Full wwPDB X-ray Structure Validation Report (i)

May 14, 2020 – 08:35 am BST

PDB ID	:	6I5D
Title	:	Crystal structure of an OXA-48 beta-lactamase synthetic mutant
Authors	:	Zavala, A.; Retailleau, P.; Dabos, L.; Naas, T.; Iorga, B.
Deposited on	:	2018-11-13
Resolution	:	1.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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.
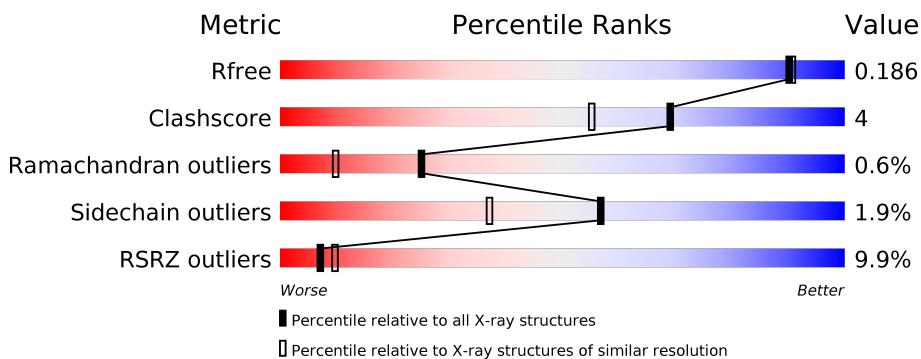
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	255	7% / 86% 9% ·
1	B	255	12% / 88% 7% 5%
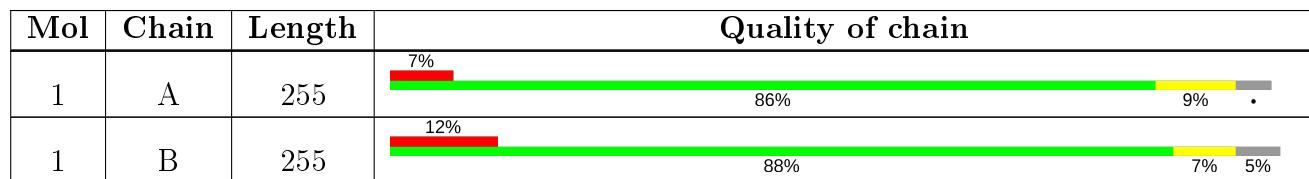
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	303	-	-	X	-
2	GOL	B	310	-	-	-	X
5	EDO	B	313	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 4660 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 Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total 2062	C 1322	N 359	O 372	S 9	0	13	0
1	B	243	Total 2063	C 1320	N 363	O 372	S 8	0	12	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	initiating methionine	UNP Q6XEC0
A	?	-	PRO	deletion	UNP Q6XEC0
A	265	PHE	-	expression tag	UNP Q6XEC0
A	266	GLU	-	expression tag	UNP Q6XEC0
A	267	HIS	-	expression tag	UNP Q6XEC0
A	268	HIS	-	expression tag	UNP Q6XEC0
A	269	HIS	-	expression tag	UNP Q6XEC0
A	270	HIS	-	expression tag	UNP Q6XEC0
A	271	HIS	-	expression tag	UNP Q6XEC0
A	272	HIS	-	expression tag	UNP Q6XEC0
A	273	HIS	-	expression tag	UNP Q6XEC0
A	274	HIS	-	expression tag	UNP Q6XEC0
B	20	MET	-	initiating methionine	UNP Q6XEC0
B	?	-	PRO	deletion	UNP Q6XEC0
B	265	PHE	-	expression tag	UNP Q6XEC0
B	266	GLU	-	expression tag	UNP Q6XEC0
B	267	HIS	-	expression tag	UNP Q6XEC0
B	268	HIS	-	expression tag	UNP Q6XEC0
B	269	HIS	-	expression tag	UNP Q6XEC0
B	270	HIS	-	expression tag	UNP Q6XEC0
B	271	HIS	-	expression tag	UNP Q6XEC0
B	272	HIS	-	expression tag	UNP Q6XEC0
B	273	HIS	-	expression tag	UNP Q6XEC0
B	274	HIS	-	expression tag	UNP Q6XEC0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
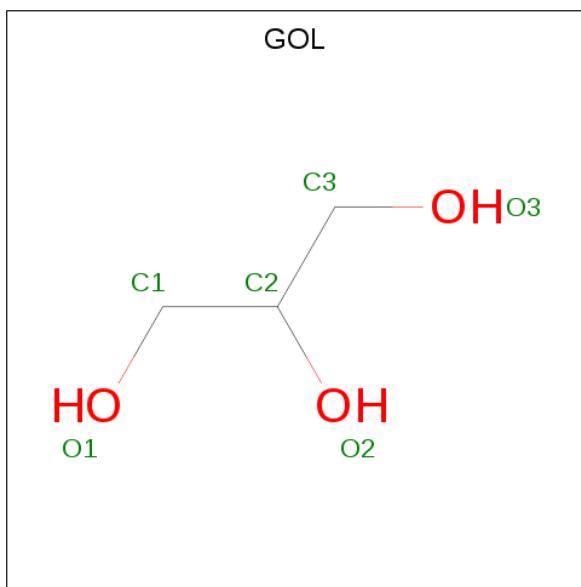
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0

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

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

- Molecule 4 is NITRATE ION (three-letter code: NO3) (formula: NO_3).
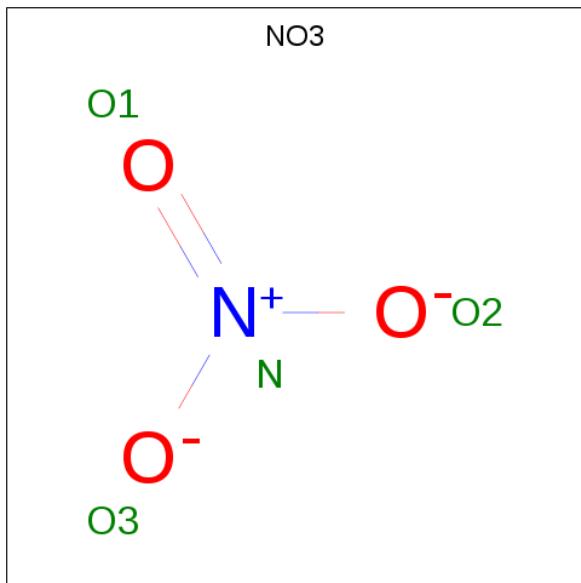
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total N O 4 1 3	0	0
4	A	1	Total N O 4 1 3	0	0
4	A	1	Total N O 4 1 3	0	0
4	A	1	Total N O 4 1 3	0	0
4	A	1	Total N O 4 1 3	0	0
4	B	1	Total N O 4 1 3	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO
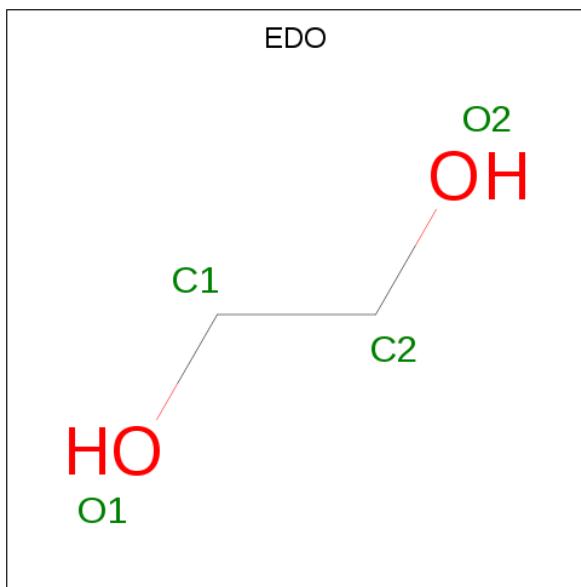
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 5	C 2	O 3	0	1
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

PEG

C4

OH O4

O2

O

C3

C1

HO

C2

O1
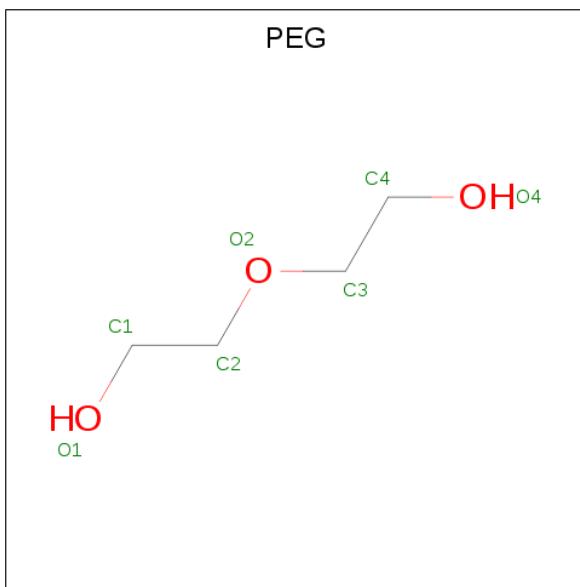
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	7	4	3	0	0

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

PO4

O3

O⁻

O2 O⁻ —— P ══ O O1

P

O⁻

O4
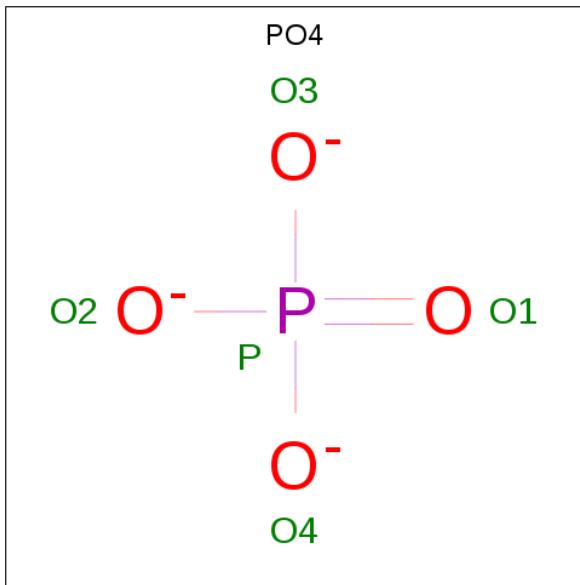
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
7	B	1	5	4	1	0	0

- Molecule 8 is water.

W O R L D W I D E
PDB
PROTEIN DATA BANK

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	194	Total O 195 195	0	1
8	B	182	Total O 184 184	0	4

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: Beta-lactamase
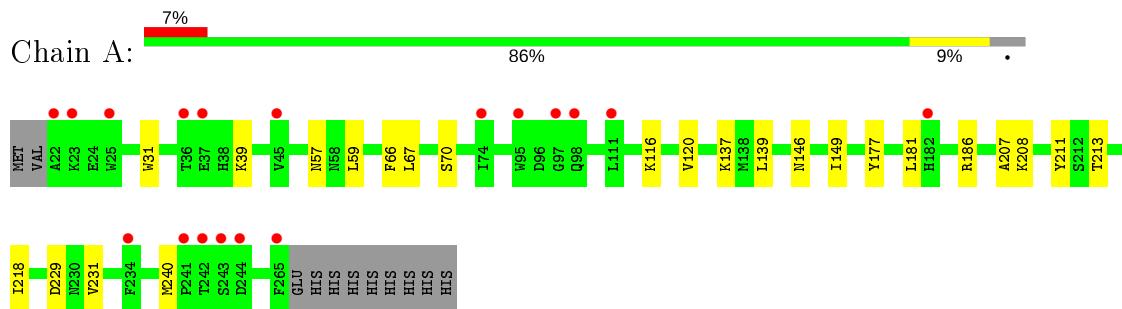
- Molecule 1: Beta-lactamase
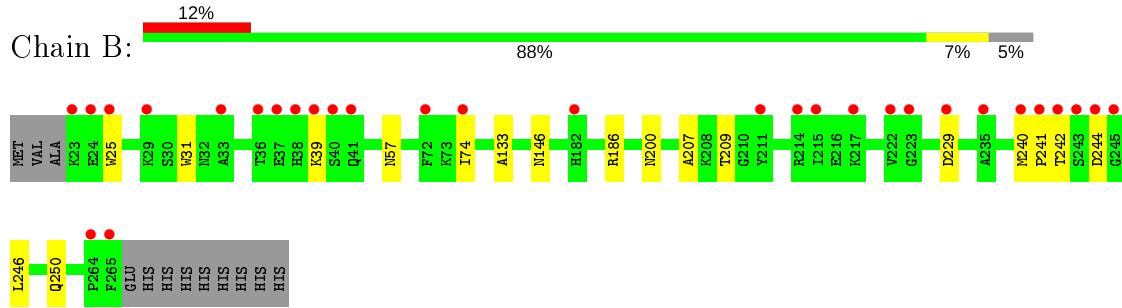
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	49.57Å 92.98Å 126.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.62 – 1.75 25.61 – 1.75	Depositor EDS
% Data completeness (in resolution range)	97.5 (25.62-1.75) 97.5 (25.61-1.75)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 1.75Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.170 , 0.185 0.169 , 0.186	Depositor DCC
R_{free} test set	2894 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	24.4	Xtriage
Anisotropy	0.597	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 53.9	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4660	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CL, PO4, EDO, PEG, NO3

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	0.51	0/2152	0.60	0/2907
1	B	0.51	0/2151	0.59	0/2905
All	All	0.51	0/4303	0.59	0/5812

There are no bond length outliers.

There are no bond angle outliers.

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	2062	0	2052	18	0
1	B	2063	0	2040	11	0
2	A	18	0	24	6	0
2	B	60	0	80	7	0
3	A	1	0	0	0	0
4	A	20	0	0	0	0
4	B	4	0	0	0	0
5	A	29	0	42	5	0
5	B	12	0	18	3	0
6	A	7	0	10	0	0
7	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	195	0	0	4	0
8	B	184	0	0	1	0
All	All	4660	0	4266	32	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 4.

All (32) 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:181:LEU:HD23	5:A:315:EDO:H21	1.74	0.69
2:A:301:GOL:H2	8:A:434:HOH:O	1.98	0.63
1:B:146:ASN:HB3	2:B:309:GOL:H11	1.83	0.61
1:B:246:LEU:HD21	5:B:315:EDO:H22	1.85	0.59
1:B:250:GLN:NE2	5:B:315:EDO:H12	2.19	0.57
1:A:146:ASN:HB3	5:A:312:EDO:H11	1.84	0.57
2:A:303:GOL:H2	1:B:186:ARG:HB2	1.87	0.56
1:A:67:LEU:H	5:A:313:EDO:H21	1.71	0.55
2:A:301:GOL:H12	8:A:544:HOH:O	2.05	0.55
1:B:25:TRP:HZ2	2:B:303:GOL:H31	1.71	0.55
1:B:200:ASN:O	2:B:307:GOL:H11	2.07	0.54
1:B:146:ASN:HD22	2:B:309:GOL:H31	1.71	0.54
1:A:116:LYS:HD2	2:B:307:GOL:H2	1.91	0.53
1:A:186:ARG:HA	2:A:303:GOL:H11	1.92	0.51
1:A:67:LEU:H	5:A:313:EDO:C2	2.24	0.51
5:B:315:EDO:H21	8:B:505:HOH:O	2.11	0.51
1:A:240[B]:MET:HE3	8:A:485[B]:HOH:O	2.12	0.50
1:A:139:LEU:HD12	1:A:149:ILE:CG2	2.43	0.49
2:A:303:GOL:H2	1:B:186:ARG:CB	2.43	0.49
1:A:70:SER:HB3	1:A:211:TYR:O	2.12	0.48
1:A:31:TRP:HB2	1:A:57:ASN:HB3	1.95	0.47
1:A:66:PHE:CD1	1:A:218:ILE:HG13	2.49	0.47
1:A:208:LYS:NZ	2:B:307:GOL:H32	2.29	0.47
1:A:177:TYR:CZ	1:A:231[B]:VAL:HG21	2.52	0.44
1:A:120:VAL:HG23	1:A:213:THR:HG21	2.00	0.44
1:B:31:TRP:HB2	1:B:57:ASN:HB3	2.00	0.43
1:A:186:ARG:HB2	2:A:303:GOL:H32	2.00	0.43
1:B:133:ALA:HB3	2:B:306:GOL:H12	2.00	0.42
1:B:74:ILE:HD11	1:B:209:THR:CG2	2.50	0.41
1:A:120:VAL:CG2	1:A:213:THR:HG21	2.51	0.41
1:A:137:LYS:HG3	8:A:512:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ILE:HB	5:A:313:EDO:H11	2.03	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	A	255/255 (100%)	244 (96%)	10 (4%)	1 (0%)	34	17
1	B	253/255 (99%)	243 (96%)	8 (3%)	2 (1%)	19	6
All	All	508/510 (100%)	487 (96%)	18 (4%)	3 (1%)	25	10

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	241	PRO
1	A	207	ALA
1	B	207	ALA

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	225/223 (101%)	221 (98%)	4 (2%)	59	40
1	B	224/223 (100%)	218 (97%)	6 (3%)	44	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	449/446 (101%)	439 (98%)	10 (2%)	57 29

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LYS
1	A	59	LEU
1	A	229[A]	ASP
1	A	229[B]	ASP
1	B	39	LYS
1	B	229[A]	ASP
1	B	229[B]	ASP
1	B	240	MET
1	B	242	THR
1	B	244	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	250	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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 33 ligands modelled in this entry, 1 is monoatomic - leaving 32 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	GOL	B	311	-	5,5,5	0.04	0	5,5,5	0.22	0
2	GOL	B	303	-	5,5,5	0.06	0	5,5,5	0.23	0
2	GOL	B	308	-	5,5,5	0.10	0	5,5,5	0.16	0
2	GOL	B	306	-	5,5,5	0.13	0	5,5,5	0.20	0
7	PO4	B	301	-	4,4,4	2.45	1 (25%)	6,6,6	0.50	0
5	EDO	A	314	-	3,3,3	0.51	0	2,2,2	0.39	0
5	EDO	A	315	-	3,3,3	0.44	0	2,2,2	0.42	0
4	NO3	A	306	-	1,3,3	0.26	0	0,3,3	0.00	-
5	EDO	A	316[B]	-	3,3,3	0.89	0	2,2,2	0.35	0
2	GOL	B	304	-	5,5,5	0.07	0	5,5,5	0.23	0
4	NO3	A	305	-	1,3,3	0.41	0	0,3,3	0.00	-
2	GOL	A	302	-	5,5,5	0.07	0	5,5,5	0.58	0
5	EDO	B	313	-	3,3,3	0.53	0	2,2,2	0.33	0
5	EDO	A	313	-	3,3,3	0.64	0	2,2,2	0.48	0
4	NO3	B	312	-	1,3,3	0.32	0	0,3,3	0.00	-
4	NO3	A	307	-	1,3,3	0.54	0	0,3,3	0.00	-
5	EDO	A	311	-	3,3,3	0.69	0	2,2,2	0.30	0
2	GOL	B	307	-	5,5,5	0.16	0	5,5,5	0.34	0
5	EDO	A	316[A]	-	3,3,3	0.88	0	2,2,2	0.52	0
2	GOL	B	310	-	5,5,5	0.06	0	5,5,5	0.24	0
5	EDO	A	312	-	3,3,3	0.50	0	2,2,2	0.51	0
5	EDO	B	314	-	3,3,3	0.45	0	2,2,2	0.50	0
6	PEG	A	317	-	6,6,6	0.09	0	5,5,5	0.09	0
4	NO3	A	309	-	1,3,3	0.06	0	0,3,3	0.00	-
2	GOL	A	301	-	5,5,5	0.12	0	5,5,5	0.25	0
2	GOL	B	305	-	5,5,5	0.05	0	5,5,5	0.16	0
5	EDO	A	310	-	3,3,3	0.72	0	2,2,2	0.48	0
2	GOL	B	309	-	5,5,5	0.09	0	5,5,5	0.32	0
5	EDO	B	315	-	3,3,3	0.53	0	2,2,2	0.30	0
2	GOL	A	303	-	5,5,5	0.23	0	5,5,5	0.85	0
2	GOL	B	302	-	5,5,5	0.05	0	5,5,5	0.19	0
4	NO3	A	308	-	1,3,3	0.42	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.

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	311	-	-	1/4/4/4	-
2	GOL	B	303	-	-	0/4/4/4	-
2	GOL	B	308	-	-	1/4/4/4	-
2	GOL	B	306	-	-	2/4/4/4	-
5	EDO	A	314	-	-	0/1/1/1	-
5	EDO	A	315	-	-	0/1/1/1	-
5	EDO	A	316[B]	-	-	1/1/1/1	-
2	GOL	B	304	-	-	0/4/4/4	-
2	GOL	A	302	-	-	0/4/4/4	-
5	EDO	B	313	-	-	0/1/1/1	-
5	EDO	A	313	-	-	0/1/1/1	-
2	GOL	B	302	-	-	0/4/4/4	-
5	EDO	A	311	-	-	0/1/1/1	-
2	GOL	B	307	-	-	4/4/4/4	-
5	EDO	A	316[A]	-	-	1/1/1/1	-
2	GOL	B	310	-	-	2/4/4/4	-
5	EDO	A	312	-	-	0/1/1/1	-
5	EDO	B	314	-	-	1/1/1/1	-
6	PEG	A	317	-	-	2/4/4/4	-
2	GOL	A	301	-	-	3/4/4/4	-
2	GOL	B	305	-	-	1/4/4/4	-
5	EDO	A	310	-	-	0/1/1/1	-
2	GOL	B	309	-	-	2/4/4/4	-
5	EDO	B	315	-	-	1/1/1/1	-
2	GOL	A	303	-	-	1/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	301	PO4	P-O1	4.06	1.60	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	307	GOL	O1-C1-C2-O2
2	B	307	GOL	O1-C1-C2-C3
2	A	301	GOL	O1-C1-C2-C3
2	B	309	GOL	O1-C1-C2-C3
2	B	306	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	A	301	GOL	O1-C1-C2-O2
2	B	309	GOL	O1-C1-C2-O2
2	B	311	GOL	C1-C2-C3-O3
2	B	308	GOL	O1-C1-C2-C3
2	B	306	GOL	O1-C1-C2-C3
2	B	307	GOL	C1-C2-C3-O3
2	B	310	GOL	O1-C1-C2-C3
2	B	305	GOL	C1-C2-C3-O3
2	A	303	GOL	O1-C1-C2-C3
2	B	307	GOL	O2-C2-C3-O3
5	A	316[A]	EDO	O1-C1-C2-O2
6	A	317	PEG	C4-C3-O2-C2
6	A	317	PEG	C1-C2-O2-C3
5	B	314	EDO	O1-C1-C2-O2
5	A	316[B]	EDO	O1-C1-C2-O2
2	B	310	GOL	O1-C1-C2-O2
2	A	301	GOL	C1-C2-C3-O3
5	B	315	EDO	O1-C1-C2-O2

There are no ring outliers.

10 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	303	GOL	1	0
2	B	306	GOL	1	0
5	A	315	EDO	1	0
5	A	313	EDO	3	0
2	B	307	GOL	3	0
5	A	312	EDO	1	0
2	A	301	GOL	2	0
2	B	309	GOL	2	0
5	B	315	EDO	3	0
2	A	303	GOL	4	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	244/255 (95%)	0.39	18 (7%)	14	19	18, 27, 50, 76	0
1	B	243/255 (95%)	0.64	30 (12%)	4	6	18, 28, 64, 87	0
All	All	487/510 (95%)	0.52	48 (9%)	7	10	18, 28, 58, 87	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	243	SER	10.4
1	B	241	PRO	9.9
1	B	215	ILE	8.9
1	B	242	THR	8.5
1	A	22	ALA	6.4
1	B	23	LYS	6.4
1	A	265	PHE	6.2
1	B	244	ASP	5.8
1	B	265	PHE	5.7
1	A	241	PRO	5.2
1	A	97	GLY	5.1
1	A	242	THR	4.5
1	B	264	PRO	4.3
1	B	36	THR	3.9
1	B	41	GLN	3.9
1	B	33	ALA	3.4
1	A	23	LYS	3.3
1	B	25	TRP	3.2
1	B	39	LYS	3.2
1	B	182[A]	HIS	3.0
1	A	98	GLN	3.0
1	B	240	MET	3.0
1	A	37	GLU	3.0
1	B	245	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	29	LYS	2.8
1	B	222	VAL	2.8
1	B	38	HIS	2.7
1	A	95	TRP	2.7
1	B	24	GLU	2.7
1	B	214[A]	ARG	2.6
1	A	111	LEU	2.5
1	A	182[A]	HIS	2.5
1	B	74	ILE	2.4
1	B	217	LYS	2.4
1	A	244	ASP	2.4
1	B	37	GLU	2.3
1	B	229[A]	ASP	2.3
1	B	211	TYR	2.3
1	A	45	VAL	2.3
1	B	235	ALA	2.3
1	B	40	SER	2.2
1	A	234	PHE	2.1
1	B	223	GLY	2.1
1	A	74	ILE	2.1
1	B	72	PHE	2.1
1	A	243	SER	2.0
1	A	25	TRP	2.0
1	A	36	THR	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 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, 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(Å²)	Q<0.9
5	EDO	B	314	4/4	0.64	0.30	51,51,52,54	0
2	GOL	B	310	6/6	0.66	0.54	54,57,58,59	6
5	EDO	A	316[B]	4/4	0.67	0.26	29,32,36,41	1
5	EDO	A	316[A]	4/4	0.67	0.26	24,32,36,41	1
2	GOL	A	303	6/6	0.68	0.24	32,39,41,45	0
2	GOL	B	304	6/6	0.70	0.32	55,59,59,60	0
2	GOL	B	309	6/6	0.73	0.26	43,52,53,56	0
2	GOL	B	305	6/6	0.74	0.21	60,66,67,68	0
5	EDO	A	313	4/4	0.74	0.21	33,35,36,46	0
2	GOL	B	308	6/6	0.74	0.32	43,58,58,62	0
6	PEG	A	317	7/7	0.75	0.27	63,67,70,70	0
5	EDO	B	313	4/4	0.78	0.42	50,52,53,57	0
2	GOL	A	302	6/6	0.81	0.19	52,54,56,57	0
7	PO4	B	301	5/5	0.81	0.22	62,63,63,63	5
4	NO3	A	308	4/4	0.81	0.37	52,52,52,53	4
2	GOL	B	306	6/6	0.82	0.28	27,47,49,52	0
2	GOL	B	303	6/6	0.82	0.16	50,56,57,59	0
2	GOL	B	311	6/6	0.83	0.23	69,69,70,71	0
2	GOL	B	307	6/6	0.83	0.20	43,53,55,55	0
5	EDO	A	312	4/4	0.83	0.24	53,53,55,56	0
2	GOL	A	301	6/6	0.83	0.16	41,46,49,50	0
5	EDO	A	311	4/4	0.85	0.12	37,41,42,43	0
5	EDO	B	315	4/4	0.85	0.14	39,44,45,46	0
2	GOL	B	302	6/6	0.86	0.29	58,62,64,66	0
5	EDO	A	315	4/4	0.88	0.36	33,43,49,51	0
4	NO3	A	309	4/4	0.89	0.33	44,48,48,51	0
5	EDO	A	310	4/4	0.89	0.11	32,35,40,42	0
5	EDO	A	314	4/4	0.90	0.25	61,61,61,61	0
4	NO3	A	307	4/4	0.95	0.32	42,46,47,49	0
4	NO3	A	305	4/4	0.96	0.07	36,39,41,43	0
4	NO3	B	312	4/4	0.97	0.07	35,38,40,41	0
4	NO3	A	306	4/4	0.97	0.17	45,47,47,48	0
3	CL	A	304	1/1	0.99	0.06	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.