	-6.38	103.64	112.19
8	B	613	JXS	C07-N22-N18	-6.33	108.06	111.73
8	E	610	JXS	C07-N22-N18	-6.28	108.08	111.73
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
5	G	607	HEM	CBA-CAA-C2A	-6.12	102.25	112.54
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
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
5	B	608	HEM	CBA-CAA-C2A	-5.56	103.20	112.54
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
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
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
8	G	612	JXS	C07-C04-C12	4.38	107.60	105.21
5	B	608	HEM	C4A-C3A-C2A	-4.38	103.95	107.00
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
8	E	610	JXS	C07-C04-C12	4.21	107.50	105.21
3	I	608	NAG	C3-C4-C5	4.21	117.86	110.23
3	B	605	NAG	C1-O5-C5	-4.18	106.58	112.19
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
8	G	612	JXS	C16-O24-C11	4.15	123.16	117.49
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
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
8	E	610	JXS	N23-C14-N19	3.99	121.54	118.24
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
8	B	613	JXS	C16-O24-C11	3.78	122.65	117.49
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
8	B	613	JXS	C07-C04-C12	3.69	107.22	105.21
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
3	G	608	NAG	O3-C3-C2	3.49	116.66	109.40
5	G	607	HEM	CHC-C4B-NB	3.46	128.16	124.44
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
8	E	610	JXS	C04-C12-C08	-3.37	125.62	128.77
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
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
8	E	610	JXS	C08-C12-N18	3.19	126.00	120.93
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
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
3	B	605	NAG	O3-C3-C4	3.11	117.70	110.38
3	B	603	NAG	C2-N2-C7	3.10	127.06	122.90
8	E	610	JXS	C04-C07-N22	3.10	108.34	106.81
3	G	602	NAG	C6-C5-C4	3.09	120.60	113.02
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
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
5	I	610	HEM	CHA-C4D-ND	3.04	128.15	124.37
4	E	608	FUC	C1-O5-C5	3.04	120.14	112.97
6	B	610	BMA	O5-C5-C6	-3.03	101.77	107.66
5	E	609	HEM	CHC-C4B-NB	3.03	127.69	124.44
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
5	I	610	HEM	CMC-C2C-C3C	2.93	130.54	124.68
3	I	606	NAG	O5-C1-C2	2.93	115.82	111.29
5	I	610	HEM	CHB-C1B-C2B	-2.90	118.72	126.94
5	G	607	HEM	CMB-C2B-C1B	2.90	129.57	125.03
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
8	B	613	JXS	C04-C07-N22	2.87	108.23	106.81
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
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	613	JXS	C04-C12-C08	-2.71	126.24	128.77
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
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
8	G	612	JXS	N23-C14-N19	2.67	120.45	118.24
6	E	601	BMA	C6-C5-C4	2.67	119.58	113.02
3	I	608	NAG	O5-C1-C2	-2.66	107.18	111.29
5	B	608	HEM	CHA-C4D-ND	2.65	127.66	124.37
8	B	613	JXS	C08-C12-N18	2.62	125.10	120.93
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
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
5	G	607	HEM	CHB-C1B-NB	2.59	127.58	124.37
3	B	603	NAG	O5-C5-C6	2.58	112.69	107.66
5	B	608	HEM	CMA-C3A-C2A	2.58	129.81	124.94
5	I	610	HEM	C4A-C3A-C2A	-2.58	105.20	107.00
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
5	I	610	HEM	C3B-C2B-C1B	-2.53	104.52	106.41
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
5	B	608	HEM	CHB-C1B-C2B	-2.51	119.83	126.94
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
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
8	G	612	JXS	C08-C05-C09	-2.49	117.88	121.20
5	G	607	HEM	CHB-C1B-C2B	-2.48	119.91	126.94
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
5	E	609	HEM	CHC-C4B-C3B	-2.46	120.81	124.57
3	G	606	NAG	C3-C4-C5	2.45	114.67	110.23
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	603	NAG	O5-C5-C4	2.43	116.74	110.83
8	G	612	JXS	C04-C07-N22	2.43	108.01	106.81
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
6	I	602	BMA	O4-C4-C3	-2.39	104.74	110.38
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
7	I	603	MAN	O5-C1-C2	2.33	116.34	110.79
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
8	B	613	JXS	N23-C14-N19	2.29	120.13	118.24
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
3	G	603	NAG	C1-O5-C5	2.24	115.19	112.19
8	G	612	JXS	C02-C08-C12	-2.24	117.74	121.28
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
6	G	609	BMA	O2-C2-C3	2.20	114.70	110.15
8	B	613	JXS	N21-N20-N17	-2.19	108.40	111.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
5	I	610	HEM	CMA-C3A-C4A	-2.17	125.28	128.46
7	G	611	MAN	O4-C4-C5	-2.17	103.99	109.32
5	I	610	HEM	CHC-C4B-NB	2.16	126.75	124.44
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
5	I	610	HEM	CMA-C3A-C2A	2.14	128.98	124.94
3	E	605	NAG	O5-C5-C6	2.14	111.83	107.66
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
7	I	604	MAN	O6-C6-C5	2.11	118.50	111.33
4	E	608	FUC	O5-C5-C6	2.10	111.95	107.40
5	B	608	HEM	CHC-C4B-NB	2.10	126.69	124.44
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
8	E	610	JXS	N21-N20-N17	-2.05	108.59	111.25
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	I	610	HEM	CHB-C1B-NB	2.04	126.90	124.37
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
8	G	612	JXS	C08-C12-N18	2.02	124.15	120.93
8	E	610	JXS	C16-O24-C11	2.02	120.24	117.49
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 (73) 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

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Mol	Chain	Res	Type	Atoms
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
3	I	607	NAG	C4-C5-C6-O6
3	B	602	NAG	O5-C5-C6-O6
7	G	611	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
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	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 98 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	603	NAG	2	0
3	I	601	NAG	4	0
7	I	604	MAN	1	0
3	I	607	NAG	1	0

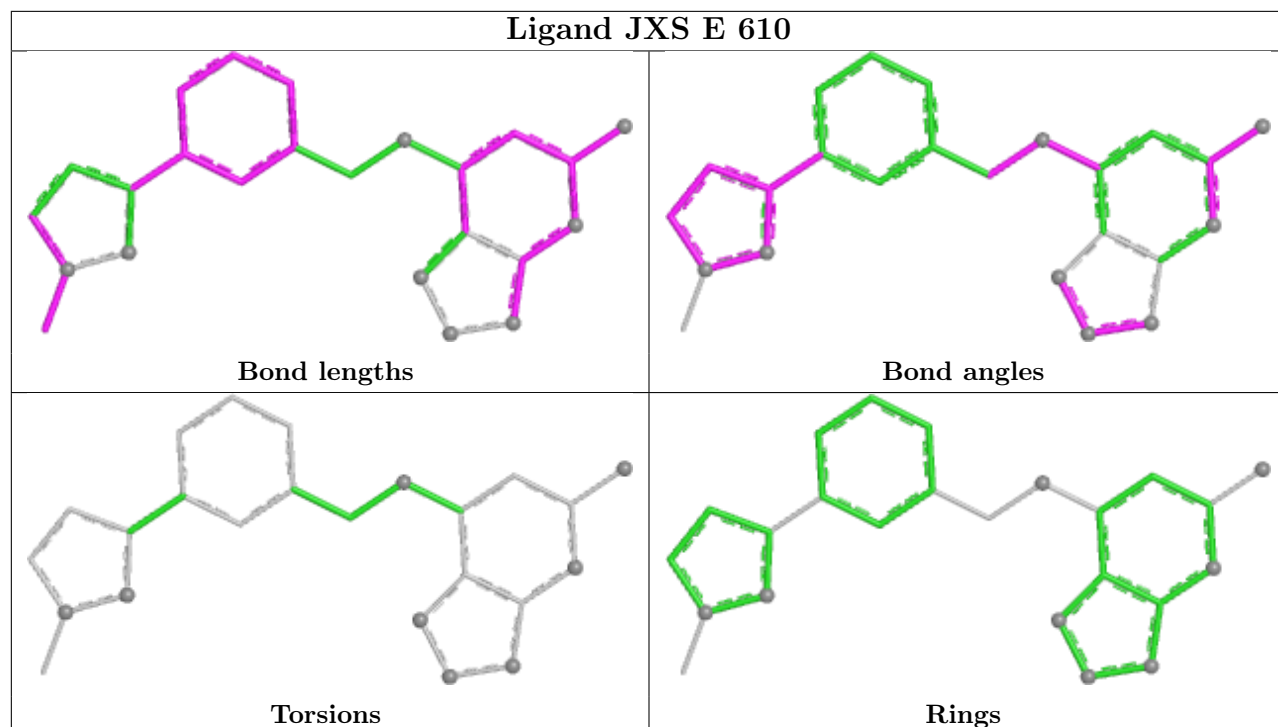
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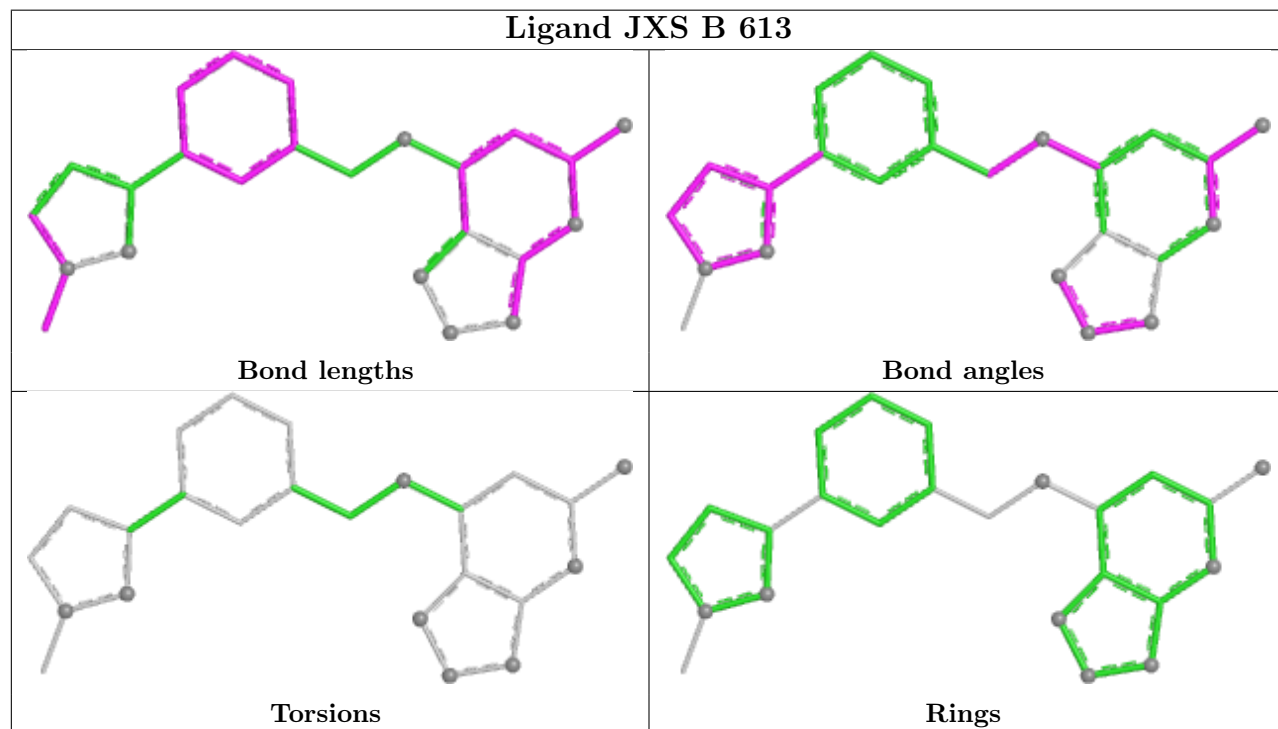
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	602	MAN	4	0
3	B	604	NAG	6	0
4	I	609	FUC	1	0
3	B	607	NAG	1	0
3	E	607	NAG	4	0
3	G	601	NAG	1	0
3	I	606	NAG	1	0
7	G	610	MAN	1	0
5	G	607	HEM	11	0
3	B	603	NAG	3	0
6	I	602	BMA	2	0
3	G	604	NAG	6	0
3	B	609	NAG	3	0
3	B	602	NAG	5	0
4	B	606	FUC	1	0
3	G	608	NAG	5	0
3	E	606	NAG	1	0
3	E	605	NAG	4	0
5	B	608	HEM	10	0
6	E	601	BMA	5	0
6	G	609	BMA	8	0
5	I	610	HEM	9	0
7	G	611	MAN	4	0
3	I	605	NAG	1	0
3	I	608	NAG	4	0
6	B	610	BMA	3	0
3	B	605	NAG	4	0
3	B	601	NAG	1	0
3	G	602	NAG	5	0
5	E	609	HEM	8	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.

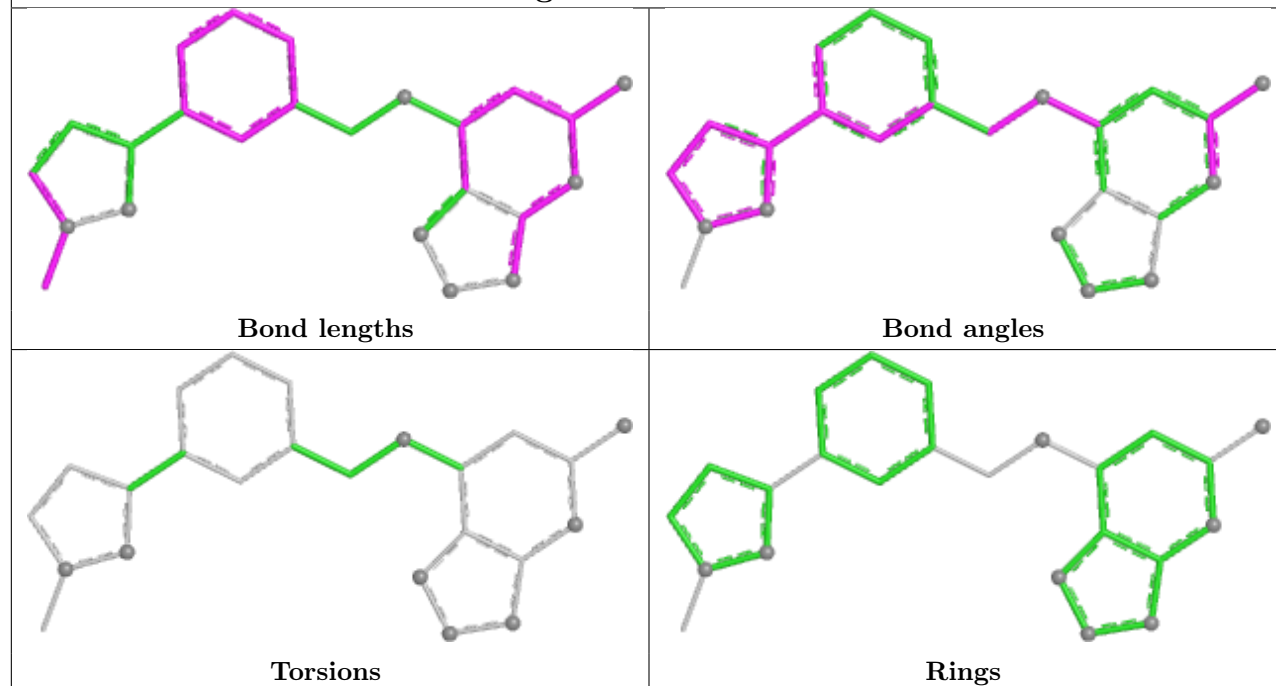
Ligand JXS E 610



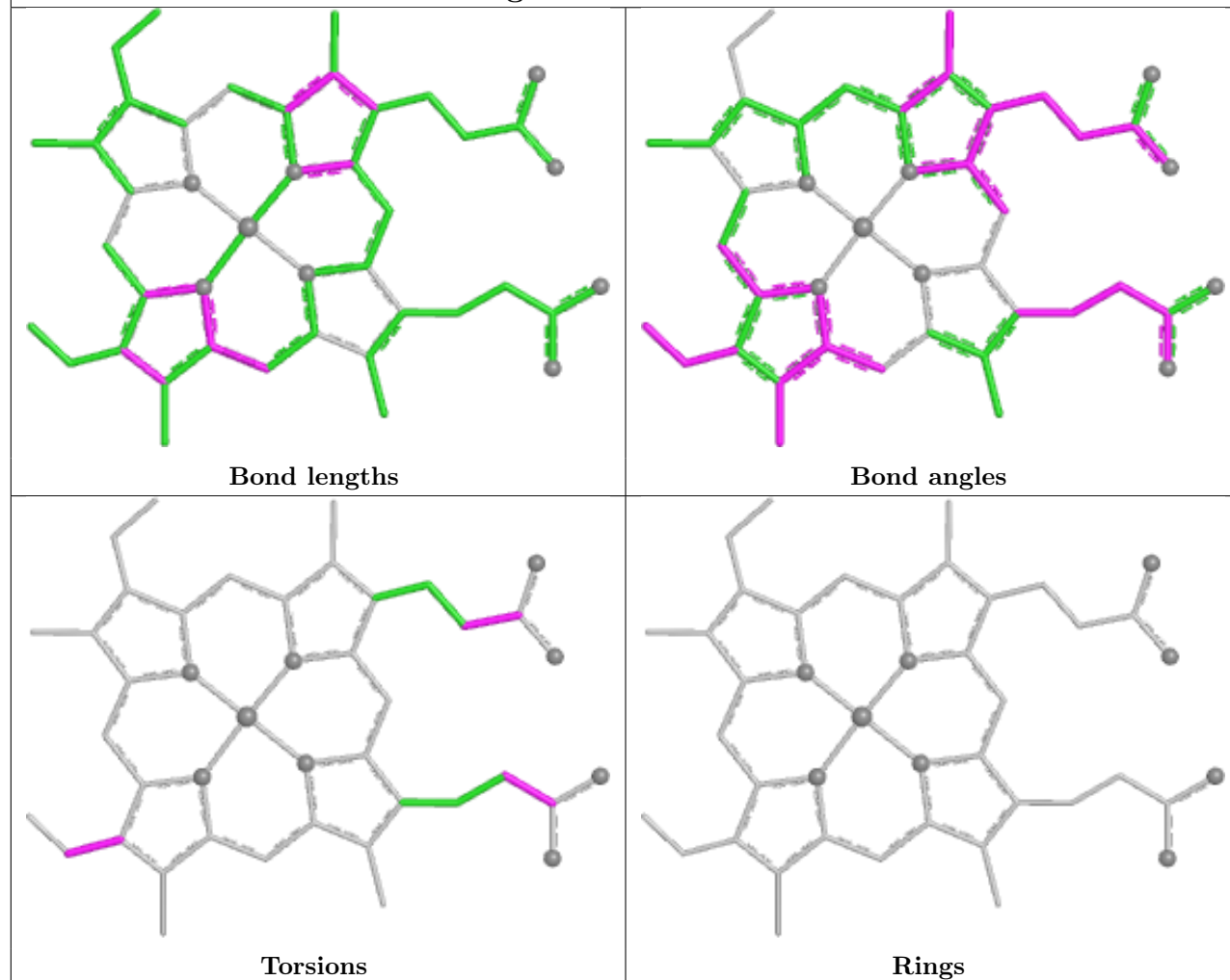
Ligand JXS B 613

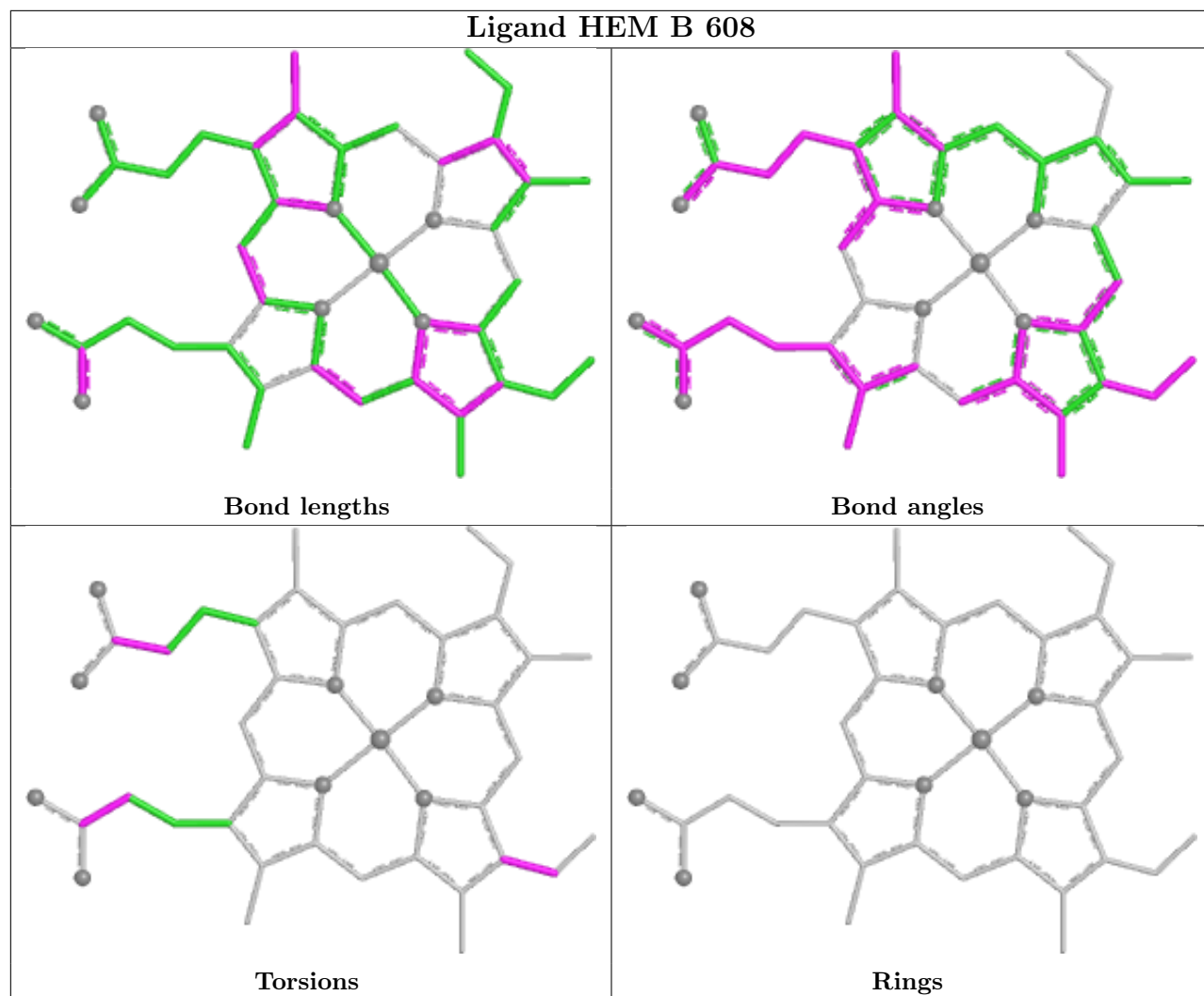


Ligand JXS G 612

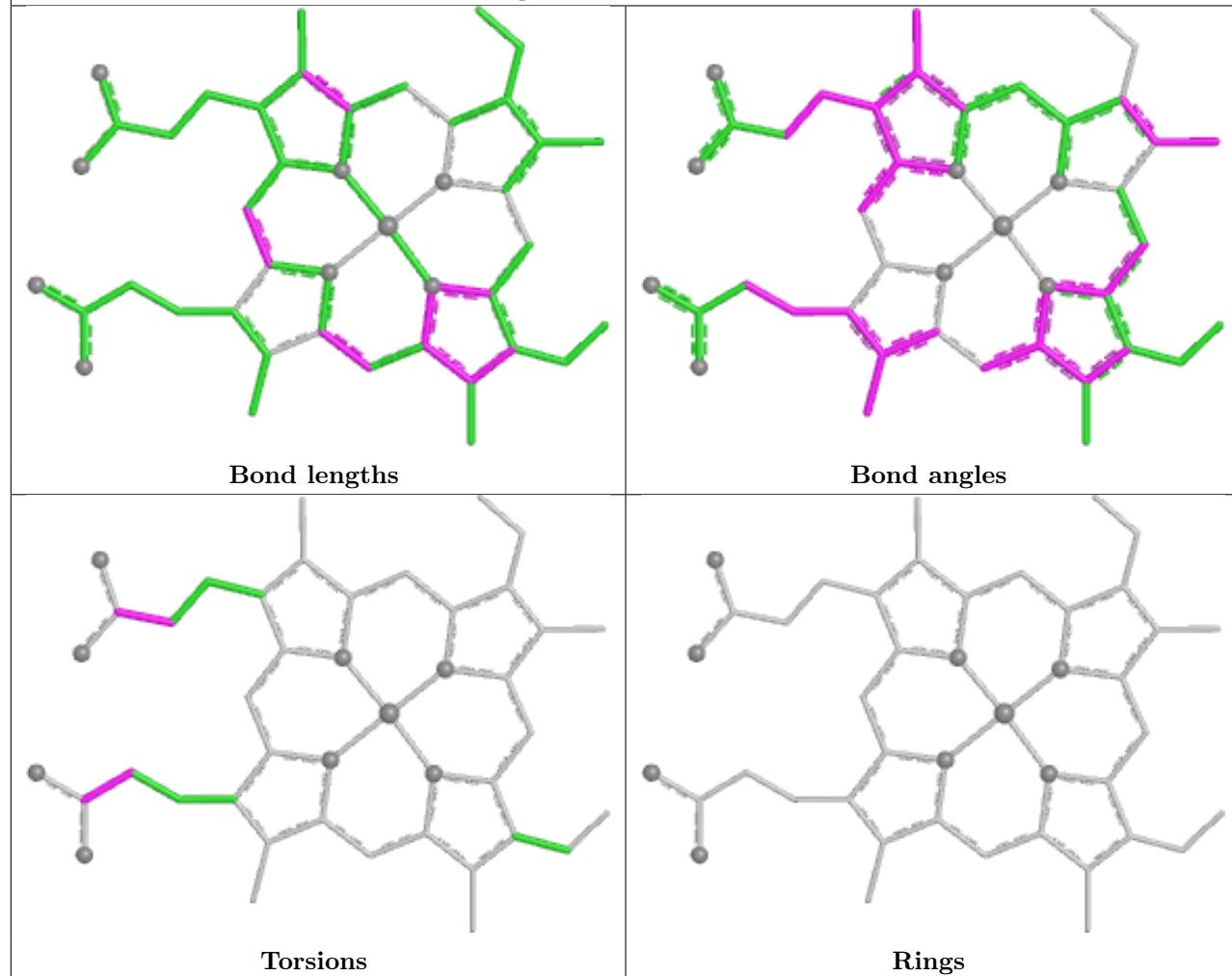


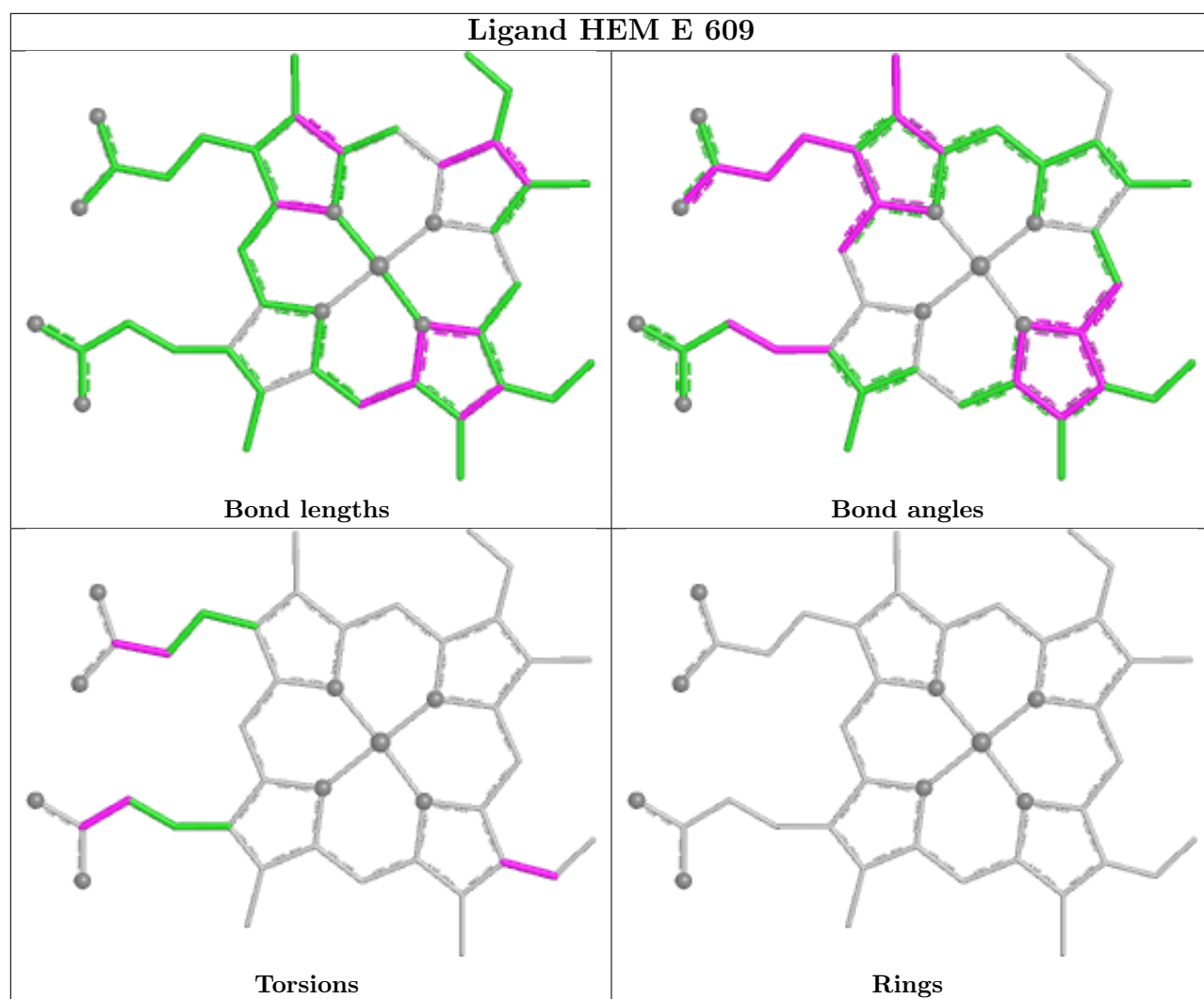
Ligand HEM G 607





Ligand HEM I 610





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%)	-0.04	0 100 100	29, 51, 77, 85	1 (0%)
1	D	103/105 (98%)	0.17	2 (1%) 66 59	38, 54, 74, 90	2 (1%)
1	F	103/105 (98%)	0.19	1 (0%) 79 73	35, 52, 70, 86	0
1	H	103/105 (98%)	0.03	1 (0%) 79 73	29, 52, 80, 95	1 (0%)
2	B	465/467 (99%)	0.29	13 (2%) 55 47	27, 58, 86, 112	7 (1%)
2	E	465/467 (99%)	0.28	10 (2%) 62 54	32, 58, 79, 90	6 (1%)
2	G	465/467 (99%)	0.11	5 (1%) 77 72	26, 54, 75, 94	7 (1%)
2	I	465/467 (99%)	0.39	14 (3%) 52 44	29, 62, 94, 111	10 (2%)
All	All	2272/2288 (99%)	0.24	46 (2%) 64 57	26, 56, 84, 112	34 (1%)

All (46) 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	3.1
2	B	348	ASN	2.9
2	B	354	GLU	2.8
2	B	248	SER	2.8
2	I	577	GLU	2.7
2	G	329	THR	2.7
2	B	113	VAL	2.7
2	B	288	VAL	2.7
2	B	331	ALA	2.7
2	G	159	THR	2.6
2	E	325	ALA	2.6
2	G	155	GLY	2.6
2	I	202	ARG	2.5
2	B	377	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	I	170	PHE	2.4
2	I	218	ASP	2.4
2	I	377	ILE	2.4
1	H	1	CYS	2.4
2	G	326	ASN	2.4
2	I	468	TYR	2.3
2	E	482	SER	2.3
2	B	251	THR	2.3
1	F	29	PHE	2.3
2	E	497	CYS	2.3
2	I	264	LEU	2.3
2	I	455	LEU	2.3
2	G	372	VAL	2.3
2	E	365	PHE	2.3
2	E	562	VAL	2.2
1	D	29	PHE	2.2
2	I	113	VAL	2.2
2	E	577	GLU	2.2
2	E	326	ASN	2.2
2	B	284	VAL	2.2
2	E	164	ILE	2.1
2	I	195	GLY	2.1
2	I	263	GLU	2.1
2	B	322	PRO	2.1
1	D	32	TRP	2.1
2	B	115	CYS	2.1
2	B	522	MET	2.0
2	E	113	VAL	2.0
2	I	574	SER	2.0
2	E	408	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	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
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

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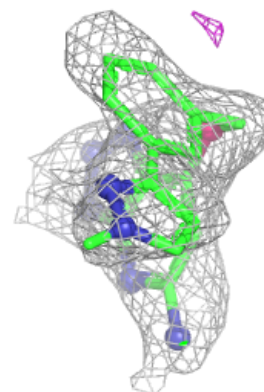
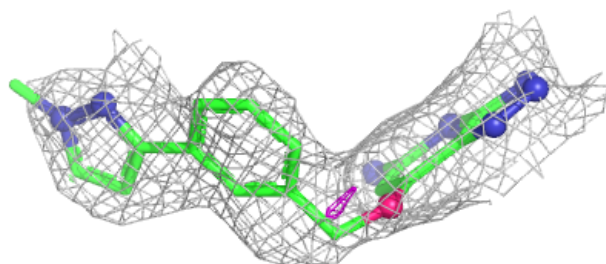
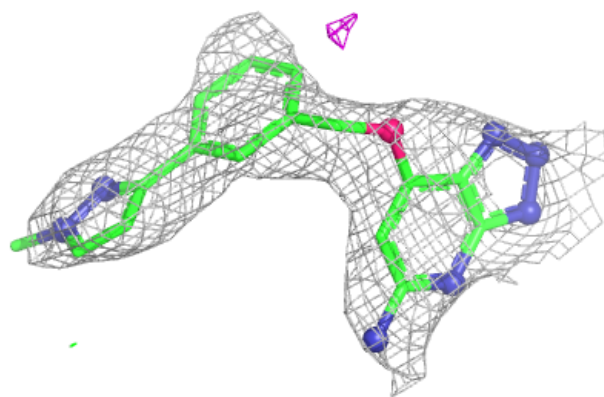
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	HEM	B	608	43/43	0.94	0.11	49,50,54,56	0
3	NAG	G	608	14/15	0.94	0.10	51,54,57,57	0
3	NAG	B	605	14/15	0.95	0.07	35,38,41,42	0
3	NAG	I	601	14/15	0.95	0.08	30,35,37,38	0
5	HEM	E	609	43/43	0.95	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
10	CL	B	615	1/1	0.96	0.26	62,62,62,62	0
4	FUC	G	605	10/11	0.96	0.09	41,41,42,42	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.

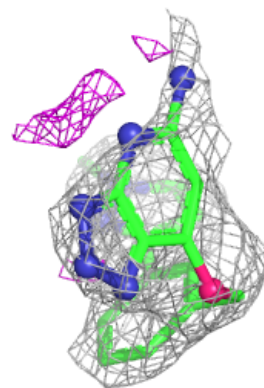
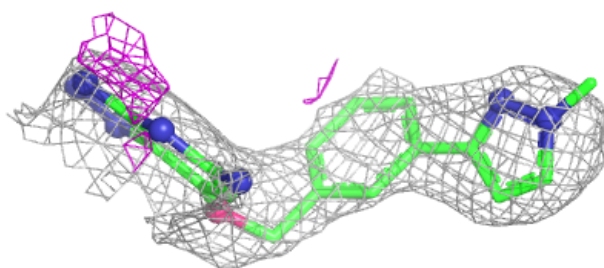
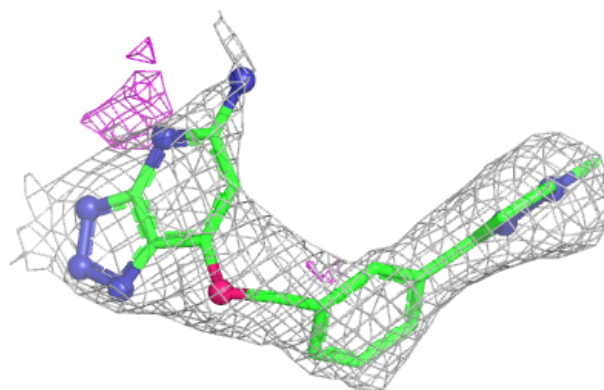
Electron density around JXS B 613:

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

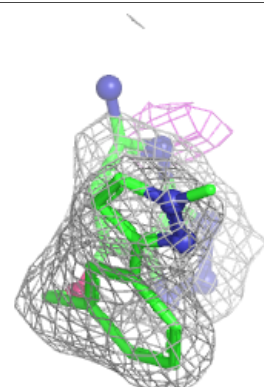
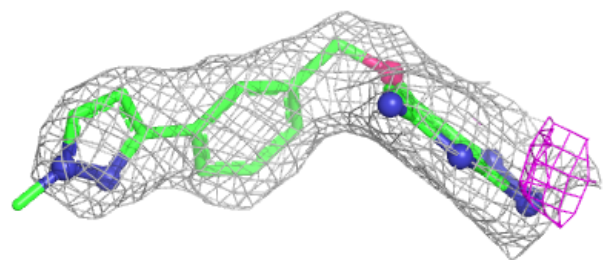
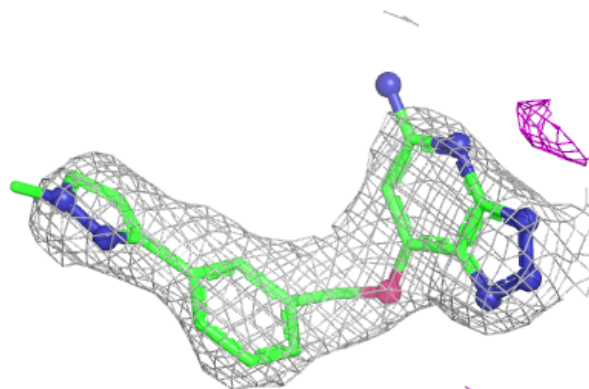


Electron density around JXS E 610:

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

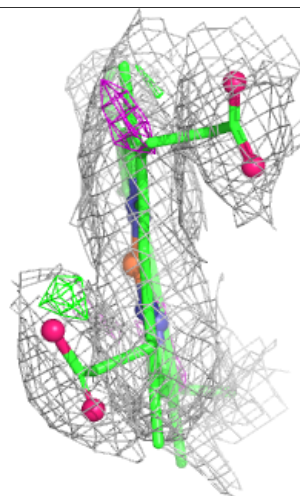
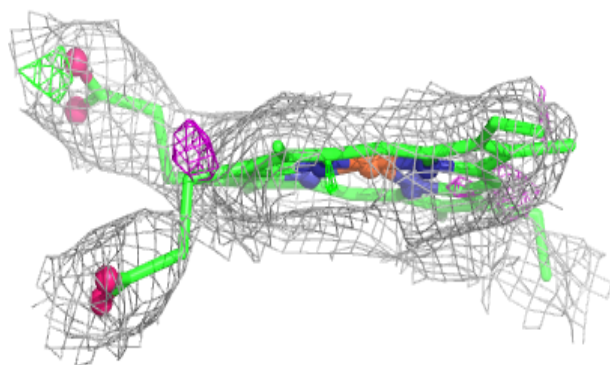
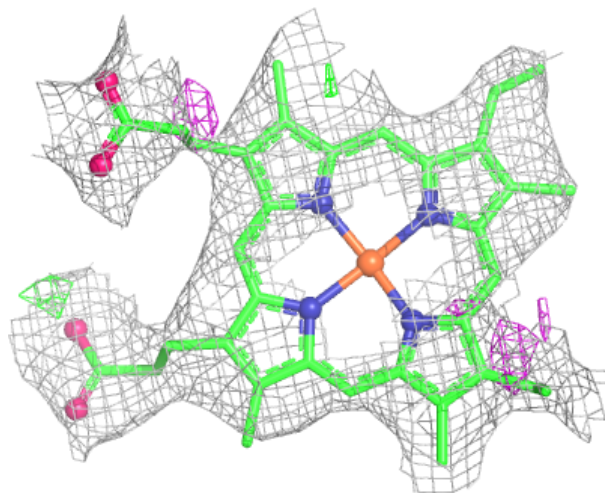
**Electron density around JXS G 612:**

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



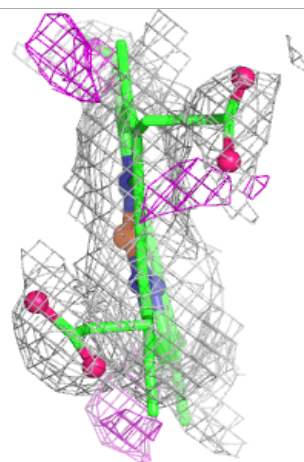
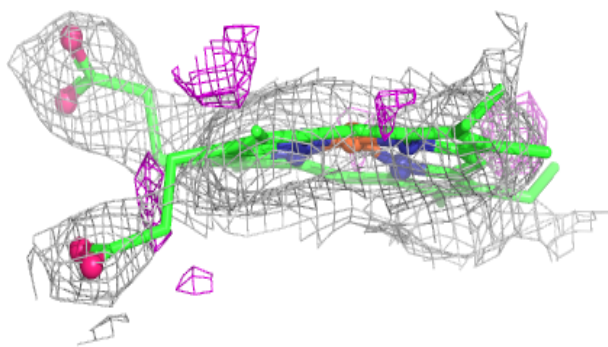
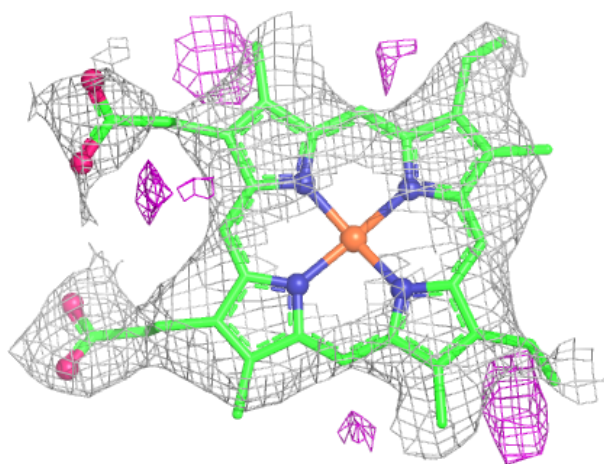
Electron density around HEM B 608:

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



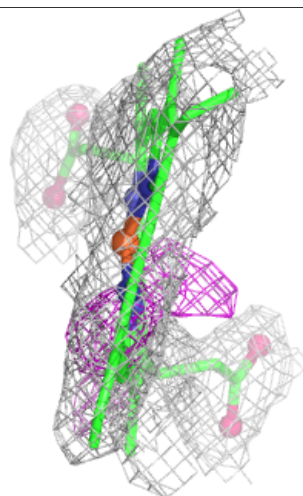
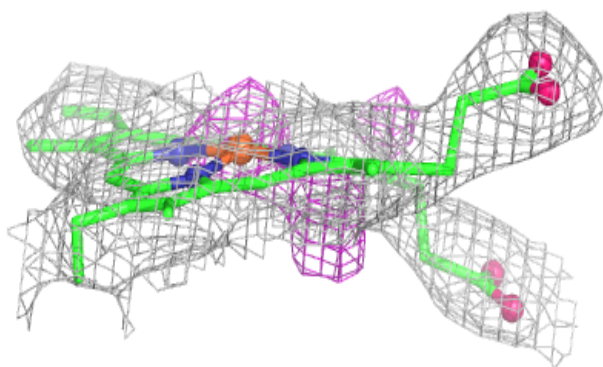
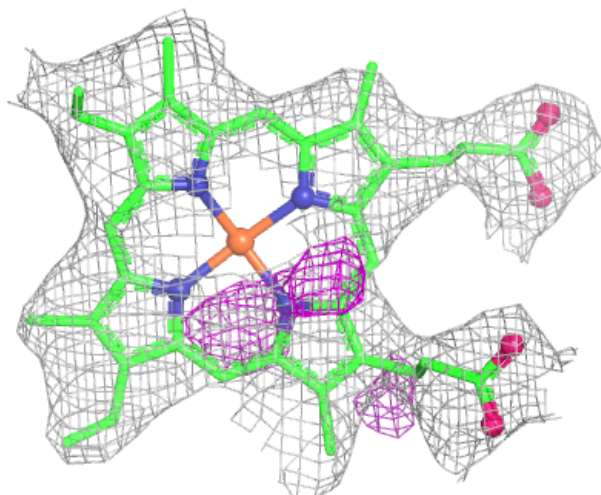
Electron density around HEM E 609:

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



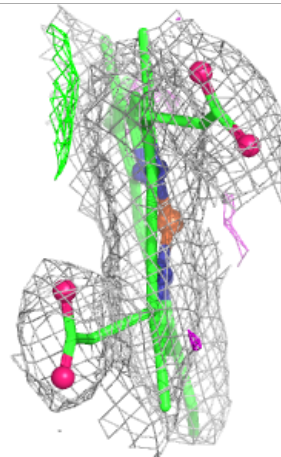
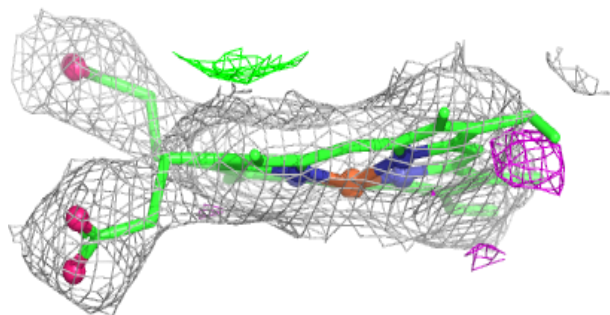
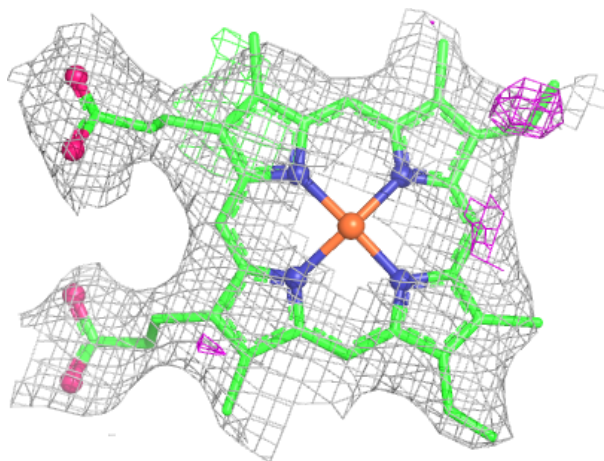
Electron density around HEM G 607:

$2mF_o-DF_c$ (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.