



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:21 AM UTC

PDB ID : 6O07 / pdb_00006o07
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

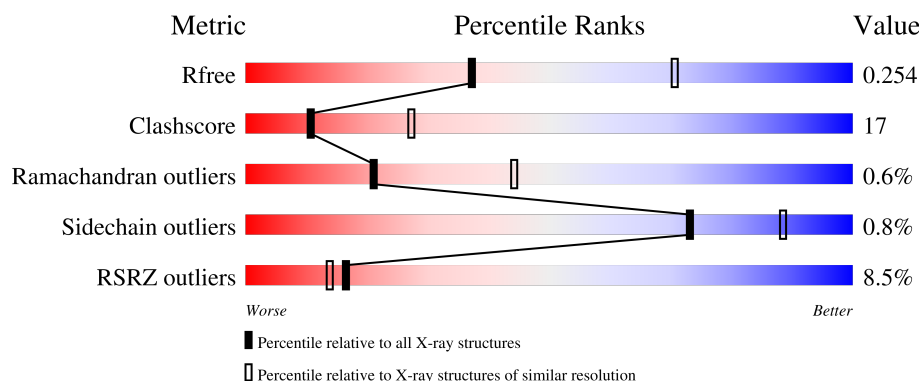
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 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	C	176	28% 47% 27% • • 21%
2	A	854	4% 63% 26% • 11%
3	B	238	4% 58% 26% 16%

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

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 (CCD ID: CL) (formula: Cl).

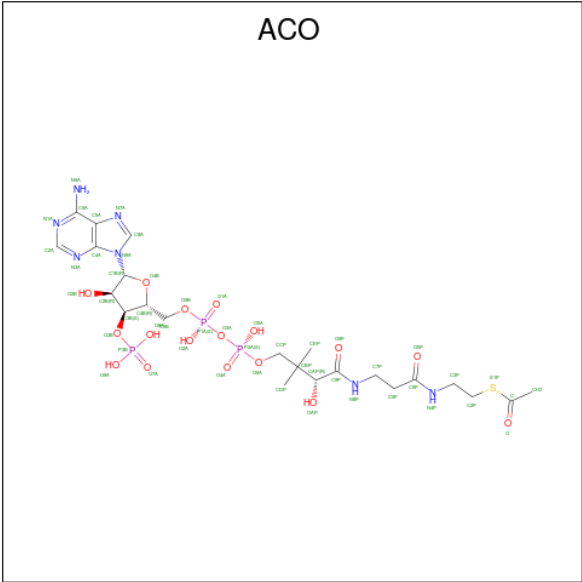
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Cl	0	0
			1	1		
4	A	11	Total	Cl	0	0
			11	11		
4	B	6	Total	Cl	0	0
			6	6		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



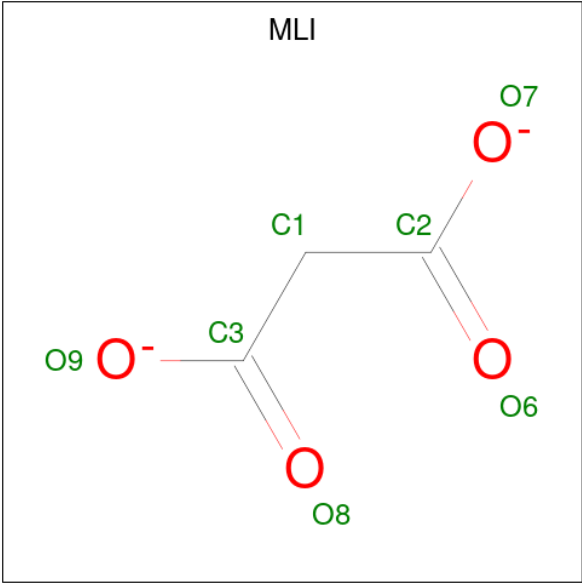
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is ACETYL COENZYME *A (CCD ID: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S).



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 (CCD ID: MLI) (formula: C₃H₂O₄).



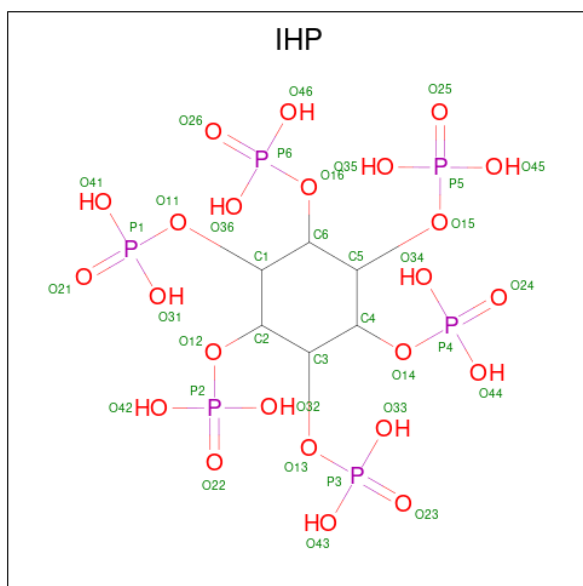
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	3	4		
7	A	1	Total	C	O	0	0
			7	3	4		
7	A	1	Total	C	O	0	0
			7	3	4		

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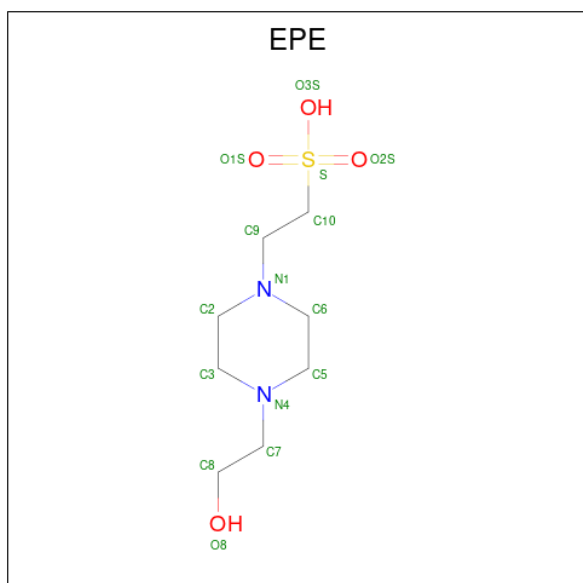
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			7	3	4		

- Molecule 8 is INOSITOL HEXAKISPHOSPHATE (CCD ID: 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		

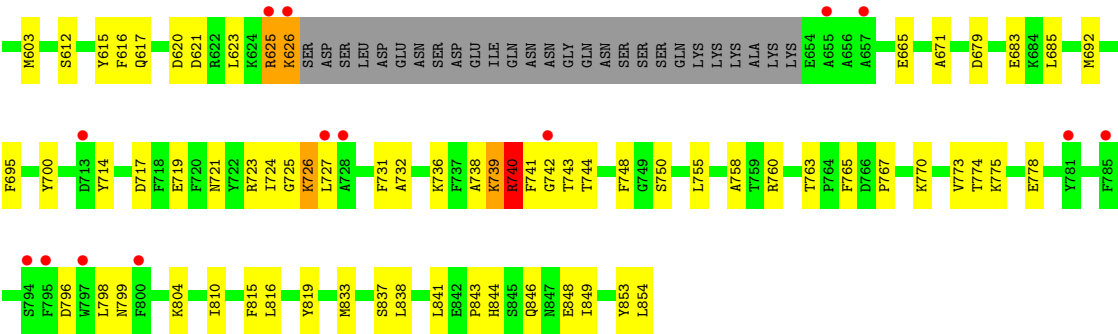
- Molecule 9 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



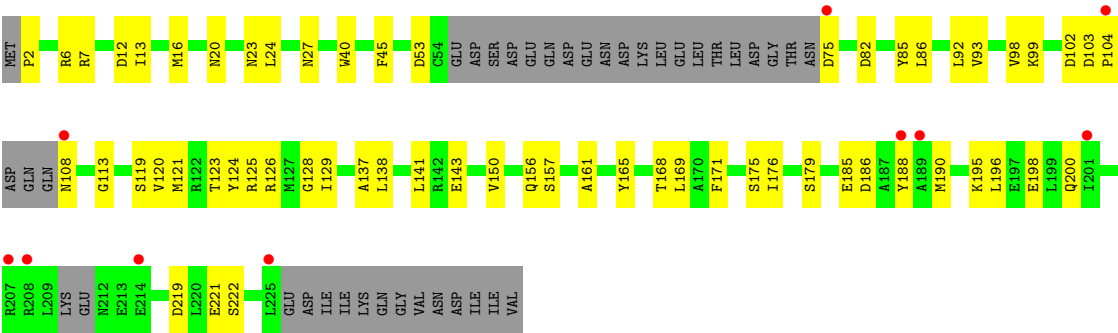
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- 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 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) 80.3 (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 0.225 , 0.254	Depositor DCC
R_{free} test set	1709 reflections (3.95%)	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)	0.29 , 37.9	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: MLI, GOL, ACO, CL, EPE, IHP

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	0.32	0/1002	1.47	15/1363 (1.1%)
2	A	0.21	0/6245	0.73	15/8447 (0.2%)
3	B	0.22	0/1589	0.39	0/2155
All	All	0.23	0/8836	0.80	30/11965 (0.3%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	377	THR	CA-C-N	29.21	167.63	121.19
2	A	377	THR	C-N-CA	29.21	167.63	121.19
1	C	151	GLY	N-CA-C	25.64	173.95	113.18
1	C	154	VAL	N-CA-C	-24.48	74.20	108.96
1	C	150	VAL	N-CA-C	-21.17	76.39	109.20
2	A	378	GLN	N-CA-CB	14.52	134.40	109.72
2	A	739	LYS	CB-CA-C	14.45	134.83	110.84
2	A	740	ARG	N-CA-C	14.02	129.32	111.24
1	C	13	ALA	CB-CA-C	-12.50	85.55	110.42
2	A	625	ARG	CB-CA-C	-12.27	86.00	110.42
2	A	623	LEU	N-CA-C	11.34	123.64	111.28
2	A	121	GLY	N-CA-C	10.70	131.16	115.32
2	A	625	ARG	N-CA-C	8.96	129.89	110.80
1	C	146	GLY	N-CA-C	-8.92	92.04	113.18
2	A	740	ARG	CB-CA-C	-8.54	96.77	110.86
1	C	105	LYS	N-CA-C	-8.14	103.37	112.57
1	C	38	ALA	CB-CA-C	8.08	126.50	110.42
2	A	377	THR	CB-CA-C	7.71	125.77	110.42
2	A	623	LEU	CB-CA-C	7.43	123.13	110.79
1	C	154	VAL	CB-CA-C	7.32	121.22	111.19
1	C	28	PRO	N-CA-CB	-7.25	95.63	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	28	PRO	N-CA-C	6.94	126.76	112.47
2	A	626	LYS	N-CA-C	-6.50	92.80	111.00
2	A	623	LEU	O-C-N	6.11	128.60	122.12
2	A	217	SER	CB-CA-C	-5.95	109.70	116.54
1	C	29	ASN	CA-C-N	5.84	128.11	120.28
1	C	29	ASN	C-N-CA	5.84	128.11	120.28
1	C	104	HIS	CB-CA-C	-5.66	102.00	111.23
1	C	158	ILE	CA-C-N	5.05	128.65	121.42
1	C	158	ILE	C-N-CA	5.05	128.65	121.42

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	54	0
2	A	6110	0	5940	187	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	288	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 17.

All (288) 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:621:ASP:O	2:A:626:LYS:C	1.85	1.18
2:A:140:ASP:OD2	10:A:1001:HOH:O	1.62	1.17
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
2:A:621:ASP:C	2:A:626:LYS:O	2.01	1.04
1:C:130:TYR:CZ	1:C:157:PHE:CZ	2.48	1.00
1:C:130:TYR:CZ	1:C:157:PHE:HZ	1.80	0.99
2:A:140:ASP:CG	10:A:1001:HOH:O	1.99	0.98
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	0.95
2:A:457:LYS:CE	8:A:920:IHP:O35	2.14	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:64:LEU:O	10:A:1005:HOH:O	1.93	0.84
2:A:537:ALA:O	2:A:540:ILE:HG22	1.78	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: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
1:C:130:TYR:CE1	1:C:157:PHE:CE1	2.71	0.78
3:B:108:ASN:N	10:B:403:HOH:O	2.14	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
1:C:130:TYR:CE2	1:C:157:PHE:CZ	2.77	0.73
2:A:549:LYS:NZ	2:A:665:GLU:OE2	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:140:ASP:OD1	10:A:1001:HOH:O	1.96	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
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
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:798:LEU:HD21	2:A:833:MET:HE1	1.77	0.66
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
1:C:30:LEU:HA	1:C:160:GLY:HA2	1.79	0.63
2:A:518:LEU:CD1	2:A:540:ILE:CD1	2.76	0.63
3:B:99:LYS:NZ	10:B:404:HOH:O	2.21	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
1:C:13:ALA:HB2	1:C:40:PHE:CG	2.38	0.59
3:B:86:LEU:HD11	3:B:92:LEU:HB2	1.85	0.59
1:C:24:HIS:O	1:C:28:PRO:CB	2.51	0.59
1:C:145:HIS:O	1:C:146:GLY:C	2.46	0.58
1:C:18:MET:HE1	2:A:447:LEU:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:HIS:C	1:C:28:PRO:HB3	2.27	0.58
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
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
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:149:LYS:NZ	10:A:1014:HOH:O	2.30	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:617:GLN:NE2	2:A:621:ASP:OD2	2.34	0.55
2:A:742:GLY:C	2:A:744:THR:H	2.14	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
2:A:55:ASP:OD2	2:A:93:CYS:HB2	2.08	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
2:A:738:ALA:O	2:A:739:LYS:C	2.52	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
3:B:219:ASP:N	3:B:219:ASP:OD1	2.41	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:270:ARG:HH22	3:B:143:GLU:CD	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:A:535:GLN:C	2:A:537:ALA:H	2.19	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
3:B:171:PHE:HB3	3:B:190:MET:HE2	1.93	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:798:LEU:HD21	2:A:833:MET:CE	2.41	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
1:C:18:MET:O	1:C:22:LEU:HD12	2.12	0.49
2:A:796:ASP:OD1	2:A:799:ASN:N	2.32	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:442:GLU:OE1	2:A:470:LYS:NZ	2.44	0.49
2:A:333:VAL:HG12	2:A:348:VAL:HG11	1.94	0.49
2:A:376:PRO:HB3	2:A:383:PHE:CE2	2.47	0.49
2:A:517:LYS:O	2:A:521:LEU:HD23	2.13	0.48
1:C:30:LEU:H	1:C:30:LEU:HD22	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
1:C:130:TYR:CG	1:C:157:PHE:CE2	3.02	0.47
2:A:740:ARG:HB3	2:A:741:PHE:CD1	2.49	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
1:C:103:ARG:HD3	6:C:203:ACO:H10	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:6:ARG:NH1	3:B:12:ASP:OD2	2.40	0.47
2:A:504:ALA:HB2	2:A:557:ARG:HB2	1.97	0.47
3:B:93:VAL:HA	3:B:121:MET:HE3	1.97	0.47
3:B:195:LYS:NZ	3:B:198:GLU:OE1	2.36	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
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
1:C:139:LYS:NZ	1:C:169:ILE:HG21	2.30	0.46
2:A:439:GLY:HA2	5:A:913:GOL:H12	1.96	0.46
1:C:130:TYR:CD2	1:C:157:PHE:CE2	3.04	0.46
2:A:369:ASP:O	2:A:372:SER:OG	2.27	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
1:C:170:LEU:C	1:C:171:LEU:HD12	2.41	0.46
2:A:200:GLU:HG3	2:A:583:GLY:HA3	1.98	0.46
1:C:31:TYR:HA	10:C:310:HOH:O	2.15	0.46
1:C:104:HIS:HA	6:C:203:ACO:C5B	2.44	0.46
2:A:741:PHE:CD1	2:A:741:PHE:N	2.83	0.46
8:A:920:IHP:O25	8:A:920:IHP:H6	2.15	0.46
2:A:61:GLY:O	2:A:65:TYR:N	2.34	0.46
2:A:273:ASP:OD1	2:A:307:ARG:NH1	2.48	0.46
3:B:156:GLN:N	10:B:402:HOH:O	2.10	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:714:TYR:CZ	2:A:736:LYS:HB3	2.51	0.46
1:C:98:VAL:HG21	1:C:108:GLY:HA2	1.97	0.45
2:A:616:PHE:CE1	2:A:692:MET:HE1	2.51	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:429:LYS:HG3	2:A:430:HIS:N	2.28	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:429:LYS:O	2:A:434:MET:HE1	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:428:LEU:HD13	2:A:436:THR:HG22	1.99	0.45
2:A:742:GLY:C	2:A:744:THR:N	2.74	0.44
3:B:124:TYR:HB3	3:B:129:ILE:HD12	1.99	0.44
2:A:216:ALA:O	2:A:217:SER:C	2.60	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:HH11	2:A:246:ARG:HG2	1.83	0.44
2:A:833:MET:HE3	2:A:833:MET:HB3	1.77	0.44
3:B:188:TYR:O	3:B:190:MET:HG3	2.18	0.44
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
1:C:12:TYR:C	1:C:14:ASN:H	2.25	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:107:TYR:OH	2:A:570:ASP:OD1	2.28	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:201:HIS:NE2	7:A:919:MLI:O7	2.49	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:313:PHE:CZ	3:B:2:PRO:HD3	2.54	0.43
3:B:222:SER:N	10:B:401:HOH:O	2.36	0.43
1:C:109:SER:HA	6:C:203:ACO:H2A	2.01	0.42
2:A:225:ASN:O	2:A:225:ASN:ND2	2.52	0.42
2:A:336:GLN:HB3	2:A:341:VAL:CG1	2.49	0.42
1:C:16:LEU:HD21	1:C:36:PHE:O	2.19	0.42
2:A:174:GLU:HB3	2:A:177:GLN:CD	2.43	0.42
3:B:179:SER:O	3:B:179:SER:OG	2.29	0.42
2:A:84:ILE:HD12	2:A:89:ALA:HB2	2.00	0.42
2:A:201:HIS:O	2:A:205:LEU:HG	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:203:ACO:H32	6:C:203:ACO:H61	1.71	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
1:C:125:HIS:O	1:C:174:HIS:HA	2.20	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: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:HD23	3:B:141:LEU:HA	1.86	0.42
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
3:B:121:MET:HE3	3:B:121:MET:HB2	1.79	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
1:C:127:VAL:O	1:C:127:VAL:HG13	2.20	0.41
2:A:267:LEU:HB3	2:A:277:TYR:CD2	2.55	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:535:GLN:C	2:A:537:ALA:N	2.78	0.41
1:C:100:PRO:HA	1:C:103:ARG:HG3	2.03	0.41
2:A:156:LEU:HD23	2:A:156:LEU:HA	1.86	0.41
2:A:222:LYS:O	2:A:222:LYS:HD3	2.21	0.41
2:A:457:LYS:HD3	10:A:1110:HOH:O	2.20	0.41
2:A:844:HIS:CE1	5:A:916:GOL:H32	2.56	0.41
3:B:156:GLN:HA	3:B:188:TYR:CE2	2.56	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:92:ILE:H	2:A:92:ILE:HD12	1.86	0.40
2:A:160:ALA:O	2:A:164:SER:OG	2.32	0.40
2:A:748:PHE:CD1	2:A:748:PHE:C	2.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:TYR:CE1	1:C:70:PRO:HG3	2.56	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
2:A:290:ASP:OD2	2:A:293:LEU:HD12	2.22	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	C	133/176 (76%)	112 (84%)	19 (14%)	2 (2%)	8	22
2	A	755/854 (88%)	710 (94%)	41 (5%)	4 (0%)	24	48
3	B	191/238 (80%)	180 (94%)	11 (6%)	0	100	100
All	All	1079/1268 (85%)	1002 (93%)	71 (7%)	6 (1%)	21	44

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 [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	C	84/153 (55%)	83 (99%)	1 (1%)	63	84
2	A	639/760 (84%)	634 (99%)	5 (1%)	73	88
3	B	163/216 (76%)	162 (99%)	1 (1%)	78	91
All	All	886/1129 (78%)	879 (99%)	7 (1%)	73	88

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	28	PRO
2	A	81	ILE
2	A	338	LYS
2	A	374	LEU
2	A	603	MET
2	A	740	ARG
3	B	23	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	10	ASN
1	C	62	GLN
2	A	184	GLN
2	A	225	ASN
2	A	288	GLN
2	A	387	ASN
2	A	455	ASN
2	A	481	ASN
2	A	559	ASN
2	A	676	GLN
2	A	793	ASN
2	A	844	HIS
2	A	846	GLN
3	B	11	ASN
3	B	20	ASN
3	B	206	HIS
3	B	212	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
6	ACO	C	203	-	51,53,53	3.33	20 (39%)	73,79,79	1.96	18 (24%)
5	GOL	A	914	-	5,5,5	0.86	0	5,5,5	1.01	0
7	MLI	A	918	-	6,6,6	1.37	0	7,7,7	1.26	0
5	GOL	B	307	-	5,5,5	0.97	0	5,5,5	1.04	0
5	GOL	A	913	-	5,5,5	0.93	0	5,5,5	1.07	0
7	MLI	A	917	-	6,6,6	1.35	0	7,7,7	1.27	0
8	IHP	A	920	-	36,36,36	1.68	6 (16%)	60,60,60	1.85	12 (20%)
7	MLI	B	309	-	6,6,6	1.35	0	7,7,7	1.36	0
7	MLI	A	919	-	6,6,6	1.35	0	7,7,7	1.25	0
5	GOL	B	308	-	5,5,5	0.99	0	5,5,5	1.08	0
9	EPE	B	310	-	15,15,15	0.82	1 (6%)	19,20,20	1.78	5 (26%)
5	GOL	A	912	-	5,5,5	0.94	0	5,5,5	1.06	0
5	GOL	A	915	-	5,5,5	0.90	0	5,5,5	1.08	0
5	GOL	A	916	-	5,5,5	0.91	0	5,5,5	1.04	0
5	GOL	C	202	-	5,5,5	0.91	0	5,5,5	1.11	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
6	ACO	C	203	-	-	21/51/67/67	0/3/3/3
5	GOL	A	914	-	-	0/4/4/4	-
7	MLI	A	918	-	-	2/4/4/4	-
5	GOL	B	307	-	-	4/4/4/4	-
5	GOL	A	913	-	-	2/4/4/4	-
7	MLI	A	917	-	-	2/4/4/4	-
8	IHP	A	920	-	-	11/30/54/54	0/1/1/1
7	MLI	B	309	-	-	0/4/4/4	-
7	MLI	A	919	-	-	2/4/4/4	-
5	GOL	B	308	-	-	0/4/4/4	-
9	EPE	B	310	-	-	6/9/19/19	0/1/1/1
5	GOL	A	912	-	-	2/4/4/4	-
5	GOL	A	915	-	-	2/4/4/4	-
5	GOL	A	916	-	-	2/4/4/4	-
5	GOL	C	202	-	-	1/4/4/4	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	203	ACO	P2A-O3A	11.78	1.72	1.59
6	C	203	ACO	O4B-C1B	10.43	1.66	1.42
6	C	203	ACO	C5P-N4P	6.96	1.49	1.33
6	C	203	ACO	O4B-C4B	-6.48	1.30	1.45
6	C	203	ACO	C2B-C1B	-5.98	1.34	1.53
8	A	920	IHP	P2-O12	5.29	1.68	1.59
6	C	203	ACO	C9P-N8P	5.25	1.45	1.33
6	C	203	ACO	P1A-O3A	5.17	1.65	1.59
6	C	203	ACO	C6A-N6A	4.94	1.46	1.34
8	A	920	IHP	P3-O13	3.62	1.65	1.59
8	A	920	IHP	P5-O15	3.47	1.65	1.59
6	C	203	ACO	O3B-C3B	-3.32	1.32	1.44
6	C	203	ACO	P3B-O3B	3.30	1.65	1.59
8	A	920	IHP	P6-O16	3.24	1.65	1.59
6	C	203	ACO	C6P-C5P	3.14	1.57	1.51
6	C	203	ACO	P2A-O6A	3.03	1.71	1.59
6	C	203	ACO	O5P-C5P	-2.90	1.17	1.23
6	C	203	ACO	C3B-C4B	2.76	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	310	EPE	C10-S	2.71	1.81	1.77
8	A	920	IHP	C4-C3	2.33	1.57	1.52
6	C	203	ACO	C5A-N7A	-2.19	1.35	1.39
6	C	203	ACO	OAP-CAP	-2.17	1.38	1.42
6	C	203	ACO	C5A-C4A	-2.15	1.35	1.39
6	C	203	ACO	C2A-N1A	2.14	1.37	1.33
6	C	203	ACO	P1A-O5B	2.11	1.67	1.59
8	A	920	IHP	C5-C4	2.07	1.56	1.52
6	C	203	ACO	O2B-C2B	2.02	1.48	1.43

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	203	ACO	N6A-C6A-N1A	-6.32	104.31	118.38
6	C	203	ACO	N3A-C2A-N1A	-5.45	120.34	128.58
6	C	203	ACO	C5A-C4A-N3A	-5.09	119.71	126.72
6	C	203	ACO	C5A-C6A-N6A	4.93	135.50	123.29
8	A	920	IHP	P4-O14-C4	-4.85	110.47	123.43
8	A	920	IHP	C5-C4-C3	4.26	119.77	110.43
8	A	920	IHP	P2-O12-C2	4.19	134.63	123.43
8	A	920	IHP	O12-C2-C1	4.16	117.61	108.76
6	C	203	ACO	N9A-C8A-N7A	-4.12	108.08	113.94
8	A	920	IHP	O15-C5-C4	4.03	117.34	108.76
9	B	310	EPE	C5-N4-C3	4.01	117.49	108.84
8	A	920	IHP	O11-C1-C6	-3.76	100.75	108.76
8	A	920	IHP	C4-C3-C2	3.65	118.42	110.43
9	B	310	EPE	C7-N4-C5	3.46	120.47	111.24
6	C	203	ACO	C2A-N3A-C4A	3.43	120.20	111.83
8	A	920	IHP	O11-C1-C2	3.17	115.51	108.76
6	C	203	ACO	C2P-C3P-N4P	-3.15	105.83	112.41
6	C	203	ACO	C3B-C2B-C1B	3.14	106.78	99.89
6	C	203	ACO	C7P-C6P-C5P	-3.04	107.32	112.39
6	C	203	ACO	C5A-N7A-C8A	3.04	108.22	103.45
6	C	203	ACO	N3A-C4A-N9A	2.95	132.19	127.17
8	A	920	IHP	C5-C6-C1	2.92	116.83	110.43
9	B	310	EPE	C7-N4-C3	2.87	118.90	111.24
8	A	920	IHP	O13-C3-C4	2.74	114.58	108.76
9	B	310	EPE	C6-N1-C2	2.62	114.48	108.84
6	C	203	ACO	C7P-N8P-C9P	-2.57	117.93	122.55
6	C	203	ACO	C3P-N4P-C5P	-2.50	118.16	122.82
8	A	920	IHP	O32-P2-O12	2.45	115.41	105.85
6	C	203	ACO	C5B-C4B-C3B	-2.42	106.33	114.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	203	ACO	C4A-C5A-N7A	-2.42	107.82	110.58
6	C	203	ACO	O2A-P1A-O3A	2.29	113.46	107.27
8	A	920	IHP	O14-C4-C3	-2.24	103.99	108.76
6	C	203	ACO	C6P-C7P-N8P	-2.11	107.50	112.00
9	B	310	EPE	O1S-S-C10	2.10	109.91	106.73
6	C	203	ACO	C5A-C4A-N9A	2.10	108.10	105.81

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	913	GOL	O1-C1-C2-C3
5	A	915	GOL	C1-C2-C3-O3
5	B	307	GOL	C1-C2-C3-O3
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
6	C	203	ACO	C9P-CAP-CBP-CEP
6	C	203	ACO	C5P-C6P-C7P-N8P
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
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	O5P-C5P-N4P-C3P
5	A	912	GOL	O1-C1-C2-O2
5	B	307	GOL	O1-C1-C2-O2
6	C	203	ACO	C3B-C4B-C5B-O5B
5	A	912	GOL	O1-C1-C2-C3
5	B	307	GOL	O1-C1-C2-C3
5	A	913	GOL	O1-C1-C2-O2
5	A	915	GOL	O2-C2-C3-O3
5	B	307	GOL	O2-C2-C3-O3
6	C	203	ACO	C2B-C1B-N9A-C8A

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Mol	Chain	Res	Type	Atoms
6	C	203	ACO	O4B-C4B-C5B-O5B
6	C	203	ACO	C4B-C5B-O5B-P1A
8	A	920	IHP	C6-O16-P6-O26
6	C	203	ACO	C2B-C1B-N9A-C4A
9	B	310	EPE	C10-C9-N1-C2
9	B	310	EPE	C10-C9-N1-C6
6	C	203	ACO	OAP-CAP-CBP-CDP
6	C	203	ACO	O-C-S1P-C2P
5	A	916	GOL	O2-C2-C3-O3
9	B	310	EPE	C9-C10-S-O1S
6	C	203	ACO	OAP-CAP-CBP-CCP
5	C	202	GOL	O1-C1-C2-O2
7	A	918	MLI	C3-C1-C2-O6
7	A	918	MLI	C3-C1-C2-O7
7	A	919	MLI	C2-C1-C3-O8
7	A	919	MLI	C2-C1-C3-O9
8	A	920	IHP	C1-C2-O12-P2
8	A	920	IHP	C4-C3-O13-P3
8	A	920	IHP	C2-O12-P2-O42
5	A	916	GOL	C1-C2-C3-O3
8	A	920	IHP	C1-O11-P1-O21
6	C	203	ACO	CH3-C-S1P-C2P
8	A	920	IHP	C1-O11-P1-O41
8	A	920	IHP	C5-O15-P5-O45
7	A	917	MLI	C3-C1-C2-O6
7	A	917	MLI	C2-C1-C3-O8

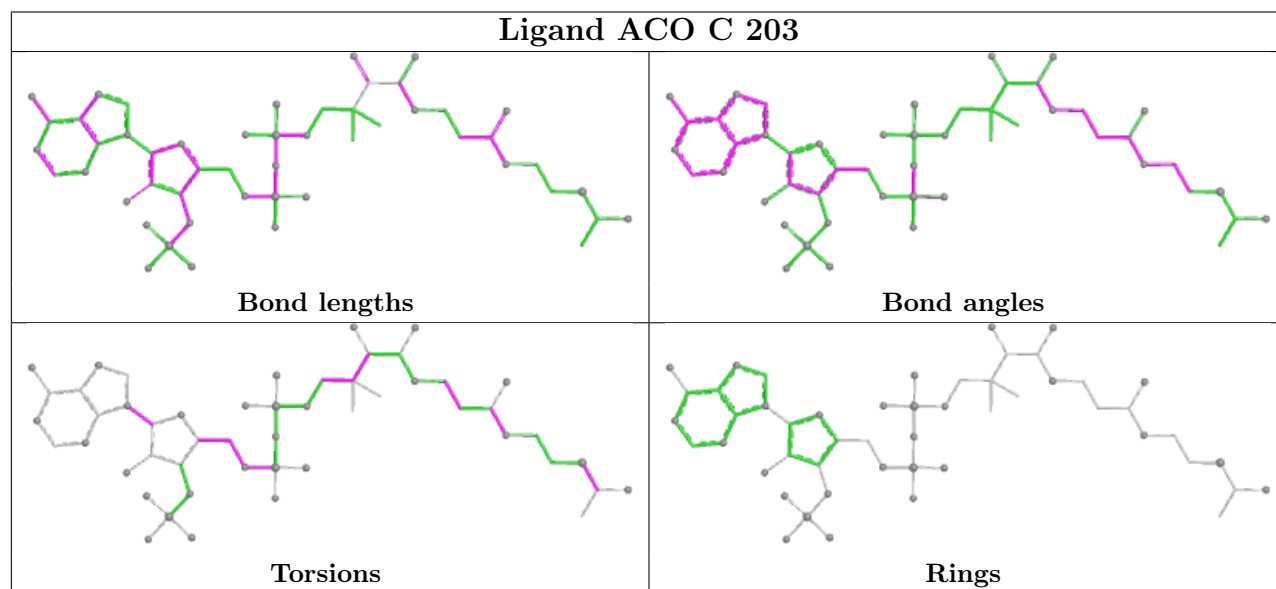
There are no ring outliers.

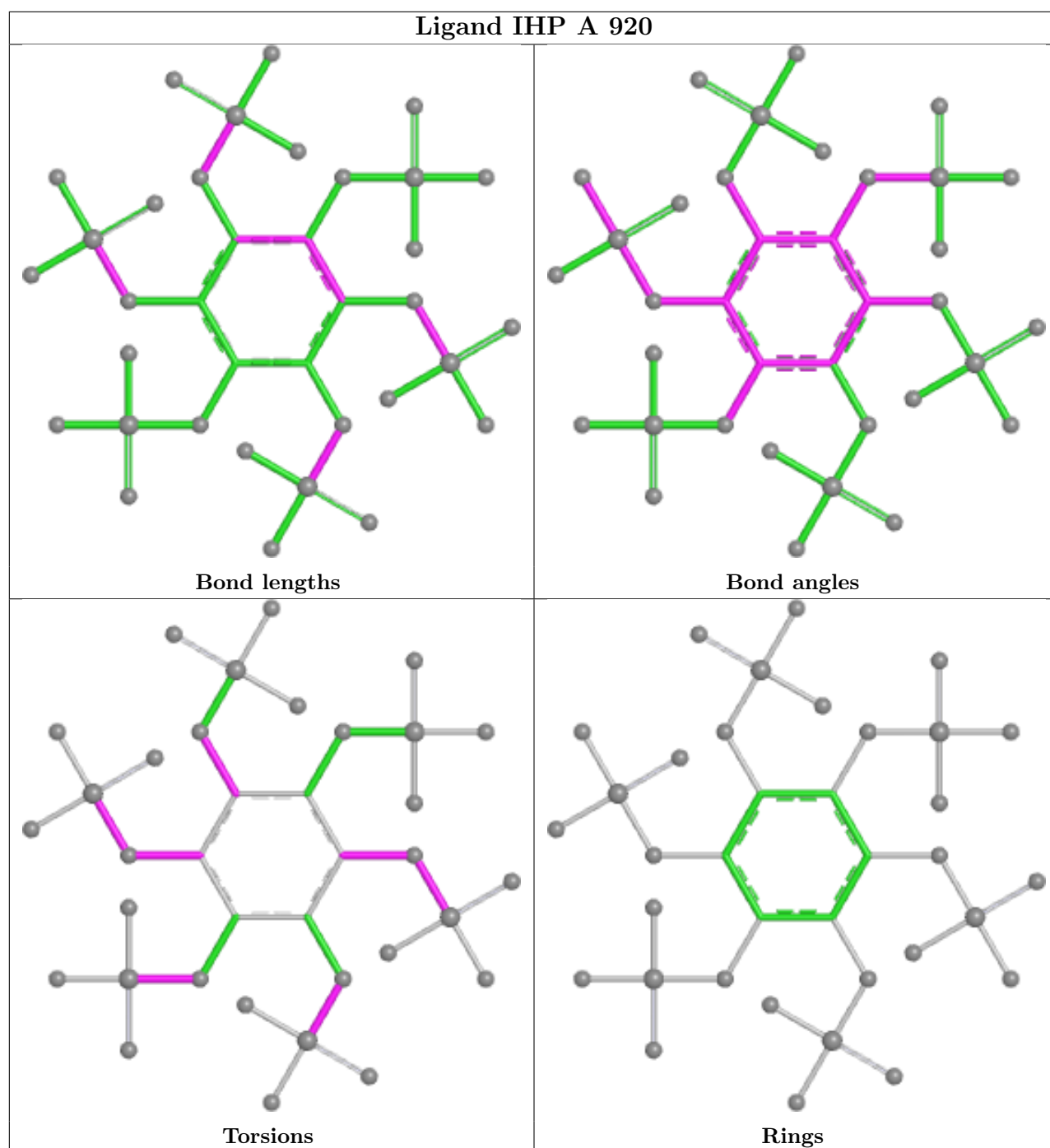
6 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	203	ACO	9	0
5	A	913	GOL	2	0
8	A	920	IHP	5	0
7	A	919	MLI	1	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%)	1.73	50 (35%) 1 0	57, 89, 105, 119	1 (0%)
2	A	763/854 (89%)	0.44	34 (4%) 38 34	26, 52, 90, 112	0
3	B	199/238 (83%)	0.47	10 (5%) 34 30	24, 45, 83, 109	0
All	All	1101/1268 (86%)	0.61	94 (8%) 16 14	24, 54, 96, 119	1 (0%)

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	154	VAL	6.1
1	C	11	VAL	4.8
2	A	387	ASN	4.5
1	C	137	LEU	4.5
3	B	188	TYR	4.2
1	C	141	TRP	4.1
2	A	742	GLY	3.8
1	C	30	LEU	3.7
2	A	524	LEU	3.7
1	C	162	ASN	3.5
1	C	74	LEU	3.4
1	C	12	TYR	3.3
3	B	225	LEU	3.3
2	A	794	SER	3.3
1	C	6	CYS	3.3
1	C	28	PRO	3.2
1	C	32	GLN	3.1
1	C	158	ILE	3.1
1	C	19	LEU	3.0
1	C	146	GLY	3.0
1	C	156	ASN	2.9
3	B	208	ARG	2.9
1	C	36	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
3	B	104	PRO	2.9
1	C	134	VAL	2.8
1	C	150	VAL	2.8
1	C	5	ILE	2.8
2	A	566	LYS	2.8
2	A	626	LYS	2.8
3	B	201	ILE	2.8
3	B	75	ASP	2.8
1	C	161	VAL	2.8
1	C	165	GLU	2.8
3	B	214	GLU	2.7
2	A	88	SER	2.7
1	C	168	ALA	2.7
2	A	785	PHE	2.7
2	A	57	LEU	2.7
2	A	536	ILE	2.6
3	B	108	ASN	2.6
1	C	7	THR	2.6
1	C	136	ASP	2.6
1	C	148	GLU	2.6
2	A	377	THR	2.6
2	A	713	ASP	2.5
1	C	22	LEU	2.5
2	A	80	ALA	2.5
1	C	175	ILE	2.5
1	C	131	LEU	2.5
1	C	26	THR	2.5
2	A	657	ALA	2.4
1	C	34	ALA	2.4
1	C	157	PHE	2.4
2	A	189	ALA	2.4
2	A	655	ALA	2.4
2	A	800	PHE	2.4
1	C	31	TYR	2.4
1	C	60	PHE	2.4
2	A	97	LEU	2.4
3	B	207	ARG	2.4
1	C	114	PHE	2.3
1	C	135	ASP	2.3
2	A	523	SER	2.3
1	C	40	PHE	2.3
2	A	727	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	93	ILE	2.3
2	A	76	TYR	2.3
2	A	121	GLY	2.2
1	C	25	VAL	2.2
1	C	153	THR	2.2
1	C	140	GLN	2.2
2	A	490	ASP	2.2
1	C	13	ALA	2.2
1	C	29	ASN	2.2
2	A	483	ASP	2.2
1	C	38	ALA	2.2
2	A	781	TYR	2.2
1	C	63	MET	2.2
2	A	201	HIS	2.2
2	A	728	ALA	2.1
1	C	164	ASP	2.1
2	A	625	ARG	2.1
1	C	151	GLY	2.1
2	A	277	TYR	2.1
2	A	241	PHE	2.1
2	A	795	PHE	2.1
3	B	189	ALA	2.1
1	C	102	TYR	2.1
1	C	169	ILE	2.1
1	C	129	VAL	2.1
1	C	159	LYS	2.0
2	A	797	TRP	2.0
2	A	91	PRO	2.0
2	A	191	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

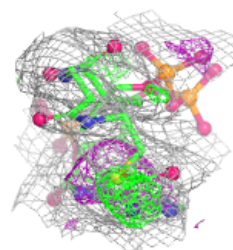
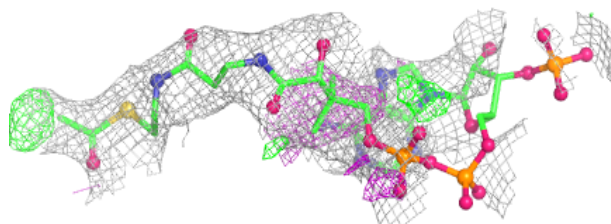
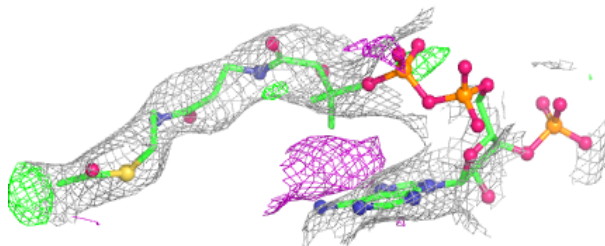
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CL	B	305	1/1	0.60	0.43	121,121,121,121	0
5	GOL	C	202	6/6	0.61	0.15	76,77,78,82	0
4	CL	C	201	1/1	0.67	0.16	102,102,102,102	0
9	EPE	B	310	15/15	0.69	0.17	49,59,100,117	0
4	CL	A	910	1/1	0.70	0.17	93,93,93,93	0
6	ACO	C	203	51/51	0.71	0.15	67,98,121,129	0
5	GOL	A	914	6/6	0.72	0.18	59,66,70,74	0
5	GOL	B	307	6/6	0.72	0.19	52,54,59,66	0
4	CL	A	904	1/1	0.74	0.17	103,103,103,103	0
5	GOL	A	915	6/6	0.77	0.12	64,66,70,79	0
4	CL	A	905	1/1	0.77	0.15	94,94,94,94	0
7	MLI	B	309	7/7	0.78	0.17	41,47,51,57	0
4	CL	B	303	1/1	0.79	0.07	99,99,99,99	0
7	MLI	A	917	7/7	0.80	0.15	65,70,74,79	0
5	GOL	A	912	6/6	0.81	0.18	47,50,58,60	0
4	CL	A	902	1/1	0.81	0.15	77,77,77,77	0
4	CL	A	907	1/1	0.81	0.22	79,79,79,79	0
4	CL	A	901	1/1	0.81	0.12	69,69,69,69	0
4	CL	B	302	1/1	0.82	0.23	90,90,90,90	0
4	CL	A	903	1/1	0.82	0.14	78,78,78,78	0
7	MLI	A	919	7/7	0.83	0.22	59,62,69,79	0
4	CL	B	306	1/1	0.84	0.13	81,81,81,81	0
4	CL	A	908	1/1	0.85	0.14	75,75,75,75	0
7	MLI	A	918	7/7	0.85	0.17	57,62,70,71	0
5	GOL	A	916	6/6	0.85	0.13	47,57,63,63	0
5	GOL	A	913	6/6	0.85	0.15	43,47,58,64	0
4	CL	A	909	1/1	0.85	0.16	65,65,65,65	0
4	CL	A	911	1/1	0.86	0.09	68,68,68,68	0
4	CL	A	906	1/1	0.88	0.15	65,65,65,65	0
4	CL	B	301	1/1	0.89	0.14	67,67,67,67	0
4	CL	B	304	1/1	0.90	0.11	80,80,80,80	0
5	GOL	B	308	6/6	0.91	0.15	44,44,48,60	0
8	IHP	A	920	36/36	0.92	0.10	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.

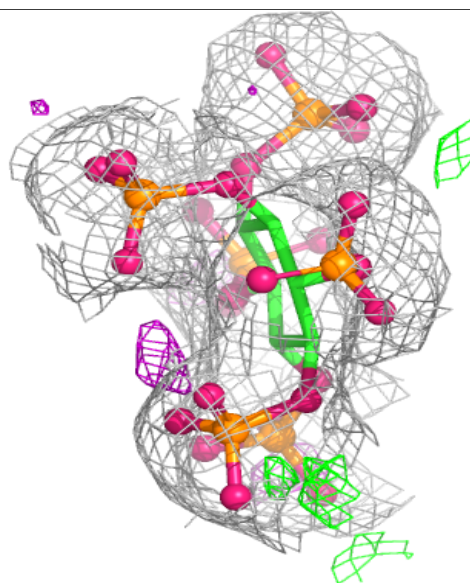
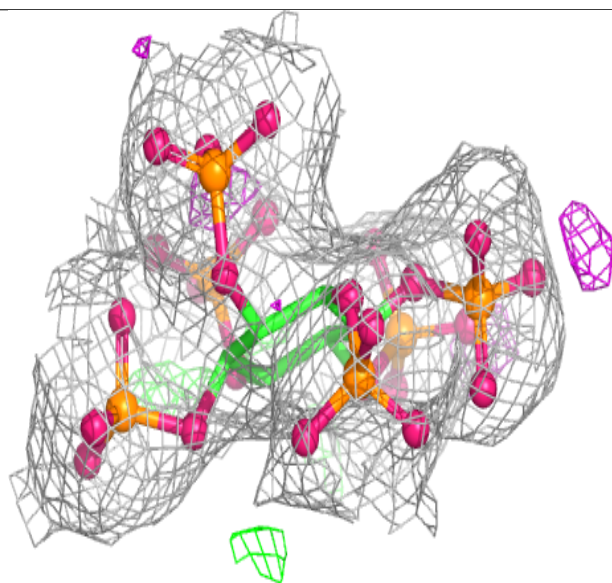
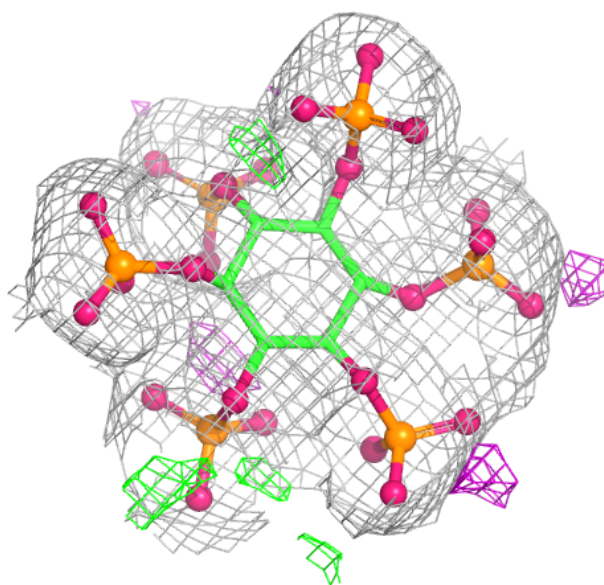
Electron density around ACO C 203:

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



Electron density around 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 ⓘ

There are no such residues in this entry.