Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 03:46 AM EDT

PDB ID	:	2IUF
Title	:	The structures of Penicillium vitale catalase: resting state, oxidised state (compound I) and complex with aminotriazole
Authors	:	Murshudov, G.; Borovik, A.; Grebenko, A.; Barynin, V.; Vagin, A.; Melik-Adamyan, W.
Deposited on	:	2006-06-02
Resolution	:	1.71 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 (i) 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 (i)) were used in the production of this report:

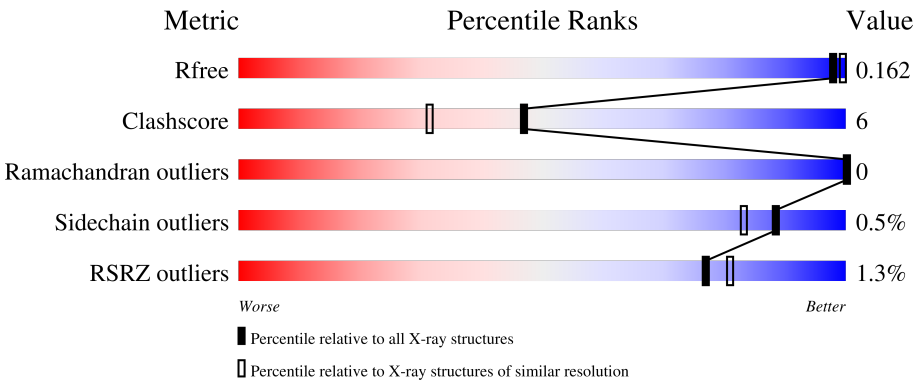
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.71 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	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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 <=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	688	% 90% 10% •
1	E	688	% 91% 8% •
2	B	2	100%

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
4	NAG	A	1693	-	-	X	-
4	NAG	A	1694	-	-	-	X
7	ACT	E	1701	-	-	X	-
7	ACT	E	1707	-	-	X	-
8	F50	E	1705	-	X	-	-
9	MPD	A	1704	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 12590 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.

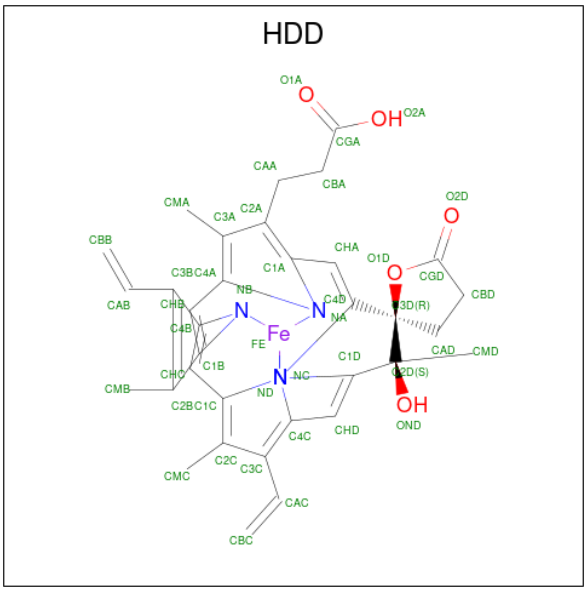
- Molecule 1 is a protein called CATALASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	688	5429	3418	960	1041	10	0	11	0
1	E	688	5402	3401	952	1039	10	0	8	0

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

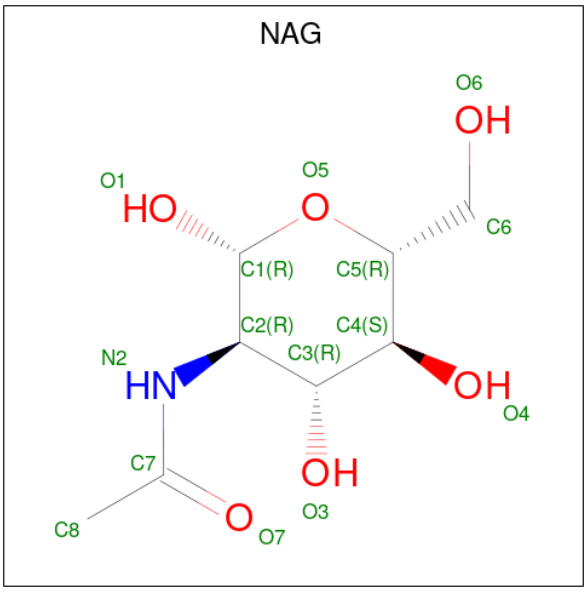
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	2	28	16	2	10	0	0	0

- Molecule 3 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (three-letter code: HDD) (formula: $C_{34}H_{32}FeN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
3	A	1	44	34	1	4	5	0	0
			Total	C	Fe	N	O		
3	E	1	44	34	1	4	5	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	14	8	1	5	0	0

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

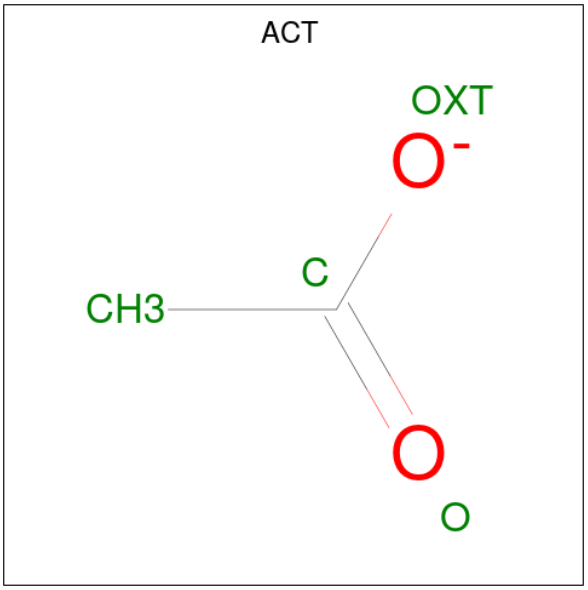
- Molecule 5 is OXYGEN ATOM (three-letter code: O) (formula: O).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 1 1	0	0
5	E	1	Total O 1 1	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

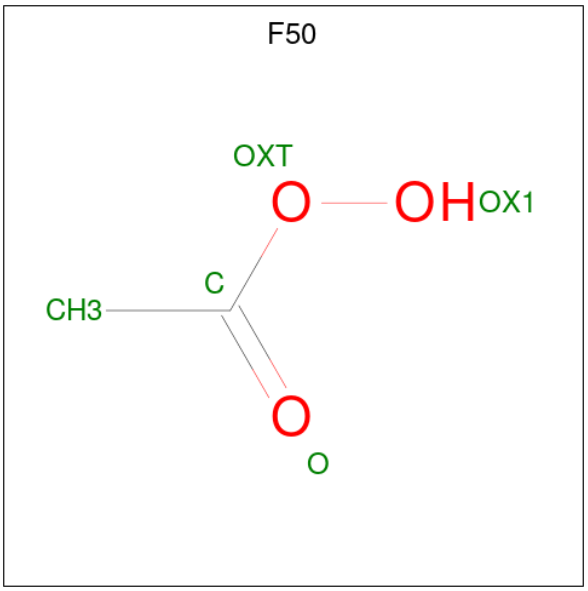
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Ca 2 2	0	0
6	E	4	Total Ca 4 4	0	0

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



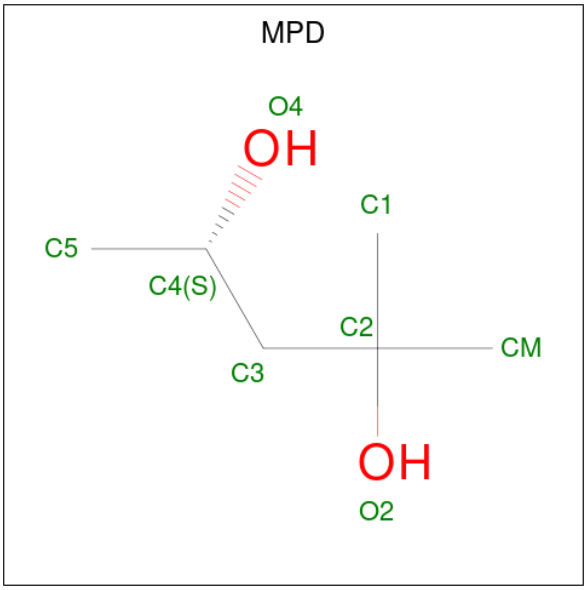
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
7	A	1	4	2	2		0	0
7	A	1	4	2	2		0	0
7	A	1	4	2	2		0	0
7	A	1	4	2	2		0	0
7	A	1	4	2	2		0	0
7	E	1	4	2	2		0	0
7	E	1	4	2	2		0	0
7	E	1	4	2	2		0	0
7	E	1	4	2	2		0	0
7	E	1	4	2	2		0	0
7	E	1	4	2	2		0	0
7	E	1	4	2	2		0	0
7	E	1	4	2	2		0	0

- Molecule 8 is ETHANEPEROXOIC ACID (three-letter code: F50) (formula: $C_2H_4O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	5	2	3	0	0
			Total	C	O		
8	E	1	5	2	3	0	0
			Total	C	O		
8	E	1	5	2	3	0	0

- Molecule 9 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	A	1	8	6	2	0	0

- Molecule 10 is water.

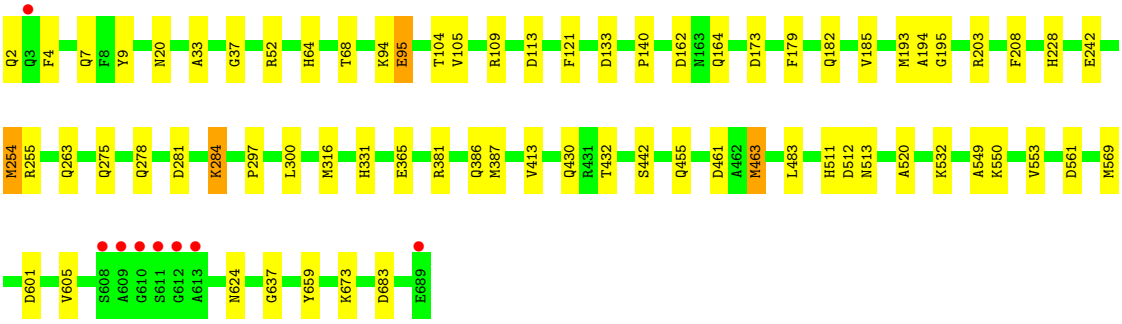
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	774	774	774	0	0
			Total	O		
10	E	716	716	716	0	0

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.

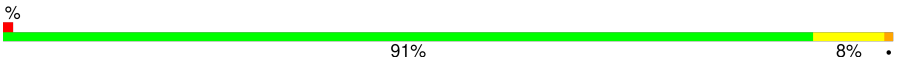
• Molecule 1: CATALASE

Chain A:



• Molecule 1: CATALASE

Chain E:



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	142.44Å 142.44Å 132.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	119.52 – 1.71 19.80 – 1.71	Depositor EDS
% Data completeness (in resolution range)	98.9 (119.52-1.71) 99.0 (19.80-1.71)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.63 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.3.0002	Depositor
R, R_{free}	0.129 , 0.154 0.139 , 0.162	Depositor DCC
R_{free} test set	8285 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	14.7	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 58.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.010 for -h,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	12590	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: HDD, MPD, F50, MHO, O, NAG, CA, ACT

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	0.90	2/5503 (0.0%)	0.86	5/7456 (0.1%)
1	E	0.90	2/5476 (0.0%)	0.87	8/7422 (0.1%)
All	All	0.90	4/10979 (0.0%)	0.87	13/14878 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	242	GLU	CB-CG	-7.50	1.37	1.52
1	A	242	GLU	CB-CG	-5.92	1.40	1.52
1	E	48	GLU	CD-OE2	5.36	1.31	1.25
1	A	95	GLU	CD-OE1	-5.12	1.20	1.25

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	631	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	A	162	ASP	CB-CG-OD1	6.69	124.32	118.30
1	E	36	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	E	79	ASP	CB-CG-OD1	6.23	123.91	118.30
1	A	683	ASP	CB-CG-OD2	6.03	123.73	118.30
1	A	203	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	E	358	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	162	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	E	152	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	E	387	MET	CG-SD-CE	5.45	108.92	100.20
1	E	288	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	381	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	E	381	ARG	NE-CZ-NH2	-5.06	117.77	120.30

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	5429	0	5242	67	0
1	E	5402	0	5205	57	2
2	B	28	0	25	3	0
3	A	44	0	31	1	0
3	E	44	0	31	1	0
4	A	42	0	39	9	2
4	E	28	0	26	0	0
5	A	1	0	0	0	0
5	E	1	0	0	0	0
6	A	2	0	0	0	0
6	E	4	0	0	0	0
7	A	20	0	15	1	0
7	E	32	0	24	9	0
8	A	5	0	4	0	0
8	E	10	0	8	0	0
9	A	8	0	14	6	0
10	A	774	0	0	25	3
10	E	716	0	0	15	2
All	All	12590	0	10664	135	5

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 6.

All (135) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:GLN:NE2	10:A:2463:HOH:O	1.81	1.12
1:A:68[A]:THR:HG21	1:A:255:ARG:HB3	1.33	1.07
4:A:1692:NAG:H82	10:A:2487:HOH:O	0.90	1.07
1:A:463:MHO:HE3	1:A:483:LEU:HD11	1.35	1.05
10:A:2697:HOH:O	7:E:1701:ACT:H2	1.55	1.04
1:A:278:GLN:OE1	9:A:1704:MPD:H51	1.58	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:463:MHO:HE3	1:E:483:LEU:HD11	1.48	0.94
1:A:95:GLU:OE1	10:A:2161:HOH:O	1.86	0.92
7:E:1707:ACT:H1	10:E:2097:HOH:O	1.69	0.91
1:A:68[A]:THR:HG21	1:A:255:ARG:CB	2.00	0.91
7:E:1701:ACT:H1	10:E:2289:HOH:O	1.74	0.87
1:E:109[A]:ARG:NH1	10:E:2149:HOH:O	2.06	0.86
1:E:179:PHE:HA	1:E:185:VAL:HG21	1.59	0.85
1:E:550:LYS:O	1:E:553:VAL:HG22	1.75	0.85
1:A:94[B]:LYS:NZ	10:A:2152:HOH:O	2.11	0.83
1:E:601:ASP:O	1:E:605[A]:VAL:HG23	1.79	0.82
1:E:506:ASN:C	1:E:506:ASN:HD22	1.84	0.82
1:A:109[B]:ARG:HH12	1:E:164:GLN:HE22	1.28	0.81
1:A:550:LYS:O	1:A:553:VAL:HG22	1.81	0.80
1:A:109[B]:ARG:NH1	10:A:2171:HOH:O	2.14	0.79
1:A:601:ASP:O	1:A:605[B]:VAL:HG23	1.81	0.79
1:A:195:GLY:H	1:A:455:GLN:HE21	1.27	0.79
1:A:113:ASP:HB3	1:A:254:MHO:HE2	1.65	0.78
1:A:455:GLN:HE22	1:A:520:ALA:H	1.32	0.77
1:E:455:GLN:HE22	1:E:520:ALA:H	1.31	0.77
1:E:373:ARG:HH22	7:E:1707:ACT:H3	1.49	0.76
9:A:1704:MPD:HM1	9:A:1704:MPD:H52	1.68	0.76
1:E:195:GLY:H	1:E:455:GLN:HE21	1.31	0.76
1:A:179:PHE:HA	1:A:185:VAL:HG21	1.68	0.74
1:A:511:HIS:HD2	1:A:513:ASN:H	1.35	0.74
4:A:1692:NAG:O6	10:A:2765:HOH:O	1.91	0.73
1:A:109[A]:ARG:NH1	10:A:2170:HOH:O	2.20	0.73
1:A:109[B]:ARG:HH12	1:E:164:GLN:NE2	1.86	0.72
4:A:1693:NAG:O7	10:A:2769:HOH:O	2.07	0.72
1:A:254:MHO:CE	10:A:2178:HOH:O	2.38	0.71
1:E:331:HIS:HE1	1:E:365:GLU:OE2	1.72	0.71
1:A:109[A]:ARG:NH2	10:A:2170:HOH:O	2.19	0.71
1:A:109[B]:ARG:NH1	1:E:164:GLN:HE22	1.89	0.69
9:A:1704:MPD:H11	10:A:2053:HOH:O	1.92	0.69
1:A:331:HIS:HE1	1:A:365:GLU:OE2	1.76	0.68
4:A:1693:NAG:C8	10:A:2769:HOH:O	2.41	0.67
4:A:1693:NAG:C7	10:A:2769:HOH:O	2.41	0.67
1:E:133:ASP:OD2	1:E:331:HIS:HD2	1.76	0.67
1:A:601:ASP:O	1:A:605[A]:VAL:HG13	1.94	0.67
10:E:2706:HOH:O	2:B:2:NAG:O7	2.12	0.67
4:A:1693:NAG:H81	10:A:2769:HOH:O	1.95	0.66
1:A:109[A]:ARG:HH21	1:E:164:GLN:HE22	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:506:ASN:OD1	10:E:2536:HOH:O	2.15	0.64
1:E:506:ASN:C	1:E:506:ASN:ND2	2.48	0.64
1:A:133:ASP:OD2	1:A:331:HIS:HD2	1.81	0.63
1:E:371[A]:ARG:NH2	10:E:2408:HOH:O	2.32	0.63
1:E:179:PHE:CA	1:E:185:VAL:HG21	2.29	0.63
1:E:428:LYS:NZ	10:E:2470:HOH:O	2.32	0.63
1:A:413:VAL:HG21	4:A:1692:NAG:H62	1.81	0.62
1:E:316:MHO:HE3	10:E:2363:HOH:O	2.00	0.61
1:A:549:ALA:O	1:A:553:VAL:HG13	2.01	0.61
1:E:182:GLN:O	1:E:185:VAL:HG22	2.01	0.61
1:A:20:ASN:HD21	1:A:52:ARG:HH11	1.48	0.60
1:E:506:ASN:HD22	1:E:507:SER:N	2.00	0.60
1:E:461:ASP:HB3	7:E:1701:ACT:H3	1.83	0.60
1:E:316:MHO:CE	10:E:2363:HOH:O	2.50	0.60
1:A:461:ASP:OD2	7:A:1700:ACT:O	2.20	0.59
1:A:463:MHO:HE3	1:A:483:LEU:CD1	2.22	0.58
1:E:549:ALA:O	1:E:553:VAL:HG13	2.03	0.58
1:E:373:ARG:HH12	7:E:1707:ACT:CH3	2.17	0.58
1:A:68[A]:THR:HG23	10:A:2177:HOH:O	2.03	0.57
1:A:195:GLY:H	1:A:455:GLN:NE2	2.01	0.57
1:A:281:ASP:OD1	1:A:284:LYS:HD3	2.05	0.57
1:A:532[A]:LYS:NZ	1:A:561:ASP:OD2	2.34	0.57
1:E:410:ASN:OD1	1:E:413[B]:VAL:HG22	2.04	0.56
10:A:2697:HOH:O	7:E:1701:ACT:CH3	2.28	0.56
4:A:1692:NAG:O5	10:A:2766:HOH:O	2.18	0.56
1:A:109[A]:ARG:CZ	10:A:2170:HOH:O	2.46	0.55
1:A:164:GLN:HE22	1:E:109[B]:ARG:HH12	1.55	0.55
1:E:20:ASN:HD21	1:E:52:ARG:HH11	1.53	0.55
1:E:260:GLN:NE2	10:E:2313:HOH:O	2.18	0.55
1:A:179:PHE:CA	1:A:185:VAL:HG21	2.37	0.55
1:A:182:GLN:O	1:A:185:VAL:HG22	2.06	0.54
1:E:373:ARG:NH2	7:E:1707:ACT:H3	2.22	0.54
1:A:2:GLN:NE2	1:A:9:TYR:OH	2.38	0.54
1:A:442:SER:O	1:A:511:HIS:HE1	1.92	0.53
1:A:228:HIS:HE1	1:A:275:GLN:OE1	1.92	0.53
1:A:278:GLN:OE1	9:A:1704:MPD:C5	2.46	0.52
1:E:193:MHO:HE2	1:E:463:MHO:HG3	1.91	0.52
1:E:373:ARG:HH22	7:E:1707:ACT:CH3	2.22	0.50
10:E:2061:HOH:O	2:B:2:NAG:H83	2.12	0.49
1:E:64:HIS:CE1	1:E:105:VAL:HG22	2.47	0.49
2:B:1:NAG:HO4	2:B:2:NAG:C1	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:228:HIS:HE1	1:E:275:GLN:OE1	1.95	0.49
1:A:20:ASN:ND2	1:A:52:ARG:HH11	2.10	0.49
9:A:1704:MPD:H13	10:A:2147:HOH:O	2.13	0.49
9:A:1704:MPD:H52	9:A:1704:MPD:CM	2.40	0.48
1:E:3:GLN:H	1:E:3:GLN:CD	2.17	0.48
1:E:637:GLY:HA2	1:E:659:TYR:O	2.14	0.48
1:A:512:ASP:HB2	4:A:1693:NAG:H81	1.96	0.47
1:E:195:GLY:H	1:E:455:GLN:NE2	2.06	0.47
3:E:1691:HDD:HMB1	3:E:1691:HDD:HBB1	1.96	0.47
1:A:64:HIS:CE1	1:A:105:VAL:HG22	2.49	0.47
1:A:263:GLN:HG3	10:A:2341:HOH:O	2.14	0.47
1:E:193:MHO:CE	1:E:463:MHO:HG3	2.45	0.47
1:A:68[A]:THR:CG2	1:A:255:ARG:HE	2.27	0.46
1:E:2:GLN:NE2	1:E:9:TYR:OH	2.42	0.46
1:A:164:GLN:NE2	1:E:109[A]:ARG:HH12	2.13	0.46
1:A:164:GLN:NE2	1:E:109[B]:ARG:HH12	2.13	0.46
1:A:164:GLN:HE22	1:E:109[A]:ARG:HH12	1.64	0.46
3:A:1691:HDD:HMB1	3:A:1691:HDD:HBB1	1.98	0.46
1:A:4:PHE:O	1:A:7:GLN:HG2	2.16	0.45
1:E:20:ASN:ND2	1:E:52:ARG:HH11	2.14	0.45
1:E:64:HIS:HA	1:E:104:THR:O	2.16	0.45
1:A:254:MHO:HE3	10:A:2178:HOH:O	2.10	0.45
1:A:387:MET:HB3	10:A:2442:HOH:O	2.15	0.45
1:E:455:GLN:NE2	1:E:520:ALA:H	2.08	0.45
1:E:387:MET:HB3	10:E:2408:HOH:O	2.16	0.44
1:A:430:GLN:HB2	1:A:432:THR:HG23	1.98	0.44
1:E:33:ALA:O	1:E:37:GLY:HA3	2.18	0.44
1:A:64:HIS:HA	1:A:104:THR:O	2.18	0.44
1:A:637:GLY:HA2	1:A:659:TYR:O	2.18	0.43
1:A:68[A]:THR:HG21	1:A:255:ARG:HB2	1.94	0.43
1:A:68[A]:THR:HG22	1:A:255:ARG:NE	2.33	0.43
1:A:164:GLN:HE22	1:E:109[A]:ARG:NH1	2.16	0.43
1:E:140:PRO:HB3	1:E:208:PHE:CD1	2.54	0.42
1:A:297:PRO:HD2	1:A:300:LEU:HD12	2.01	0.42
1:A:673:LYS:CE	10:A:2743:HOH:O	2.67	0.42
1:E:553:VAL:HG13	10:E:2578:HOH:O	2.18	0.42
1:E:659:TYR:CD1	1:E:671:ASP:HB3	2.55	0.42
1:E:4:PHE:O	1:E:7:GLN:HG2	2.20	0.41
1:E:331:HIS:CE1	1:E:365:GLU:OE2	2.63	0.41
1:A:194:ALA:HB1	1:A:455:GLN:HE21	1.85	0.41
1:A:140:PRO:HB3	1:A:208:PHE:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:GLN:NE2	1:A:520:ALA:H	2.09	0.41
1:A:624:ASN:ND2	10:A:2702:HOH:O	2.49	0.41
1:E:415:LYS:HB2	1:E:415:LYS:HE3	1.93	0.41
1:E:553:VAL:CG1	10:E:2578:HOH:O	2.69	0.41
1:A:68[B]:THR:CG2	10:E:2209:HOH:O	2.68	0.40
1:A:33:ALA:O	1:A:37:GLY:HA3	2.21	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:415:LYS:NZ	4:A:1693:NAG:O3[4_455]	1.74	0.46
1:E:129[B]:GLU:OE2	4:A:1693:NAG:O3[4_455]	1.76	0.44
10:A:2150:HOH:O	10:A:2723:HOH:O[2_665]	2.05	0.15
10:A:2769:HOH:O	10:E:2457:HOH:O[4_565]	2.05	0.15
10:A:2156:HOH:O	10:E:2137:HOH:O[4_565]	2.13	0.07

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	692/688 (101%)	672 (97%)	20 (3%)	0	100	100
1	E	689/688 (100%)	672 (98%)	17 (2%)	0	100	100
All	All	1381/1376 (100%)	1344 (97%)	37 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	570/559 (102%)	567 (100%)	3 (0%)	88 83
1	E	567/559 (101%)	564 (100%)	3 (0%)	88 83
All	All	1137/1118 (102%)	1131 (100%)	6 (0%)	88 83

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	PHE
1	A	173	ASP
1	A	284	LYS
1	E	173	ASP
1	E	242	GLU
1	E	506	ASN

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

Mol	Chain	Res	Type
1	A	2	GLN
1	A	26	GLN
1	A	228	HIS
1	A	260	GLN
1	A	263	GLN
1	A	314	ASN
1	A	331	HIS
1	A	455	GLN
1	A	511	HIS
1	A	624	ASN
1	A	650	GLN
1	E	26	GLN
1	E	164	GLN
1	E	228	HIS
1	E	244	GLN
1	E	331	HIS
1	E	455	GLN
1	E	506	ASN
1	E	571	ASN
1	E	624	ASN

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Mol	Chain	Res	Type
1	E	650	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	MHO	A	316	1	6,8,9	4.83	2 (33%)	3,9,11	3.49	2 (66%)
1	MHO	A	569	1	6,8,9	4.39	2 (33%)	3,9,11	2.80	2 (66%)
1	MHO	E	254	1	6,8,9	2.50	1 (16%)	3,9,11	1.34	0
1	MHO	E	193	1	6,8,9	5.01	2 (33%)	3,9,11	3.03	2 (66%)
1	MHO	E	316	1	6,8,9	4.80	2 (33%)	3,9,11	4.12	2 (66%)
1	MHO	A	254	1	6,8,9	5.22	2 (33%)	3,9,11	2.58	2 (66%)
1	MHO	A	193	1	6,8,9	4.86	2 (33%)	3,9,11	2.64	2 (66%)
1	MHO	E	569	1	6,8,9	4.78	2 (33%)	3,9,11	2.43	2 (66%)
1	MHO	E	463	1	6,8,9	4.64	2 (33%)	3,9,11	3.30	2 (66%)
1	MHO	A	463	1	6,8,9	4.59	3 (50%)	3,9,11	2.62	2 (66%)

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
1	MHO	A	316	1	-	1/6/7/9	-
1	MHO	A	569	1	-	2/6/7/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MHO	E	254	1	-	0/6/7/9	-
1	MHO	E	193	1	-	1/6/7/9	-
1	MHO	E	316	1	-	2/6/7/9	-
1	MHO	A	254	1	-	1/6/7/9	-
1	MHO	A	193	1	-	1/6/7/9	-
1	MHO	E	569	1	-	2/6/7/9	-
1	MHO	E	463	1	-	1/6/7/9	-
1	MHO	A	463	1	-	1/6/7/9	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	254	MHO	OD1-SD	11.64	1.84	1.50
1	E	193	MHO	OD1-SD	11.57	1.83	1.50
1	A	316	MHO	OD1-SD	11.21	1.82	1.50
1	E	569	MHO	OD1-SD	11.08	1.82	1.50
1	A	193	MHO	OD1-SD	11.00	1.82	1.50
1	E	316	MHO	OD1-SD	10.94	1.82	1.50
1	E	463	MHO	OD1-SD	10.49	1.80	1.50
1	A	463	MHO	OD1-SD	10.17	1.79	1.50
1	A	569	MHO	OD1-SD	10.09	1.79	1.50
1	E	254	MHO	OD1-SD	5.57	1.66	1.50
1	A	254	MHO	CE-SD	-4.98	1.53	1.77
1	A	193	MHO	CE-SD	-4.29	1.56	1.77
1	E	316	MHO	CE-SD	-4.15	1.57	1.77
1	E	463	MHO	CE-SD	-3.97	1.58	1.77
1	A	463	MHO	CE-SD	-3.90	1.58	1.77
1	E	193	MHO	CE-SD	-3.74	1.59	1.77
1	A	316	MHO	CE-SD	-3.56	1.60	1.77
1	A	569	MHO	CE-SD	-3.37	1.61	1.77
1	E	569	MHO	CE-SD	-3.09	1.62	1.77
1	A	463	MHO	CB-CA	-2.44	1.49	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	316	MHO	OD1-SD-CG	-6.82	88.00	105.89
1	A	316	MHO	OD1-SD-CG	-4.42	94.28	105.89
1	E	463	MHO	OD1-SD-CG	-4.39	94.35	105.89
1	E	193	MHO	OD1-SD-CG	-4.24	94.76	105.89
1	A	316	MHO	CE-SD-CG	4.02	107.50	97.45
1	A	254	MHO	CE-SD-CG	3.88	107.16	97.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	463	MHO	OD1-SD-CG	-3.67	96.26	105.89
1	E	463	MHO	CE-SD-CG	3.57	106.39	97.45
1	A	569	MHO	OD1-SD-CG	-3.56	96.54	105.89
1	A	193	MHO	CE-SD-CG	3.25	105.58	97.45
1	A	569	MHO	CE-SD-CG	3.17	105.38	97.45
1	A	193	MHO	OD1-SD-CG	-3.09	97.78	105.89
1	E	569	MHO	CE-SD-CG	3.09	105.17	97.45
1	E	193	MHO	CE-SD-CG	2.98	104.89	97.45
1	E	569	MHO	OD1-SD-CG	-2.86	98.38	105.89
1	A	463	MHO	CE-SD-CG	2.58	103.91	97.45
1	A	254	MHO	OD1-SD-CG	-2.19	100.14	105.89
1	E	316	MHO	CE-SD-CG	2.10	102.70	97.45

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	569	MHO	CB-CG-SD-OD1
1	E	193	MHO	CB-CG-SD-OD1
1	E	569	MHO	CB-CG-SD-OD1
1	A	193	MHO	CB-CG-SD-OD1
1	A	463	MHO	CB-CG-SD-OD1
1	A	254	MHO	CB-CG-SD-CE
1	A	569	MHO	CA-CB-CG-SD
1	E	569	MHO	CA-CB-CG-SD
1	E	316	MHO	CB-CG-SD-CE
1	A	316	MHO	CB-CG-SD-OD1
1	E	316	MHO	CB-CG-SD-OD1
1	E	463	MHO	CB-CG-SD-OD1

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	193	MHO	2	0
1	E	316	MHO	2	0
1	A	254	MHO	3	0
1	E	463	MHO	3	0
1	A	463	MHO	2	0

5.5 Carbohydrates (i)

2 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	$\#\|Z\| > 2$
2	NAG	B	1	2,1	14,14,15	0.76	0	17,19,21	2.52	9 (52%)
2	NAG	B	2	2	14,14,15	0.74	1 (7%)	17,19,21	1.75	4 (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
2	NAG	B	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	O5-C1	-2.04	1.40	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	NAG	C1-C2-N2	4.65	117.76	110.43
2	B	1	NAG	C4-C3-C2	-4.10	105.00	111.02
2	B	2	NAG	C4-C3-C2	-3.99	105.17	111.02
2	B	1	NAG	C1-O5-C5	3.67	117.11	112.19
2	B	2	NAG	C1-O5-C5	3.62	117.04	112.19
2	B	1	NAG	C6-C5-C4	-3.20	105.16	113.02
2	B	1	NAG	O5-C5-C4	3.01	118.15	110.83
2	B	1	NAG	O7-C7-N2	2.81	126.95	121.98
2	B	1	NAG	O6-C6-C5	-2.60	102.48	111.33
2	B	2	NAG	C6-C5-C4	-2.56	106.73	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	NAG	O5-C1-C2	-2.44	107.52	111.29
2	B	1	NAG	O7-C7-C8	-2.34	117.89	122.05
2	B	1	NAG	C2-N2-C7	2.31	126.00	122.90

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C1-C2-N2-C7
2	B	2	NAG	C1-C2-N2-C7
2	B	1	NAG	O5-C5-C6-O6
2	B	2	NAG	C3-C2-N2-C7

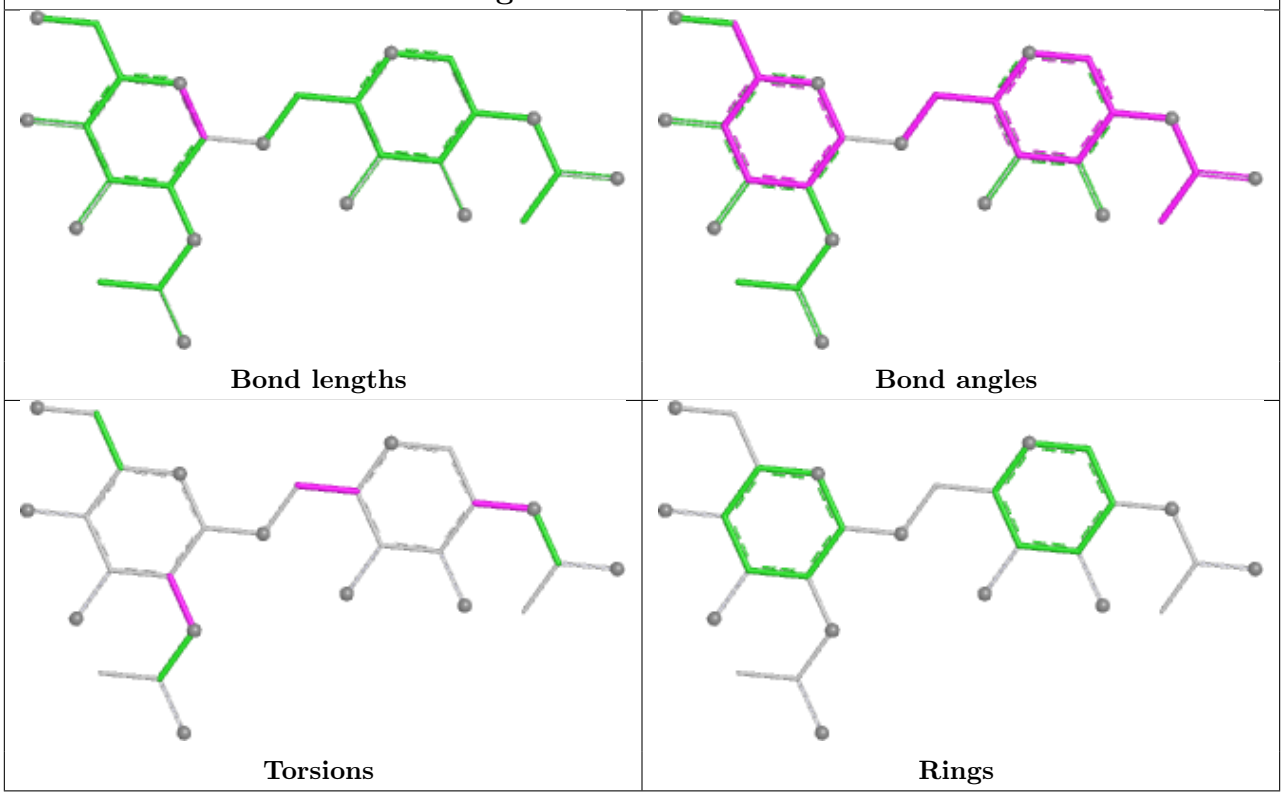
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	1	0
2	B	2	NAG	3	0

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

Oligosaccharide Chain B



5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 8 are monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	ACT	A	1702	-	3,3,3	0.86	0	3,3,3	1.05	0
7	ACT	A	1703	-	3,3,3	1.47	1 (33%)	3,3,3	1.78	1 (33%)
9	MPD	A	1704	-	7,7,7	0.29	0	9,10,10	0.65	0
7	ACT	E	1706	-	3,3,3	0.81	0	3,3,3	1.66	1 (33%)
4	NAG	A	1692	1	14,14,15	0.72	0	17,19,21	2.13	5 (29%)
7	ACT	E	1699	-	3,3,3	1.03	0	3,3,3	0.66	0
4	NAG	E	1693	1	14,14,15	0.55	0	17,19,21	1.22	3 (17%)
7	ACT	A	1700	-	3,3,3	1.16	0	3,3,3	1.71	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	ACT	E	1701	-	3,3,3	0.97	0	3,3,3	1.86	1 (33%)
3	HDD	A	1691	5,1	41,52,52	1.67	8 (19%)	34,89,89	1.58	7 (20%)
7	ACT	E	1704	-	3,3,3	1.04	0	3,3,3	2.76	2 (66%)
8	F50	A	1699	-	4,4,4	2.01	1 (25%)	4,4,4	6.64	2 (50%)
7	ACT	E	1707	-	3,3,3	1.01	0	3,3,3	1.01	0
7	ACT	E	1703	-	3,3,3	0.92	0	3,3,3	1.20	0
7	ACT	E	1712	-	3,3,3	0.92	0	3,3,3	1.19	0
4	NAG	E	1694	1	14,14,15	0.61	0	17,19,21	2.35	4 (23%)
8	F50	E	1700	-	4,4,4	2.04	1 (25%)	4,4,4	7.22	1 (25%)
4	NAG	A	1693	1	14,14,15	0.76	0	17,19,21	1.95	5 (29%)
7	ACT	E	1702	-	3,3,3	1.85	1 (33%)	3,3,3	1.11	0
8	F50	E	1705	-	4,4,4	1.82	1 (25%)	4,4,4	5.50	3 (75%)
7	ACT	A	1698	-	3,3,3	0.57	0	3,3,3	1.29	0
7	ACT	A	1701	-	3,3,3	1.85	1 (33%)	3,3,3	1.17	0
3	HDD	E	1691	5,1	41,52,52	1.81	7 (17%)	34,89,89	1.57	6 (17%)
4	NAG	A	1694	1	14,14,15	0.40	0	17,19,21	1.51	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
4	NAG	E	1693	1	-	2/6/23/26	0/1/1/1
8	F50	A	1699	-	-	0/0/2/2	-
8	F50	E	1705	-	-	0/0/2/2	-
4	NAG	E	1694	1	-	3/6/23/26	0/1/1/1
9	MPD	A	1704	-	-	2/5/5/5	-
3	HDD	A	1691	5,1	-	2/5/89/89	0/1/9/9
3	HDD	E	1691	5,1	-	2/5/89/89	0/1/9/9
8	F50	E	1700	-	-	0/0/2/2	-
4	NAG	A	1694	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1692	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1693	1	-	2/6/23/26	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1691	HDD	C3C-C2C	-4.67	1.34	1.40
3	A	1691	HDD	FE-ND	4.34	2.12	1.95
3	A	1691	HDD	O1D-C3D	-4.30	1.39	1.46
3	E	1691	HDD	C3B-C4B	4.04	1.47	1.41
3	E	1691	HDD	O1D-C3D	-3.88	1.40	1.46
8	E	1700	F50	OXT-C	3.80	1.46	1.35
3	E	1691	HDD	FE-ND	3.77	2.09	1.95
3	E	1691	HDD	C3B-C2B	-3.72	1.35	1.40
8	A	1699	F50	OXT-C	3.67	1.45	1.35
8	E	1705	F50	OXT-C	3.59	1.45	1.35
3	E	1691	HDD	CMD-C2D	3.31	1.57	1.53
3	A	1691	HDD	C3B-CAB	3.26	1.55	1.47
3	A	1691	HDD	C3B-C4B	3.22	1.46	1.41
3	A	1691	HDD	C3C-C2C	-3.08	1.36	1.40
3	A	1691	HDD	C3B-C2B	-2.71	1.36	1.40
7	E	1702	ACT	OXT-C	-2.68	1.18	1.30
3	A	1691	HDD	CMD-C2D	2.63	1.56	1.53
7	A	1701	ACT	OXT-C	-2.58	1.18	1.30
7	A	1703	ACT	OXT-C	-2.40	1.19	1.30
3	E	1691	HDD	C3B-CAB	2.32	1.52	1.47
3	A	1691	HDD	C1C-NC	2.29	1.41	1.36

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	E	1700	F50	OX1-OXT-C	14.29	128.84	110.12
8	A	1699	F50	OX1-OXT-C	12.94	127.07	110.12
8	E	1705	F50	OX1-OXT-C	8.38	121.11	110.12
4	E	1694	NAG	C1-O5-C5	7.14	121.75	112.19
8	E	1705	F50	OXT-C-O	-5.34	117.91	124.12
3	A	1691	HDD	O1D-CGD-O2D	5.06	125.07	120.81
8	E	1705	F50	OXT-C-CH3	4.67	119.42	111.09
4	A	1692	NAG	C3-C4-C5	-4.67	101.77	110.23
4	A	1693	NAG	C1-O5-C5	4.31	117.96	112.19
3	E	1691	HDD	O1D-CGD-O2D	4.02	124.19	120.81
4	A	1694	NAG	C1-O5-C5	3.82	117.30	112.19
4	A	1692	NAG	O5-C5-C4	-3.77	101.65	110.83
3	E	1691	HDD	CMC-C2C-C1C	-3.70	123.03	128.46
4	E	1694	NAG	C4-C3-C2	3.51	116.16	111.02
7	E	1704	ACT	OXT-C-O	-3.50	109.05	122.03
4	A	1692	NAG	O5-C1-C2	-3.46	105.94	111.29
3	E	1691	HDD	CMC-C2C-C3C	3.43	131.53	124.68
4	A	1694	NAG	C1-C2-N2	-3.40	105.08	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1694	NAG	C3-C4-C5	3.37	116.33	110.23
7	E	1704	ACT	OXT-C-CH3	3.27	128.76	115.05
4	A	1692	NAG	O5-C5-C6	3.27	114.02	107.66
4	A	1693	NAG	C3-C4-C5	-3.21	104.42	110.23
4	A	1693	NAG	O5-C5-C4	-3.19	103.06	110.83
4	A	1692	NAG	C4-C3-C2	-3.08	106.50	111.02
3	E	1691	HDD	O1A-CGA-CBA	-2.90	113.89	123.09
4	E	1694	NAG	C1-C2-N2	-2.89	105.89	110.43
4	E	1693	NAG	C1-O5-C5	2.60	115.68	112.19
4	E	1693	NAG	O7-C7-C8	-2.56	117.50	122.05
7	A	1703	ACT	OXT-C-O	-2.51	112.70	122.03
4	A	1693	NAG	C4-C3-C2	2.51	114.69	111.02
3	A	1691	HDD	CMA-C3A-C4A	-2.46	124.85	128.46
7	E	1701	ACT	O-C-CH3	-2.46	112.45	122.53
8	A	1699	F50	OXT-C-CH3	2.33	115.24	111.09
3	A	1691	HDD	CHD-C1D-ND	2.32	127.48	124.28
7	A	1700	ACT	OXT-C-O	-2.29	113.54	122.03
3	A	1691	HDD	C4C-CHD-C1D	-2.25	125.74	130.04
7	E	1706	ACT	OXT-C-O	-2.25	113.69	122.03
3	A	1691	HDD	CAA-CBA-CGA	-2.20	107.92	113.83
3	E	1691	HDD	O2A-CGA-CBA	2.18	120.89	114.00
3	A	1691	HDD	O1D-C3D-CAD	2.18	107.09	103.06
4	A	1693	NAG	C2-N2-C7	-2.18	119.98	122.90
3	E	1691	HDD	CMD-C2D-C1D	-2.16	109.02	112.68
3	A	1691	HDD	CMA-C3A-C2A	2.14	128.97	124.94
4	E	1693	NAG	O7-C7-N2	2.02	125.55	121.98

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1704	MPD	C2-C3-C4-O4
9	A	1704	MPD	C2-C3-C4-C5
4	A	1693	NAG	C4-C5-C6-O6
4	E	1693	NAG	O5-C5-C6-O6
4	E	1693	NAG	C4-C5-C6-O6
4	A	1692	NAG	C8-C7-N2-C2
4	A	1693	NAG	O5-C5-C6-O6
4	A	1692	NAG	O7-C7-N2-C2
4	E	1694	NAG	C4-C5-C6-O6
4	E	1694	NAG	C8-C7-N2-C2
4	E	1694	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	A	1691	HDD	CAA-CBA-CGA-O1A
3	E	1691	HDD	CAA-CBA-CGA-O1A
3	A	1691	HDD	CAA-CBA-CGA-O2A
3	E	1691	HDD	CAA-CBA-CGA-O2A

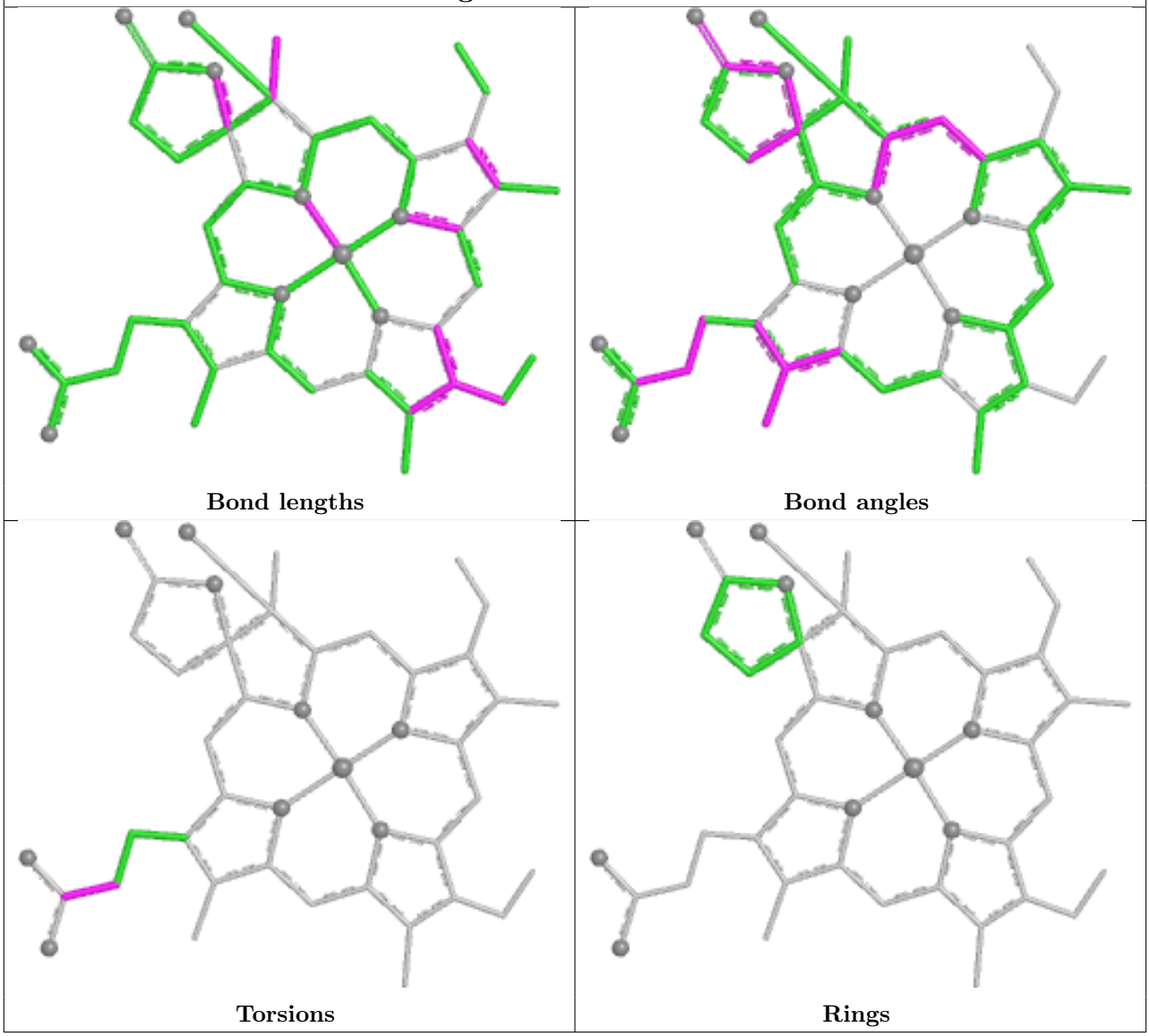
There are no ring outliers.

8 monomers are involved in 29 short contacts:

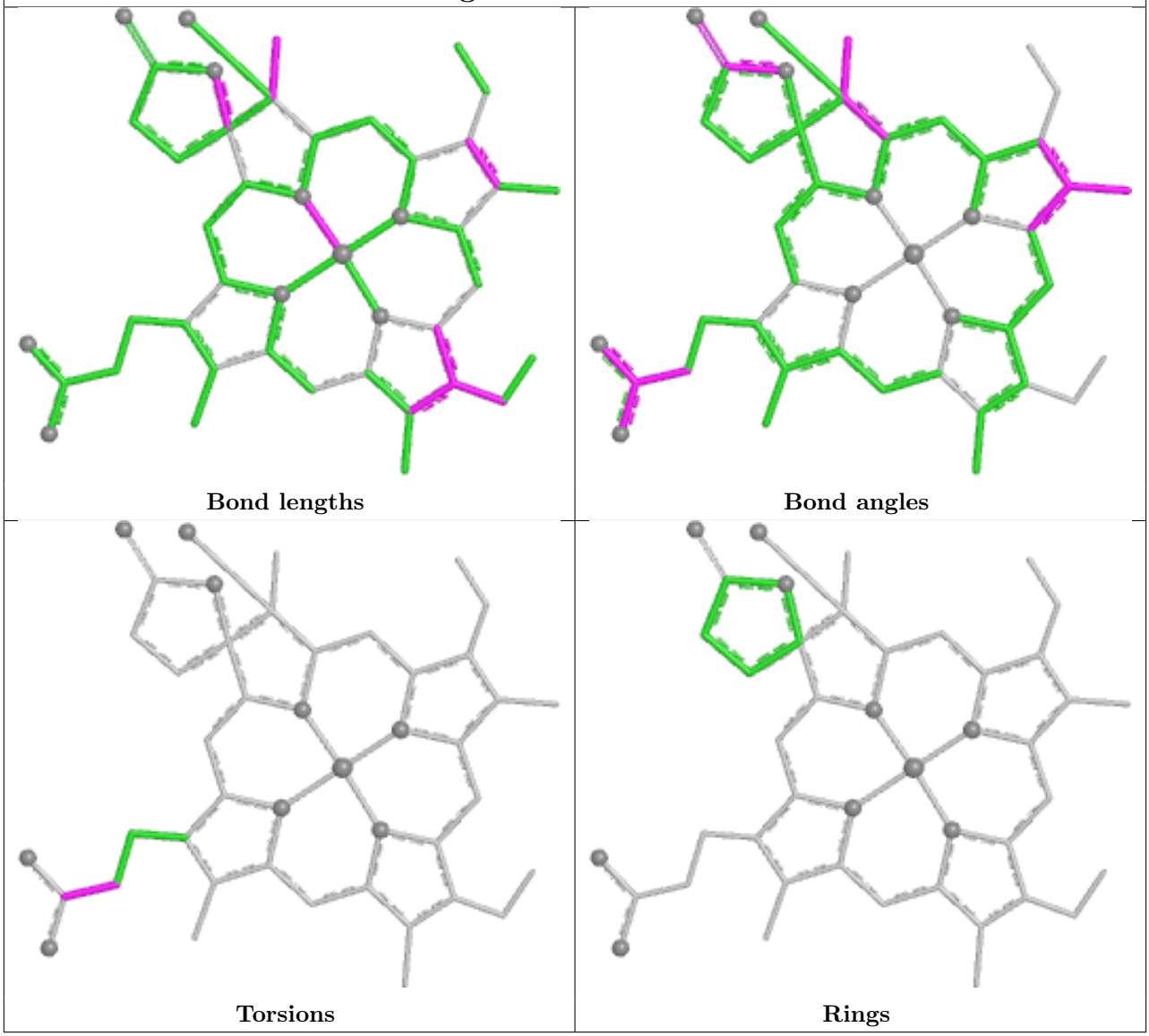
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1704	MPD	6	0
4	A	1692	NAG	4	0
7	A	1700	ACT	1	0
7	E	1701	ACT	4	0
3	A	1691	HDD	1	0
7	E	1707	ACT	5	0
4	A	1693	NAG	5	2
3	E	1691	HDD	1	0

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 then 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 HDD A 1691



Ligand HDD E 1691



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	683/688 (99%)	-0.62	8 (1%)	79	83	8, 13, 22, 37	1 (0%)
1	E	683/688 (99%)	-0.54	10 (1%)	73	78	9, 14, 25, 45	0
All	All	1366/1376 (99%)	-0.58	18 (1%)	77	81	8, 13, 24, 45	1 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	609	ALA	4.8
1	E	612	GLY	4.7
1	E	2	GLN	4.7
1	A	610	GLY	4.5
1	A	609	ALA	4.5
1	E	601	ASP	3.7
1	A	3	GLN	3.4
1	A	611	SER	3.2
1	E	3	GLN	3.1
1	E	689	GLU	3.0
1	A	612	GLY	2.8
1	E	662	LYS	2.6
1	A	689	GLU	2.5
1	E	611	SER	2.3
1	E	610	GLY	2.2
1	E	613	ALA	2.2
1	A	613	ALA	2.1
1	A	608	SER	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	MHO	E	569	9/10	0.95	0.09	17,20,26,26	0
1	MHO	E	316	9/10	0.96	0.07	11,12,23,31	0
1	MHO	A	463	9/10	0.98	0.06	9,11,13,18	0
1	MHO	A	569	9/10	0.98	0.06	16,18,24,25	0
1	MHO	E	193	9/10	0.98	0.05	8,12,15,18	0
1	MHO	E	254	9/10	0.98	0.06	11,11,15,17	0
1	MHO	A	193	9/10	0.98	0.05	8,10,14,21	0
1	MHO	E	463	9/10	0.98	0.06	12,12,15,23	0
1	MHO	A	316	9/10	0.98	0.06	10,11,23,30	0
1	MHO	A	254	9/10	0.99	0.05	11,12,15,19	0

6.3 Carbohydrates (i)

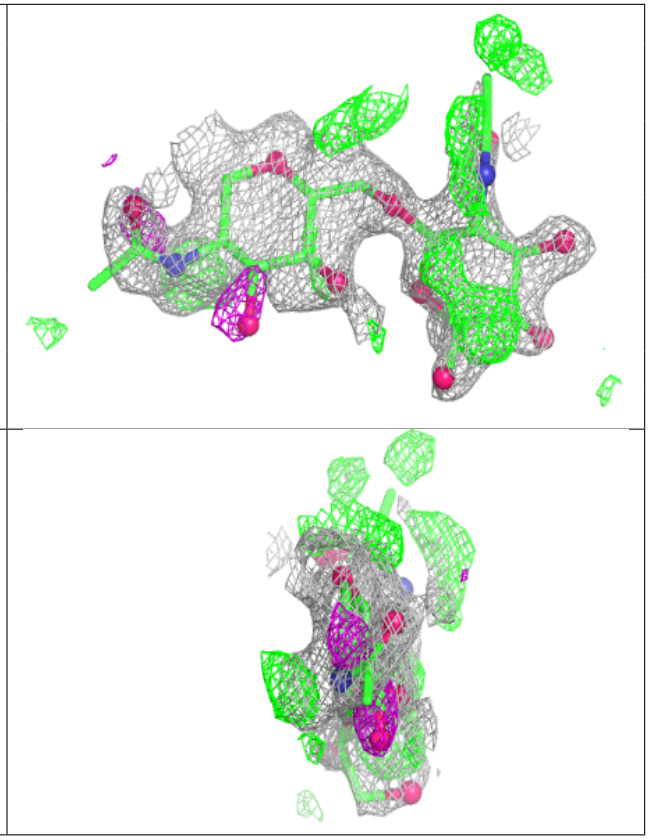
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	B	2	14/15	0.67	0.27	31,37,39,40	14
2	NAG	B	1	14/15	0.73	0.25	36,42,49,50	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.

Electron density around Chain B:

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



6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	F50	E	1705	5/5	0.58	0.23	38,39,39,39	5
4	NAG	E	1694	14/15	0.63	0.40	45,50,54,54	0
7	ACT	E	1707	4/4	0.64	0.35	28,29,30,30	4
4	NAG	A	1694	14/15	0.69	0.42	45,52,55,56	0
4	NAG	A	1693	14/15	0.76	0.28	32,36,39,41	0
4	NAG	E	1693	14/15	0.78	0.33	50,57,59,61	0
4	NAG	A	1692	14/15	0.81	0.21	30,36,43,44	0
7	ACT	A	1700	4/4	0.81	0.17	16,23,24,24	0
7	ACT	E	1706	4/4	0.84	0.23	29,30,31,32	0
8	F50	E	1700	5/5	0.86	0.16	32,32,34,35	0
8	F50	A	1699	5/5	0.86	0.16	31,31,33,35	0
7	ACT	A	1701	4/4	0.88	0.31	26,28,29,29	0
7	ACT	E	1702	4/4	0.91	0.25	28,28,29,29	0
7	ACT	E	1701	4/4	0.91	0.10	22,25,26,26	0

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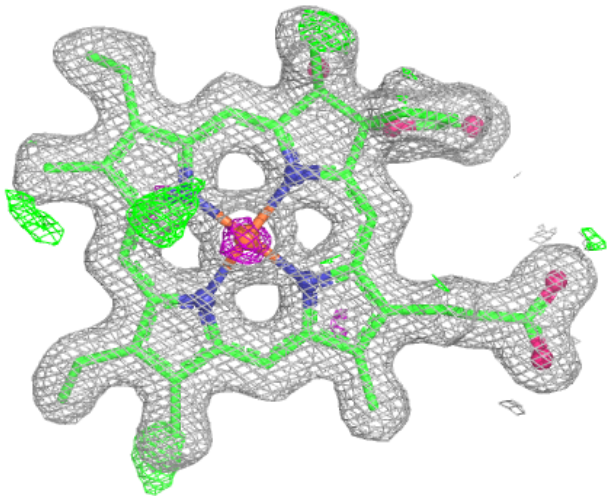
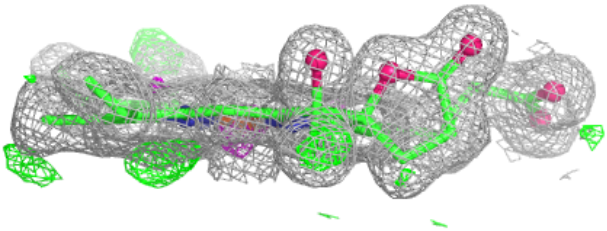
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	ACT	E	1704	4/4	0.93	0.16	22,23,24,25	0
9	MPD	A	1704	8/8	0.93	0.18	23,31,34,38	0
7	ACT	E	1703	4/4	0.94	0.10	20,21,21,22	0
7	ACT	A	1703	4/4	0.95	0.14	24,24,24,25	0
7	ACT	E	1712	4/4	0.95	0.11	46,46,46,46	0
5	O	A	1695	1/1	0.97	0.08	12,12,12,12	0
7	ACT	A	1702	4/4	0.97	0.06	17,18,19,19	0
5	O	E	1696	1/1	0.97	0.09	12,12,12,12	0
7	ACT	E	1699	4/4	0.97	0.06	13,15,16,16	0
3	HDD	A	1691	44/44	0.97	0.07	8,11,14,16	0
6	CA	E	1697	1/1	0.98	0.28	32,32,32,32	0
6	CA	E	1710	1/1	0.98	0.15	35,35,35,35	0
6	CA	E	1711	1/1	0.98	0.23	29,29,29,29	1
7	ACT	A	1698	4/4	0.98	0.04	13,14,15,15	0
3	HDD	E	1691	44/44	0.98	0.06	8,11,16,21	0
6	CA	E	1698	1/1	0.99	0.11	21,21,21,21	0
6	CA	A	1696	1/1	0.99	0.19	23,23,23,23	0
6	CA	A	1697	1/1	1.00	0.10	19,19,19,19	0

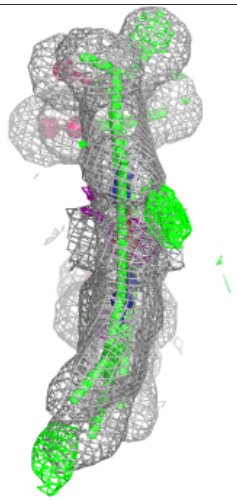
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HDD A 1691:

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

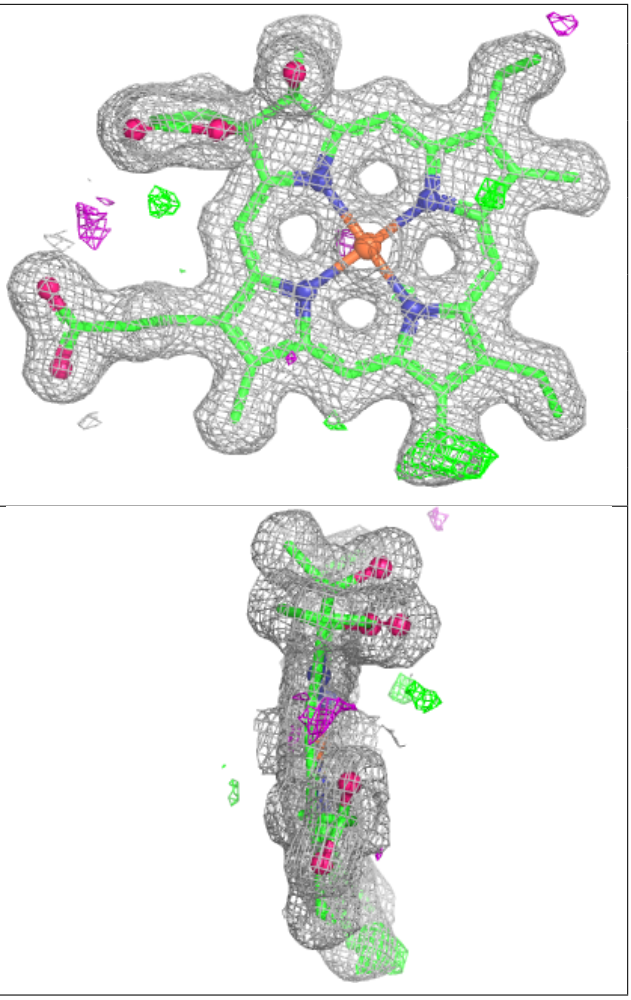






Electron density around HDD E 1691:

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.