



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 12, 2021 – 10:15 AM EDT

PDB ID : 7LAE
Title : CRYSTAL STRUCTURE OF MYELOPEROXIDASE SUBFORM C (MPO)
COMPLEX WITH Compound-4
Authors : Khan, J.A.
Deposited on : 2021-01-06
Resolution : 2.97 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

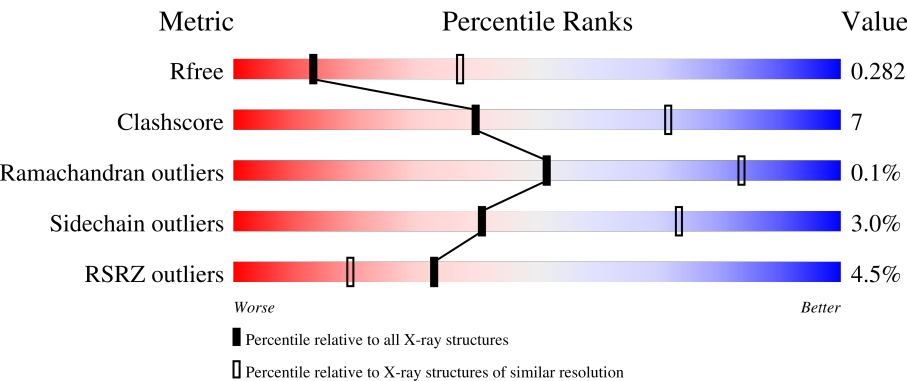
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.18
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.18

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.97 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}	130704	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	105	
1	D	105	
2	B	466	
2	E	466	
3	C	2	

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Mol	Chain	Length	Quality of chain
3	F	2	

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 9149 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 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	103	Total	C	N	O	S	0	0	0
			806	512	143	147	4			
1	D	103	Total	C	N	O	S	0	0	0
			799	508	139	147	5			

- Molecule 2 is a protein called Isoform H14 of Myeloperoxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	464	Total	C	N	O	S	6	0	0
			3551	2235	643	646	27			
2	E	465	Total	C	N	O	S	25	0	0
			3627	2298	650	652	27			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

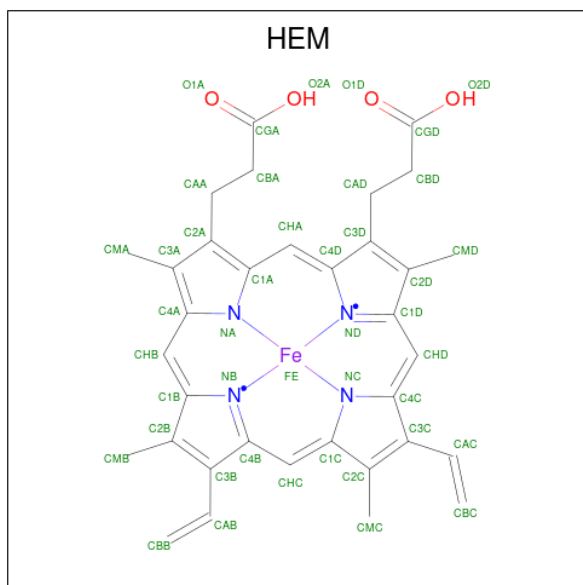
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

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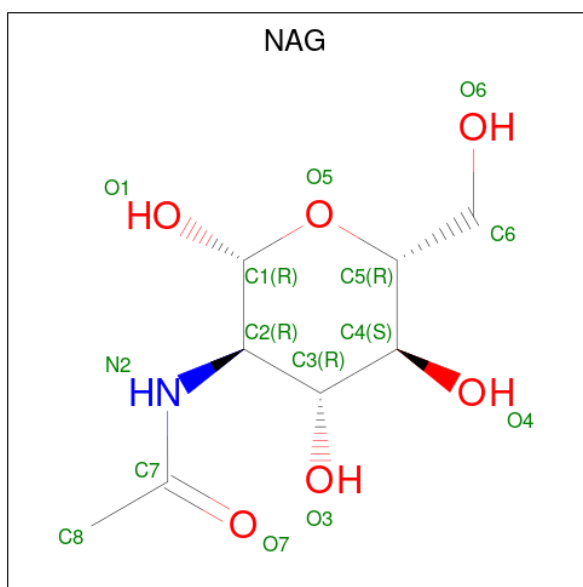
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	Cl			0	0
			1	1				

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



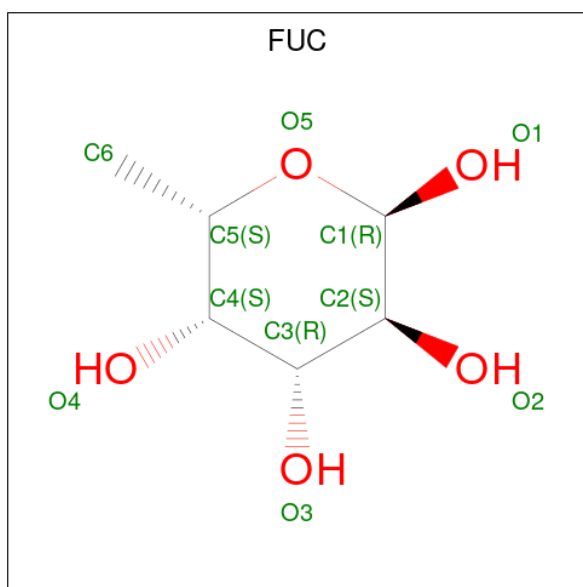
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
5	E	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



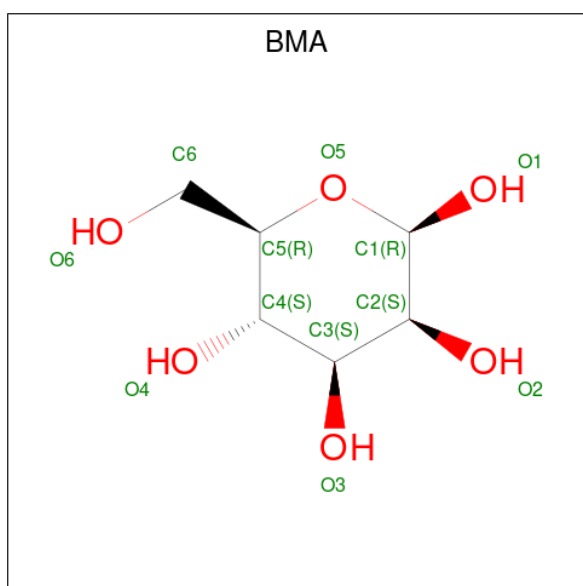
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is alpha-L-fucopyranose (three-letter code: FUC) (formula: C₆H₁₂O₅).



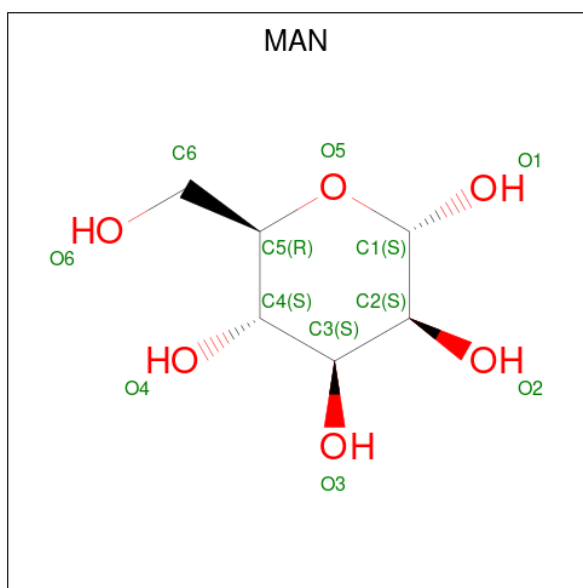
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			10	6	4		
7	E	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



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

- Molecule 9 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).

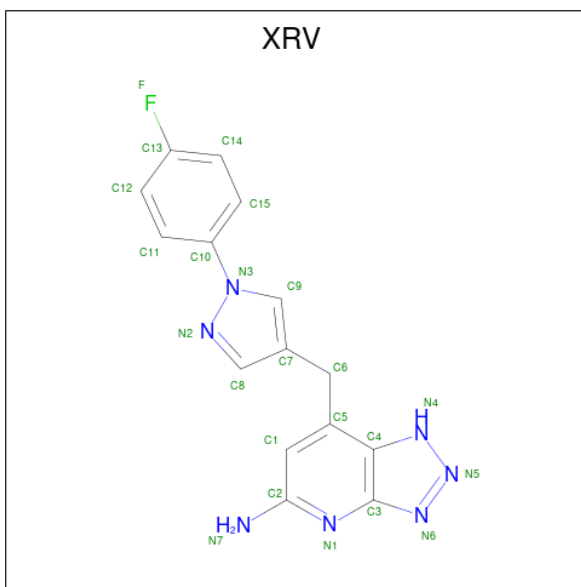


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			11	6	5		
9	B	1	Total	C	O	0	0
			11	6	5		
9	E	1	Total	C	O	0	0
			11	6	5		
9	E	1	Total	C	O	0	0
			11	6	5		

- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	Ca	0	0
			1	1		
10	E	1	Total	Ca	0	0
			1	1		

- Molecule 11 is 7-{[1-(4-fluorophenyl)-1H-pyrazol-4-yl]methyl}-1H-[1,2,3]triazolo[4,5-b]pyridine-5-amine (three-letter code: XRV) (formula: C₁₅H₁₂FN₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	F	N	0	0
			23	15	1	7		
11	E	1	Total	C	F	N	0	0
			23	15	1	7		

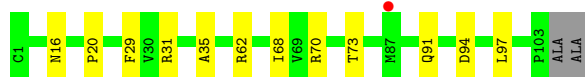
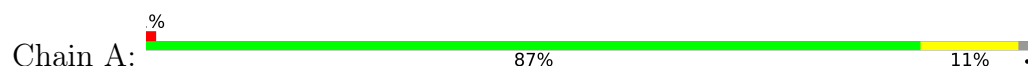
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	B	1	Total	O	0	0
			1	1		
12	D	1	Total	O	0	0
			1	1		
12	E	2	Total	O	0	0
			2	2		

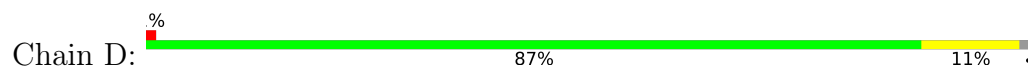
3 Residue-property plots [i](#)

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.

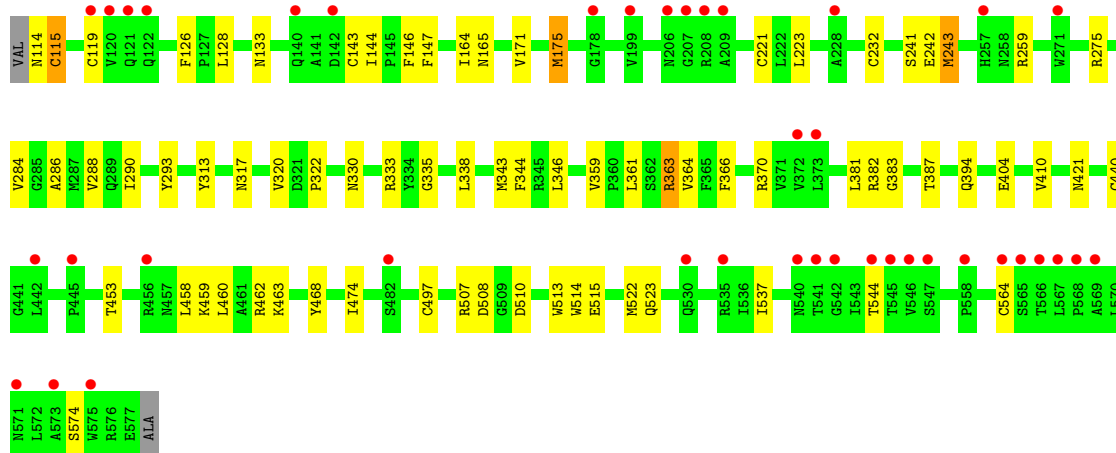
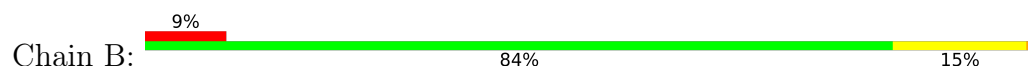
- Molecule 1: Myeloperoxidase light chain



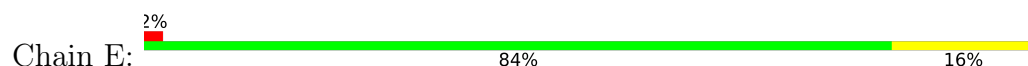
- Molecule 1: Myeloperoxidase light chain

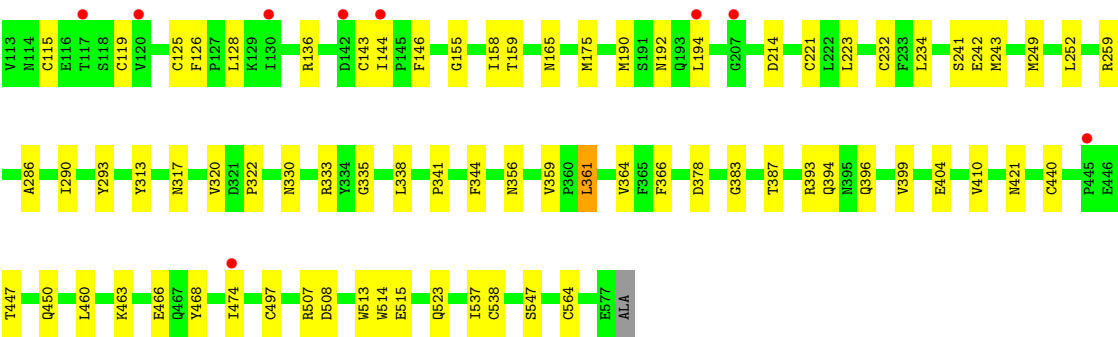


- Molecule 2: Isoform H14 of Myeloperoxidase



- Molecule 2: Isoform H14 of Myeloperoxidase





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	106.92Å 106.92Å 238.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.28 – 2.97 48.80 – 2.97	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.28-2.97) 100.0 (48.80-2.97)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.58 (at 2.96Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.216 , 0.267 0.227 , 0.282	Depositor DCC
R_{free} test set	1496 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	69.4	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9149	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: XRV, MAN, FUC, CA, CL, BMA, HEM, 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	0.51	0/831	0.73	0/1135
1	D	0.50	0/824	0.75	0/1128
2	B	0.52	0/3637	0.70	0/4953
2	E	0.53	0/3712	0.70	0/5051
All	All	0.52	0/9004	0.71	0/12267

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	806	0	750	13	0
1	D	799	0	738	11	0
2	B	3551	0	3364	50	0
2	E	3627	0	3553	46	0
3	C	28	0	25	4	0
3	F	28	0	25	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	43	0	30	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	43	0	30	10	0
6	B	42	0	39	0	0
6	E	42	0	39	0	0
7	B	10	0	10	1	0
7	E	10	0	10	1	0
8	B	11	0	10	2	0
8	E	11	0	10	2	0
9	B	22	0	20	1	0
9	E	22	0	20	1	0
10	B	1	0	0	0	0
10	E	1	0	0	0	0
11	B	23	0	0	0	0
11	E	23	0	0	0	0
12	B	1	0	0	0	0
12	D	1	0	0	0	0
12	E	2	0	0	0	0
All	All	9149	0	8673	121	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 7.

All (121) 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:E:317:ASN:HD21	3:F:1:NAG:C1	1.50	1.24
5:E:604:HEM:HBB2	5:E:604:HEM:HHC	1.32	1.09
2:B:243:MET:SD	5:B:601:HEM:HBB1	1.95	1.04
2:E:119:CYS:HG	2:E:143:CYS:HG	1.09	1.00
2:E:115:CYS:HG	2:E:125:CYS:HG	1.04	0.99
1:D:94:ASP:OD2	5:E:604:HEM:HMD3	1.60	0.99
2:E:317:ASN:ND2	3:F:1:NAG:C1	2.31	0.93
2:B:317:ASN:ND2	3:C:1:NAG:C1	2.33	0.92
1:D:94:ASP:OD2	5:E:604:HEM:CMD	2.18	0.90
2:B:242:GLU:OE2	5:B:601:HEM:HMB1	1.72	0.89
2:B:440:CYS:HG	2:B:497:CYS:HG	1.03	0.86
2:E:242:GLU:OE2	5:E:604:HEM:HMB1	1.79	0.83
1:A:94:ASP:OD2	5:B:601:HEM:HMD3	1.78	0.82
2:B:317:ASN:HD21	3:C:1:NAG:C1	1.95	0.79
2:E:538:CYS:HG	2:E:564:CYS:HG	1.23	0.78
5:E:604:HEM:HHC	5:E:604:HEM:CBB	2.09	0.78
1:A:94:ASP:OD2	5:B:601:HEM:CMD	2.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:221:CYS:HG	2:B:232:CYS:HG	0.77	0.76
7:B:605:FUC:C1	3:C:1:NAG:O6	2.37	0.73
7:E:608:FUC:C1	3:F:1:NAG:O6	2.37	0.73
5:E:604:HEM:HBB2	5:E:604:HEM:CHC	2.07	0.72
2:B:313:TYR:CD1	2:B:507:ARG:HD3	2.28	0.69
2:E:313:TYR:CD1	2:E:507:ARG:HD3	2.28	0.68
2:E:333:ARG:HH11	2:E:421:ASN:HD22	1.43	0.67
1:D:94:ASP:CG	5:E:604:HEM:HMD3	2.15	0.66
2:B:333:ARG:HH11	2:B:421:ASN:HD22	1.42	0.66
2:B:343:MET:HB3	2:B:359:VAL:HG13	1.78	0.65
2:B:164:ILE:HG12	2:E:158:ILE:HG21	1.78	0.64
2:B:119:CYS:HG	2:B:143:CYS:HG	0.65	0.63
2:E:192:ASN:OD1	2:E:194:LEU:HB2	1.99	0.62
2:B:544:THR:HA	2:B:564:CYS:SG	2.38	0.61
2:B:344:PHE:O	2:B:383:GLY:HA3	2.01	0.61
2:B:440:CYS:HA	8:B:606:BMA:H61	1.82	0.60
2:B:313:TYR:HD1	2:B:507:ARG:HD3	1.68	0.59
2:E:344:PHE:O	2:E:383:GLY:HA3	2.02	0.59
2:B:243:MET:SD	5:B:601:HEM:CBB	2.81	0.59
2:E:356:ASN:HB3	2:E:359:VAL:HG22	1.85	0.58
5:E:604:HEM:HBC2	5:E:604:HEM:HMC2	1.85	0.58
2:B:510:ASP:HB3	2:B:513:TRP:HB2	1.86	0.58
8:B:606:BMA:H3	9:B:607:MAN:C1	2.34	0.57
2:B:223:LEU:HB2	2:B:410:VAL:HG12	1.87	0.57
8:E:601:BMA:H3	9:E:602:MAN:C1	2.36	0.56
2:E:313:TYR:HD1	2:E:507:ARG:HD3	1.69	0.56
2:E:223:LEU:HB2	2:E:410:VAL:HG12	1.87	0.55
5:B:601:HEM:HBC2	5:B:601:HEM:HMC2	1.88	0.55
2:B:363:ARG:HB3	2:B:370:ARG:HH12	1.72	0.55
2:B:242:GLU:OE2	5:B:601:HEM:CMB	2.53	0.55
2:E:128:LEU:HB2	2:E:144:ILE:HB	1.89	0.55
1:A:68:ILE:HD12	2:B:463:LYS:HB3	1.89	0.54
2:E:286:ALA:O	2:E:290:ILE:HD12	2.07	0.54
2:B:128:LEU:HB2	2:B:144:ILE:HB	1.90	0.54
2:B:286:ALA:O	2:B:290:ILE:HD12	2.08	0.53
1:D:84:LEU:HD22	1:D:87:MET:HE2	1.90	0.53
1:A:91:GLN:NE2	5:B:601:HEM:HBB2	2.24	0.52
2:B:394:GLN:HB3	2:B:460:LEU:HD22	1.92	0.52
2:B:381:LEU:HD22	2:B:537:ILE:HG12	1.92	0.52
2:B:458:LEU:O	2:B:462:ARG:HG3	2.10	0.51
2:E:394:GLN:HB3	2:E:460:LEU:HD22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:VAL:O	2:B:322:PRO:HD3	2.12	0.50
2:E:221:CYS:CB	2:E:232:CYS:HG	2.24	0.50
2:E:252:LEU:HD11	2:E:537:ILE:HA	1.94	0.49
2:B:333:ARG:HH11	2:B:421:ASN:ND2	2.10	0.49
2:E:356:ASN:HB3	2:E:359:VAL:CG2	2.42	0.49
2:B:507:ARG:HD2	2:B:508:ASP:OD1	2.12	0.49
2:E:507:ARG:HD2	2:E:508:ASP:OD1	2.12	0.48
2:B:241:SER:O	2:B:366:PHE:HA	2.14	0.48
1:D:94:ASP:OD2	5:E:604:HEM:HMD2	2.07	0.48
2:B:221:CYS:CB	2:B:232:CYS:HG	2.23	0.48
2:B:333:ARG:NH1	2:B:421:ASN:HD22	2.12	0.47
2:B:514:TRP:CE2	2:B:515:GLU:HG3	2.49	0.47
1:D:62:ARG:NH2	2:E:404:GLU:OE1	2.45	0.47
2:E:119:CYS:HG	2:E:143:CYS:CB	2.25	0.46
1:A:94:ASP:CG	5:B:601:HEM:HMD3	2.36	0.46
2:B:317:ASN:CG	3:C:1:NAG:C1	2.83	0.46
5:E:604:HEM:HBC2	5:E:604:HEM:CMC	2.46	0.46
2:E:126:PHE:O	2:E:146:PHE:HB3	2.16	0.46
2:E:440:CYS:HA	8:E:601:BMA:H61	1.98	0.46
2:E:514:TRP:CE2	2:E:515:GLU:HG3	2.50	0.46
1:D:68:ILE:CD1	2:E:463:LYS:HB3	2.46	0.46
2:E:333:ARG:NH1	2:E:421:ASN:HD22	2.12	0.45
2:E:344:PHE:CD1	2:E:387:THR:HG21	2.52	0.45
2:B:126:PHE:O	2:B:146:PHE:HB3	2.16	0.45
2:B:175:MET:N	2:B:175:MET:SD	2.86	0.45
2:E:241:SER:O	2:E:366:PHE:HA	2.16	0.45
2:E:335:GLY:HA2	2:E:338:LEU:HD12	1.98	0.45
2:B:346:LEU:HB2	2:B:382:ARG:HB3	1.99	0.45
1:D:16:ASN:O	1:D:20:PRO:HA	2.17	0.45
2:B:335:GLY:HA2	2:B:338:LEU:HD12	1.99	0.45
1:A:91:GLN:HG3	5:B:601:HEM:C1C	2.52	0.44
2:E:214:ASP:HB2	2:E:234:LEU:HB2	1.99	0.44
2:E:341:PRO:HG3	2:E:399:VAL:HG11	1.99	0.44
1:D:92:LEU:HD22	2:E:249:MET:HB3	1.99	0.43
2:E:393:ARG:HB2	2:E:396:GLN:HB2	2.00	0.43
1:A:97:LEU:HD21	2:B:171:VAL:HG22	2.01	0.43
2:B:293:TYR:CD1	2:B:513:TRP:HH2	2.36	0.43
2:B:468:TYR:CD2	2:B:474:ILE:HG12	2.53	0.43
1:A:29:PHE:CE1	2:B:165:ASN:HB2	2.53	0.43
2:E:333:ARG:HH11	2:E:421:ASN:ND2	2.10	0.43
2:B:361:LEU:HA	2:B:364:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ARG:NH2	2:B:404:GLU:OE1	2.52	0.42
2:B:284:VAL:O	2:B:288:VAL:HG23	2.20	0.42
2:E:468:TYR:CD2	2:E:474:ILE:HG12	2.54	0.42
2:B:115:CYS:HB2	2:B:147:PHE:CE1	2.54	0.42
2:E:361:LEU:HA	2:E:364:VAL:HG22	2.02	0.42
2:E:440:CYS:CB	2:E:497:CYS:HG	2.31	0.42
1:D:29:PHE:CE1	2:E:165:ASN:HB2	2.54	0.42
2:E:447:THR:H	2:E:450:GLN:NE2	2.17	0.42
2:E:523:GLN:NE2	2:E:523:GLN:H	2.17	0.42
2:B:344:PHE:CD1	2:B:387:THR:HG21	2.55	0.42
1:A:68:ILE:CD1	2:B:463:LYS:HB3	2.50	0.41
1:A:16:ASN:O	1:A:20:PRO:HA	2.19	0.41
1:D:31:ARG:CZ	1:D:35:ALA:HB2	2.50	0.41
2:B:333:ARG:HD3	2:B:421:ASN:ND2	2.35	0.41
1:A:91:GLN:HB2	5:B:601:HEM:HMC1	2.01	0.41
1:A:31:ARG:CZ	1:A:35:ALA:HB2	2.51	0.41
2:E:293:TYR:CD1	2:E:513:TRP:HH2	2.39	0.41
2:B:459:LYS:HA	2:B:462:ARG:CZ	2.51	0.41
2:E:320:VAL:O	2:E:322:PRO:HD3	2.21	0.40
5:B:601:HEM:HBC2	5:B:601:HEM:CMC	2.50	0.40
2:E:333:ARG:HD3	2:E:421:ASN:ND2	2.36	0.40
2:E:440:CYS:HG	2:E:497:CYS:CB	2.33	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%)	95 (94%)	6 (6%)	0	100	100
1	D	101/105 (96%)	97 (96%)	4 (4%)	0	100	100
2	B	462/466 (99%)	439 (95%)	23 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	E	463/466 (99%)	439 (95%)	23 (5%)	1 (0%)	47 80
All	All	1127/1142 (99%)	1070 (95%)	56 (5%)	1 (0%)	51 83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	155	GLY

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	82/90 (91%)	80 (98%)	2 (2%)	49 78
1	D	82/90 (91%)	81 (99%)	1 (1%)	71 89
2	B	364/411 (89%)	351 (96%)	13 (4%)	35 68
2	E	385/411 (94%)	374 (97%)	11 (3%)	42 74
All	All	913/1002 (91%)	886 (97%)	27 (3%)	41 73

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ARG
1	A	73	THR
2	B	114	ASN
2	B	115	CYS
2	B	133	ASN
2	B	175	MET
2	B	243	MET
2	B	259	ARG
2	B	275	ARG
2	B	330	ASN
2	B	363	ARG
2	B	453	THR
2	B	522	MET

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Mol	Chain	Res	Type
2	B	523	GLN
2	B	574	SER
1	D	73	THR
2	E	136	ARG
2	E	159	THR
2	E	175	MET
2	E	190	MET
2	E	243	MET
2	E	259	ARG
2	E	330	ASN
2	E	361	LEU
2	E	378	ASP
2	E	466	GLU
2	E	547	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	140	GLN
2	B	421	ASN
2	B	450	GLN
2	E	121	GLN
2	E	140	GLN
2	E	200	ASN
2	E	317	ASN
2	E	421	ASN
2	E	450	GLN
2	E	523	GLN
2	E	563	ASN

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

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAG	C	1	3	14,14,15	0.42	0	17,19,21	1.20	1 (5%)
3	NAG	C	2	3	14,14,15	0.29	0	17,19,21	0.51	0
3	NAG	F	1	3	14,14,15	0.27	0	17,19,21	1.25	1 (5%)
3	NAG	F	2	3	14,14,15	0.28	0	17,19,21	0.66	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	3	-	1/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	3	-	1/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	NAG	C1-C2-N2	-4.86	102.19	110.49
3	C	1	NAG	C1-C2-N2	-4.21	103.30	110.49

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C3-C2-N2-C7
3	F	1	NAG	C3-C2-N2-C7

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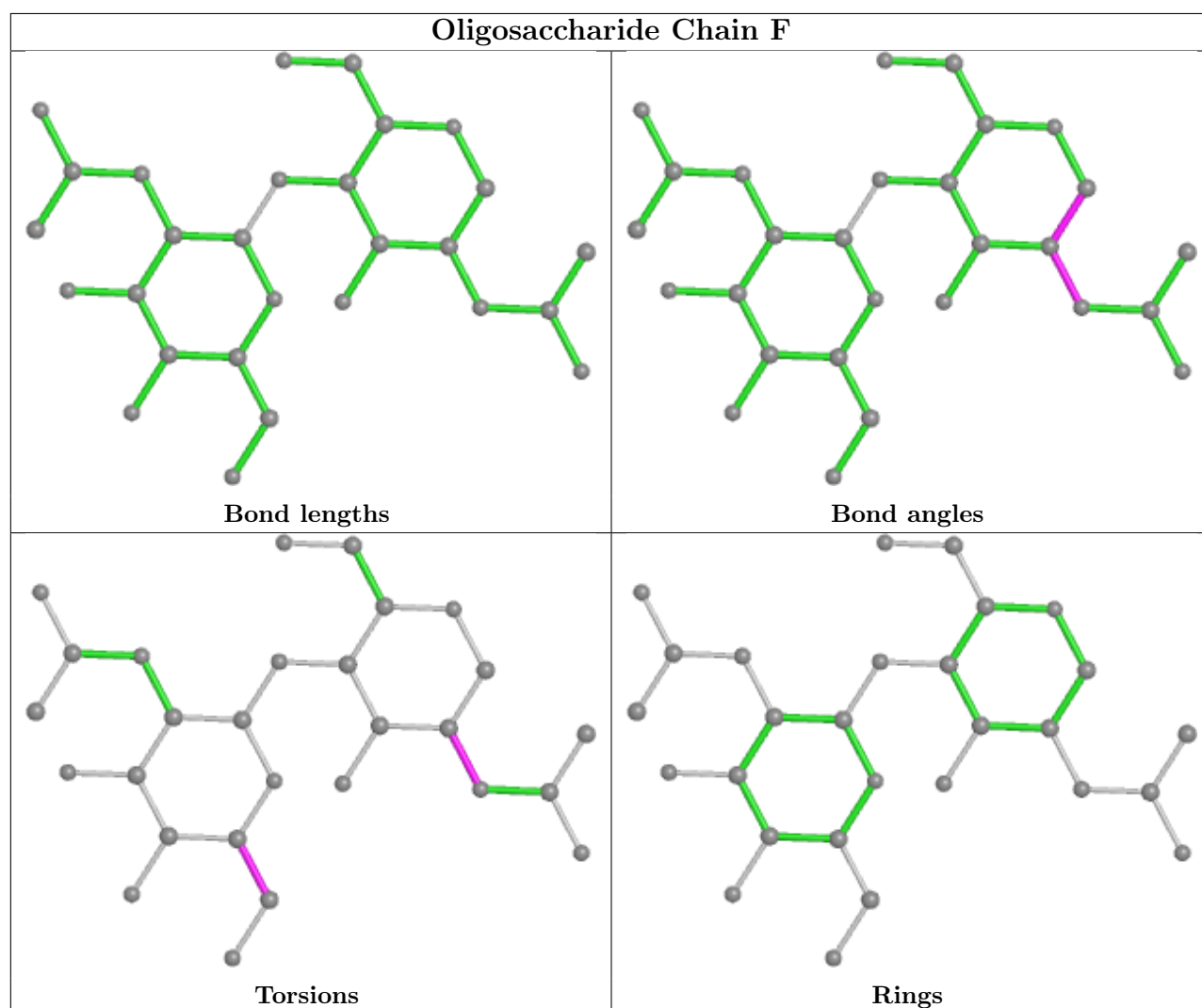
Mol	Chain	Res	Type	Atoms
3	C	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	NAG	3	0
3	C	1	NAG	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry

Of 22 ligands modelled in this entry, 4 are monoatomic - leaving 18 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
6	NAG	B	603	-	14,14,15	0.31	0	17,19,21	0.87	1 (5%)
5	HEM	B	601	2	27,50,50	2.00	6 (22%)	17,82,82	2.06	4 (23%)
8	BMA	E	601	-	11,11,12	0.25	0	15,15,17	0.70	0
5	HEM	E	604	2	27,50,50	1.47	3 (11%)	17,82,82	2.08	4 (23%)
11	XRV	B	611	-	23,26,26	1.24	4 (17%)	24,37,37	1.57	5 (20%)
9	MAN	E	603	-	11,11,12	0.36	0	15,15,17	0.97	1 (6%)
11	XRV	E	610	-	23,26,26	1.57	3 (13%)	24,37,37	1.30	1 (4%)
8	BMA	B	606	-	11,11,12	0.23	0	15,15,17	0.67	0
6	NAG	E	607	-	14,14,15	0.26	0	17,19,21	1.35	3 (17%)
6	NAG	B	602	2	14,14,15	0.30	0	17,19,21	1.02	2 (11%)
6	NAG	E	606	-	14,14,15	0.28	0	17,19,21	0.90	1 (5%)
9	MAN	B	608	-	11,11,12	0.34	0	15,15,17	1.12	1 (6%)
7	FUC	E	608	-	10,10,11	0.44	0	14,14,16	1.24	2 (14%)
9	MAN	E	602	-	11,11,12	0.31	0	15,15,17	0.82	1 (6%)
7	FUC	B	605	-	10,10,11	0.48	0	14,14,16	1.32	2 (14%)
9	MAN	B	607	-	11,11,12	0.29	0	15,15,17	0.86	1 (6%)
6	NAG	E	605	2	14,14,15	0.28	0	17,19,21	0.88	2 (11%)
6	NAG	B	604	-	14,14,15	0.28	0	17,19,21	1.35	2 (11%)

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
6	NAG	B	603	-	-	0/6/23/26	0/1/1/1
5	HEM	B	601	2	-	0/6/54/54	-
8	BMA	E	601	-	-	2/2/19/22	0/1/1/1

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

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	601	HEM	C3B-C2B	-7.23	1.30	1.40
11	E	610	XRV	C3-N6	5.69	1.43	1.34
5	E	604	HEM	C3B-C2B	-5.17	1.33	1.40
5	B	601	HEM	C3B-CAB	-3.84	1.40	1.47
11	B	611	XRV	C3-N6	3.23	1.39	1.34
5	B	601	HEM	C3D-C2D	-2.98	1.28	1.37
5	E	604	HEM	C3D-C2D	-2.79	1.29	1.37
11	B	611	XRV	C8-C7	2.56	1.44	1.37
5	B	601	HEM	C1A-CHA	-2.49	1.34	1.41
11	E	610	XRV	C4-N4	2.44	1.42	1.37
5	B	601	HEM	CMD-C2D	-2.41	1.46	1.51
5	E	604	HEM	C1A-CHA	-2.32	1.34	1.41
11	B	611	XRV	C2-N1	2.22	1.36	1.33
11	E	610	XRV	C8-C7	2.17	1.43	1.37
5	B	601	HEM	C4A-NA	2.15	1.40	1.36
11	B	611	XRV	C4-N4	2.15	1.41	1.37

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	604	HEM	CBA-CAA-C2A	-5.34	102.64	112.49
5	B	601	HEM	CBA-CAA-C2A	-5.04	103.20	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	E	610	XRV	C8-N2-N3	4.90	107.27	103.70
6	B	604	NAG	O5-C1-C2	-4.60	104.03	111.29
6	E	607	NAG	O5-C1-C2	-4.43	104.30	111.29
5	B	601	HEM	CBD-CAD-C3D	-4.16	104.81	112.48
11	B	611	XRV	C8-N2-N3	4.14	106.71	103.70
7	B	605	FUC	C1-C2-C3	3.65	114.15	109.67
5	E	604	HEM	CBD-CAD-C3D	-3.55	105.94	112.48
5	E	604	HEM	C4A-C3A-C2A	-3.40	104.63	107.00
9	B	608	MAN	C1-O5-C5	3.24	116.58	112.19
6	E	606	NAG	C1-C2-N2	-3.08	105.23	110.49
7	E	608	FUC	C1-C2-C3	3.01	113.37	109.67
5	B	601	HEM	CMC-C2C-C3C	2.95	130.20	124.68
11	B	611	XRV	C10-N3-N2	2.95	121.42	118.80
6	B	603	NAG	C1-C2-N2	-2.81	105.69	110.49
6	B	602	NAG	C1-O5-C5	2.76	115.93	112.19
7	E	608	FUC	C1-O5-C5	2.72	118.94	112.78
9	E	603	MAN	C1-O5-C5	2.71	115.87	112.19
6	E	605	NAG	O5-C1-C2	-2.69	107.03	111.29
11	B	611	XRV	C9-N3-N2	-2.68	109.99	112.72
11	B	611	XRV	C2-N1-C3	-2.55	115.31	119.22
7	B	605	FUC	C1-O5-C5	2.46	118.34	112.78
6	B	602	NAG	O5-C1-C2	-2.43	107.45	111.29
9	B	607	MAN	C1-O5-C5	2.43	115.48	112.19
9	E	602	MAN	C1-O5-C5	2.40	115.44	112.19
5	B	601	HEM	C4A-C3A-C2A	-2.37	105.35	107.00
5	E	604	HEM	CMC-C2C-C3C	2.37	129.10	124.68
6	E	607	NAG	C1-O5-C5	2.20	115.18	112.19
6	E	607	NAG	C1-C2-N2	2.20	114.25	110.49
11	B	611	XRV	N7-C2-N1	-2.10	116.52	118.26
6	B	604	NAG	C1-O5-C5	2.07	115.00	112.19
6	E	605	NAG	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	E	601	BMA	O5-C5-C6-O6
8	B	606	BMA	O5-C5-C6-O6
8	E	601	BMA	C4-C5-C6-O6
8	B	606	BMA	C4-C5-C6-O6
11	E	610	XRV	C15-C10-N3-C9
11	B	611	XRV	C15-C10-N3-C9

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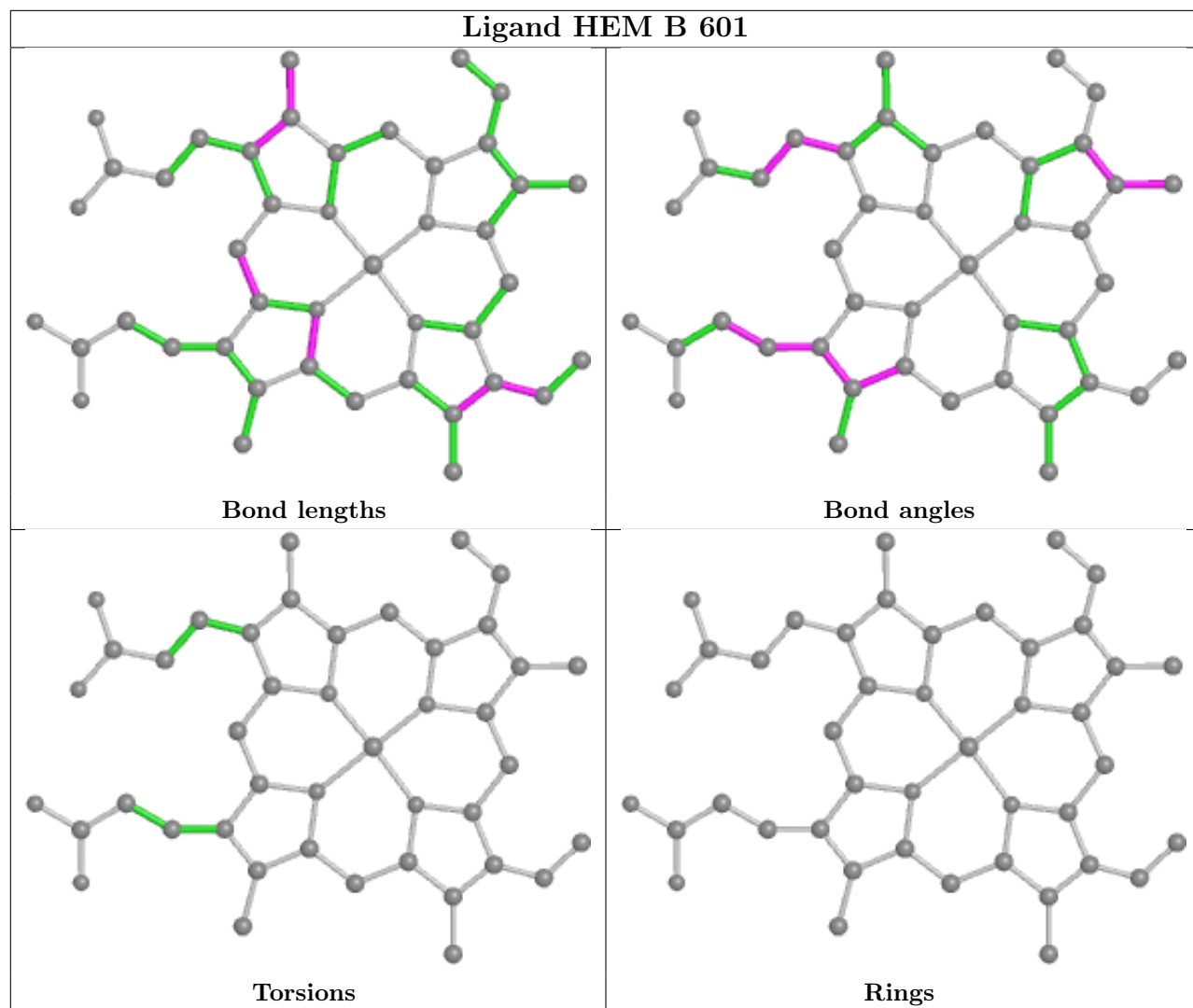
Mol	Chain	Res	Type	Atoms
11	B	611	XRV	C11-C10-N3-C9
11	B	611	XRV	C5-C6-C7-C8
11	E	610	XRV	C11-C10-N3-C9

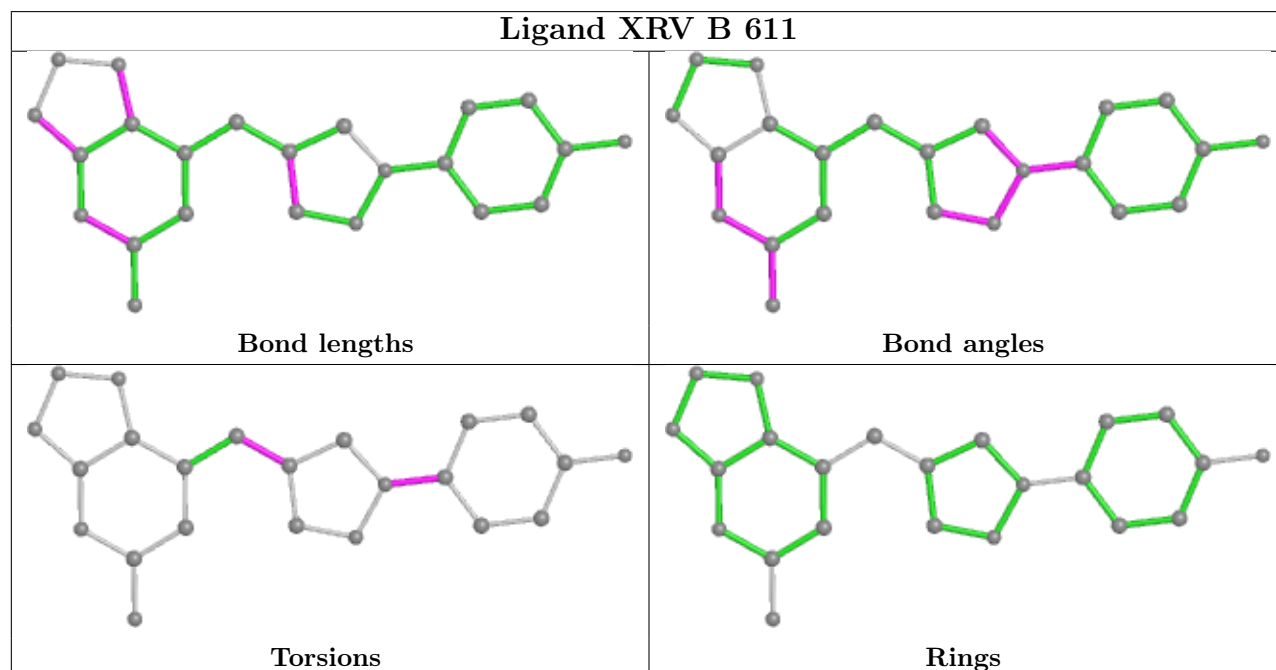
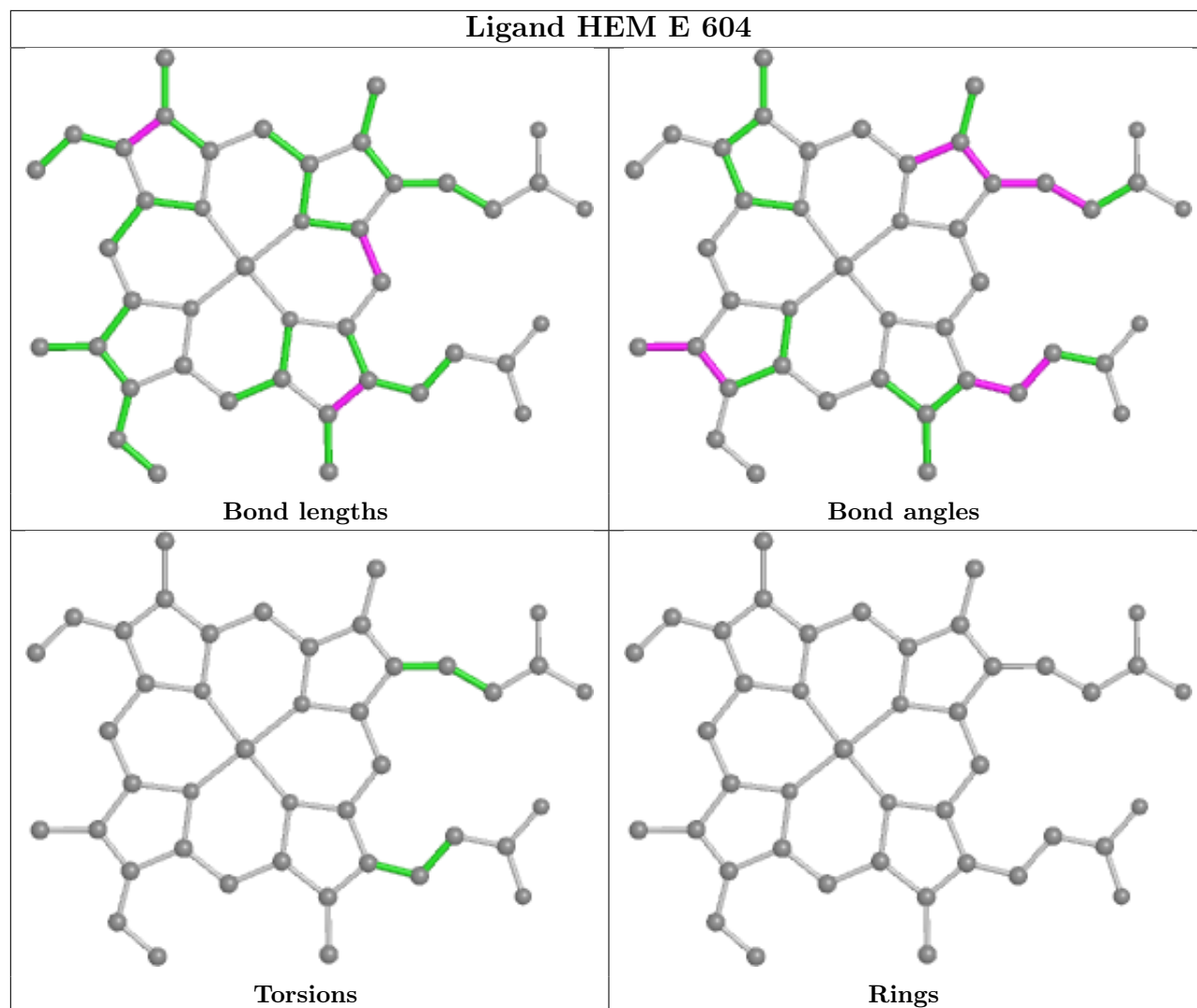
There are no ring outliers.

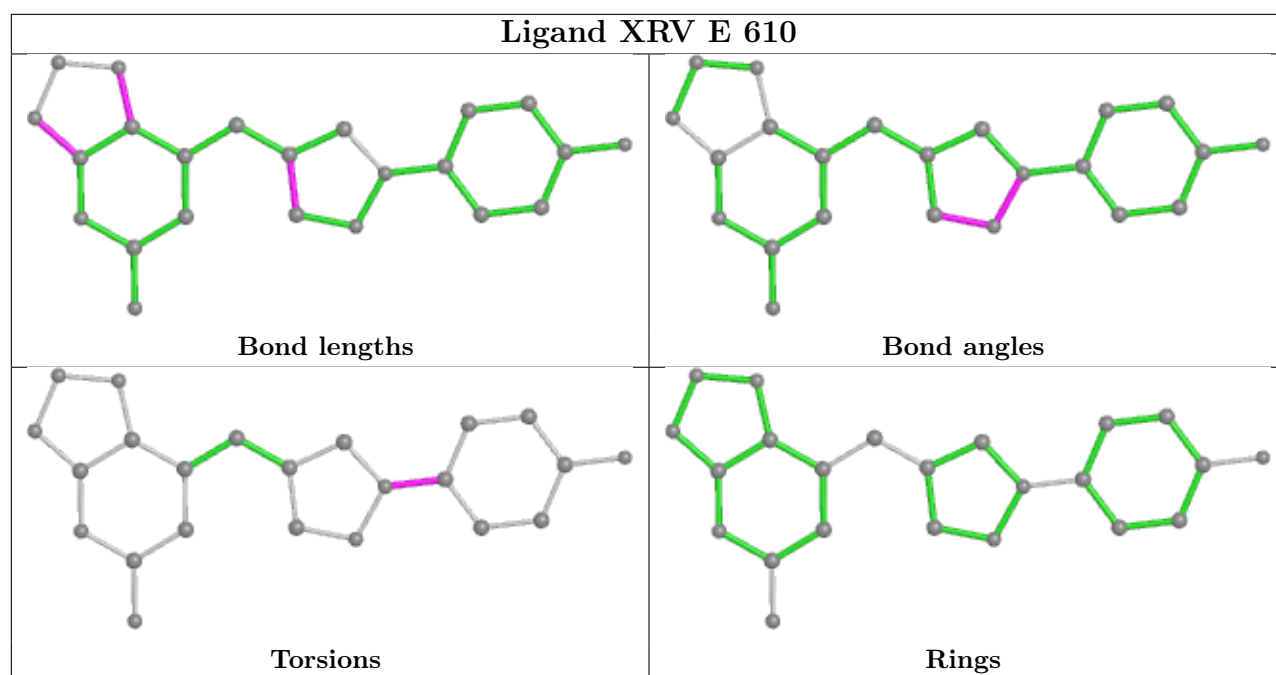
8 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	601	HEM	12	0
8	E	601	BMA	2	0
5	E	604	HEM	10	0
8	B	606	BMA	2	0
7	E	608	FUC	1	0
9	E	602	MAN	1	0
7	B	605	FUC	1	0
9	B	607	MAN	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.







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%)	0.05	1 (0%)	82 66	44, 63, 85, 102	0
1	D	103/105 (98%)	-0.07	1 (0%)	82 66	39, 57, 78, 84	0
2	B	464/466 (99%)	0.32	40 (8%)	10 5	42, 74, 100, 111	2 (0%)
2	E	465/466 (99%)	0.03	9 (1%)	66 46	41, 63, 81, 107	8 (1%)
All	All	1135/1142 (99%)	0.14	51 (4%)	33 19	39, 66, 95, 111	10 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	209	ALA	5.5
2	B	546	VAL	5.2
2	B	121	GLN	4.4
2	B	567	LEU	4.2
2	B	540	ASN	4.1
2	B	573	ALA	3.9
2	B	545	THR	3.9
2	B	206	ASN	3.7
2	B	456	ARG	3.7
2	E	207	GLY	3.6
2	B	568	PRO	3.6
1	A	87	MET	3.4
2	B	207	GLY	3.4
2	B	445	PRO	3.4
2	B	564	CYS	3.2
2	B	120	VAL	3.2
2	E	194	LEU	3.1
2	B	541	THR	3.0
2	E	445	PRO	2.9
2	B	530	GLN	2.9
2	B	482	SER	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	208	ARG	2.9
2	B	178	GLY	2.6
2	B	119	CYS	2.6
2	B	558	PRO	2.5
2	B	544	THR	2.5
2	B	372	VAL	2.5
2	B	373	LEU	2.4
2	B	565	SER	2.4
2	E	120	VAL	2.4
2	B	566	THR	2.3
2	E	474	ILE	2.3
2	B	271	TRP	2.3
2	B	142	ASP	2.3
2	B	569	ALA	2.3
2	B	257	HIS	2.3
2	B	199	VAL	2.2
2	B	122	GLN	2.2
2	E	142	ASP	2.2
2	B	228	ALA	2.2
2	E	130	ILE	2.2
1	D	83	SER	2.1
2	B	140	GLN	2.1
2	B	542	GLY	2.1
2	B	442	LEU	2.1
2	E	117	THR	2.1
2	B	575	TRP	2.0
2	B	547	SER	2.0
2	B	535	ARG	2.0
2	B	571	ASN	2.0
2	E	144	ILE	2.0

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

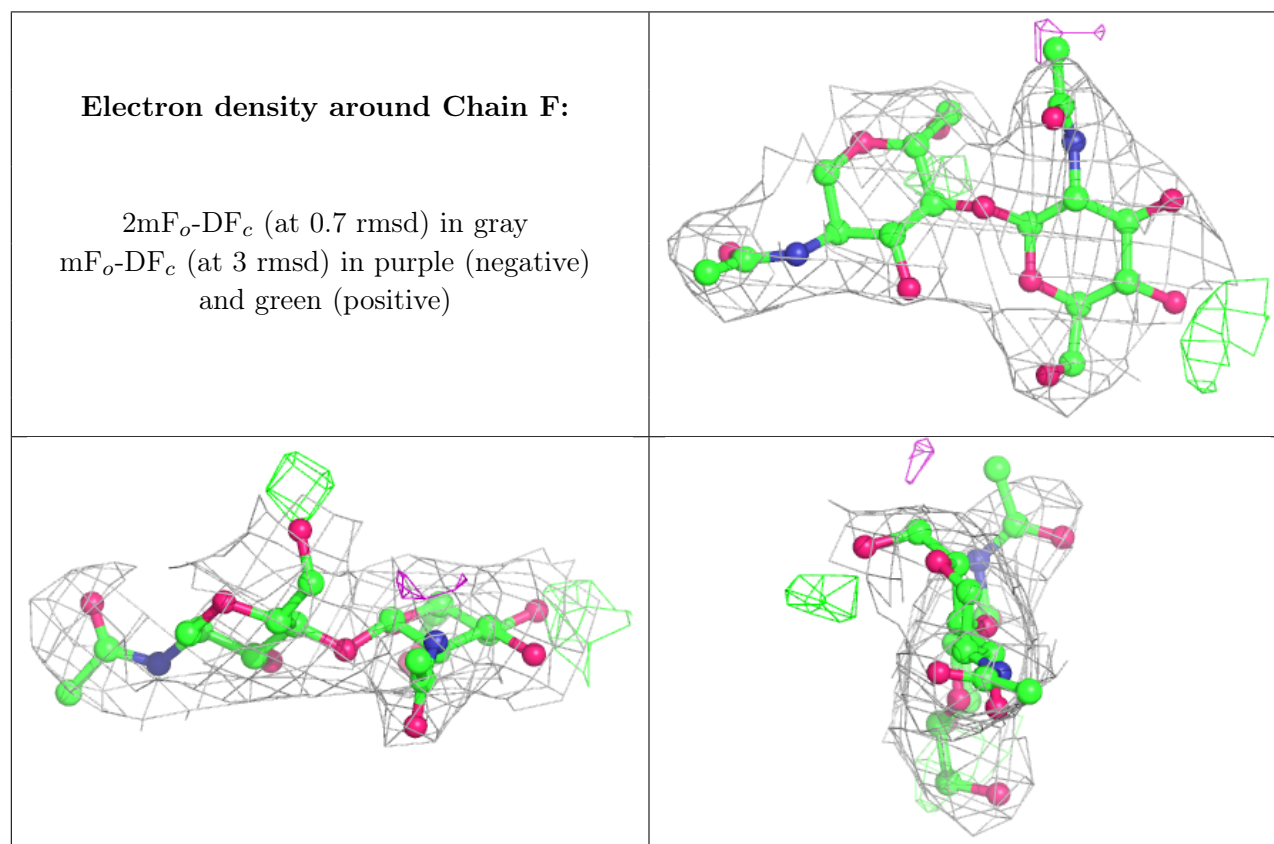
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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(\AA^2)	Q<0.9
3	NAG	C	1	14/15	0.90	0.20	52,57,68,69	0
3	NAG	F	1	14/15	0.92	0.15	59,61,66,66	0
3	NAG	C	2	14/15	0.93	0.16	50,59,61,62	0
3	NAG	F	2	14/15	0.94	0.21	61,62,63,66	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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.

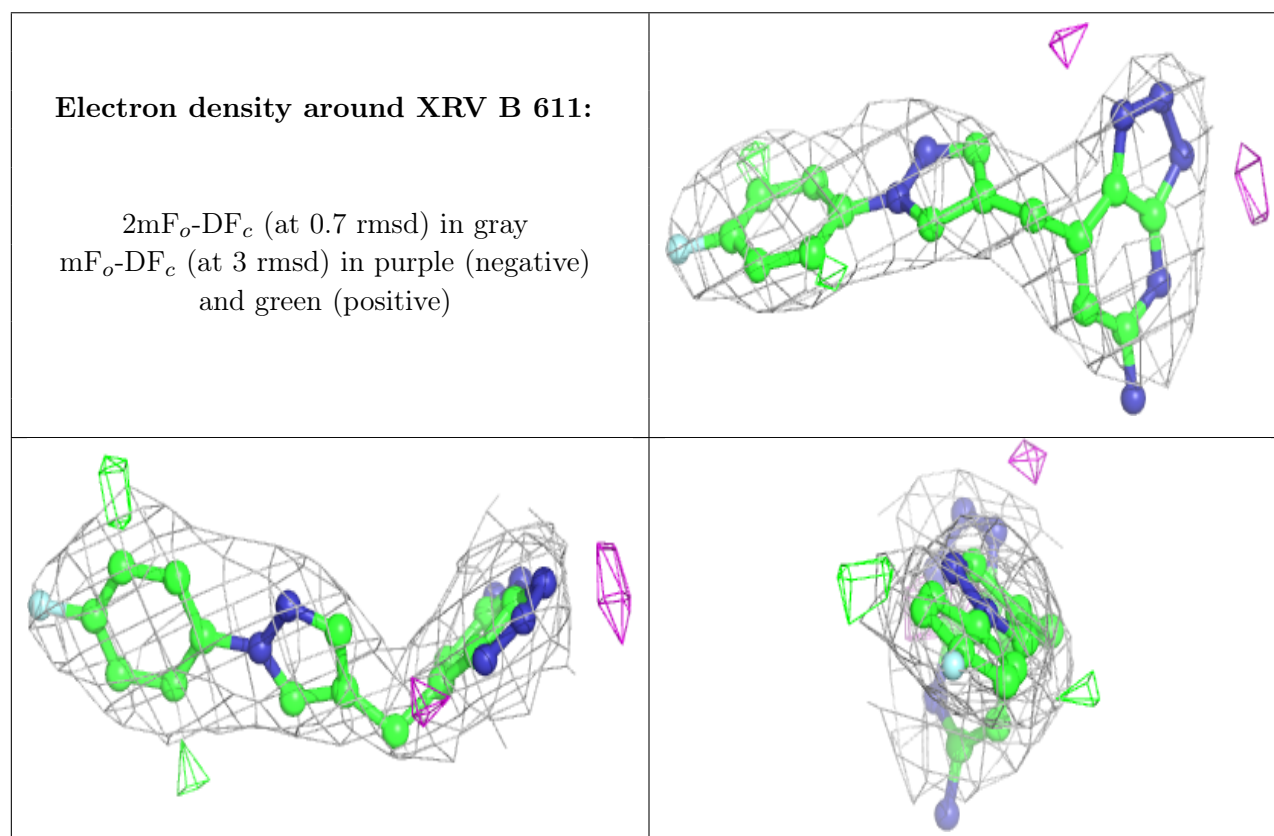
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	NAG	B	604	14/15	0.64	0.24	117,128,131,133	0
6	NAG	E	607	14/15	0.75	0.17	102,118,122,123	0
6	NAG	B	603	14/15	0.81	0.23	113,117,120,120	0
6	NAG	B	602	14/15	0.83	0.24	89,102,104,104	0
8	BMA	B	606	11/12	0.84	0.26	128,129,131,133	0

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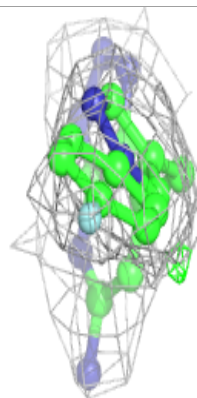
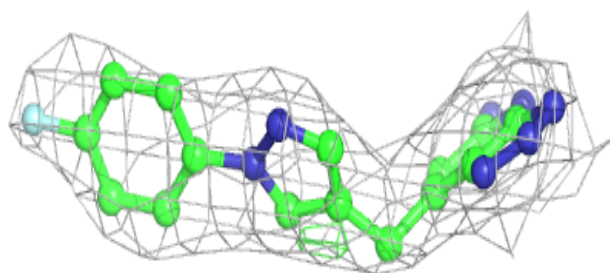
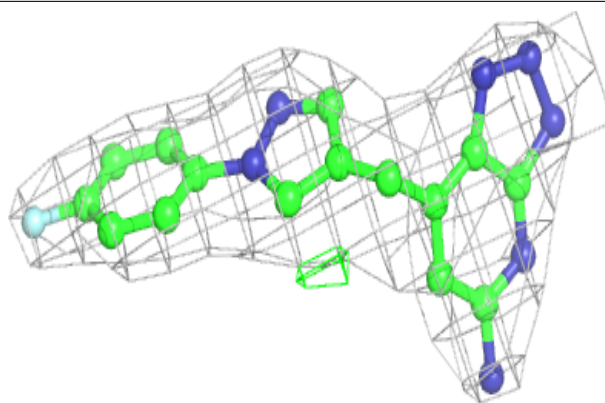
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CL	B	610	1/1	0.85	0.21	72,72,72,72	0
8	BMA	E	601	11/12	0.85	0.38	120,124,127,128	0
9	MAN	B	607	11/12	0.87	0.18	103,104,106,109	0
6	NAG	E	605	14/15	0.88	0.41	67,80,83,84	0
9	MAN	E	603	11/12	0.89	0.19	53,63,69,69	0
9	MAN	E	602	11/12	0.90	0.18	115,115,116,117	0
7	FUC	B	605	10/11	0.91	0.17	58,68,70,71	0
6	NAG	E	606	14/15	0.92	0.15	100,107,109,110	0
9	MAN	B	608	11/12	0.92	0.17	45,54,59,62	0
4	CL	A	201	1/1	0.93	0.25	61,61,61,61	0
11	XRV	B	611	23/23	0.93	0.19	63,72,78,78	0
7	FUC	E	608	10/11	0.94	0.18	56,65,69,73	0
11	XRV	E	610	23/23	0.95	0.17	58,63,75,77	0
5	HEM	B	601	43/43	0.96	0.21	70,71,74,78	0
5	HEM	E	604	43/43	0.97	0.19	47,48,52,61	0
10	CA	E	609	1/1	0.97	0.13	49,49,49,49	0
10	CA	B	609	1/1	0.98	0.16	60,60,60,60	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.

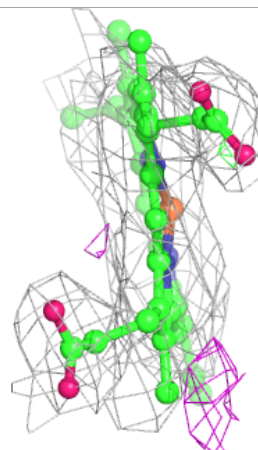
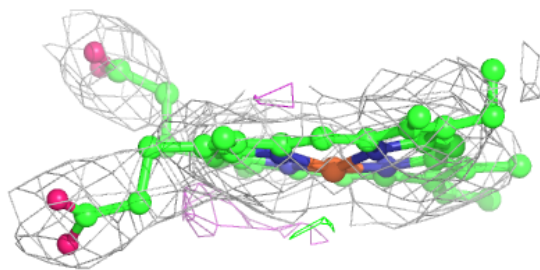
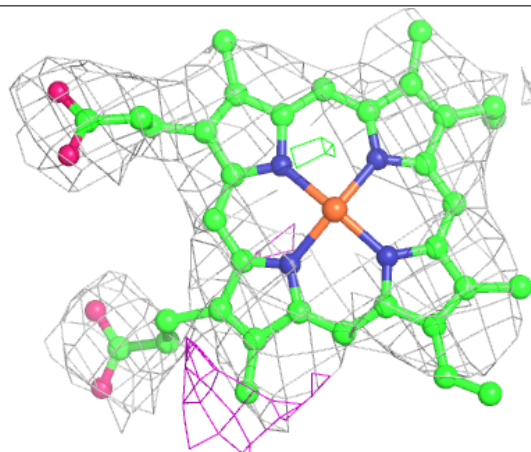


Electron density around XRV E 610:

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

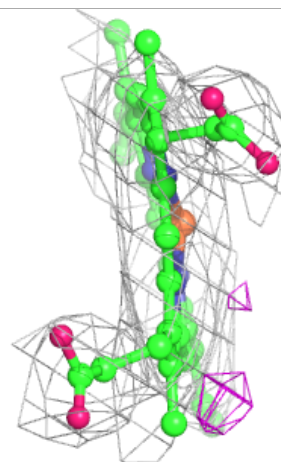
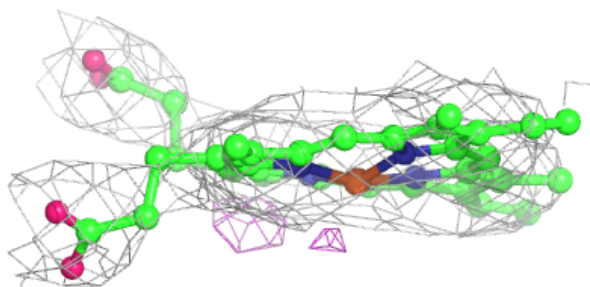
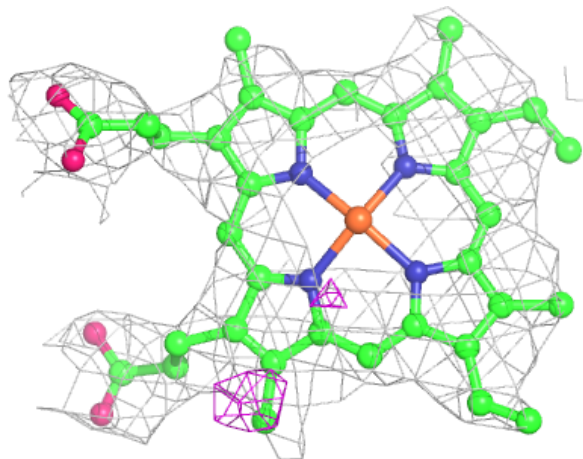
**Electron density around HEM B 601:**

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



Electron density around HEM E 604:

$2mF_o-DF_c$ (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.