



Full wwPDB X-ray Structure Validation Report i

Sep 1, 2021 – 01:08 am BST

PDB ID : 6YRS
Title : Structure of a new variant of GNCA ancestral beta-lactamase
Authors : Gavira, J.A.; Risso, V.; Martinez-Rodriguez, S.; Sanchez-Ruiz, J.M.; Modi, T.; Ozkan, S.B.
Deposited on : 2020-04-20
Resolution : 1.70 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 i symbol.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.1.3
EDS : 2.23.1
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) : 2.23.1

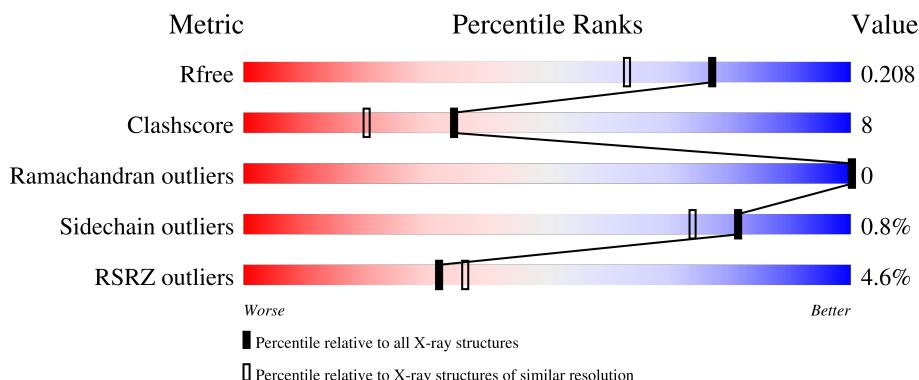
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

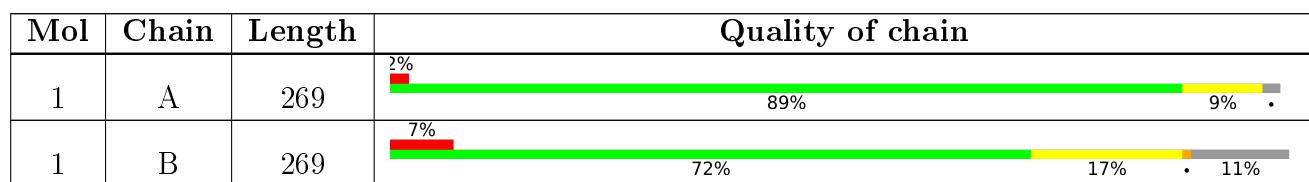
The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 <=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.



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
6	PEG	B	307	-	-	X	-

2 Entry composition [\(i\)](#)

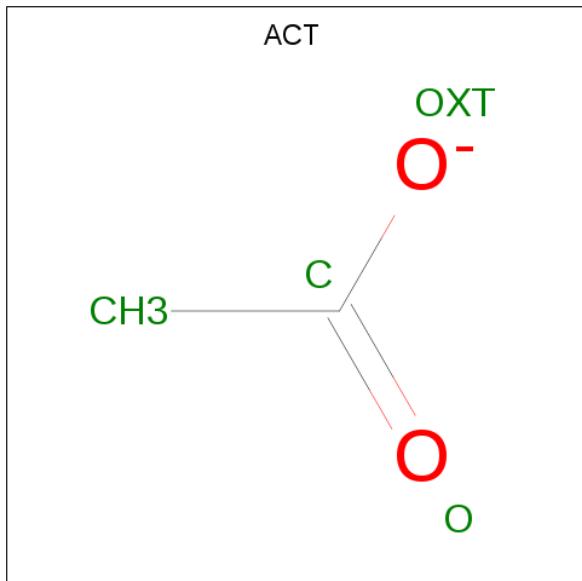
There are 7 unique types of molecules in this entry. The entry contains 8738 atoms, of which 4300 are hydrogens and 0 are deuteriums.

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 ancestral beta-lactamase.

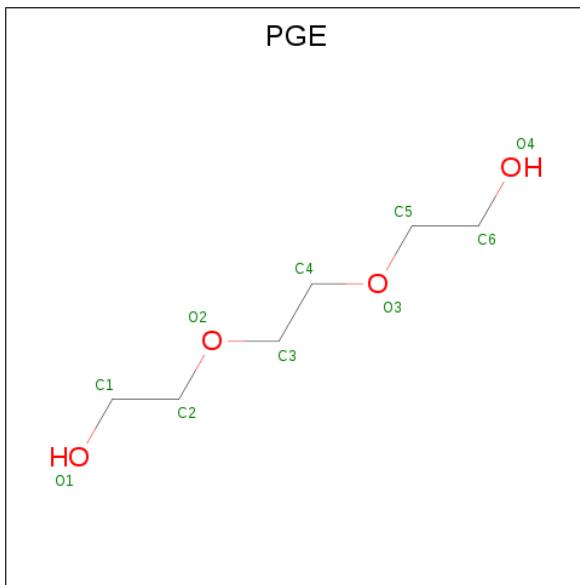
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	264	Total	C	H	N	O	S	0	28	0
			4269	1315	2147	390	411	6			
1	B	240	Total	C	H	N	O	S	0	23	0
			3898	1198	1971	354	368	7			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂⁻).



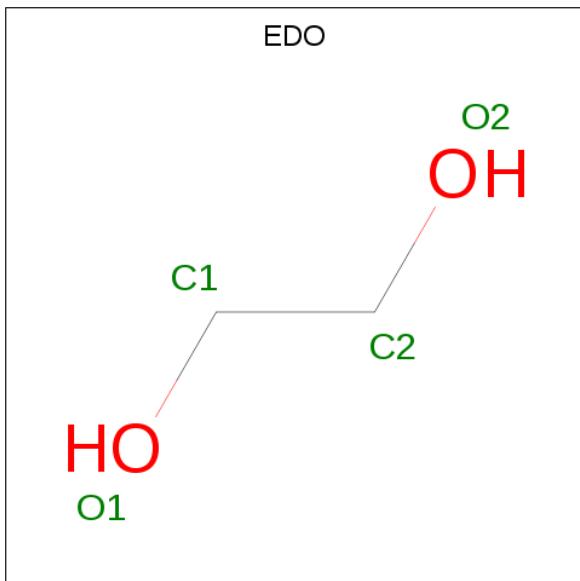
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			7	2	3	2		
2	A	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



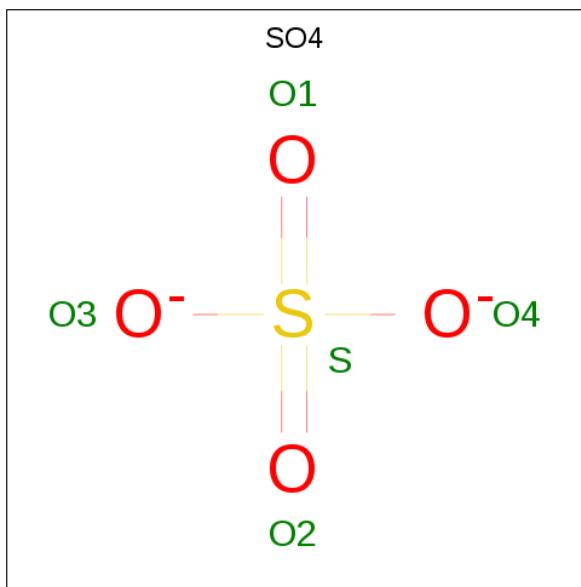
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 24 6 14 4	0	0
3	A	1	Total C H O 24 6 14 4	0	0
3	A	1	Total C H O 24 6 14 4	0	0
3	A	1	Total C H O 48 12 28 8	0	1
3	A	1	Total C H O 24 6 14 4	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



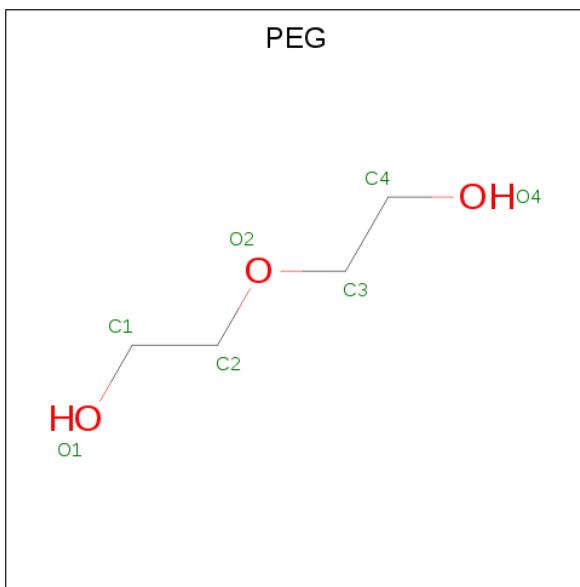
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	A	1	10	2	6	2	0	0
4	A	1	10	2	6	2	0	0
4	A	1	10	2	6	2	0	0
4	A	1	10	2	6	2	0	0
4	B	1	10	2	6	2	0	0
4	B	1	10	2	6	2	0	0
4	B	1	10	2	6	2	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	H	O	
			17	4	10	3	0
6	B	1	Total	C	H	O	
			17	4	10	3	0
6	B	1	Total	C	H	O	
			17	4	10	3	0
6	B	1	Total	C	H	O	
			17	4	10	3	0
6	B	1	Total	C	H	O	
			17	4	10	3	0

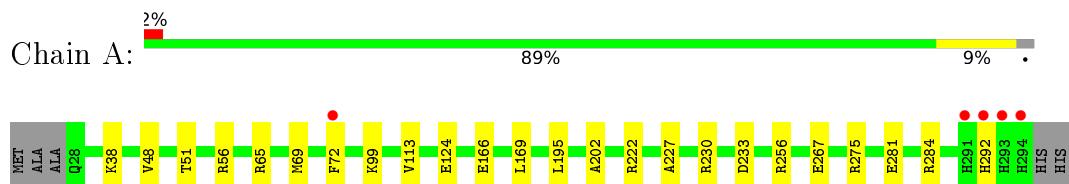
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	163	Total	O		
			163	163	0	0
7	B	90	Total	O		
			90	90	0	0

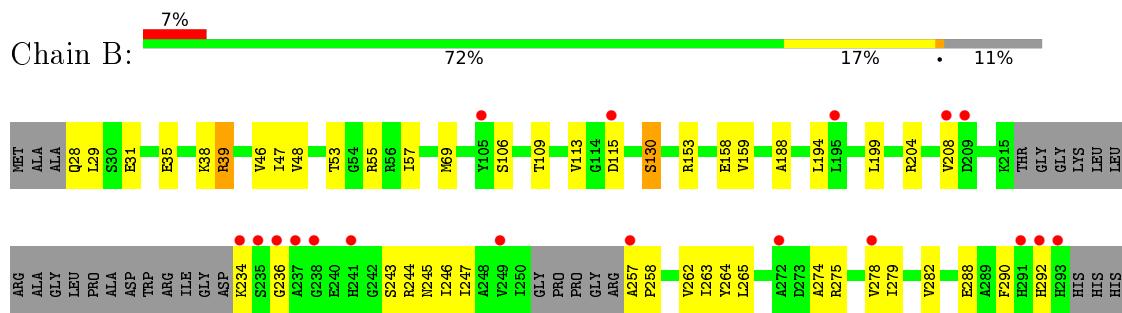
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: ancestral beta-lactamase



- Molecule 1: ancestral beta-lactamase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.35 Å 81.40 Å 61.04 Å 90.00° 94.58° 90.00°	Depositor
Resolution (Å)	48.73 – 1.70 48.73 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.7 (48.73-1.70) 97.7 (48.73-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	1.50 (at 1.70 Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R , R_{free}	0.176 , 0.208 0.176 , 0.208	Depositor DCC
R_{free} test set	2531 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 54.7	EDS
L-test for twinning ²	$< L > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8738	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ACT, EDO, PEG, SO4, PGE

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	0.58	0/2255	0.73	2/3057 (0.1%)
1	B	0.51	0/2037	0.68	0/2753
All	All	0.55	0/4292	0.71	2/5810 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	275	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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	2122	2147	2040	17	2
1	B	1927	1971	1888	52	1
2	A	8	6	6	0	0
3	A	60	84	84	0	0
4	A	16	24	24	2	0
4	B	12	18	18	1	0
5	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	7	10	10	0	0
6	B	28	40	40	6	0
7	A	163	0	0	5	1
7	B	90	0	0	2	0
All	All	4438	4300	4110	70	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 8.

All (70) 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:38:LYS:NZ	7:A:401:HOH:O	1.88	1.03
1:B:48:VAL:HB	1:B:57:ILE:HG22	1.56	0.85
1:A:267[A]:GLU:OE2	7:A:402:HOH:O	2.02	0.77
1:B:28:GLN:N	1:B:31[A]:GLU:OE2	2.20	0.74
1:B:257:ALA:HB1	1:B:258:PRO:HD3	1.69	0.74
1:A:69:MET:O	1:A:72:PHE:HD1	1.70	0.73
1:A:65[A]:ARG:NH2	7:A:403:HOH:O	2.21	0.73
1:B:48:VAL:HB	1:B:57:ILE:CG2	2.19	0.72
1:B:246:ILE:HD11	1:B:263:ILE:HD12	1.73	0.70
1:B:188:ALA:HB3	6:B:307:PEG:H41	1.75	0.68
1:B:234[A]:LYS:N	1:B:247:ILE:O	2.27	0.67
1:B:257:ALA:HB1	1:B:258:PRO:CD	2.24	0.67
1:B:69[B]:MET:HG3	1:B:245:ASN:OD1	1.95	0.67
1:B:158:GLU:H	6:B:307:PEG:C1	2.10	0.64
1:B:113:VAL:HG22	7:B:403:HOH:O	1.99	0.62
1:A:256[B]:ARG:NH1	7:A:404:HOH:O	2.32	0.61
1:B:158:GLU:H	6:B:307:PEG:H12	1.66	0.60
1:B:257:ALA:CB	1:B:258:PRO:CD	2.81	0.58
1:B:47:ILE:HB	1:B:262[A]:VAL:HG22	1.86	0.57
1:A:281:GLU:OE1	1:A:284:ARG:NH2	2.33	0.57
1:B:46[B]:VAL:HG21	1:B:282:VAL:CG1	2.35	0.56
1:B:265:LEU:HD22	1:B:278:VAL:HG11	1.87	0.56
1:B:288:GLU:O	1:B:292:HIS:ND1	2.38	0.56
1:B:69[A]:MET:HE1	1:B:243:SER:HB3	1.89	0.54
1:B:35:GLU:OE1	1:B:38:LYS:NZ	2.27	0.54
1:B:234[B]:LYS:N	1:B:247:ILE:O	2.41	0.53
1:A:202:ALA:HB1	4:A:304:EDO:H22	1.91	0.51
1:B:244:ARG:HG3	1:B:279:ILE:HG13	1.92	0.51
1:B:130:SER:CB	1:B:234[A]:LYS:HZ1	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230[A]:ARG:HH21	1:A:230[A]:ARG:HG3	1.76	0.50
1:B:158:GLU:HB2	6:B:307:PEG:H11	1.93	0.50
1:B:46[B]:VAL:HG21	1:B:282:VAL:HG11	1.94	0.50
1:B:275:ARG:O	1:B:278:VAL:CG1	2.59	0.50
4:A:309:EDO:H12	1:B:153:ARG:HE	1.77	0.50
1:A:69:MET:O	1:A:72:PHE:CD1	2.60	0.49
1:B:234[A]:LYS:HB3	1:B:247:ILE:HG13	1.94	0.49
1:A:99:LYS:HG2	1:A:113:VAL:HG21	1.95	0.48
1:B:234[A]:LYS:HB3	1:B:247:ILE:CG1	2.43	0.48
1:A:72:PHE:CE1	1:A:166:GLU:OE1	2.66	0.48
1:A:99:LYS:CE	7:A:429:HOH:O	2.63	0.46
1:A:72:PHE:HE1	1:A:166:GLU:OE1	1.97	0.46
1:B:35:GLU:OE1	1:B:38:LYS:HD2	2.16	0.45
1:B:106:SER:HB3	1:B:109:THR:OG1	2.17	0.44
1:B:204:ARG:O	1:B:208:VAL:HG23	2.17	0.44
1:B:69[A]:MET:HE3	1:B:69[A]:MET:HB2	1.94	0.43
1:B:39[B]:ARG:NH1	7:B:410:HOH:O	2.52	0.42
1:A:48:VAL:O	1:A:56:ARG:HA	2.19	0.42
1:B:262[B]:VAL:CG1	1:B:264:TYR:CE2	3.02	0.42
1:B:130:SER:HA	1:B:234[A]:LYS:HZ3	1.84	0.42
4:B:301:EDO:C1	6:B:307:PEG:H32	2.49	0.42
1:A:72:PHE:CZ	1:A:169:LEU:HD21	2.55	0.42
1:B:194:LEU:HD22	1:B:208:VAL:HG22	2.02	0.42
1:B:29:LEU:HD23	1:B:57:ILE:HD11	2.02	0.42
1:B:244:ARG:C	1:B:245:ASN:HD22	2.23	0.42
1:B:46[B]:VAL:CG2	1:B:282:VAL:HG11	2.50	0.41
1:B:47:ILE:HB	1:B:262[A]:VAL:CG2	2.50	0.41
1:B:53:THR:CG2	1:B:55[A]:ARG:HB2	2.50	0.41
1:B:275:ARG:O	1:B:278:VAL:HG12	2.21	0.41
1:B:39[A]:ARG:NE	1:B:39[A]:ARG:HA	2.36	0.41
1:B:55[A]:ARG:NH2	1:B:290:PHE:O	2.52	0.41
1:B:243:SER:HA	1:B:265:LEU:O	2.21	0.41
1:B:159:VAL:HG23	6:B:307:PEG:H22	2.02	0.41
1:B:199:LEU:HB2	1:B:204:ARG:HG3	2.02	0.41
1:B:274:ALA:O	1:B:278:VAL:HG12	2.21	0.41
1:A:51:THR:HG21	1:A:195:LEU:HD13	2.03	0.40
1:B:247:ILE:HG22	1:B:262[B]:VAL:HG13	2.04	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:124:GLU:OE2	7:A:401:HOH:O[1_655]	2.07	0.13
1:A:227:ALA:H	1:B:115:ASP:OD2[1_454]	1.47	0.13

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	290/269 (108%)	284 (98%)	6 (2%)	0	100 100
1	B	256/269 (95%)	252 (98%)	4 (2%)	0	100 100
All	All	546/538 (102%)	536 (98%)	10 (2%)	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	228/206 (111%)	227 (100%)	1 (0%)	91 87
1	B	210/206 (102%)	207 (99%)	3 (1%)	67 53
All	All	438/412 (106%)	434 (99%)	4 (1%)	81 70

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	292	HIS
1	B	39[A]	ARG

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Mol	Chain	Res	Type
1	B	39[B]	ARG
1	B	130	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

21 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	PGE	A	308[A]	-	9,9,9	0.38	0	8,8,8	0.39	0
2	ACT	A	301	-	1,3,3	5.05	1 (100%)	0,3,3	0.00	-
3	PGE	A	306	-	9,9,9	0.33	0	8,8,8	0.25	0
4	EDO	B	305	-	3,3,3	0.53	0	2,2,2	0.21	0
3	PGE	A	303	-	9,9,9	0.32	0	8,8,8	0.32	0
3	PGE	A	311	-	9,9,9	0.30	0	8,8,8	0.29	0
4	EDO	A	304	-	3,3,3	0.45	0	2,2,2	0.30	0
4	EDO	A	309	-	3,3,3	0.48	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PEG	A	313	-	6,6,6	0.49	0	5,5,5	0.35	0
4	EDO	B	303	-	3,3,3	0.44	0	2,2,2	0.28	0
6	PEG	B	306	-	6,6,6	0.48	0	5,5,5	0.44	0
2	ACT	A	302	-	1,3,3	4.76	1 (100%)	0,3,3	0.00	-
4	EDO	A	312	-	3,3,3	0.52	0	2,2,2	0.24	0
4	EDO	B	301	-	3,3,3	0.52	0	2,2,2	0.03	0
3	PGE	A	307	-	9,9,9	0.29	0	8,8,8	0.34	0
6	PEG	B	307	-	6,6,6	0.53	0	5,5,5	0.34	0
3	PGE	A	308[B]	-	9,9,9	0.34	0	8,8,8	0.42	0
4	EDO	A	305	-	3,3,3	0.49	0	2,2,2	0.19	0
6	PEG	B	304	-	6,6,6	0.50	0	5,5,5	0.29	0
6	PEG	B	302	-	6,6,6	0.50	0	5,5,5	0.43	0
5	SO4	A	310	-	4,4,4	0.14	0	6,6,6	0.14	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
4	EDO	A	305	-	-	1/1/1/1	-
6	PEG	B	304	-	-	1/4/4/4	-
4	EDO	A	312	-	-	1/1/1/1	-
4	EDO	A	304	-	-	1/1/1/1	-
3	PGE	A	308[A]	-	-	2/7/7/7	-
4	EDO	A	309	-	-	1/1/1/1	-
3	PGE	A	306	-	-	3/7/7/7	-
4	EDO	B	301	-	-	1/1/1/1	-
4	EDO	B	305	-	-	1/1/1/1	-
6	PEG	A	313	-	-	3/4/4/4	-
3	PGE	A	303	-	-	3/7/7/7	-
6	PEG	B	302	-	-	2/4/4/4	-
4	EDO	B	303	-	-	1/1/1/1	-
3	PGE	A	307	-	-	7/7/7/7	-
6	PEG	B	307	-	-	2/4/4/4	-
3	PGE	A	308[B]	-	-	3/7/7/7	-
6	PEG	B	306	-	-	2/4/4/4	-
3	PGE	A	311	-	-	4/7/7/7	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	ACT	CH3-C	5.05	1.55	1.48
2	A	302	ACT	CH3-C	4.76	1.54	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	307	PEG	C1-C2-O2-C3
3	A	308[B]	PGE	O3-C5-C6-O4
6	B	302	PEG	O2-C3-C4-O4
3	A	308[B]	PGE	O2-C3-C4-O3
3	A	308[A]	PGE	O1-C1-C2-O2
3	A	311	PGE	O1-C1-C2-O2
6	A	313	PEG	O1-C1-C2-O2
6	B	306	PEG	O2-C3-C4-O4
4	A	305	EDO	O1-C1-C2-O2
6	B	307	PEG	O2-C3-C4-O4
6	B	304	PEG	O1-C1-C2-O2
4	A	304	EDO	O1-C1-C2-O2
3	A	303	PGE	O1-C1-C2-O2
3	A	306	PGE	O1-C1-C2-O2
6	B	302	PEG	C4-C3-O2-C2
3	A	306	PGE	O2-C3-C4-O3
3	A	307	PGE	O1-C1-C2-O2
3	A	311	PGE	O3-C5-C6-O4
3	A	307	PGE	C3-C4-O3-C5
3	A	308[B]	PGE	C4-C3-O2-C2
3	A	307	PGE	C1-C2-O2-C3
3	A	307	PGE	O3-C5-C6-O4
3	A	306	PGE	C4-C3-O2-C2
6	A	313	PEG	C1-C2-O2-C3
4	B	305	EDO	O1-C1-C2-O2
6	B	306	PEG	O1-C1-C2-O2
3	A	307	PGE	C4-C3-O2-C2
3	A	308[A]	PGE	O2-C3-C4-O3
3	A	311	PGE	C6-C5-O3-C4
4	A	309	EDO	O1-C1-C2-O2
4	A	312	EDO	O1-C1-C2-O2
6	A	313	PEG	C4-C3-O2-C2
3	A	307	PGE	C6-C5-O3-C4
3	A	303	PGE	C6-C5-O3-C4

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Mol	Chain	Res	Type	Atoms
4	B	301	EDO	O1-C1-C2-O2
4	B	303	EDO	O1-C1-C2-O2
3	A	307	PGE	O2-C3-C4-O3
3	A	311	PGE	O2-C3-C4-O3
3	A	303	PGE	O2-C3-C4-O3

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	304	EDO	1	0
4	A	309	EDO	1	0
4	B	301	EDO	1	0
6	B	307	PEG	6	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	264/269 (98%)	-0.18	5 (1%) 66 70	23, 33, 51, 100	0
1	B	240/269 (89%)	0.29	18 (7%) 14 16	25, 43, 75, 102	0
All	All	504/538 (93%)	0.05	23 (4%) 32 36	23, 36, 68, 102	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	236	GLY	6.3
1	A	292	HIS	5.3
1	B	238	GLY	5.0
1	B	235[A]	SER	4.9
1	B	237	ALA	4.4
1	B	293	HIS	4.2
1	A	291	HIS	3.2
1	B	278	VAL	3.2
1	B	291	HIS	3.2
1	B	292	HIS	3.2
1	B	241	HIS	3.0
1	A	294	HIS	3.0
1	A	293	HIS	2.8
1	B	272	ALA	2.7
1	A	72	PHE	2.7
1	B	249	VAL	2.5
1	B	234[A]	LYS	2.3
1	B	208	VAL	2.3
1	B	105	TYR	2.2
1	B	257	ALA	2.2
1	B	209	ASP	2.2
1	B	115	ASP	2.1
1	B	195	LEU	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 monosaccharides in this entry.

6.4 Ligands [\(i\)](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PEG	A	313	7/7	0.38	0.20	81,97,100,100	0
4	EDO	A	312	4/4	0.47	0.20	83,100,102,102	0
4	EDO	B	305	4/4	0.56	0.21	70,84,87,87	0
6	PEG	B	302	7/7	0.58	0.15	65,78,84,84	0
6	PEG	B	304	7/7	0.61	0.16	77,93,94,94	0
3	PGE	A	308[B]	10/10	0.63	0.26	44,54,56,57	24
3	PGE	A	308[A]	10/10	0.63	0.26	37,47,57,57	24
6	PEG	B	306	7/7	0.65	0.21	70,84,91,91	0
6	PEG	B	307	7/7	0.73	0.32	75,90,95,95	0
4	EDO	A	305	4/4	0.76	0.14	62,75,77,77	0
3	PGE	A	306	10/10	0.78	0.14	64,77,80,80	0
3	PGE	A	303	10/10	0.80	0.12	59,71,78,79	0
2	ACT	A	302	4/4	0.81	0.12	58,58,70,70	0
4	EDO	B	301	4/4	0.83	0.11	56,67,68,70	0
3	PGE	A	311	10/10	0.84	0.14	69,83,89,89	0
4	EDO	A	309	4/4	0.85	0.12	77,92,93,93	0
3	PGE	A	307	10/10	0.86	0.12	63,76,80,80	0
4	EDO	A	304	4/4	0.86	0.16	47,57,59,59	0
4	EDO	B	303	4/4	0.87	0.10	54,65,65,66	0
5	SO4	A	310	5/5	0.92	0.17	95,95,96,96	0
2	ACT	A	301	4/4	0.94	0.12	48,49,58,58	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.