



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2020 – 01:01 PM EDT

PDB ID : 6O07
Title : Structure and mechanism of acetylation by the N-terminal dual enzyme NatA/Naa50 complex
Authors : Deng, S.; Marmorstein, R.
Deposited on : 2019-02-15
Resolution : 2.70 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	:	2.14.6
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)	:	2.14.6

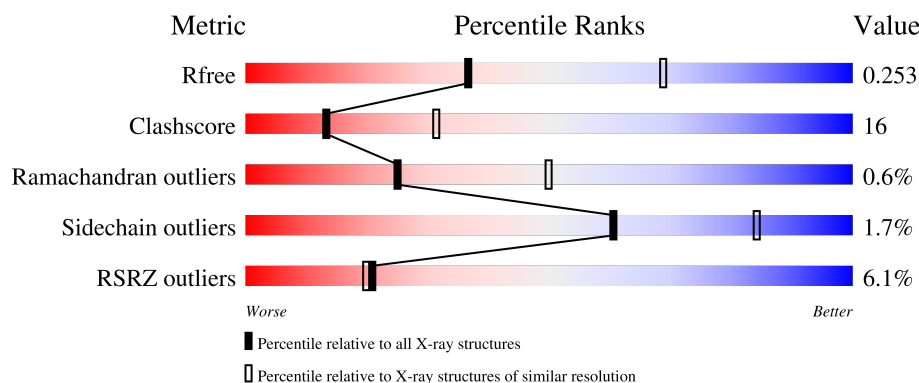
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on 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	C	176	
2	A	854	
3	B	238	

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	CL	B	305	-	-	-	X

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 9036 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 N-terminal acetyltransferase A complex subunit NAT5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	139	Total	C	N	O	S	0	0	0
			982	629	168	181	4			

- Molecule 2 is a protein called Naa15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	763	Total	C	N	O	S	0	0	0
			6110	3935	1015	1137	23			

- Molecule 3 is a protein called N-terminal acetyltransferase A complex catalytic subunit ARD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	199	Total	C	N	O	S	0	0	0
			1560	991	267	291	11			

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

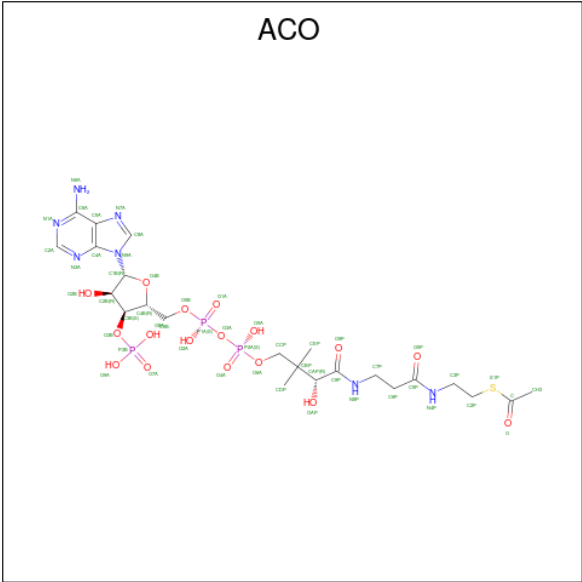
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	6	Total	Cl	0	0
			6	6		
4	A	11	Total	Cl	0	0
			11	11		
4	C	1	Total	Cl	0	0
			1	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



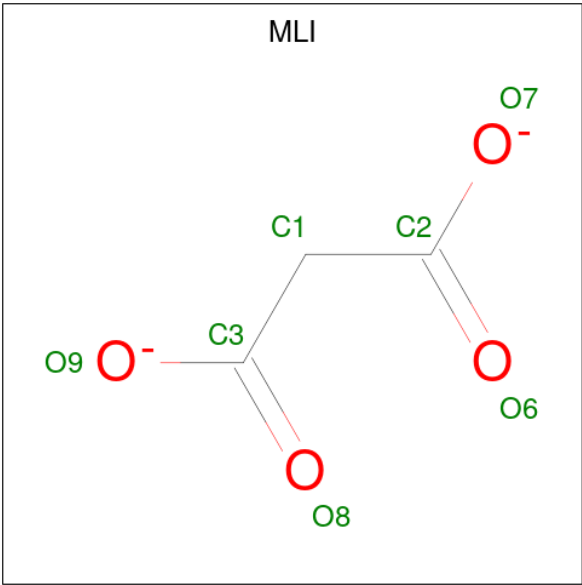
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is ACETYL COENZYME *A (three-letter code: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
6	C	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

- Molecule 7 is MALONATE ION (three-letter code: MLI) (formula: C₃H₂O₄).



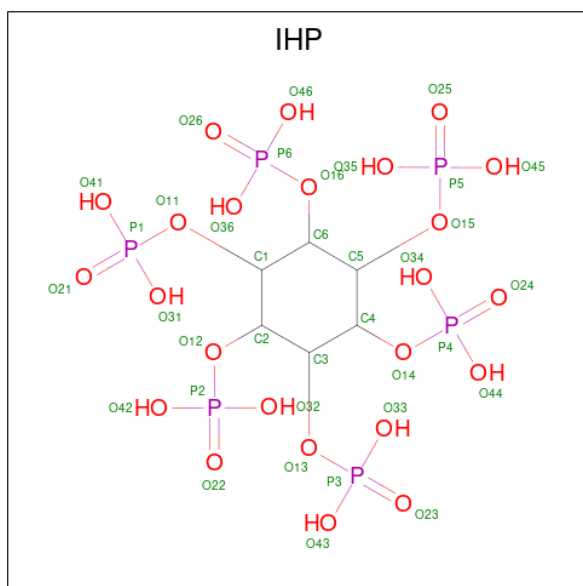
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	3	4		
7	A	1	Total	C	O	0	0
			7	3	4		
7	A	1	Total	C	O	0	0
			7	3	4		

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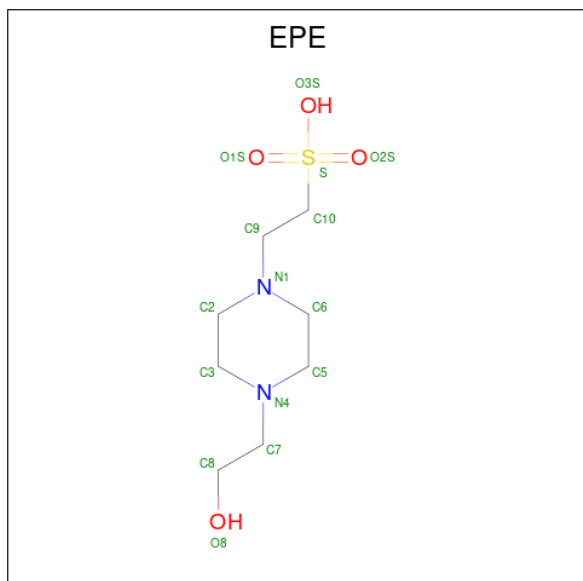
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			7	3	4		

- Molecule 8 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	O	P	0	0
			36	6	24	6		

- Molecule 9 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



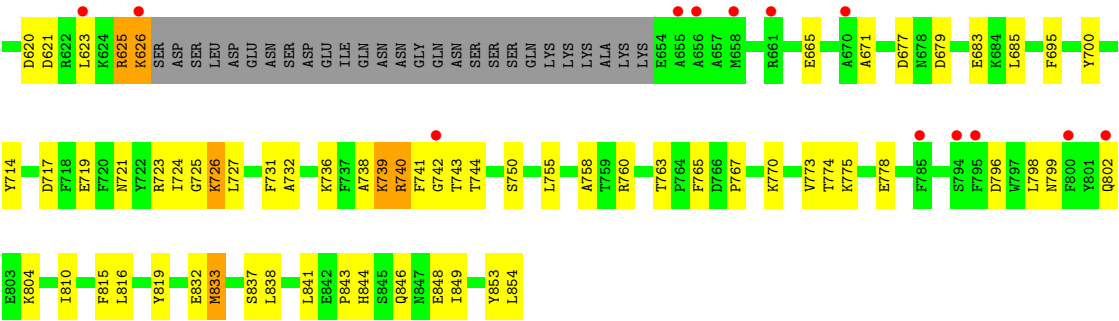
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 10 is water.

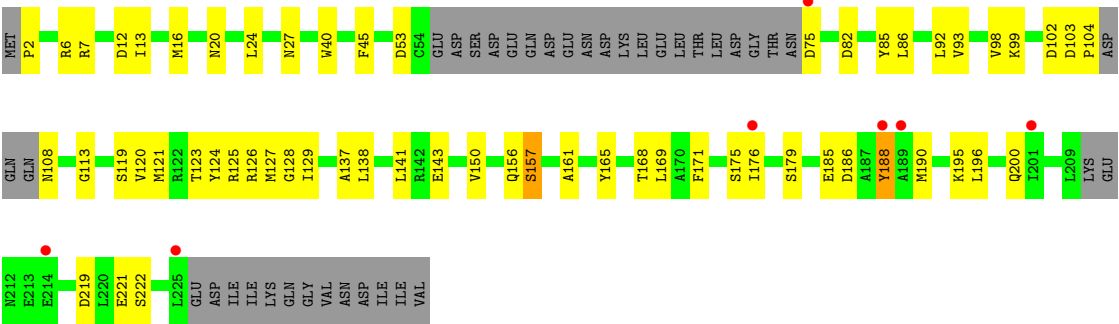
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	C	12	Total	O	0	0
			12	12		
10	A	132	Total	O	0	0
			132	132		
10	B	44	Total	O	0	0
			44	44		

- Molecule 1: N-terminal acetyltransferase A complex subunit NAT5





● Molecule 3: N-terminal acetyltransferase A complex catalytic subunit ARD1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.44Å 125.73Å 145.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.66 – 2.70 47.66 – 2.70	Depositor EDS
% Data completeness (in resolution range)	80.3 (47.66-2.70) 80.4 (47.66-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.222 , 0.250 0.224 , 0.253	Depositor DCC
R_{free} test set	1709 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	54.1	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9036	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CL, IHP, MLI, ACO, EPE

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	C	0.31	0/1002	1.20	9/1363 (0.7%)
2	A	0.28	0/6245	0.57	13/8447 (0.2%)
3	B	0.26	0/1589	0.44	0/2155
All	All	0.28	0/8836	0.65	22/11965 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	151	GLY	N-CA-C	24.34	173.95	113.10
2	A	377	THR	C-N-CA	18.37	167.63	121.70
1	C	13	ALA	CB-CA-C	-16.36	85.55	110.10
1	C	154	VAL	N-CA-C	-13.63	74.20	111.00
2	A	378	GLN	N-CA-CB	13.22	134.40	110.60
1	C	150	VAL	N-CA-C	-12.82	76.39	111.00
2	A	739	LYS	CB-CA-C	12.22	134.83	110.40
2	A	625	ARG	CB-CA-C	-12.20	86.00	110.40
1	C	38	ALA	CB-CA-C	10.94	126.50	110.10
1	C	146	GLY	N-CA-C	-8.42	92.04	113.10
2	A	121	GLY	N-CA-C	7.22	131.16	113.10
2	A	625	ARG	N-CA-C	7.00	129.89	111.00
2	A	740	ARG	CB-CA-C	-6.81	96.77	110.40
2	A	623	LEU	CB-CA-C	6.80	123.13	110.20
2	A	740	ARG	N-CA-C	6.79	129.32	111.00
2	A	626	LYS	N-CA-C	-6.74	92.80	111.00
1	C	28	PRO	N-CA-CB	-6.33	95.63	102.60
1	C	28	PRO	N-CA-C	5.64	126.76	112.10
2	A	540	ILE	CG1-CB-CG2	-5.44	99.43	111.40
2	A	429	LYS	CD-CE-NZ	-5.40	99.28	111.70
2	A	377	THR	CB-CA-C	5.25	125.77	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	154	VAL	CB-CA-C	5.17	121.22	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	982	0	843	53	0
2	A	6110	0	5940	179	0
3	B	1560	0	1500	53	0
4	A	11	0	0	1	0
4	B	6	0	0	2	0
4	C	1	0	0	0	0
5	A	30	0	40	5	0
5	B	12	0	16	0	0
5	C	6	0	8	0	0
6	C	51	0	34	9	0
7	A	21	0	6	1	0
7	B	7	0	2	0	0
8	A	36	0	6	5	0
9	B	15	0	14	3	0
10	A	132	0	0	22	0
10	B	44	0	0	10	0
10	C	12	0	0	5	0
All	All	9036	0	8409	279	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (279) 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)
6:C:203:ACO:O4B	6:C:203:ACO:C1B	1.66	1.23
2:A:140:ASP:OD2	10:A:1001:HOH:O	1.62	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:621:ASP:O	2:A:626:LYS:C	1.85	1.13
2:A:457:LYS:HE3	8:A:920:IHP:O35	1.46	1.13
1:C:153:THR:HG22	1:C:154:VAL:O	1.50	1.12
1:C:130:TYR:CZ	1:C:157:PHE:CZ	2.48	1.00
2:A:621:ASP:C	2:A:626:LYS:O	2.01	0.99
1:C:130:TYR:CZ	1:C:157:PHE:HZ	1.80	0.99
1:C:130:TYR:CE1	1:C:157:PHE:CZ	2.52	0.97
2:A:270:ARG:NH2	3:B:143:GLU:OE2	1.98	0.96
2:A:621:ASP:O	2:A:626:LYS:O	1.82	0.96
2:A:457:LYS:CE	8:A:920:IHP:O35	2.14	0.94
2:A:140:ASP:CG	10:A:1001:HOH:O	1.99	0.94
3:B:219:ASP:OD2	10:B:401:HOH:O	1.84	0.94
2:A:371:LEU:HA	2:A:374:LEU:HD22	1.51	0.91
2:A:521:LEU:HD11	2:A:540:ILE:HD13	1.49	0.91
2:A:377:THR:O	10:A:1002:HOH:O	1.91	0.88
1:C:68:GLU:OE1	3:B:126:ARG:NH2	2.07	0.87
3:B:186:ASP:O	10:B:402:HOH:O	1.92	0.86
2:A:442:GLU:OE2	10:A:1003:HOH:O	1.92	0.85
2:A:495:GLU:OE2	10:A:1004:HOH:O	1.93	0.85
2:A:405:GLU:O	10:A:1006:HOH:O	1.94	0.85
2:A:340:GLY:O	3:B:126:ARG:NH1	2.10	0.84
2:A:537:ALA:O	2:A:540:ILE:HG22	1.78	0.84
2:A:64:LEU:O	10:A:1005:HOH:O	1.93	0.84
1:C:149:GLN:HG2	1:C:150:VAL:O	1.77	0.84
2:A:300:LYS:O	10:A:1007:HOH:O	1.95	0.84
2:A:143:SER:HB2	10:A:1001:HOH:O	1.77	0.83
2:A:140:ASP:OD1	10:A:1001:HOH:O	1.96	0.83
2:A:143:SER:CB	10:A:1001:HOH:O	2.25	0.80
1:C:109:SER:OG	6:C:203:ACO:O1A	1.99	0.80
3:B:108:ASN:N	10:B:403:HOH:O	2.14	0.78
1:C:130:TYR:CE1	1:C:157:PHE:CE1	2.71	0.78
2:A:700:TYR:OH	2:A:717:ASP:OD1	2.05	0.75
2:A:216:ALA:HB2	2:A:222:LYS:HD2	1.69	0.75
2:A:518:LEU:HD12	2:A:540:ILE:CD1	2.18	0.74
2:A:118:LEU:HD23	2:A:122:SER:HB3	1.69	0.73
2:A:549:LYS:NZ	2:A:665:GLU:OE2	2.20	0.73
1:C:130:TYR:CE2	1:C:157:PHE:CZ	2.77	0.73
1:C:130:TYR:CE2	1:C:157:PHE:HZ	2.05	0.73
1:C:104:HIS:HA	6:C:203:ACO:H52A	1.72	0.72
2:A:69:GLU:N	10:A:1005:HOH:O	2.24	0.70
3:B:20:ASN:ND2	10:B:406:HOH:O	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:157:SER:HB3	3:B:185:GLU:OE2	1.93	0.68
2:A:514:ARG:NH1	10:A:1012:HOH:O	2.27	0.68
1:C:77:LYS:O	1:C:92:GLN:N	2.27	0.67
2:A:286:GLY:HA2	2:A:288:GLN:HE21	1.60	0.67
3:B:93:VAL:HA	3:B:121:MET:HE3	1.76	0.67
1:C:139:LYS:O	1:C:143:ILE:N	2.27	0.67
2:A:841:LEU:O	2:A:846:GLN:NE2	2.28	0.67
2:A:220:GLN:HG3	2:A:254:LEU:HD23	1.78	0.66
1:C:149:GLN:CG	1:C:150:VAL:O	2.43	0.66
2:A:370:TYR:O	2:A:374:LEU:HD13	1.95	0.66
2:A:620:ASP:OD2	2:A:723:ARG:NH2	2.29	0.65
1:C:29:ASN:OD1	1:C:161:VAL:N	2.19	0.65
2:A:719:GLU:OE2	2:A:819:TYR:OH	2.07	0.65
1:C:60:PHE:N	10:C:303:HOH:O	2.29	0.65
2:A:89:ALA:O	2:A:120:ASN:ND2	2.27	0.64
1:C:130:TYR:CD1	1:C:157:PHE:CZ	2.84	0.64
3:B:185:GLU:HG2	10:B:402:HOH:O	1.97	0.64
2:A:518:LEU:CD1	2:A:540:ILE:CD1	2.76	0.63
1:C:30:LEU:HA	1:C:160:GLY:HA2	1.79	0.63
3:B:138:LEU:HD22	3:B:150:VAL:HG11	1.80	0.63
2:A:472:VAL:HG22	2:A:488:ILE:HD11	1.80	0.63
1:C:24:HIS:O	1:C:28:PRO:HB3	1.97	0.63
2:A:518:LEU:HD12	2:A:540:ILE:HD12	1.81	0.63
2:A:804:LYS:NZ	10:A:1017:HOH:O	2.31	0.63
2:A:615:TYR:CG	2:A:695:PHE:HB2	2.34	0.62
2:A:426:ARG:HD2	8:A:920:IHP:O25	1.99	0.61
2:A:220:GLN:NE2	2:A:253:LYS:O	2.34	0.61
1:C:61:THR:O	1:C:62:GLN:NE2	2.35	0.60
2:A:521:LEU:CD1	2:A:540:ILE:HD13	2.29	0.60
1:C:33:ASP:O	10:C:301:HOH:O	2.17	0.59
3:B:86:LEU:HD11	3:B:92:LEU:HB2	1.85	0.59
1:C:13:ALA:HB2	1:C:40:PHE:CG	2.38	0.59
2:A:149:LYS:NZ	10:A:1014:HOH:O	2.30	0.59
1:C:24:HIS:O	1:C:28:PRO:CB	2.51	0.59
2:A:462:PHE:HE1	5:A:913:GOL:H32	1.69	0.58
2:A:518:LEU:CD1	2:A:540:ILE:HD11	2.34	0.58
2:A:549:LYS:HE2	2:A:550:TYR:CE1	2.39	0.58
1:C:18:MET:HE1	2:A:447:LEU:HD13	1.86	0.58
2:A:518:LEU:CD1	2:A:540:ILE:HD12	2.33	0.58
2:A:767:PRO:HA	2:A:770:LYS:HD2	1.86	0.57
2:A:457:LYS:NZ	8:A:920:IHP:O15	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:724:ILE:HG13	2:A:726:LYS:HG2	1.87	0.57
3:B:98:VAL:HG21	3:B:137:ALA:HB1	1.87	0.57
3:B:125:ARG:HH11	3:B:126:ARG:NH2	2.01	0.57
2:A:848:GLU:OE1	5:A:916:GOL:O3	2.22	0.56
2:A:282:GLU:OE1	2:A:298:TYR:OH	2.13	0.56
2:A:562:PRO:O	2:A:566:LYS:HG3	2.05	0.56
2:A:727:LEU:HB3	2:A:773:VAL:HG21	1.88	0.55
1:C:12:TYR:O	1:C:14:ASN:N	2.38	0.55
2:A:721:ASN:HA	2:A:724:ILE:HG12	1.88	0.55
2:A:798:LEU:HD21	2:A:833:MET:HE1	1.87	0.55
2:A:617:GLN:NE2	2:A:621:ASP:OD2	2.34	0.55
2:A:518:LEU:HD12	2:A:540:ILE:HD11	1.87	0.54
3:B:20:ASN:HD21	3:B:27:ASN:HA	1.72	0.54
1:C:145:HIS:O	1:C:146:GLY:C	2.46	0.54
2:A:55:ASP:OD2	2:A:93:CYS:HB2	2.08	0.54
1:C:24:HIS:C	1:C:28:PRO:HB3	2.27	0.54
1:C:106:SER:O	1:C:110:LYS:HE3	2.08	0.54
2:A:352:TYR:O	2:A:356:LYS:HB2	2.08	0.53
3:B:219:ASP:OD1	3:B:219:ASP:N	2.41	0.53
1:C:131:LEU:O	1:C:169:ILE:N	2.38	0.53
2:A:64:LEU:O	2:A:67:VAL:HG22	2.09	0.53
3:B:120:VAL:HG11	9:B:310:EPE:H61	1.90	0.53
2:A:407:ILE:HD13	2:A:423:LEU:HD23	1.91	0.53
2:A:445:ARG:HB3	10:A:1003:HOH:O	2.07	0.53
2:A:286:GLY:HA2	2:A:288:GLN:NE2	2.22	0.52
2:A:732:ALA:N	10:A:1008:HOH:O	2.20	0.52
2:A:280:LEU:O	2:A:283:VAL:HG12	2.09	0.52
2:A:168:ALA:O	2:A:172:ASN:ND2	2.31	0.52
2:A:423:LEU:O	2:A:427:ILE:HG13	2.10	0.52
3:B:221:GLU:HB2	10:B:401:HOH:O	2.10	0.52
2:A:354:ARG:NH1	3:B:53:ASP:OD1	2.43	0.51
3:B:168:THR:HG21	4:B:306:CL:CL	2.47	0.51
3:B:196:LEU:O	3:B:200:GLN:HG2	2.11	0.51
3:B:82:ASP:HB3	3:B:85:TYR:HD1	1.76	0.51
3:B:165:TYR:O	3:B:171:PHE:HB2	2.11	0.51
2:A:117:ALA:O	2:A:122:SER:HB2	2.11	0.50
2:A:798:LEU:HD21	2:A:833:MET:CE	2.41	0.50
3:B:82:ASP:HB3	3:B:85:TYR:CD1	2.46	0.50
2:A:177:GLN:OE1	2:A:177:GLN:N	2.37	0.50
3:B:128:GLY:H	9:B:310:EPE:H82	1.76	0.50
1:C:108:GLY:N	6:C:203:ACO:O2A	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:742:GLY:C	2:A:744:THR:H	2.14	0.50
2:A:60:LYS:O	2:A:64:LEU:HB2	2.12	0.50
3:B:113:GLY:HA3	3:B:141:LEU:HD13	1.94	0.50
2:A:283:VAL:HA	2:A:288:GLN:HG2	1.93	0.50
2:A:424:LYS:HG2	2:A:440:ILE:HG21	1.93	0.50
2:A:774:THR:O	2:A:778:GLU:HG3	2.11	0.50
2:A:183:SER:O	2:A:187:LYS:HD3	2.11	0.49
3:B:102:ASP:HB2	10:B:404:HOH:O	2.12	0.49
3:B:13:ILE:HA	3:B:16:MET:HB2	1.94	0.49
2:A:224:GLN:HG3	2:A:228:LYS:HE3	1.95	0.49
2:A:796:ASP:OD1	2:A:799:ASN:N	2.32	0.49
3:B:99:LYS:NZ	10:B:404:HOH:O	2.21	0.49
1:C:18:MET:O	1:C:22:LEU:HD12	2.12	0.49
2:A:445:ARG:NE	10:A:1003:HOH:O	2.45	0.49
2:A:765:PHE:HB2	2:A:770:LYS:HE2	1.93	0.49
2:A:294:LYS:HB3	2:A:318:PHE:CZ	2.48	0.49
2:A:354:ARG:NH1	3:B:75:ASP:O	2.46	0.49
2:A:333:VAL:HG12	2:A:348:VAL:HG11	1.94	0.49
2:A:738:ALA:O	2:A:739:LYS:C	2.52	0.49
2:A:376:PRO:HB3	2:A:383:PHE:CE2	2.47	0.49
2:A:429:LYS:HG3	2:A:430:HIS:N	2.28	0.49
2:A:517:LYS:O	2:A:521:LEU:HD23	2.13	0.48
1:C:30:LEU:HD22	1:C:30:LEU:H	1.78	0.48
3:B:7:ARG:HG2	3:B:45:PHE:CE2	2.49	0.48
2:A:352:TYR:HB3	2:A:396:PHE:CE2	2.48	0.48
2:A:760:ARG:O	2:A:770:LYS:NZ	2.47	0.48
2:A:327:LYS:O	2:A:331:GLU:HG3	2.14	0.48
2:A:555:LEU:HD23	2:A:685:LEU:HB3	1.95	0.48
3:B:24:LEU:HD11	3:B:119:SER:HB2	1.96	0.48
2:A:270:ARG:HH22	3:B:143:GLU:CD	2.13	0.47
2:A:740:ARG:HB3	2:A:741:PHE:CD1	2.49	0.47
1:C:130:TYR:CG	1:C:157:PHE:CE2	3.02	0.47
2:A:84:ILE:CD1	2:A:89:ALA:HB2	2.45	0.47
2:A:315:PRO:HA	2:A:318:PHE:CZ	2.49	0.47
3:B:6:ARG:NH1	3:B:12:ASP:OD2	2.40	0.47
1:C:103:ARG:HD3	6:C:203:ACO:H10	1.96	0.47
2:A:442:GLU:OE1	2:A:470:LYS:NZ	2.44	0.47
2:A:504:ALA:HB2	2:A:557:ARG:HB2	1.97	0.47
3:B:179:SER:OG	3:B:179:SER:O	2.29	0.47
2:A:229:HIS:O	2:A:233:ILE:HG12	2.15	0.47
2:A:431:LEU:HA	2:A:843:PRO:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:165:TYR:O	3:B:169:LEU:HB2	2.15	0.46
2:A:295:LYS:HG3	2:A:296:ALA:N	2.29	0.46
2:A:485:VAL:HG13	2:A:486:ASN:H	1.79	0.46
2:A:810:ILE:HD13	2:A:838:LEU:HD23	1.97	0.46
2:A:439:GLY:HA2	5:A:913:GOL:H12	1.96	0.46
1:C:139:LYS:NZ	1:C:169:ILE:HG21	2.30	0.46
1:C:130:TYR:CD2	1:C:157:PHE:CE2	3.04	0.46
2:A:175:ARG:O	2:A:179:ILE:HG13	2.16	0.46
2:A:507:TYR:HB3	2:A:554:ALA:HB2	1.97	0.46
2:A:200:GLU:HG3	2:A:583:GLY:HA3	1.98	0.46
2:A:741:PHE:N	2:A:741:PHE:CD1	2.83	0.46
8:A:920:IHP:O25	8:A:920:IHP:H6	2.15	0.46
1:C:104:HIS:HA	6:C:203:ACO:C5B	2.44	0.46
1:C:31:TYR:HA	10:C:310:HOH:O	2.15	0.46
2:A:273:ASP:OD1	2:A:307:ARG:NH1	2.48	0.46
2:A:61:GLY:O	2:A:65:TYR:N	2.34	0.46
3:B:156:GLN:N	10:B:402:HOH:O	2.10	0.46
3:B:171:PHE:HB3	3:B:190:MET:HE2	1.98	0.46
2:A:159:ARG:HD2	2:A:185:PHE:CE1	2.51	0.46
2:A:279:LYS:HA	2:A:282:GLU:HG3	1.97	0.46
2:A:535:GLN:C	2:A:537:ALA:H	2.19	0.46
2:A:714:TYR:CZ	2:A:736:LYS:HB3	2.51	0.46
3:B:127:MET:HE2	3:B:129:ILE:HD11	1.98	0.46
1:C:98:VAL:HG21	1:C:108:GLY:HA2	1.97	0.45
2:A:411:LEU:HG	2:A:420:PHE:HB3	1.98	0.45
1:C:132:PRO:O	10:C:302:HOH:O	2.21	0.45
2:A:224:GLN:O	2:A:228:LYS:HG2	2.17	0.45
2:A:246:ARG:O	2:A:250:ILE:HG13	2.16	0.45
2:A:445:ARG:HB2	2:A:454:ILE:HG22	1.97	0.45
2:A:740:ARG:HB3	2:A:741:PHE:H	1.67	0.45
1:C:36:PHE:N	10:C:301:HOH:O	2.48	0.45
2:A:621:ASP:HB3	2:A:626:LYS:O	2.17	0.45
2:A:250:ILE:O	2:A:254:LEU:N	2.42	0.45
2:A:428:LEU:HD13	2:A:436:THR:HG22	1.99	0.45
3:B:124:TYR:HB3	3:B:129:ILE:HD12	1.99	0.44
2:A:549:LYS:HE2	2:A:550:TYR:HE1	1.81	0.44
2:A:679:ASP:OD1	2:A:683:GLU:N	2.50	0.44
2:A:216:ALA:CB	2:A:222:LYS:HD2	2.45	0.44
2:A:403:ALA:HB1	2:A:427:ILE:HD13	1.98	0.44
2:A:246:ARG:HG2	2:A:246:ARG:HH11	1.83	0.44
3:B:188:TYR:O	3:B:190:MET:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:402:LYS:HA	2:A:405:GLU:HB3	1.99	0.44
2:A:492:HIS:CD2	2:A:671:ALA:HB1	2.53	0.44
1:C:109:SER:H	6:C:203:ACO:P1A	2.40	0.44
2:A:838:LEU:HD21	2:A:849:ILE:HG21	2.00	0.44
2:A:374:LEU:HD23	2:A:383:PHE:HA	2.00	0.43
2:A:615:TYR:CD2	2:A:695:PHE:HB2	2.53	0.43
2:A:750:SER:HB2	2:A:815:PHE:HD2	1.82	0.43
2:A:209:ASN:ND2	2:A:226:VAL:HG23	2.33	0.43
3:B:123:THR:HG23	3:B:124:TYR:CD2	2.54	0.43
2:A:329:LEU:HD13	2:A:363:LEU:HG	2.00	0.43
1:C:130:TYR:CD2	1:C:157:PHE:CZ	3.05	0.43
1:C:69:ILE:HG12	2:A:417:LEU:HD21	2.01	0.43
2:A:441:LEU:HD21	2:A:457:LYS:HG3	1.98	0.43
2:A:549:LYS:CE	2:A:665:GLU:OE2	2.66	0.43
2:A:853:TYR:O	2:A:854:LEU:HD23	2.19	0.43
2:A:201:HIS:NE2	7:A:919:MLI:O7	2.49	0.43
3:B:222:SER:N	10:B:401:HOH:O	2.36	0.43
2:A:313:PHE:CZ	3:B:2:PRO:HD3	2.54	0.43
2:A:225:ASN:ND2	2:A:225:ASN:O	2.52	0.42
2:A:336:GLN:HB3	2:A:341:VAL:CG1	2.49	0.42
1:C:109:SER:HA	6:C:203:ACO:H2A	2.01	0.42
1:C:16:LEU:HD21	1:C:36:PHE:O	2.19	0.42
2:A:201:HIS:O	2:A:205:LEU:HG	2.19	0.42
2:A:84:ILE:HD12	2:A:89:ALA:HB2	2.00	0.42
3:B:175:SER:OG	3:B:176:ILE:N	2.53	0.42
1:C:101:ASN:O	10:A:1002:HOH:O	2.21	0.42
2:A:283:VAL:HA	2:A:288:GLN:CG	2.49	0.42
2:A:333:VAL:CG1	2:A:348:VAL:HG11	2.50	0.42
2:A:758:ALA:HA	2:A:763:THR:HG21	2.01	0.42
6:C:203:ACO:H61	6:C:203:ACO:H32	1.71	0.42
2:A:273:ASP:OD1	10:A:1009:HOH:O	2.21	0.42
3:B:40:TRP:CZ3	3:B:99:LYS:HB2	2.55	0.42
1:C:125:HIS:O	1:C:174:HIS:HA	2.20	0.42
1:C:98:VAL:HG21	1:C:108:GLY:CA	2.49	0.42
2:A:731:PHE:HB2	2:A:755:LEU:HD21	2.01	0.42
3:B:103:ASP:HA	3:B:104:PRO:HD3	1.95	0.42
2:A:124:ASN:O	2:A:127:ILE:HG13	2.19	0.42
2:A:371:LEU:HB2	2:A:386:THR:HG21	2.01	0.42
3:B:161:ALA:HB2	4:B:305:CL:CL	2.56	0.42
2:A:612:SER:OG	4:A:908:CL:CL	2.73	0.42
3:B:141:LEU:HA	3:B:141:LEU:HD23	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:725:GLY:O	2:A:727:LEU:N	2.53	0.41
2:A:64:LEU:CD2	2:A:69:GLU:HB2	2.50	0.41
2:A:442:GLU:HA	10:A:1003:HOH:O	2.20	0.41
2:A:810:ILE:HD11	2:A:837:SER:O	2.21	0.41
2:A:267:LEU:HB3	2:A:277:TYR:CD2	2.55	0.41
1:C:127:VAL:O	1:C:127:VAL:HG13	2.20	0.41
1:C:170:LEU:C	1:C:171:LEU:HD12	2.41	0.41
2:A:287:ILE:H	2:A:287:ILE:HG13	1.62	0.41
2:A:775:LYS:HB2	2:A:775:LYS:HE3	1.61	0.41
2:A:509:ARG:HD3	5:A:916:GOL:H2	2.01	0.41
2:A:222:LYS:O	2:A:222:LYS:HD3	2.21	0.41
2:A:844:HIS:CE1	5:A:916:GOL:H32	2.56	0.41
2:A:156:LEU:HA	2:A:156:LEU:HD23	1.86	0.41
2:A:457:LYS:HD3	10:A:1110:HOH:O	2.20	0.41
2:A:556:LYS:HZ1	2:A:677:ASP:CG	2.24	0.41
3:B:156:GLN:HA	3:B:188:TYR:CE2	2.56	0.41
1:C:100:PRO:HA	1:C:103:ARG:HG3	2.03	0.41
2:A:252:MET:SD	2:A:257:LEU:HD22	2.61	0.41
3:B:195:LYS:HB3	3:B:195:LYS:HE2	1.69	0.41
2:A:457:LYS:HD2	2:A:460:LYS:HE2	2.04	0.40
2:A:750:SER:HA	2:A:816:LEU:HD21	2.03	0.40
2:A:160:ALA:O	2:A:164:SER:OG	2.32	0.40
2:A:92:ILE:HD12	2:A:92:ILE:H	1.86	0.40
3:B:126:ARG:HA	9:B:310:EPE:H81	1.90	0.40
2:A:268:ILE:HD11	2:A:278:TYR:HA	2.03	0.40
2:A:742:GLY:C	2:A:744:THR:N	2.74	0.40
3:B:121:MET:HE3	3:B:121:MET:HB2	1.97	0.40
2:A:223:LEU:HA	2:A:226:VAL:HG12	2.03	0.40
2:A:479:THR:OG1	2:A:481:ASN:ND2	2.54	0.40
1:C:65:TYR:CE1	1:C:70:PRO:HG3	2.56	0.40
2:A:290:ASP:OD2	2:A:293:LEU:HD12	2.22	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	C	133/176 (76%)	112 (84%)	19 (14%)	2 (2%)	10	26
2	A	755/854 (88%)	710 (94%)	41 (5%)	4 (0%)	29	54
3	B	191/238 (80%)	180 (94%)	11 (6%)	0	100	100
All	All	1079/1268 (85%)	1002 (93%)	71 (7%)	6 (1%)	25	50

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	13	ALA
1	C	31	TYR
2	A	743	THR
2	A	625	ARG
2	A	726	LYS
2	A	287	ILE

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	C	84/153 (55%)	83 (99%)	1 (1%)	71	88
2	A	639/760 (84%)	627 (98%)	12 (2%)	57	82
3	B	163/216 (76%)	161 (99%)	2 (1%)	71	88
All	All	886/1129 (78%)	871 (98%)	15 (2%)	60	84

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	28	PRO
2	A	90	SER
2	A	93	CYS
2	A	187	LYS

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Mol	Chain	Res	Type
2	A	241	PHE
2	A	338	LYS
2	A	358	LYS
2	A	424	LYS
2	A	511	TYR
2	A	603	MET
2	A	802	GLN
2	A	832	GLU
2	A	833	MET
3	B	157	SER
3	B	188	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	225	ASN
2	A	288	GLN
2	A	481	ASN
2	A	844	HIS
3	B	20	ASN
3	B	206	HIS
3	B	212	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 18 are monoatomic - leaving 15 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	MLI	A	917	-	0,6,6	0.00	-	0,7,7	0.00	-
7	MLI	A	918	-	0,6,6	0.00	-	0,7,7	0.00	-
5	GOL	A	912	-	5,5,5	0.91	0	5,5,5	0.98	0
5	GOL	A	915	-	5,5,5	0.88	0	5,5,5	1.00	0
5	GOL	B	308	-	5,5,5	0.96	0	5,5,5	1.00	0
5	GOL	A	913	-	5,5,5	0.89	0	5,5,5	0.99	0
6	ACO	C	203	-	45,53,53	4.00	18 (40%)	56,79,79	2.21	11 (19%)
5	GOL	C	202	-	5,5,5	0.89	0	5,5,5	1.03	0
7	MLI	A	919	-	0,6,6	0.00	-	0,7,7	0.00	-
8	IHP	A	920	-	36,36,36	1.63	6 (16%)	54,60,60	1.60	9 (16%)
9	EPE	B	310	-	15,15,15	0.83	1 (6%)	18,20,20	1.89	6 (33%)
7	MLI	B	309	-	0,6,6	0.00	-	0,7,7	0.00	-
5	GOL	B	307	-	5,5,5	0.93	0	5,5,5	0.97	0
5	GOL	A	914	-	5,5,5	0.84	0	5,5,5	0.93	0
5	GOL	A	916	-	5,5,5	0.89	0	5,5,5	0.97	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
7	MLI	A	917	-	-	0/0/4/4	-
7	MLI	A	918	-	-	0/0/4/4	-
5	GOL	A	912	-	-	3/4/4/4	-
5	GOL	A	915	-	-	2/4/4/4	-
5	GOL	B	308	-	-	0/4/4/4	-
5	GOL	A	913	-	-	2/4/4/4	-
6	ACO	C	203	-	-	20/47/67/67	0/3/3/3
5	GOL	C	202	-	-	1/4/4/4	-
7	MLI	A	919	-	-	0/0/4/4	-
8	IHP	A	920	-	-	14/30/54/54	0/1/1/1
9	EPE	B	310	-	-	7/9/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MLI	B	309	-	-	0/0/4/4	-
5	GOL	B	307	-	-	4/4/4/4	-
5	GOL	A	914	-	-	1/4/4/4	-
5	GOL	A	916	-	-	2/4/4/4	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	203	ACO	O4B-C1B	17.94	1.66	1.41
6	C	203	ACO	C2B-C1B	-12.57	1.34	1.53
6	C	203	ACO	C5P-N4P	7.26	1.49	1.33
6	C	203	ACO	O4B-C4B	-6.45	1.30	1.45
6	C	203	ACO	C9P-N8P	5.64	1.45	1.33
8	A	920	IHP	P2-O12	5.03	1.68	1.59
6	C	203	ACO	C6A-N6A	3.50	1.46	1.34
8	A	920	IHP	P3-O13	3.48	1.65	1.59
8	A	920	IHP	P5-O15	3.34	1.65	1.59
6	C	203	ACO	C6P-C5P	3.30	1.57	1.51
6	C	203	ACO	P3B-O3B	3.17	1.65	1.59
6	C	203	ACO	O3B-C3B	-3.12	1.32	1.44
8	A	920	IHP	P6-O16	3.12	1.65	1.59
6	C	203	ACO	P2A-O6A	2.96	1.71	1.59
6	C	203	ACO	O5P-C5P	-2.84	1.17	1.23
9	B	310	EPE	C10-S	2.73	1.81	1.77
6	C	203	ACO	C3B-C4B	2.67	1.60	1.52
8	A	920	IHP	C4-C3	2.31	1.57	1.52
6	C	203	ACO	C2A-N3A	2.25	1.35	1.32
6	C	203	ACO	C5A-C4A	-2.15	1.35	1.40
6	C	203	ACO	O2B-C2B	2.12	1.48	1.43
6	C	203	ACO	OAP-CAP	-2.08	1.38	1.42
6	C	203	ACO	P1A-O5B	2.06	1.67	1.59
8	A	920	IHP	C5-C4	2.06	1.56	1.52
6	C	203	ACO	C2A-N1A	2.06	1.37	1.33

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	203	ACO	C5A-C6A-N6A	9.97	135.50	120.35
6	C	203	ACO	N6A-C6A-N1A	-6.87	104.31	118.57
6	C	203	ACO	N3A-C2A-N1A	-5.34	120.34	128.68
8	A	920	IHP	C5-C4-C3	4.27	119.77	110.41
6	C	203	ACO	P2A-O3A-P1A	-3.98	119.17	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	310	EPE	C5-N4-C3	3.85	117.49	108.83
8	A	920	IHP	O12-C2-C1	3.78	117.61	108.69
8	A	920	IHP	O15-C5-C4	3.67	117.34	108.69
8	A	920	IHP	C4-C3-C2	3.66	118.42	110.41
9	B	310	EPE	C7-N4-C5	3.61	120.47	111.23
8	A	920	IHP	O11-C1-C6	-3.37	100.75	108.69
6	C	203	ACO	C2P-C3P-N4P	-3.13	105.83	112.42
6	C	203	ACO	C3B-C2B-C1B	3.11	106.78	99.89
6	C	203	ACO	C7P-C6P-C5P	-3.02	107.32	112.36
9	B	310	EPE	C7-N4-C3	3.00	118.90	111.23
8	A	920	IHP	C5-C6-C1	2.93	116.83	110.41
8	A	920	IHP	O11-C1-C2	2.89	115.51	108.69
6	C	203	ACO	C7P-N8P-C9P	-2.61	117.93	122.59
6	C	203	ACO	C3P-N4P-C5P	-2.52	118.16	122.84
9	B	310	EPE	C6-N1-C2	2.51	114.48	108.83
8	A	920	IHP	O13-C3-C4	2.50	114.58	108.69
9	B	310	EPE	O1S-S-C10	2.48	109.91	106.92
6	C	203	ACO	C5B-C4B-C3B	-2.44	106.33	114.40
9	B	310	EPE	O2S-S-C10	2.22	109.58	106.92
6	C	203	ACO	C6P-C7P-N8P	-2.18	107.50	111.90
8	A	920	IHP	O32-P2-O12	2.10	115.41	105.99

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	307	GOL	C1-C2-C3-O3
5	A	915	GOL	C1-C2-C3-O3
5	A	913	GOL	O1-C1-C2-C3
8	A	920	IHP	C3-C2-O12-P2
8	A	920	IHP	C2-C3-O13-P3
8	A	920	IHP	C4-C5-O15-P5
8	A	920	IHP	C6-C5-O15-P5
8	A	920	IHP	C6-O16-P6-O26
6	C	203	ACO	C5B-O5B-P1A-O1A
6	C	203	ACO	C5B-O5B-P1A-O3A
6	C	203	ACO	CDP-CBP-CCP-O6A
6	C	203	ACO	CEP-CBP-CCP-O6A
6	C	203	ACO	CAP-CBP-CCP-O6A
6	C	203	ACO	C9P-CAP-CBP-CCP
6	C	203	ACO	C9P-CAP-CBP-CDP
6	C	203	ACO	OAP-CAP-CBP-CEP

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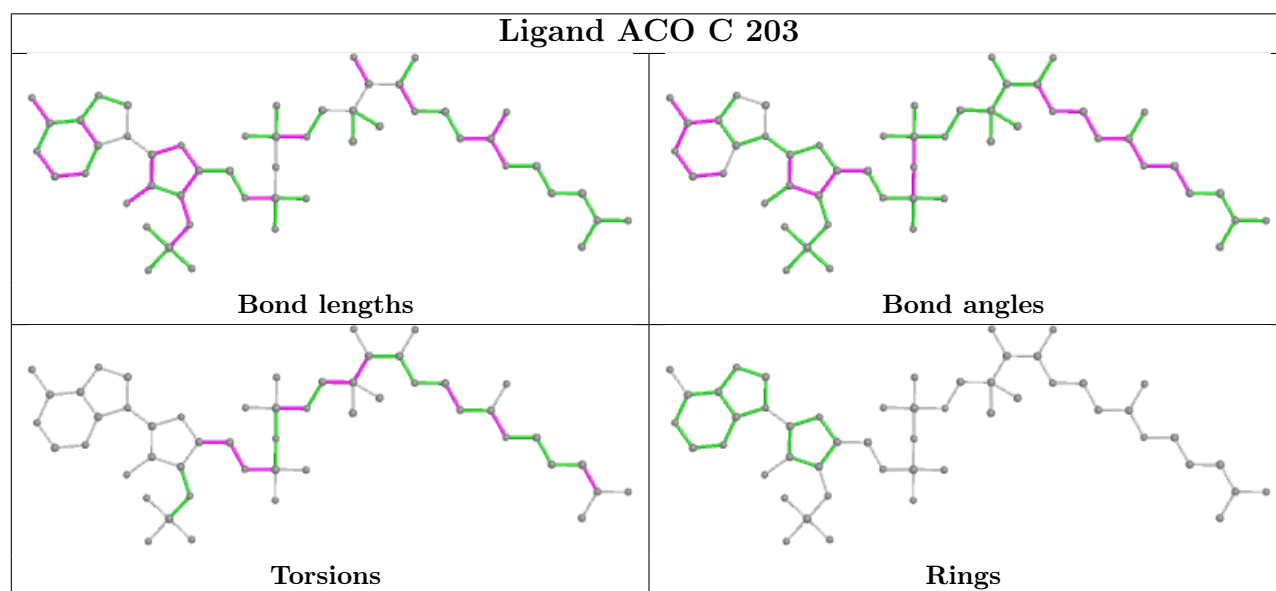
Mol	Chain	Res	Type	Atoms
6	C	203	ACO	C9P-CAP-CBP-CEP
6	C	203	ACO	C5P-C6P-C7P-N8P
9	B	310	EPE	C8-C7-N4-C5
9	B	310	EPE	C9-C10-S-O2S
9	B	310	EPE	C9-C10-S-O3S
6	C	203	ACO	C6P-C5P-N4P-C3P
6	C	203	ACO	C3B-C4B-C5B-O5B
6	C	203	ACO	O5P-C5P-N4P-C3P
5	A	912	GOL	O1-C1-C2-O2
5	B	307	GOL	O1-C1-C2-O2
5	A	912	GOL	O1-C1-C2-C3
5	B	307	GOL	O1-C1-C2-C3
5	B	307	GOL	O2-C2-C3-O3
5	A	915	GOL	O2-C2-C3-O3
5	A	913	GOL	O1-C1-C2-O2
6	C	203	ACO	O4B-C4B-C5B-O5B
6	C	203	ACO	C4B-C5B-O5B-P1A
6	C	203	ACO	OAP-CAP-CBP-CDP
9	B	310	EPE	C10-C9-N1-C2
9	B	310	EPE	C10-C9-N1-C6
6	C	203	ACO	O-C-S1P-C2P
5	A	916	GOL	O2-C2-C3-O3
8	A	920	IHP	C2-O12-P2-O42
8	A	920	IHP	C5-O15-P5-O45
5	A	916	GOL	C1-C2-C3-O3
9	B	310	EPE	C9-C10-S-O1S
6	C	203	ACO	OAP-CAP-CBP-CCP
8	A	920	IHP	C1-C2-O12-P2
8	A	920	IHP	C4-C3-O13-P3
5	C	202	GOL	O1-C1-C2-O2
9	B	310	EPE	S-C10-C9-N1
8	A	920	IHP	C1-O11-P1-O21
8	A	920	IHP	C1-O11-P1-O31
8	A	920	IHP	C1-O11-P1-O41
8	A	920	IHP	C3-O13-P3-O43
8	A	920	IHP	C6-O16-P6-O36
6	C	203	ACO	CCP-O6A-P2A-O3A
5	A	912	GOL	C1-C2-C3-O3
5	A	914	GOL	C1-C2-C3-O3
6	C	203	ACO	CH3-C-S1P-C2P

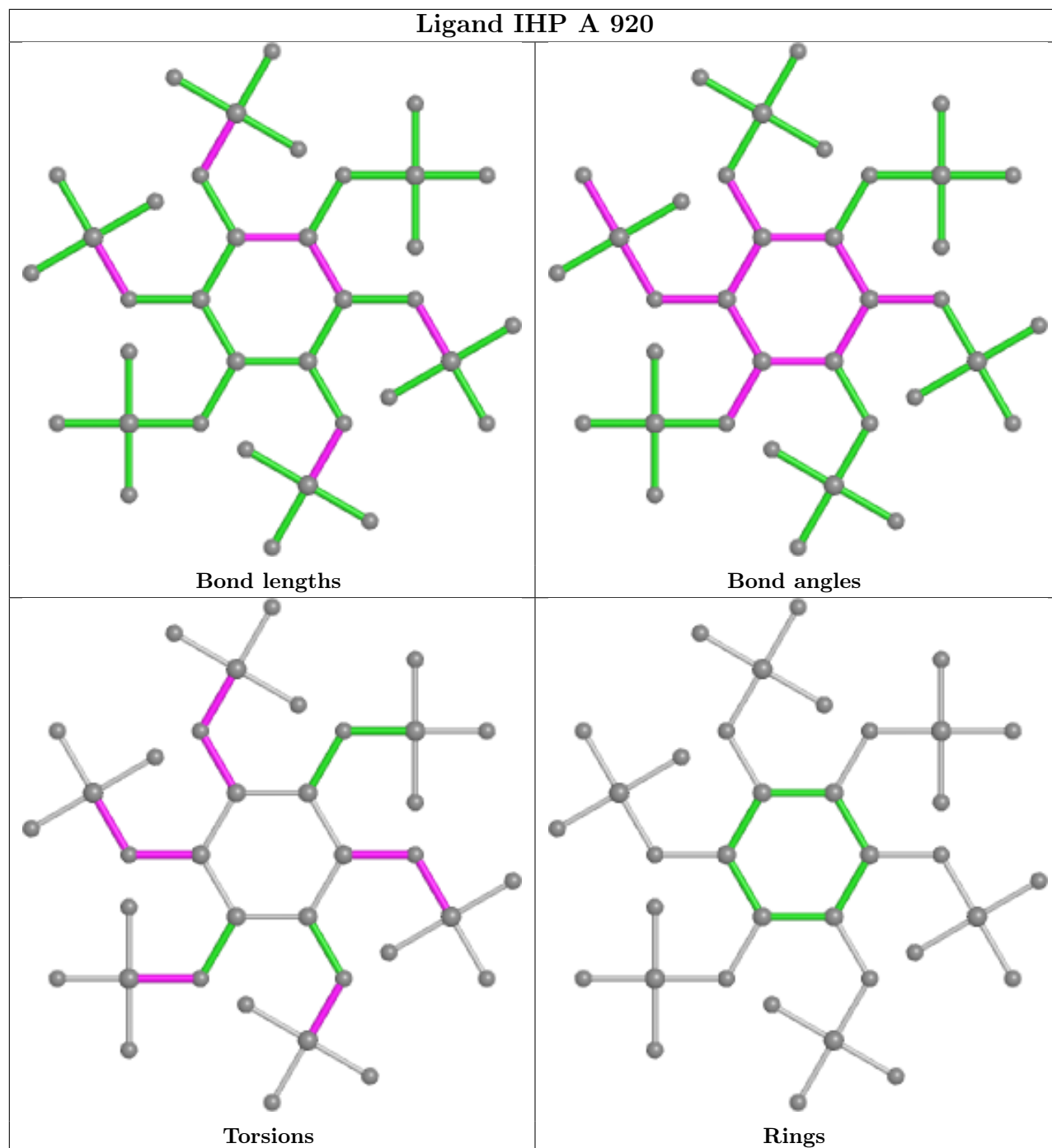
There are no ring outliers.

6 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	913	GOL	2	0
6	C	203	ACO	9	0
7	A	919	MLI	1	0
8	A	920	IHP	5	0
9	B	310	EPE	3	0
5	A	916	GOL	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 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	C	139/176 (78%)	1.02	31 (22%) 0 0	57, 89, 105, 119	1 (0%)
2	A	763/854 (89%)	0.10	29 (3%) 40 39	26, 52, 90, 112	0
3	B	199/238 (83%)	0.10	7 (3%) 44 44	24, 45, 83, 109	0
All	All	1101/1268 (86%)	0.21	67 (6%) 21 20	24, 54, 96, 119	1 (0%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	123	HIS	5.5
1	C	154	VAL	5.4
2	A	57	LEU	4.9
1	C	60	PHE	4.7
1	C	129	VAL	4.6
1	C	157	PHE	4.3
1	C	74	LEU	4.3
1	C	119	CYS	4.2
2	A	58	ALA	4.2
1	C	148	GLU	4.0
1	C	77	LYS	3.6
1	C	35	PHE	3.6
1	C	93	ILE	3.4
2	A	59	LEU	3.4
2	A	80	ALA	3.3
2	A	91	PRO	3.3
3	B	225	LEU	3.3
1	C	169	ILE	3.2
1	C	114	PHE	3.2
1	C	12	TYR	3.2
2	A	84	ILE	3.2
2	A	661	ARG	3.2
2	A	794	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	11	VAL	3.1
2	A	742	GLY	3.1
2	A	76	TYR	3.0
2	A	88	SER	3.0
1	C	19	LEU	3.0
1	C	168	ALA	2.9
2	A	656	ALA	2.9
2	A	785	PHE	2.9
1	C	102	TYR	2.8
1	C	163	GLY	2.8
2	A	655	ALA	2.8
1	C	94	GLU	2.7
1	C	130	TYR	2.7
1	C	103	ARG	2.7
2	A	623	LEU	2.7
2	A	97	LEU	2.6
2	A	71	ASP	2.6
2	A	658	MET	2.6
2	A	670	ALA	2.6
1	C	164	ASP	2.5
1	C	151	GLY	2.5
2	A	795	PHE	2.4
1	C	141	TRP	2.4
2	A	626	LYS	2.4
3	B	214	GLU	2.4
1	C	120	SER	2.3
3	B	189	ALA	2.3
3	B	176	ILE	2.3
1	C	150	VAL	2.3
1	C	153	THR	2.3
2	A	54	VAL	2.3
2	A	802	GLN	2.3
1	C	78	LEU	2.3
2	A	77	VAL	2.3
3	B	75	ASP	2.3
3	B	188	TYR	2.3
1	C	28	PRO	2.2
2	A	285	LEU	2.2
2	A	800	PHE	2.2
3	B	201	ILE	2.2
1	C	122	CYS	2.2
2	A	262	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	A	75	SER	2.1
2	A	387	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

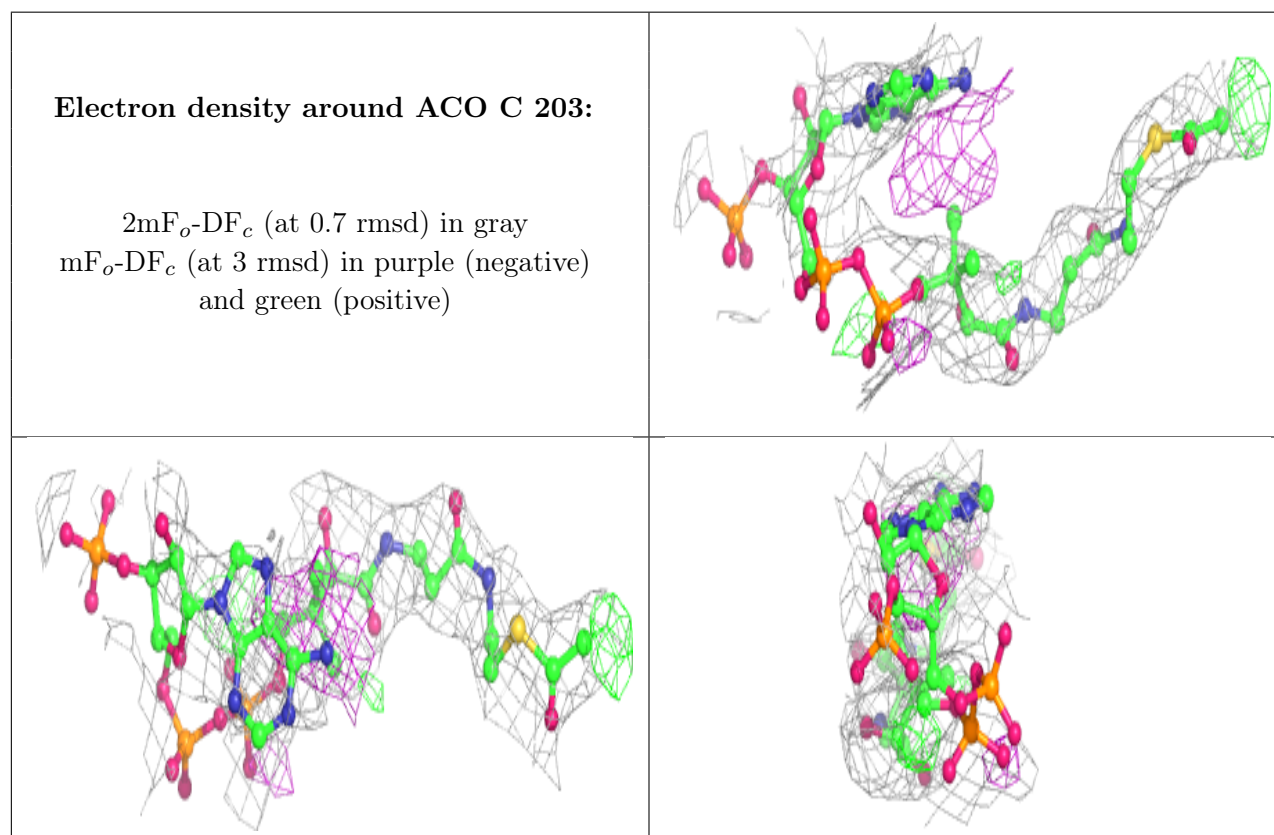
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CL	B	305	1/1	0.43	1.18	121,121,121,121	0
4	CL	A	910	1/1	0.65	0.21	93,93,93,93	0
5	GOL	A	914	6/6	0.77	0.24	59,66,70,74	0
9	EPE	B	310	15/15	0.77	0.29	49,59,100,117	0
6	ACO	C	203	51/51	0.79	0.23	67,98,121,129	0
4	CL	B	301	1/1	0.79	0.14	67,67,67,67	0
4	CL	A	904	1/1	0.80	0.09	103,103,103,103	0
4	CL	B	304	1/1	0.81	0.27	80,80,80,80	0
5	GOL	B	307	6/6	0.81	0.50	52,54,59,66	0
4	CL	A	905	1/1	0.81	0.10	94,94,94,94	0
4	CL	C	201	1/1	0.82	0.10	102,102,102,102	0
5	GOL	A	912	6/6	0.83	0.29	47,50,58,60	0
7	MLI	A	917	7/7	0.83	0.34	65,70,74,79	0
4	CL	A	902	1/1	0.84	0.12	77,77,77,77	0
4	CL	A	903	1/1	0.85	0.14	78,78,78,78	0
4	CL	A	907	1/1	0.85	0.57	79,79,79,79	0
4	CL	A	911	1/1	0.87	0.15	68,68,68,68	0
7	MLI	A	919	7/7	0.87	0.40	59,62,69,79	0
4	CL	B	306	1/1	0.88	0.12	81,81,81,81	0
5	GOL	A	915	6/6	0.88	0.25	64,66,70,79	0
5	GOL	A	913	6/6	0.88	0.24	43,47,58,64	0

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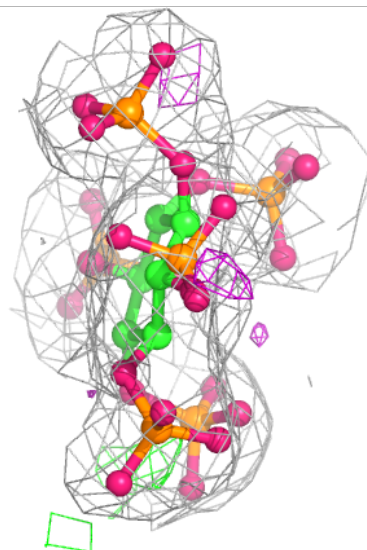
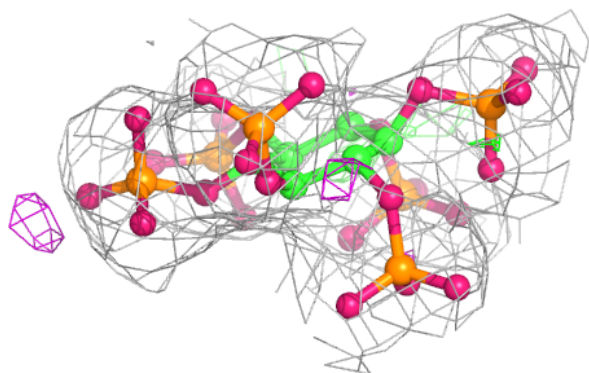
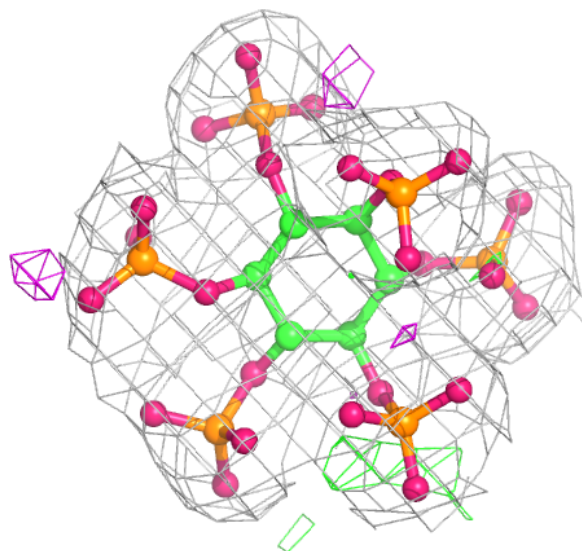
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CL	A	906	1/1	0.88	0.25	65,65,65,65	0
7	MLI	A	918	7/7	0.90	0.27	57,62,70,71	0
5	GOL	A	916	6/6	0.90	0.19	47,57,63,63	0
5	GOL	C	202	6/6	0.90	0.16	76,77,78,82	0
4	CL	B	303	1/1	0.90	0.28	99,99,99,99	0
4	CL	A	908	1/1	0.91	0.20	75,75,75,75	0
7	MLI	B	309	7/7	0.91	0.21	41,47,51,57	0
4	CL	A	901	1/1	0.92	0.31	69,69,69,69	0
4	CL	B	302	1/1	0.93	0.09	90,90,90,90	0
5	GOL	B	308	6/6	0.94	0.27	44,44,48,60	0
4	CL	A	909	1/1	0.94	0.37	65,65,65,65	0
8	IHP	A	920	36/36	0.96	0.20	41,54,64,66	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 IHP A 920:

$2mF_o-DF_c$ (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.