



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:45 pm BST

PDB ID : 2WLF  
Title : Crystallographic analysis of the polysialic acid O-acetyltransferase OatWY  
Authors : Lee, H.J.; Rakic, B.; Gilbert, M.; Wakarchuk, W.W.; Withers, S.G.; Strynadka, N.C.J.  
Deposited on : 2009-06-23  
Resolution : 2.35 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](mailto: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.

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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 : 2.11  
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) : 2.11

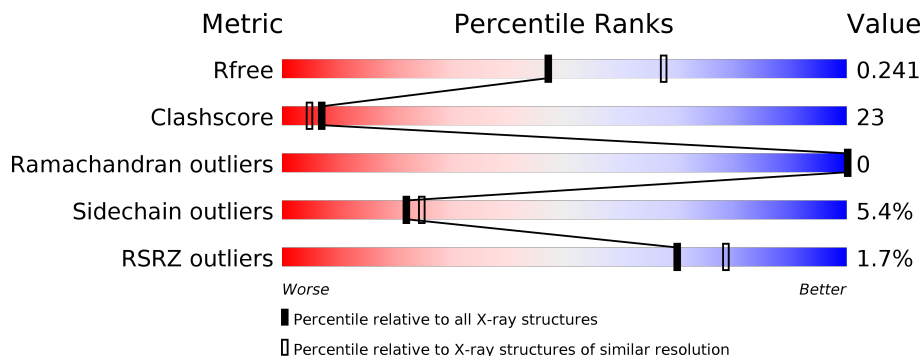
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	215	
1	B	215	
1	C	215	

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
2	ACT	A	1215	-	-	X	-
3	EDO	A	1217	-	-	X	-
4	ACO	A	1221	X	-	-	-
4	ACO	B	1218	X	-	-	-
4	ACO	C	1218	X	-	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5349 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.

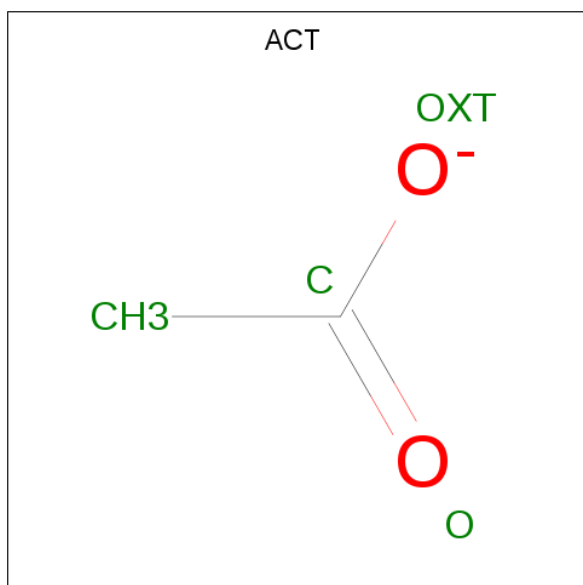
- Molecule 1 is a protein called POLYSIALIC ACID O-ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	210	Total 1631	C 1021	N 281	O 314	S 15	0	5	0
1	B	211	Total 1635	C 1024	N 284	O 313	S 14	6	2	0
1	C	211	Total 1638	C 1027	N 283	O 313	S 15	0	3	0

There are 3 discrepancies between the modelled and reference sequences:

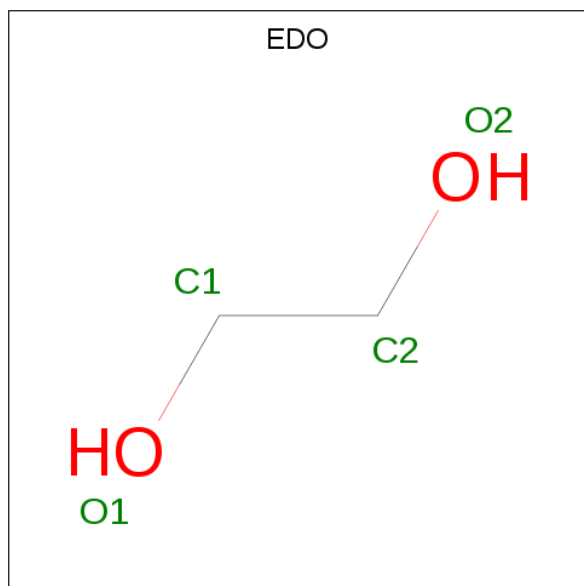
Chain	Residue	Modelled	Actual	Comment	Reference
A	67	ILE	ASN	engineered mutation	UNP Q93S40
B	67	ILE	ASN	engineered mutation	UNP Q93S40
C	67	ILE	ASN	engineered mutation	UNP Q93S40

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



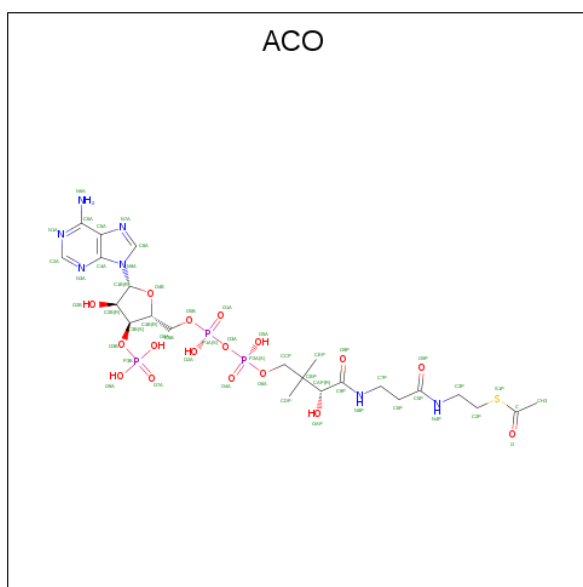
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0

- Molecule 4 is ACETYL COENZYME \*A (three-letter code: ACO) (formula: C<sub>23</sub>H<sub>38</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>S).



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

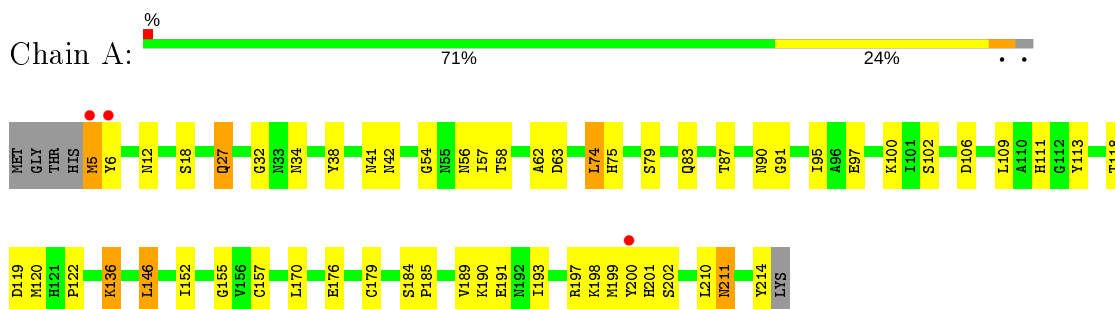
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	117	117	117	0	0
5	B	58	58	58	0	0
5	C	77	77	77	0	0

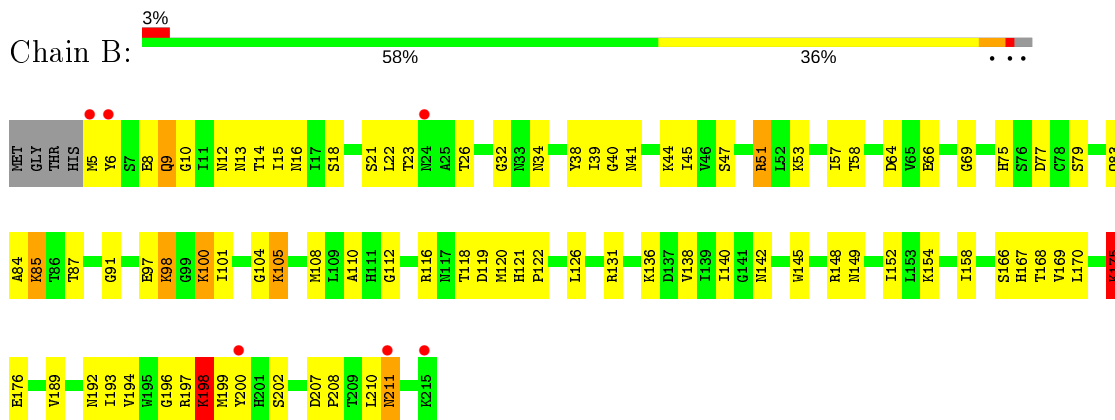
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

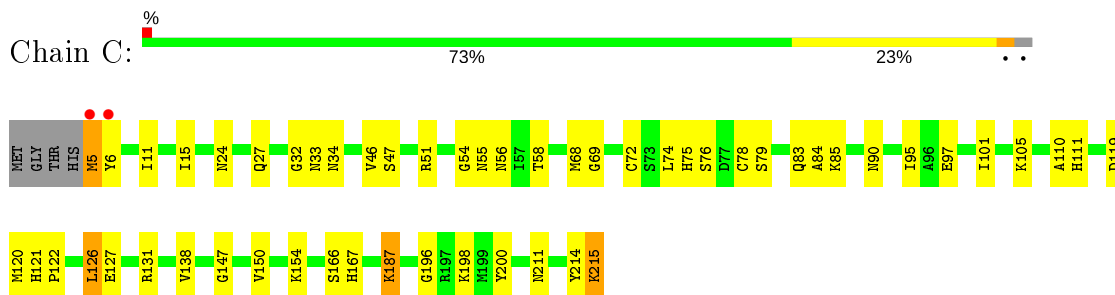
- Molecule 1: POLYSIALIC ACID O-ACETYLTRANSFERASE



- Molecule 1: POLYSIALIC ACID O-ACETYLTRANSFERASE



- Molecule 1: POLYSIALIC ACID O-ACETYLTRANSFERASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.86Å 94.66Å 100.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.35 40.58 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.00-2.35) 100.0 (40.58-2.35)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.75 (at 2.34Å)	Xtrriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.183 , 0.231 0.196 , 0.241	Depositor DCC
$R_{free}$ test set	1631 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.4	Xtrriage
Anisotropy	0.638	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 43.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5349	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ACO, EDO, 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	0.47	0/1674	0.60	0/2267
1	B	0.49	2/1667 (0.1%)	0.58	1/2257 (0.0%)
1	C	0.42	0/1673	0.55	0/2264
All	All	0.46	2/5014 (0.0%)	0.58	1/6788 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	175	LYS	CG-CD	8.93	1.82	1.52
1	B	198	LYS	CG-CD	-8.58	1.23	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	LYS	CB-CG-CD	-6.59	94.45	111.60

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	1631	0	1643	72	1
1	B	1635	0	1646	103	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1638	0	1654	70	0
2	A	8	0	6	5	0
2	C	4	0	3	1	0
3	A	16	0	24	15	0
3	B	8	0	12	3	0
3	C	4	0	6	0	0
4	A	51	0	34	1	0
4	B	51	0	34	10	1
4	C	51	0	34	10	0
5	A	117	0	0	8	0
5	B	58	0	0	2	0
5	C	77	0	0	10	0
All	All	5349	0	5096	233	2

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 23.

All (233) 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)
4:C:1218:ACO:C2P	5:C:2075:HOH:O	1.75	1.33
4:C:1218:ACO:HH31	5:C:2072:HOH:O	1.28	1.28
1:C:6:TYR:OH	1:C:15:ILE:HD12	1.18	1.26
4:B:1218:ACO:C5B	4:B:1218:ACO:H8A	1.73	1.17
4:B:1218:ACO:H52A	4:B:1218:ACO:H8A	1.21	1.15
1:B:91:GLY:HA2	3:B:1217:EDO:H22	1.19	1.15
1:B:199:MET:CE	1:C:131:ARG:NH2	2.11	1.12
1:A:62:ALA:HB1	3:A:1217:EDO:H12	1.28	1.11
1:A:199:MET:N	2:A:1215:ACT:O	1.84	1.09
1:A:62:ALA:HB1	3:A:1217:EDO:C1	1.84	1.07
4:C:1218:ACO:H22	5:C:2075:HOH:O	1.37	1.07
1:B:199:MET:CE	1:C:131:ARG:HH22	1.68	1.05
1:C:214:TYR:O	1:C:215:LYS:HB3	1.57	1.04
1:A:199:MET:CE	1:B:131:ARG:NH2	2.21	1.02
1:C:90:ASN:H	1:C:111:HIS:CD2	1.78	1.01
1:A:176:GLU:HG2	1:A:179[B]:CYS:SG	2.02	1.00
1:A:12:ASN:HB3	5:A:2017:HOH:O	1.61	0.99
1:C:105:LYS:HD2	5:C:2024:HOH:O	1.59	0.99
1:A:199:MET:HE2	1:B:131:ARG:NH2	1.77	0.98
1:C:55:ASN:H	1:C:76:SER:HB2	1.29	0.97
1:C:6:TYR:OH	1:C:15:ILE:CD1	2.13	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1215:ACT:H1	5:A:2110:HOH:O	1.68	0.94
4:C:1218:ACO:H21	5:C:2075:HOH:O	1.49	0.91
1:C:90:ASN:H	1:C:111:HIS:HD2	0.95	0.91
1:B:199:MET:HE3	1:C:131:ARG:HH22	1.35	0.90
1:A:90:ASN:H	1:A:111:HIS:HD2	1.14	0.90
1:A:63:ASP:H	3:A:1217:EDO:H11	1.35	0.90
1:B:199:MET:HE3	1:C:131:ARG:NH2	1.87	0.90
1:A:90:ASN:H	1:A:111:HIS:CD2	1.89	0.89
1:A:62:ALA:CB	3:A:1217:EDO:H12	2.03	0.89
1:C:5:MET:N	1:C:5:MET:CE	2.36	0.88
1:C:90:ASN:N	1:C:111:HIS:HD2	1.73	0.87
4:B:1218:ACO:C5B	4:B:1218:ACO:C8A	2.52	0.87
4:B:1218:ACO:H52A	4:B:1218:ACO:C8A	2.02	0.87
1:A:176:GLU:CG	1:A:179[B]:CYS:SG	2.63	0.86
1:C:105:LYS:CD	5:C:2024:HOH:O	2.16	0.86
1:B:112:GLY:HA2	3:B:1217:EDO:H11	1.58	0.86
4:B:1218:ACO:H51A	4:B:1218:ACO:H8A	1.58	0.85
1:A:199:MET:HE1	1:B:131:ARG:NH2	1.92	0.83
1:A:199:MET:CE	1:B:131:ARG:HH22	1.87	0.83
1:C:11:ILE:HG12	1:C:33:ASN:OD1	1.79	0.83
1:A:199:MET:HE2	1:B:131:ARG:CZ	2.09	0.82
1:B:79:SER:OG	1:B:100:LYS:HD3	1.81	0.81
1:A:190:LYS:HG3	5:B:2057:HOH:O	1.79	0.81
1:B:199:MET:CE	1:C:131:ARG:CZ	2.58	0.81
1:C:6:TYR:CZ	1:C:15:ILE:HD12	2.16	0.81
1:A:63:ASP:N	3:A:1217:EDO:H11	1.95	0.80
1:C:5:MET:N	1:C:5:MET:HE1	1.96	0.80
1:B:199:MET:HE1	1:C:131:ARG:HH12	1.47	0.79
1:B:8:GLU:HG2	1:B:9:GLN:N	1.98	0.79
1:B:207:ASP:OD2	1:B:210:LEU:HG	1.84	0.77
1:C:6:TYR:HH	1:C:15:ILE:HD12	1.50	0.77
1:B:199:MET:HE1	1:C:131:ARG:NH1	2.00	0.76
1:B:194:VAL:HG12	1:C:126:LEU:HD13	1.66	0.75
1:C:6:TYR:HE2	1:C:15:ILE:HD13	1.51	0.74
1:B:199:MET:HE1	1:C:131:ARG:HH22	1.51	0.74
1:A:157[B]:CYS:SG	5:A:2094:HOH:O	2.47	0.73
1:A:199:MET:HE1	1:B:131:ARG:HH22	1.47	0.73
1:B:211:ASN:H	1:B:211:ASN:HD22	1.35	0.72
1:A:12:ASN:CB	5:A:2017:HOH:O	2.29	0.72
1:B:166:SER:OG	1:B:167:HIS:HD2	1.71	0.72
1:B:207:ASP:HB3	1:B:210:LEU:HD12	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ALA:CB	3:A:1217:EDO:C1	2.65	0.71
4:C:1218:ACO:H131	4:C:1218:ACO:N8P	2.04	0.71
1:B:8:GLU:HG2	1:B:9:GLN:H	1.55	0.71
1:C:119:ASP:OD2	1:C:154:LYS:NZ	2.22	0.71
1:A:63:ASP:H	3:A:1217:EDO:C1	2.04	0.70
1:B:199:MET:HE1	1:C:131:ARG:NH2	2.03	0.70
1:B:208:PRO:O	1:B:211:ASN:ND2	2.25	0.69
1:C:97:GLU:O	5:C:2020:HOH:O	2.10	0.69
1:B:44:LYS:HB2	1:B:66:GLU:HG2	1.75	0.68
1:B:167:HIS:HE1	5:B:2041:HOH:O	1.77	0.67
1:C:6:TYR:CE2	1:C:15:ILE:HD13	2.29	0.67
1:A:18:SER:OG	1:A:41:ASN:ND2	2.27	0.67
1:B:105:LYS:HG2	1:B:142:ASN:OD1	1.94	0.66
4:C:1218:ACO:CDP	4:C:1218:ACO:N8P	2.58	0.66
1:C:214:TYR:O	1:C:215:LYS:CB	2.37	0.65
1:B:6:TYR:OH	1:B:15:ILE:HD12	1.96	0.65
1:A:201:HIS:O	1:A:202:SER:C	2.36	0.65
1:C:214:TYR:HD2	1:C:215:LYS:HE2	1.62	0.64
1:C:5:MET:N	1:C:5:MET:SD	2.70	0.64
1:B:211:ASN:N	1:B:211:ASN:HD22	1.93	0.64
1:B:58:THR:HB	1:B:79:SER:CB	2.28	0.64
1:B:6:TYR:CZ	1:B:15:ILE:HD12	2.33	0.63
1:B:199:MET:HE2	1:C:131:ARG:CZ	2.27	0.63
1:A:198:LYS:HB3	1:A:200:TYR:CE2	2.33	0.63
1:C:46:VAL:HG23	1:C:68[A]:MET:SD	2.38	0.62
1:C:6:TYR:CE2	1:C:15:ILE:CD1	2.82	0.62
1:A:62:ALA:HB1	3:A:1217:EDO:H11	1.79	0.62
1:A:211:ASN:HD22	1:A:211:ASN:N	1.96	0.62
1:C:95:ILE:HG12	1:C:101:ILE:HD12	1.83	0.61
1:B:84:ALA:O	1:B:85:LYS:HB2	2.00	0.60
1:B:91:GLY:HA2	3:B:1217:EDO:C2	2.12	0.60
1:C:166:SER:OG	1:C:167:HIS:HD2	1.85	0.60
1:A:200:TYR:CD2	2:A:1215:ACT:H3	2.37	0.60
1:B:193:ILE:C	1:B:193:ILE:HD12	2.23	0.59
1:A:87:THR:OG1	1:A:197:ARG:NH2	2.35	0.59
1:C:154:LYS:HE2	5:C:2036:HOH:O	2.03	0.59
4:C:1218:ACO:HN8	4:C:1218:ACO:CDP	2.15	0.59
1:A:176:GLU:HG3	1:A:179[B]:CYS:SG	2.41	0.59
1:C:101:ILE:HG12	1:C:138:VAL:HB	1.83	0.59
1:B:199:MET:HE1	1:C:131:ARG:CZ	2.27	0.58
4:B:1218:ACO:H51A	4:B:1218:ACO:C8A	2.26	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:GLN:HA	1:A:27:GLN:OE1	2.04	0.58
1:C:58:THR:OG1	1:C:79:SER:CB	2.52	0.58
1:B:87:THR:CG2	1:B:197:ARG:NH2	2.67	0.58
4:B:1218:ACO:O2B	4:B:1218:ACO:O7A	2.22	0.57
1:C:5:MET:HE2	1:C:27:GLN:HE22	1.69	0.57
1:C:55:ASN:H	1:C:76:SER:CB	2.12	0.57
1:C:58:THR:OG1	1:C:79:SER:HB2	2.03	0.57
1:B:97:GLU:O	1:B:98:LYS:HG2	2.05	0.57
1:A:32:GLY:HA3	1:A:54:GLY:O	2.05	0.57
1:B:194:VAL:CG1	1:C:126:LEU:HD13	2.35	0.57
1:A:42:ASN:OD1	5:A:2023:HOH:O	2.17	0.56
1:B:198:LYS:HG2	1:B:200:TYR:OH	2.05	0.56
1:A:58:THR:CG2	3:A:1220:EDO:H21	2.36	0.56
1:A:193:ILE:C	1:A:193:ILE:HD12	2.26	0.56
1:C:84:ALA:O	1:C:85:LYS:HB2	2.06	0.55
1:A:136:LYS:HB3	1:A:155:GLY:CA	2.37	0.55
1:A:136:LYS:HB3	1:A:155:GLY:HA2	1.88	0.55
1:A:211:ASN:ND2	1:A:211:ASN:N	2.54	0.55
1:C:46:VAL:CG2	1:C:68[A]:MET:SD	2.95	0.55
1:B:199:MET:CE	1:C:131:ARG:NH1	2.64	0.55
1:A:90:ASN:N	1:A:111:HIS:HD2	1.96	0.54
1:C:211:ASN:HD22	1:C:211:ASN:N	2.04	0.54
1:B:5:MET:HG3	1:B:26:THR:O	2.08	0.54
1:B:199:MET:HE2	1:C:131:ARG:NH2	2.12	0.54
1:C:6:TYR:CZ	1:C:15:ILE:CD1	2.86	0.54
1:C:198:LYS:HD3	1:C:200:TYR:CE2	2.43	0.53
1:B:23:THR:HA	1:B:45:ILE:O	2.09	0.53
1:B:83:GLN:HB2	1:B:104:GLY:C	2.29	0.53
1:A:83:GLN:NE2	5:A:2042:HOH:O	2.26	0.53
1:B:12:ASN:O	1:B:34:ASN:HA	2.07	0.53
1:B:8:GLU:OE2	1:B:13:ASN:HB2	2.08	0.53
1:B:148:ARG:HG2	4:C:1218:ACO:H31	1.91	0.53
1:B:8:GLU:CG	1:B:9:GLN:H	2.21	0.53
1:A:91:GLY:HA3	1:A:113:TYR:CE2	2.44	0.52
1:B:58:THR:HB	1:B:79:SER:HB2	1.91	0.52
1:B:207:ASP:OD2	1:B:210:LEU:CG	2.57	0.52
1:B:21:SER:OG	1:B:40:GLY:O	2.27	0.52
1:A:152:ILE:HD12	1:A:170:LEU:HD12	1.91	0.52
1:C:187:LYS:HG2	5:C:2059:HOH:O	2.09	0.52
1:B:47:SER:O	1:B:69:GLY:HA2	2.09	0.52
1:C:83:GLN:HG2	5:C:2023:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:ASP:HB2	1:B:98:LYS:HB3	1.92	0.51
1:B:101:ILE:HG12	1:B:138:VAL:HB	1.92	0.51
1:B:196:GLY:O	1:C:122:PRO:HD2	2.10	0.51
1:B:8:GLU:CG	1:B:9:GLN:N	2.69	0.51
1:B:58:THR:HB	1:B:79:SER:HB3	1.92	0.51
1:A:106:ASP:OD1	1:A:197:ARG:NH1	2.44	0.50
1:A:62:ALA:CA	3:A:1217:EDO:H11	2.41	0.50
1:B:10:GLY:HA3	1:B:32:GLY:O	2.11	0.50
4:A:1221:ACO:O5A	5:A:2116:HOH:O	2.20	0.50
1:B:140:ILE:HG12	1:B:158:ILE:HD12	1.94	0.50
1:C:34:ASN:O	1:C:56:ASN:HA	2.12	0.50
1:B:87:THR:OG1	1:B:197:ARG:NH2	2.44	0.50
1:B:6:TYR:OH	1:B:15:ILE:CD1	2.59	0.50
1:B:58:THR:O	1:B:79:SER:HA	2.12	0.49
1:B:108:MET:CE	1:C:121:HIS:CE1	2.95	0.49
1:B:84:ALA:O	1:B:85:LYS:CB	2.60	0.49
1:A:34:ASN:O	3:A:1220:EDO:H11	2.13	0.49
1:B:16[B]:ASN:ND2	1:B:38:TYR:HD1	2.11	0.49
1:C:119:ASP:O	1:C:120:MET:HB2	2.13	0.49
1:B:16[B]:ASN:HD21	1:B:38:TYR:HD1	1.60	0.49
1:A:184:SER:HA	1:A:185:PRO:C	2.33	0.48
1:C:110:ALA:HA	2:C:1216:ACT:H1	1.93	0.48
1:A:122:PRO:HD2	1:C:196:GLY:O	2.13	0.48
1:A:34:ASN:HB2	1:A:56:ASN:HD22	1.79	0.48
1:B:149:ASN:O	1:B:167:HIS:HA	2.14	0.48
1:A:63:ASP:HB2	3:A:1217:EDO:H22	1.94	0.48
1:B:211:ASN:H	1:B:211:ASN:ND2	2.09	0.48
1:A:211:ASN:H	1:A:211:ASN:ND2	2.12	0.47
1:B:108:MET:HE2	1:C:121:HIS:CE1	2.49	0.47
1:A:198:LYS:HB3	1:A:200:TYR:CZ	2.49	0.47
1:B:23:THR:O	1:B:26:THR:HB	2.14	0.47
1:C:32:GLY:HA3	1:C:54:GLY:O	2.14	0.47
1:A:79[B]:SER:HB3	1:A:100:LYS:HB3	1.97	0.47
1:B:57:ILE:HG12	1:B:75:HIS:O	2.15	0.47
1:C:72:CYS:SG	1:C:74:LEU:HD13	2.55	0.47
1:A:200:TYR:HD2	2:A:1215:ACT:H3	1.79	0.46
1:B:6:TYR:CE1	1:B:15:ILE:CD1	2.98	0.46
1:B:6:TYR:CZ	1:B:15:ILE:CD1	2.98	0.46
1:A:34:ASN:HB2	1:A:56:ASN:ND2	2.31	0.46
1:A:5:MET:O	1:A:6:TYR:HB3	2.15	0.46
1:A:57:ILE:HG12	1:A:75:HIS:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:LYS:HB3	1:C:187:LYS:HE3	1.50	0.46
1:A:199:MET:HE2	1:B:131:ARG:NH1	2.31	0.45
1:B:136:LYS:HE2	1:B:154:LYS:HD2	1.98	0.45
1:B:145:TRP:C	1:B:145:TRP:CD1	2.88	0.45
1:B:110:ALA:HB2	4:C:1218:ACO:HH33	1.98	0.45
1:B:121:HIS:NE2	4:B:1218:ACO:O	2.42	0.45
1:A:5:MET:HB3	1:A:6:TYR:H	1.69	0.44
1:B:14:THR:HG23	1:B:14:THR:O	2.18	0.44
1:B:6:TYR:OH	1:B:8:GLU:HB2	2.16	0.44
1:B:154:LYS:NZ	4:B:1218:ACO:O5A	2.47	0.44
1:B:85:LYS:HE2	1:B:85:LYS:HB3	1.83	0.44
1:B:16[B]:ASN:ND2	1:B:38:TYR:CD1	2.86	0.44
1:A:176:GLU:OE2	1:A:191:GLU:OE2	2.35	0.44
1:A:34:ASN:HD22	1:A:56:ASN:HD21	1.65	0.44
1:B:51:ARG:HH22	1:B:53:LYS:HE3	1.83	0.44
1:A:119:ASP:O	1:A:120:MET:HB2	2.18	0.44
1:C:90:ASN:N	1:C:111:HIS:CD2	2.60	0.44
1:C:126:LEU:HD12	1:C:126:LEU:HA	1.70	0.43
1:B:152:ILE:HD12	1:B:158:ILE:HD11	1.99	0.43
4:C:1218:ACO:HN8	4:C:1218:ACO:H132	1.82	0.43
1:A:38:TYR:OH	5:A:2021:HOH:O	2.19	0.43
1:C:147:GLY:O	1:C:150:VAL:HG23	2.18	0.43
1:A:199:MET:HB3	1:B:122:PRO:HD3	2.00	0.43
1:B:39:ILE:HD13	1:B:45:ILE:HD12	2.00	0.42
1:A:199:MET:HG2	2:A:1215:ACT:O	2.18	0.42
1:B:207:ASP:OD2	1:B:210:LEU:CD1	2.68	0.42
4:B:1218:ACO:P3B	4:B:1218:ACO:HO2A	2.41	0.42
1:B:64:ASP:O	1:B:85:LYS:HA	2.19	0.42
1:B:116:ARG:HD3	1:B:118:THR:O	2.19	0.42
1:A:58:THR:HG23	3:A:1220:EDO:H21	2.01	0.42
1:C:47:SER:O	1:C:69:GLY:HA2	2.20	0.42
1:C:75:HIS:O	1:C:78:CYS:HB2	2.20	0.42
1:A:109:LEU:HG	1:A:146:LEU:HD22	2.00	0.42
1:B:87:THR:HG21	1:B:197:ARG:NH2	2.34	0.42
1:B:194:VAL:CG1	1:C:126:LEU:CD1	2.97	0.41
1:B:211:ASN:N	1:B:211:ASN:ND2	2.64	0.41
1:B:119:ASP:O	1:B:120:MET:HB2	2.20	0.41
1:A:211:ASN:HA	1:A:214:TYR:CE1	2.56	0.41
1:B:168:THR:HG22	1:B:169:VAL:N	2.35	0.41
1:A:62:ALA:CB	3:A:1217:EDO:H11	2.43	0.41
1:B:18:SER:HB3	1:B:41:ASN:HD22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:GLU:C	1:B:98:LYS:HG2	2.41	0.41
1:A:63:ASP:H	3:A:1217:EDO:C2	2.34	0.41
1:A:74:LEU:HD12	1:A:95:ILE:HB	2.02	0.41
1:A:97:GLU:OE2	1:A:118:THR:OG1	2.33	0.41
1:B:192:ASN:ND2	1:C:127:GLU:HG3	2.36	0.41
1:A:197:ARG:O	1:B:121:HIS:ND1	2.54	0.40
1:B:16[A]:ASN:HA	1:B:16[A]:ASN:HD22	1.71	0.40

All (2) 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:A:200:TYR:CB	1:A:200:TYR:CB[3_654]	1.86	0.34
1:B:175:LYS:CD	4:B:1218:ACO:O8A[2_645]	2.12	0.08

## 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	213/215 (99%)	207 (97%)	6 (3%)	0	100	100
1	B	211/215 (98%)	202 (96%)	9 (4%)	0	100	100
1	C	212/215 (99%)	207 (98%)	5 (2%)	0	100	100
All	All	636/645 (99%)	616 (97%)	20 (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	190/189 (100%)	181 (95%)	9 (5%)	26	31
1	B	188/189 (100%)	173 (92%)	15 (8%)	12	12
1	C	189/189 (100%)	183 (97%)	6 (3%)	39	47
All	All	567/567 (100%)	537 (95%)	30 (5%)	22	26

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MET
1	A	27	GLN
1	A	74	LEU
1	A	102	SER
1	A	136	LYS
1	A	146	LEU
1	A	189	VAL
1	A	210	LEU
1	A	211	ASN
1	B	9	GLN
1	B	22	LEU
1	B	51	ARG
1	B	85	LYS
1	B	98	LYS
1	B	100	LYS
1	B	105	LYS
1	B	126	LEU
1	B	170	LEU
1	B	175	LYS
1	B	176	GLU
1	B	189	VAL
1	B	198	LYS
1	B	202	SER
1	B	211	ASN
1	C	5	MET
1	C	24	ASN
1	C	51	ARG
1	C	126	LEU
1	C	187	LYS
1	C	215	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	41	ASN
1	A	42	ASN
1	A	56	ASN
1	A	111	HIS
1	A	211	ASN
1	B	34	ASN
1	B	41	ASN
1	B	75	HIS
1	B	90	ASN
1	B	167	HIS
1	B	192	ASN
1	B	211	ASN
1	C	12	ASN
1	C	27	GLN
1	C	34	ASN
1	C	41	ASN
1	C	81	GLN
1	C	90	ASN
1	C	111	HIS
1	C	134	HIS
1	C	149	ASN
1	C	167	HIS
1	C	211	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 carbohydrates in this entry.

## 5.6 Ligand geometry i

13 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	A	1217	-	3,3,3	0.37	0	2,2,2	0.36	0
3	EDO	A	1219	-	3,3,3	0.41	0	2,2,2	0.65	0
2	ACT	A	1216	-	1,3,3	1.67	0	0,3,3	0.00	-
2	ACT	C	1216	-	1,3,3	1.17	0	0,3,3	0.00	-
3	EDO	C	1217	-	3,3,3	0.39	0	2,2,2	0.42	0
4	ACO	B	1218	-	45,53,53	1.10	3 (6%)	56,79,79	3.14	12 (21%)
3	EDO	B	1216	-	3,3,3	0.63	0	2,2,2	0.14	0
3	EDO	B	1217	-	3,3,3	0.46	0	2,2,2	0.35	0
4	ACO	C	1218	-	45,53,53	1.21	3 (6%)	56,79,79	1.19	3 (5%)
4	ACO	A	1221	-	45,53,53	1.31	6 (13%)	56,79,79	3.28	11 (19%)
3	EDO	A	1220	-	3,3,3	0.43	0	2,2,2	0.24	0
3	EDO	A	1218	-	3,3,3	0.45	0	2,2,2	0.29	0
2	ACT	A	1215	-	1,3,3	1.82	0	0,3,3	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	1217	-	-	1/1/1/1	-
3	EDO	A	1219	-	-	1/1/1/1	-
3	EDO	B	1217	-	-	0/1/1/1	-
3	EDO	C	1217	-	-	1/1/1/1	-
4	ACO	B	1218	-	1/1/12/14	19/47/67/67	0/3/3/3
3	EDO	B	1216	-	-	1/1/1/1	-
4	ACO	A	1221	-	1/1/12/14	16/47/67/67	0/3/3/3
3	EDO	A	1220	-	-	1/1/1/1	-
3	EDO	A	1218	-	-	1/1/1/1	-
4	ACO	C	1218	-	1/1/12/14	14/47/67/67	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1218	ACO	O4B-C1B	4.04	1.46	1.41
4	B	1218	ACO	P3B-O7A	3.95	1.63	1.50
4	C	1218	ACO	P3B-O7A	3.89	1.63	1.50
4	A	1221	ACO	P3B-O7A	3.71	1.62	1.50
4	A	1221	ACO	P2A-O6A	2.72	1.70	1.59
4	A	1221	ACO	CDP-CBP	2.43	1.59	1.53
4	C	1218	ACO	P3B-O8A	2.39	1.64	1.54
4	B	1218	ACO	O4B-C1B	2.37	1.44	1.41
4	A	1221	ACO	O6A-CCP	2.32	1.51	1.43
4	B	1218	ACO	P3B-O8A	2.17	1.63	1.54
4	A	1221	ACO	C6P-C5P	2.06	1.55	1.51
4	A	1221	ACO	P3B-O8A	2.04	1.62	1.54

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1218	ACO	CDP-CBP-CCP	-13.28	86.57	108.23
4	A	1221	ACO	CEP-CBP-CCP	-12.55	87.76	108.23
4	B	1218	ACO	CEP-CBP-CCP	-12.06	88.56	108.23
4	A	1221	ACO	CDP-CBP-CCP	-11.20	89.97	108.23
4	A	1221	ACO	CEP-CBP-CAP	8.99	124.41	108.82
4	A	1221	ACO	CEP-CBP-CDP	8.81	127.11	109.17
4	B	1218	ACO	CEP-CBP-CAP	7.29	121.47	108.82
4	B	1218	ACO	CDP-CBP-CAP	5.83	118.93	108.82
4	B	1218	ACO	O5B-P1A-O1A	-5.72	86.71	109.07
4	A	1221	ACO	O5B-P1A-O1A	-5.28	88.44	109.07
4	A	1221	ACO	O2A-P1A-O5B	-5.03	84.37	107.75
4	B	1218	ACO	CEP-CBP-CDP	4.93	119.21	109.17
4	A	1221	ACO	N3A-C2A-N1A	-4.70	121.33	128.68
4	A	1221	ACO	O6A-CCP-CBP	4.52	117.82	110.55
4	C	1218	ACO	N3A-C2A-N1A	-4.47	121.69	128.68
4	B	1218	ACO	N3A-C2A-N1A	-4.44	121.74	128.68
4	A	1221	ACO	P2A-O3A-P1A	-3.87	119.55	132.83
4	B	1218	ACO	O2A-P1A-O5B	-3.86	89.81	107.75
4	B	1218	ACO	P2A-O3A-P1A	-3.11	122.15	132.83
4	C	1218	ACO	C5B-C4B-C3B	-3.05	104.30	114.40
4	A	1221	ACO	OAP-CAP-CBP	2.73	116.67	110.25
4	B	1218	ACO	C5B-C4B-C3B	-2.34	106.63	114.40
4	A	1221	ACO	O2A-P1A-O1A	2.32	123.72	112.24
4	C	1218	ACO	P2A-O3A-P1A	-2.23	125.16	132.83
4	B	1218	ACO	O6A-CCP-CBP	2.12	113.95	110.55
4	B	1218	ACO	O2A-P1A-O1A	2.05	122.39	112.24

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	1218	ACO	CAP
4	C	1218	ACO	CAP
4	A	1221	ACO	CAP

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1218	ACO	C5B-O5B-P1A-O3A
4	B	1218	ACO	CDP-CBP-CCP-O6A
4	B	1218	ACO	CAP-CBP-CCP-O6A
4	B	1218	ACO	OAP-CAP-CBP-CCP
4	B	1218	ACO	OAP-CAP-CBP-CDP
4	B	1218	ACO	C9P-CAP-CBP-CDP
4	B	1218	ACO	O9P-C9P-CAP-CBP
4	B	1218	ACO	N8P-C9P-CAP-CBP
4	B	1218	ACO	O9P-C9P-CAP-OAP
4	B	1218	ACO	N8P-C9P-CAP-OAP
4	C	1218	ACO	OAP-CAP-CBP-CCP
4	C	1218	ACO	OAP-CAP-CBP-CDP
4	C	1218	ACO	C9P-CAP-CBP-CDP
4	C	1218	ACO	O9P-C9P-CAP-CBP
4	C	1218	ACO	N8P-C9P-CAP-CBP
4	C	1218	ACO	O9P-C9P-CAP-OAP
4	C	1218	ACO	N8P-C9P-CAP-OAP
4	A	1221	ACO	CAP-CBP-CCP-O6A
4	A	1221	ACO	OAP-CAP-CBP-CCP
4	A	1221	ACO	OAP-CAP-CBP-CDP
4	A	1221	ACO	C9P-CAP-CBP-CDP
4	A	1221	ACO	O9P-C9P-CAP-CBP
4	A	1221	ACO	N8P-C9P-CAP-CBP
4	A	1221	ACO	N8P-C9P-CAP-OAP
4	A	1221	ACO	O-C-S1P-C2P
4	A	1221	ACO	CH3-C-S1P-C2P
4	B	1218	ACO	C3B-C4B-C5B-O5B
4	B	1218	ACO	CEP-CBP-CCP-O6A
4	A	1221	ACO	CEP-CBP-CCP-O6A
3	C	1217	EDO	O1-C1-C2-O2
3	B	1216	EDO	O1-C1-C2-O2
4	B	1218	ACO	O-C-S1P-C2P
4	B	1218	ACO	CH3-C-S1P-C2P
4	C	1218	ACO	O-C-S1P-C2P
4	A	1221	ACO	O9P-C9P-CAP-OAP

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms
4	A	1221	ACO	CDP-CBP-CCP-O6A
4	C	1218	ACO	OAP-CAP-CBP-CEP
3	A	1218	EDO	O1-C1-C2-O2
4	C	1218	ACO	CH3-C-S1P-C2P
4	B	1218	ACO	O4B-C4B-C5B-O5B
4	C	1218	ACO	C3B-O3B-P3B-O7A
4	A	1221	ACO	CCP-O6A-P2A-O3A
4	B	1218	ACO	C5B-O5B-P1A-O1A
4	A	1221	ACO	P1A-O3A-P2A-O5A
3	A	1219	EDO	O1-C1-C2-O2
4	B	1218	ACO	C3P-C2P-S1P-C
4	C	1218	ACO	C3P-C2P-S1P-C
4	A	1221	ACO	C3P-C2P-S1P-C
3	A	1217	EDO	O1-C1-C2-O2
3	A	1220	EDO	O1-C1-C2-O2
4	C	1218	ACO	C9P-CAP-CBP-CEP
4	B	1218	ACO	CCP-O6A-P2A-O3A
4	B	1218	ACO	CCP-O6A-P2A-O4A
4	A	1221	ACO	CCP-O6A-P2A-O4A
4	C	1218	ACO	C9P-CAP-CBP-CCP

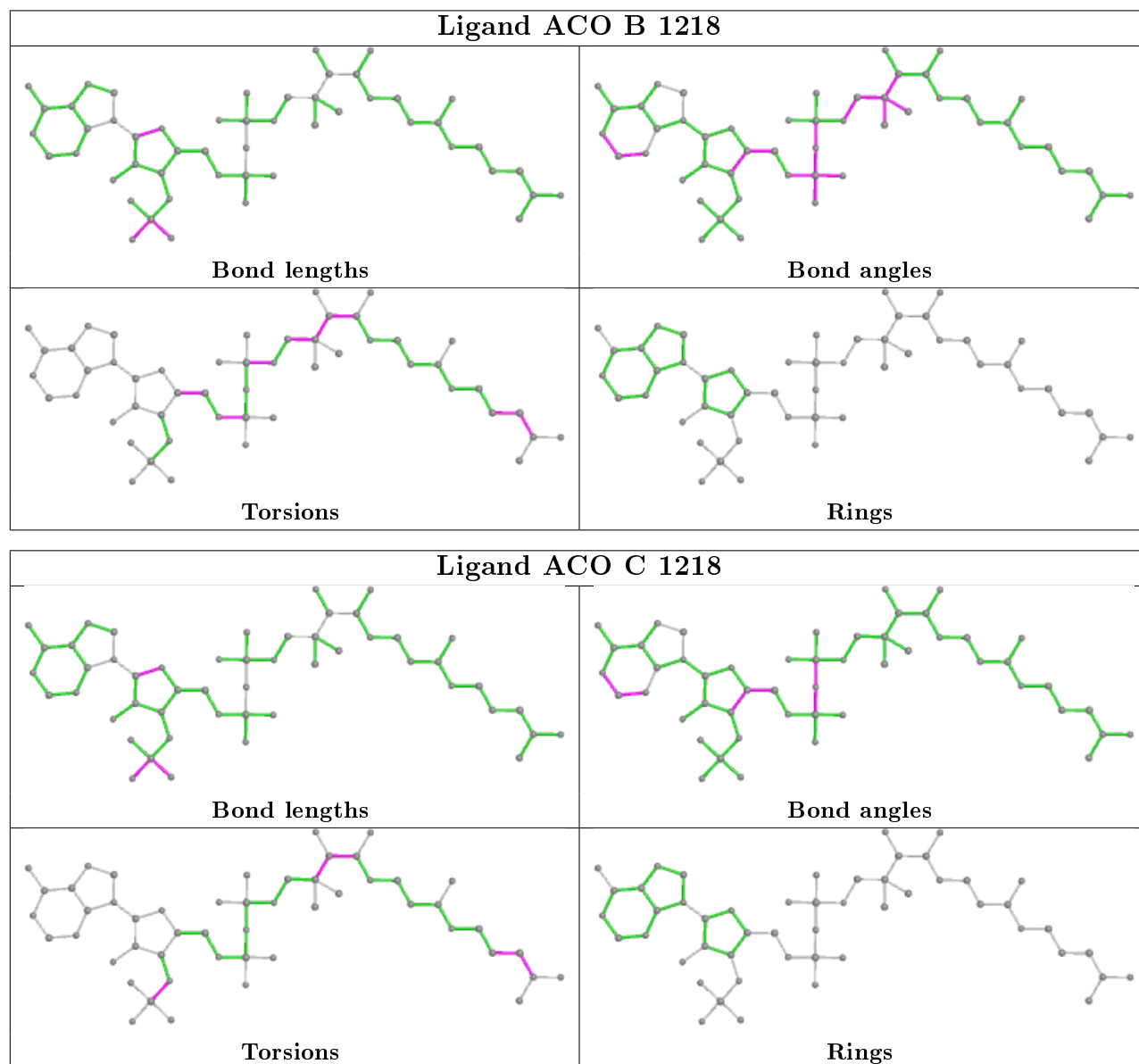
There are no ring outliers.

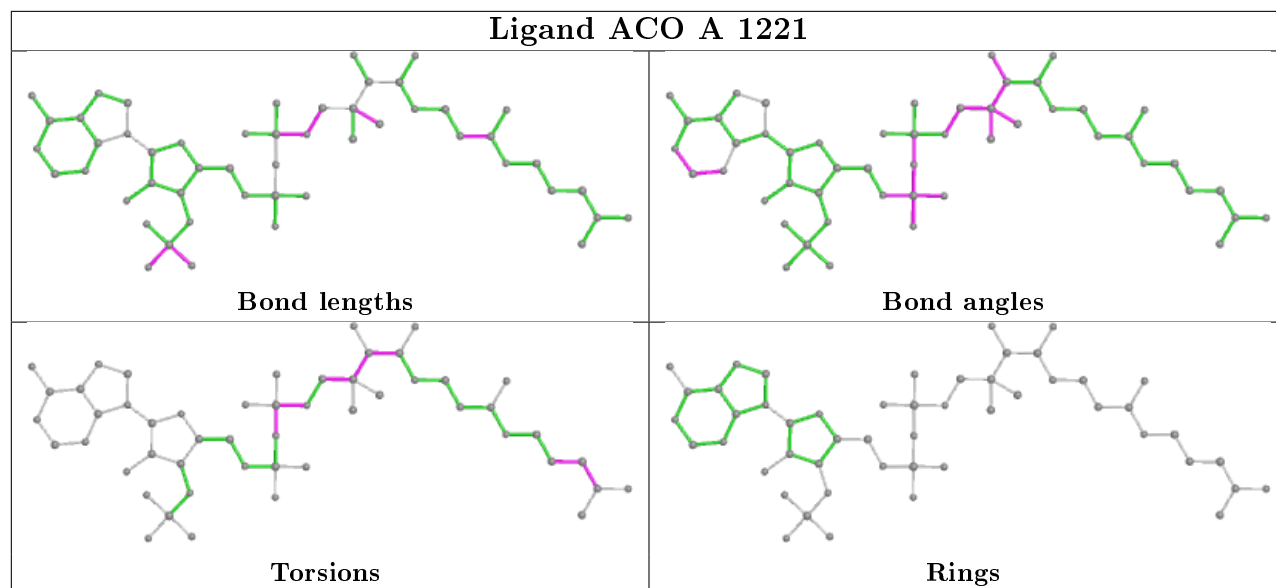
8 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1217	EDO	12	0
2	C	1216	ACT	1	0
4	B	1218	ACO	10	1
3	B	1217	EDO	3	0
4	C	1218	ACO	10	0
4	A	1221	ACO	1	0
3	A	1220	EDO	3	0
2	A	1215	ACT	5	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	210/215 (97%)	-0.11	3 (1%) 75 83	2, 10, 18, 46	1 (0%)
1	B	211/215 (98%)	-0.09	6 (2%) 53 64	7, 12, 22, 44	3 (1%)
1	C	211/215 (98%)	-0.22	2 (0%) 84 90	6, 12, 17, 44	0
All	All	632/645 (97%)	-0.14	11 (1%) 70 78	2, 12, 20, 46	4 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	200	TYR	7.0
1	C	5	MET	5.6
1	A	5	MET	4.3
1	B	215	LYS	3.8
1	C	6	TYR	3.3
1	B	6	TYR	3.1
1	A	6	TYR	2.8
1	B	24	ASN	2.7
1	B	200	TYR	2.5
1	B	211	ASN	2.1
1	B	5	MET	2.1

### 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 carbohydrates in this entry.

## 6.4 Ligands

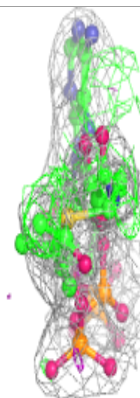
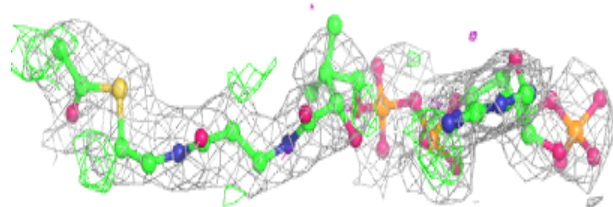
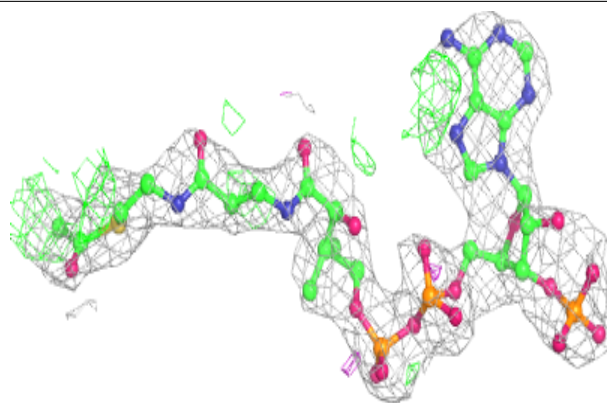
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ACT	A	1215	4/4	0.51	0.40	55,56,56,56	0
3	EDO	B	1216	4/4	0.79	0.21	44,45,45,46	0
3	EDO	A	1218	4/4	0.80	0.19	58,58,58,59	0
4	ACO	B	1218	51/51	0.82	0.18	57,68,82,82	0
2	ACT	A	1216	4/4	0.84	0.26	50,50,50,50	0
2	ACT	C	1216	4/4	0.91	0.24	46,46,46,47	0
4	ACO	C	1218	51/51	0.91	0.13	37,42,52,54	0
3	EDO	C	1217	4/4	0.93	0.18	45,46,46,46	0
4	ACO	A	1221	51/51	0.93	0.12	26,36,46,48	0
3	EDO	A	1217	4/4	0.94	0.16	38,39,39,40	0
3	EDO	A	1220	4/4	0.94	0.17	44,45,46,47	0
3	EDO	B	1217	4/4	0.94	0.35	41,42,42,43	0
3	EDO	A	1219	4/4	0.94	0.16	46,47,47,48	0

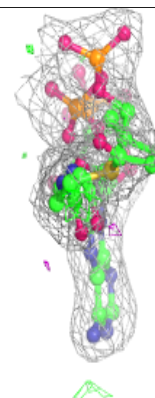
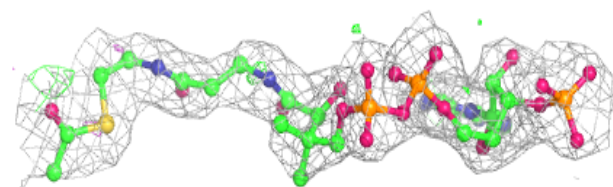
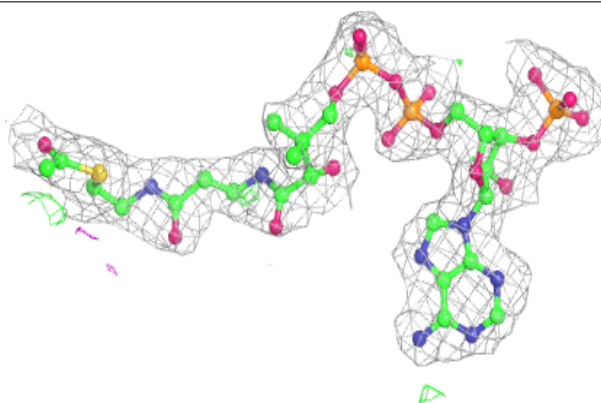
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

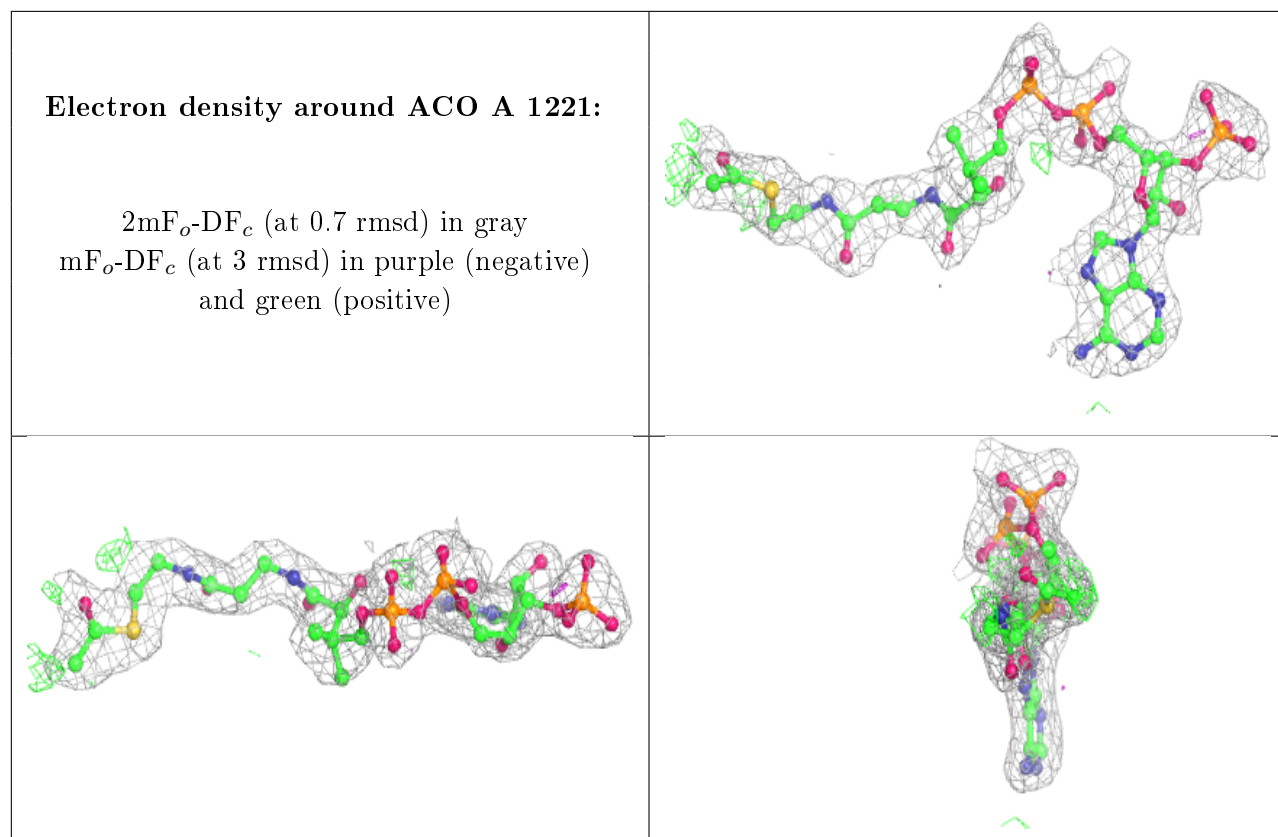
**Electron density around ACO B 1218:**

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

**Electron density around ACO C 1218:**

$2mF_o-DF_c$  (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.