



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 11:47 pm BST

PDB ID : 4AHU  
Title : Parallel screening of a low molecular weight compound library: do differences in methodology affect hit identification  
Authors : Wielens, J.; Heady, S.J.; Rhodes, D.I.; Mulder, R.J.; Dolezal, O.; Deadman, J.J.; Newman, J.; Chalmers, D.K.; Parker, M.W.; Peat, T.S.; Scanlon, M.J.  
Deposited on : 2012-02-07  
Resolution : 1.90 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
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

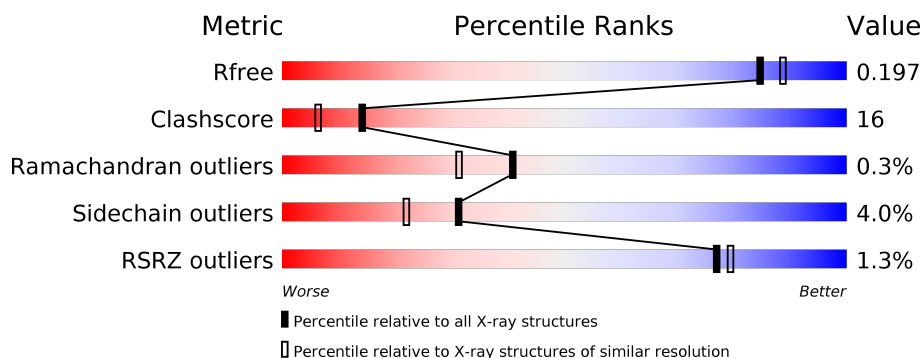
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	183	<div> <div> <div></div> <div>66%</div> <div>15%</div> <div>••</div> <div>16%</div> </div> </div>
1	B	183	<div> <div> <div>2%</div> <div>64%</div> <div>17%</div> <div>•</div> <div>16%</div> </div> </div>

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	GOL	A	1215	-	-	X	-
4	GOL	A	1216	-	X	X	-
4	GOL	B	1218	-	-	X	-
6	ACY	B	1215	-	-	X	-
7	EDO	B	1216	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 2761 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 INTEGRASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	11	0
			1247	795	215	233	4			
1	B	153	Total	C	N	O	S	0	11	0
			1249	797	216	232	4			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	expression tag	UNP P12497
A	31	GLY	-	expression tag	UNP P12497
A	32	SER	-	expression tag	UNP P12497
A	33	SER	-	expression tag	UNP P12497
A	34	HIS	-	expression tag	UNP P12497
A	35	HIS	-	expression tag	UNP P12497
A	36	HIS	-	expression tag	UNP P12497
A	37	HIS	-	expression tag	UNP P12497
A	38	HIS	-	expression tag	UNP P12497
A	39	HIS	-	expression tag	UNP P12497
A	40	SER	-	expression tag	UNP P12497
A	41	SER	-	expression tag	UNP P12497
A	42	GLY	-	expression tag	UNP P12497
A	43	LEU	-	expression tag	UNP P12497
A	44	VAL	-	expression tag	UNP P12497
A	45	PRO	-	expression tag	UNP P12497
A	46	ARG	-	expression tag	UNP P12497
A	47	GLY	-	expression tag	UNP P12497
A	48	SER	-	expression tag	UNP P12497
A	49	HIS	-	expression tag	UNP P12497
A	56	SER	CYS	engineered mutation	UNP P12497
A	139	ASP	PHE	engineered mutation	UNP P12497
A	185	HIS	PHE	engineered mutation	UNP P12497
B	30	MET	-	expression tag	UNP P12497
B	31	GLY	-	expression tag	UNP P12497

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Chain	Residue	Modelled	Actual	Comment	Reference
B	32	SER	-	expression tag	UNP P12497
B	33	SER	-	expression tag	UNP P12497
B	34	HIS	-	expression tag	UNP P12497
B	35	HIS	-	expression tag	UNP P12497
B	36	HIS	-	expression tag	UNP P12497
B	37	HIS	-	expression tag	UNP P12497
B	38	HIS	-	expression tag	UNP P12497
B	39	HIS	-	expression tag	UNP P12497
B	40	SER	-	expression tag	UNP P12497
B	41	SER	-	expression tag	UNP P12497
B	42	GLY	-	expression tag	UNP P12497
B	43	LEU	-	expression tag	UNP P12497
B	44	VAL	-	expression tag	UNP P12497
B	45	PRO	-	expression tag	UNP P12497
B	46	ARG	-	expression tag	UNP P12497
B	47	GLY	-	expression tag	UNP P12497
B	48	SER	-	expression tag	UNP P12497
B	49	HIS	-	expression tag	UNP P12497
B	56	SER	CYS	engineered mutation	UNP P12497
B	139	ASP	PHE	engineered mutation	UNP P12497
B	185	HIS	PHE	engineered mutation	UNP P12497

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

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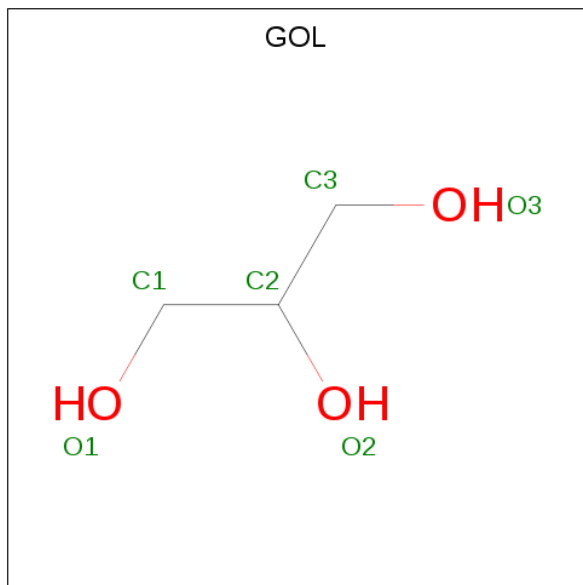
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



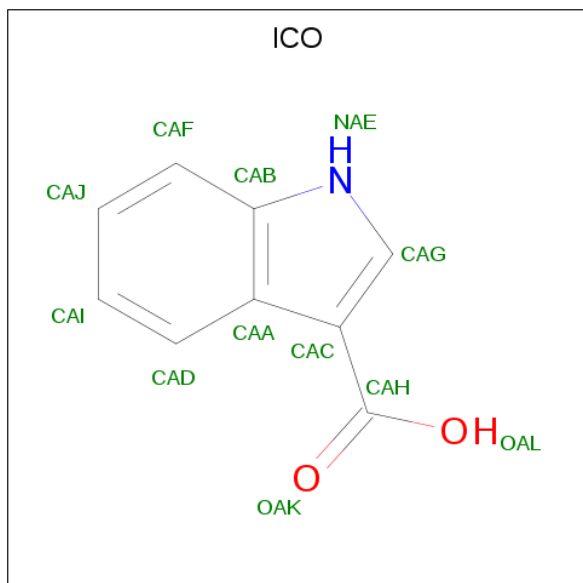
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

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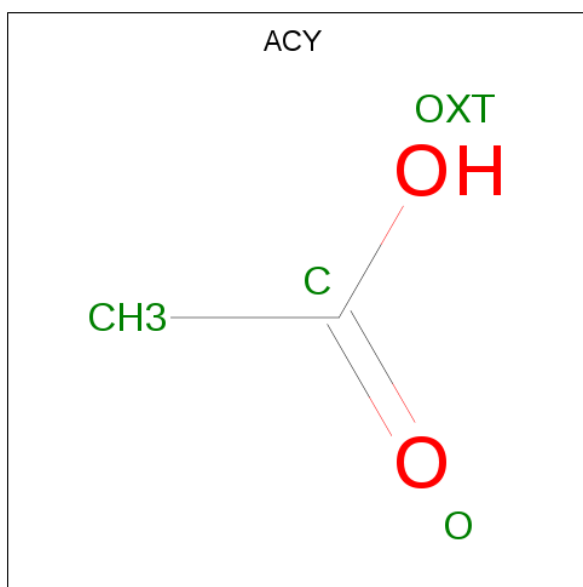
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 1H-INDOLE-3-CARBOXYLIC ACID (three-letter code: ICO) (formula:  $C_9H_7NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			12	9	1	2		
5	B	1	Total	C	N	O	0	0
			12	9	1	2		

- Molecule 6 is ACETIC ACID (three-letter code: ACY) (formula:  $C_2H_4O_2$ ).



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

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

- Molecule 8 is water.

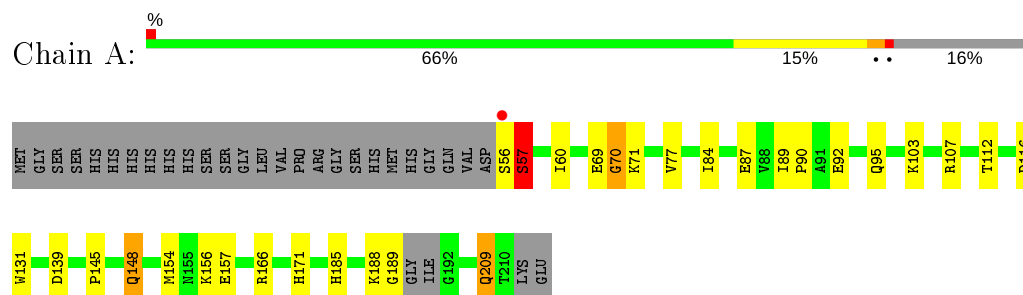


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	99	Total 99	O 99	0	0
8	B	78	Total 78	O 78	0	0

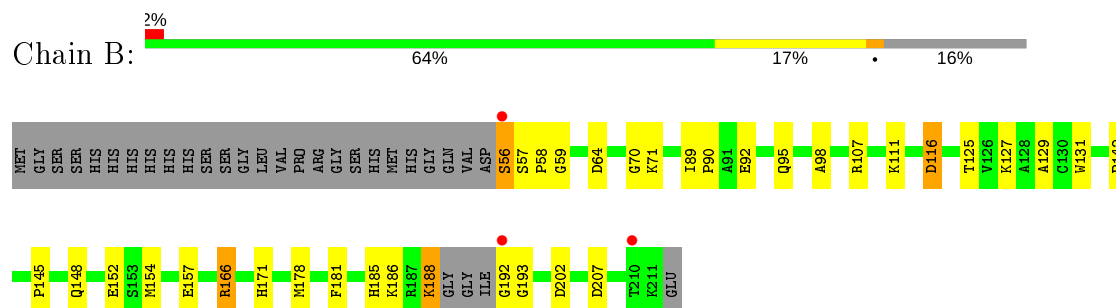
### 3 Residue-property plots [i](#)

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: INTEGRASE



- Molecule 1: INTEGRASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.70 Å 70.70 Å 66.73 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.61 – 1.90 29.30 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.7 (30.61-1.90) 94.7 (29.30-1.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.08 (at 1.91 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.160 , 0.198 0.159 , 0.197	Depositor DCC
$R_{free}$ test set	1416 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.1	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 27.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l 0.488 for h,-h-k,-l 0.027 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	2761	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.99% 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: GOL, ICO, CL, EDO, SO4, ACY

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	1.23	3/1295 (0.2%)	1.07	2/1755 (0.1%)
1	B	1.23	3/1303 (0.2%)	1.05	4/1763 (0.2%)
All	All	1.23	6/2598 (0.2%)	1.06	6/3518 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	TRP	CD2-CE2	6.90	1.49	1.41
1	B	131	TRP	CD2-CE2	6.76	1.49	1.41
1	B	157	GLU	CG-CD	6.26	1.61	1.51
1	A	107	ARG	CZ-NH1	5.99	1.40	1.33
1	B	107	ARG	CZ-NH1	5.76	1.40	1.33
1	A	157	GLU	CD-OE1	5.41	1.31	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	ASP	CB-CG-OD1	7.49	125.05	118.30
1	B	157	GLU	OE1-CD-OE2	-6.97	114.93	123.30
1	B	154	MET	CG-SD-CE	6.67	110.88	100.20
1	A	139	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	B	107	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	57	SER	CB-CA-C	5.54	120.63	110.10

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	A	1247	0	1267	38	0
1	B	1249	0	1280	36	0
2	A	15	0	0	1	0
2	B	15	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	12	0	16	15	0
4	B	12	0	16	7	0
5	A	12	0	6	2	0
5	B	12	0	6	1	0
6	B	4	0	3	4	0
7	B	4	0	6	4	0
8	A	99	0	0	16	1
8	B	78	0	0	13	1
All	All	2761	0	2600	81	1

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:SER:HA	8:A:2001:HOH:O	1.39	1.21
1:A:57:SER:OG	8:A:2005:HOH:O	1.60	1.17
1:B:56:SER:HA	8:B:2001:HOH:O	1.52	1.07
4:B:1218:GOL:O1	8:B:2023:HOH:O	1.71	1.03
1:A:69:GLU:HA	8:A:2013:HOH:O	1.69	0.92
1:A:71:LYS:NZ	4:A:1216:GOL:H31	1.84	0.90
1:A:69:GLU:CA	8:A:2013:HOH:O	2.19	0.88
1:B:95[A]:GLN:HG3	8:B:2023:HOH:O	1.74	0.87
1:A:69:GLU:N	8:A:2013:HOH:O	2.11	0.83
1:A:71:LYS:HD3	8:A:2019:HOH:O	1.80	0.80
1:A:71:LYS:HZ3	4:A:1216:GOL:H31	1.45	0.79
1:A:127:LYS:HE3	8:A:2058:HOH:O	1.81	0.78
1:B:111:LYS:CE	8:B:2006:HOH:O	2.31	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:HIS:CD2	6:B:1215:ACY:H3	2.21	0.75
1:A:125[B]:THR:CG2	4:A:1215:GOL:H32	2.16	0.75
4:A:1215:GOL:O3	8:A:2033:HOH:O	1.77	0.73
1:B:127:LYS:HE3	8:B:2043:HOH:O	1.89	0.72
8:A:2084:HOH:O	7:B:1216:EDO:H11	1.88	0.72
1:A:77[B]:VAL:HG12	1:A:84:ILE:HG22	1.71	0.71
1:A:71:LYS:NZ	4:A:1216:GOL:C3	2.53	0.71
1:A:71:LYS:HZ3	4:A:1216:GOL:C3	2.03	0.70
1:B:171:HIS:HD2	6:B:1215:ACY:H3	1.57	0.70
1:A:60[A]:ILE:HD13	1:A:112:THR:HB	1.72	0.70
1:A:95[A]:GLN:HG3	8:A:2033:HOH:O	1.91	0.70
1:B:178:MET:CE	4:B:1219:GOL:H2	2.23	0.68
1:B:111:LYS:HE2	8:B:2006:HOH:O	1.91	0.66
8:A:2079:HOH:O	7:B:1216:EDO:H22	1.95	0.66
1:B:111:LYS:HE3	8:B:2006:HOH:O	1.91	0.66
1:B:59:GLY:HA3	1:B:111:LYS:HE3	1.78	0.66
1:A:125[B]:THR:HG21	4:A:1215:GOL:H32	1.79	0.63
1:A:71:LYS:HB3	8:A:2014:HOH:O	1.98	0.63
1:B:125[B]:THR:H	4:B:1218:GOL:H31	1.65	0.61
1:A:71:LYS:HZ1	4:A:1216:GOL:H31	1.65	0.60
1:B:125[A]:THR:OG1	4:B:1218:GOL:H11	2.01	0.59
1:B:125[A]:THR:H	4:B:1218:GOL:H31	1.66	0.59
1:B:188:LYS:O	1:B:188:LYS:HD3	2.03	0.58
1:B:181:PHE:O	1:B:185:HIS:HD2	1.87	0.58
1:A:56:SER:O	8:A:2002:HOH:O	2.17	0.58
1:A:125[A]:THR:H	4:A:1215:GOL:H12	1.69	0.57
1:B:71:LYS:NZ	6:B:1215:ACY:OXT	2.38	0.56
1:A:125[B]:THR:H	4:A:1215:GOL:H12	1.70	0.55
1:A:209:GLN:NE2	1:B:202[B]:ASP:OD1	2.40	0.54
8:A:2084:HOH:O	7:B:1216:EDO:C1	2.51	0.54
1:B:59:GLY:CA	1:B:111:LYS:HE3	2.40	0.51
1:A:57:SER:H	1:A:60[B]:ILE:HD12	1.77	0.49
1:A:125[B]:THR:HG22	4:A:1215:GOL:H32	1.92	0.49
1:B:71:LYS:HG2	8:B:2011:HOH:O	2.13	0.48
1:A:171:HIS:CD2	4:A:1216:GOL:O2	2.66	0.48
5:B:1220:ICO:HAD	8:B:2074:HOH:O	2.13	0.48
1:A:95[A]:GLN:HG2	1:A:125[A]:THR:HG21	1.96	0.48
1:B:148:GLN:O	1:B:152:GLU:HG3	2.14	0.47
1:A:171:HIS:HB3	4:A:1216:GOL:H2	1.96	0.47
1:B:178:MET:HE3	4:B:1219:GOL:H2	1.95	0.47
1:B:70:GLY:N	8:B:2008:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:LYS:HE3	8:B:2058:HOH:O	2.16	0.46
1:B:178:MET:HE1	4:B:1219:GOL:H2	1.95	0.46
1:A:92:GLU:OE2	1:A:116:ASP:OD2	2.34	0.45
1:A:145:PRO:O	1:A:148:GLN:HG3	2.17	0.44
1:B:58:PRO:HG3	1:B:207:ASP:CG	2.38	0.44
1:A:87[B]:GLU:OE2	1:A:89:ILE:HG21	2.18	0.44
1:A:77[B]:VAL:HG11	1:A:154:MET:HE1	1.99	0.44
1:B:166[A]:ARG:HD2	1:B:166[A]:ARG:HA	1.62	0.44
1:B:95[B]:GLN:HG3	8:B:2024:HOH:O	2.17	0.44
1:A:185:HIS:CE1	5:A:1217:ICO:HAI	2.54	0.43
1:B:92:GLU:OE2	1:B:116:ASP:OD2	2.36	0.43
1:B:89:ILE:HB	1:B:90:PRO:HD2	2.01	0.43
1:B:171:HIS:HD2	6:B:1215:ACY:CH3	2.29	0.43
7:B:1216:EDO:H12	8:B:2045:HOH:O	2.19	0.42
1:A:171:HIS:HD2	4:A:1216:GOL:O2	2.00	0.42
1:B:188:LYS:O	1:B:188:LYS:CD	2.67	0.42
1:B:98:ALA:HB1	1:B:129:ALA:HB2	2.01	0.42
1:A:188:LYS:HA	1:A:189:GLY:HA2	1.60	0.42
1:B:58:PRO:HG2	1:B:111:LYS:NZ	2.35	0.42
1:B:192:GLY:N	1:B:193:GLY:HA2	2.36	0.41
1:A:89:ILE:HB	1:A:90:PRO:HD2	2.02	0.41
1:A:103[A]:LYS:HE3	2:A:1213:SO4:O1	2.21	0.41
5:A:1217:ICO:HAD	8:A:2092:HOH:O	2.20	0.41
1:A:70:GLY:HA2	8:A:2012:HOH:O	2.21	0.40
1:B:142:PRO:HG3	1:B:148:GLN:HG3	2.02	0.40
1:A:71:LYS:HZ1	4:A:1216:GOL:C3	2.26	0.40
1:B:145:PRO:HA	1:B:148:GLN:NE2	2.37	0.40

All (1) 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)
8:A:2030:HOH:O	8:B:2073:HOH:O[3_564]	1.93	0.27

## 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	160/183 (87%)	158 (99%)	1 (1%)	1 (1%)	25	15
1	B	160/183 (87%)	160 (100%)	0	0	100	100
All	All	320/366 (87%)	318 (99%)	1 (0%)	1 (0%)	41	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	70	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	136/150 (91%)	130 (96%)	6 (4%)	28	19
1	B	137/150 (91%)	131 (96%)	6 (4%)	28	19
All	All	273/300 (91%)	261 (96%)	12 (4%)	31	19

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	SER
1	A	148	GLN
1	A	156	LYS
1	A	166[A]	ARG
1	A	166[B]	ARG
1	A	209	GLN
1	B	56	SER
1	B	57	SER
1	B	64	ASP
1	B	166[A]	ARG
1	B	166[B]	ARG

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Mol	Chain	Res	Type
1	B	188	LYS

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

Mol	Chain	Res	Type
1	A	62	GLN
1	A	171	HIS
1	A	209	GLN
1	B	148	GLN
1	B	155	ASN
1	B	171	HIS
1	B	185	HIS

### 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](#)

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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	$\# Z  > 2$
2	SO4	A	1211	-	4,4,4	0.43	0	6,6,6	1.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	B	1213	-	4,4,4	0.26	0	6,6,6	1.03	0
7	EDO	B	1216	-	3,3,3	0.49	0	2,2,2	0.26	0
4	GOL	A	1216	-	5,5,5	0.79	0	5,5,5	2.26	3 (60%)
2	SO4	B	1214	-	4,4,4	0.63	0	6,6,6	0.80	0
5	ICO	A	1217	-	10,13,13	3.35	1 (10%)	11,18,18	0.52	0
2	SO4	A	1213	-	4,4,4	0.84	0	6,6,6	0.78	0
4	GOL	A	1215	-	5,5,5	0.69	0	5,5,5	0.54	0
4	GOL	B	1218	-	5,5,5	0.77	0	5,5,5	0.64	0
6	ACY	B	1215	-	1,3,3	0.31	0	0,3,3	0.00	-
2	SO4	B	1212	-	4,4,4	0.69	0	6,6,6	0.93	0
2	SO4	A	1212	-	4,4,4	0.20	0	6,6,6	1.96	2 (33%)
5	ICO	B	1220	-	10,13,13	2.97	1 (10%)	11,18,18	0.84	0
4	GOL	B	1219	-	5,5,5	0.76	0	5,5,5	1.43	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	EDO	B	1216	-	-	0/1/1/1	-
4	GOL	A	1216	-	-	4/4/4/4	-
5	ICO	A	1217	-	-	0/0/4/4	0/2/2/2
4	GOL	A	1215	-	-	0/4/4/4	-
4	GOL	B	1218	-	-	0/4/4/4	-
5	ICO	B	1220	-	-	0/0/4/4	0/2/2/2
4	GOL	B	1219	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1217	ICO	CAC-CAH	10.24	1.57	1.47
5	B	1220	ICO	CAC-CAH	8.87	1.56	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1216	GOL	O2-C2-C3	-3.31	94.56	109.12
2	A	1212	SO4	O4-S-O3	-3.07	95.94	109.06
2	A	1212	SO4	O4-S-O2	2.93	124.61	109.31
4	A	1216	GOL	O3-C3-C2	-2.56	97.92	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1216	GOL	O2-C2-C1	2.28	119.16	109.12

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1216	GOL	O1-C1-C2-C3
4	A	1216	GOL	O2-C2-C3-O3
4	A	1216	GOL	C1-C2-C3-O3
4	A	1216	GOL	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1216	EDO	4	0
4	A	1216	GOL	9	0
5	A	1217	ICO	2	0
2	A	1213	SO4	1	0
4	A	1215	GOL	6	0
4	B	1218	GOL	4	0
6	B	1215	ACY	4	0
5	B	1220	ICO	1	0
4	B	1219	GOL	3	0

## 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	153/183 (83%)	-0.62	1 (0%) 87 88	8, 15, 37, 61	11 (7%)
1	B	153/183 (83%)	-0.61	3 (1%) 65 68	8, 15, 40, 59	12 (7%)
All	All	306/366 (83%)	-0.62	4 (1%) 77 79	8, 15, 40, 61	23 (7%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	56	SER	3.3
1	B	56	SER	3.0
1	B	210	THR	2.6
1	B	192	GLY	2.2

### 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 [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, 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
5	ICO	A	1217	12/12	0.84	0.18	32,35,52,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	ICO	B	1220	12/12	0.87	0.16	27,31,46,52	0
4	GOL	B	1219	6/6	0.88	0.12	40,42,44,45	0
4	GOL	A	1215	6/6	0.93	0.07	26,29,35,40	0
4	GOL	A	1216	6/6	0.94	0.07	29,39,41,50	0
2	SO4	B	1214	5/5	0.94	0.15	27,27,42,44	5
4	GOL	B	1218	6/6	0.94	0.09	27,29,36,40	0
2	SO4	A	1213	5/5	0.95	0.10	26,27,39,40	5
3	CL	A	1214	1/1	0.95	0.08	44,44,44,44	0
7	EDO	B	1216	4/4	0.95	0.09	36,39,44,51	0
6	ACY	B	1215	4/4	0.97	0.08	36,38,39,50	0
2	SO4	B	1212	5/5	0.98	0.12	19,21,25,27	5
2	SO4	A	1212	5/5	0.98	0.11	22,27,28,30	5
3	CL	B	1217	1/1	0.98	0.06	42,42,42,42	0
2	SO4	A	1211	5/5	0.98	0.12	20,22,25,26	5
2	SO4	B	1213	5/5	0.99	0.09	30,37,41,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.