



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:46 AM UTC

PDB ID : 5HAP / pdb_00005hap
Title : OXA-48 beta-lactamase - S70A mutant
Authors : Stojanoski, V.; Adamski, C.J.; Hu, L.; Mehta, S.C.; Sankaran, B.; Prasad, B.V.V.; Palzkill, T.G.
Deposited on : 2015-12-30
Resolution : 1.89 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

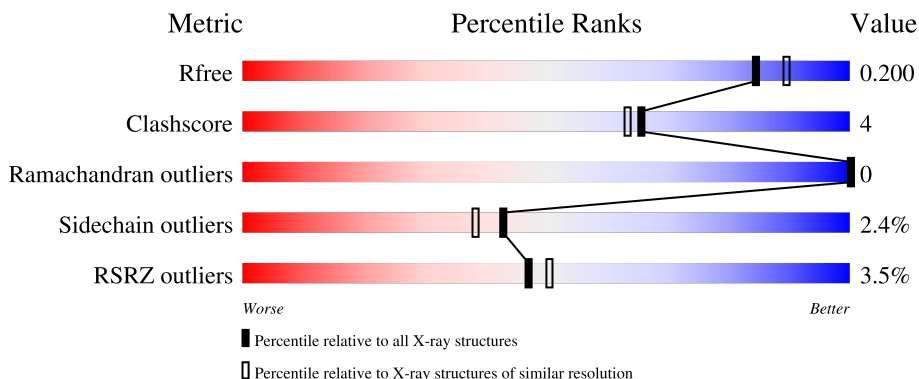
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	241	
1	B	241	

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	A	309	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 4371 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
			Total	C	N	O	S			
1	A	241	1989	1267	351	364	7	0	3	0
1	B	241	1973	1257	348	361	7	0	0	0

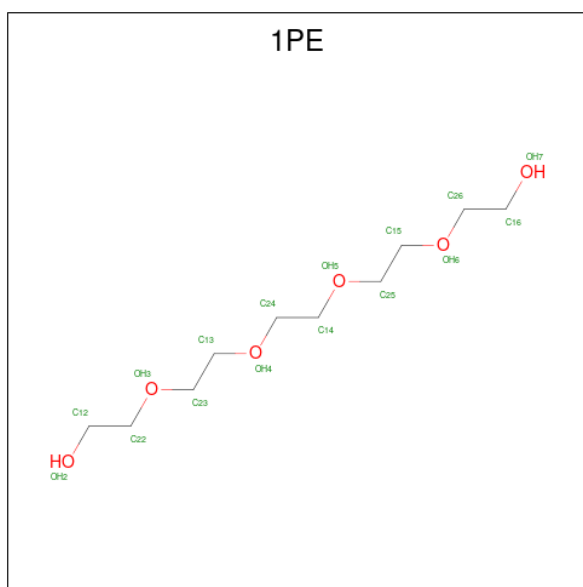
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	70	ALA	SER	engineered mutation	UNP Q6XEC0
B	70	ALA	SER	engineered mutation	UNP Q6XEC0

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

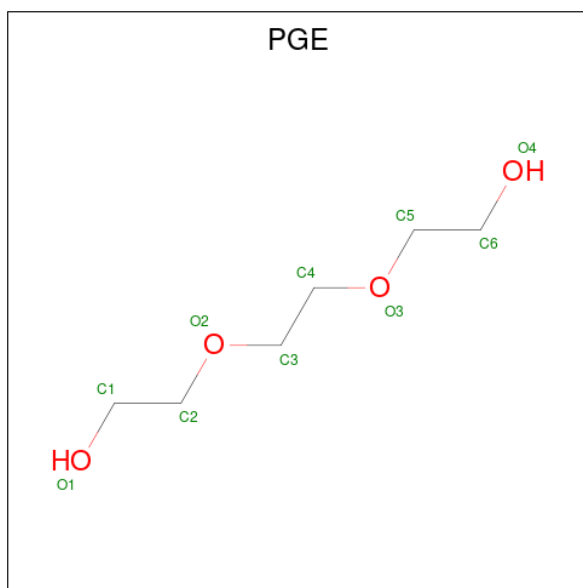
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).

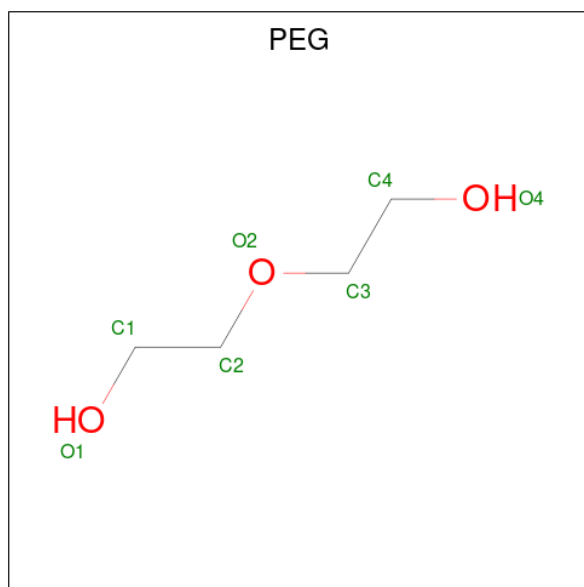


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

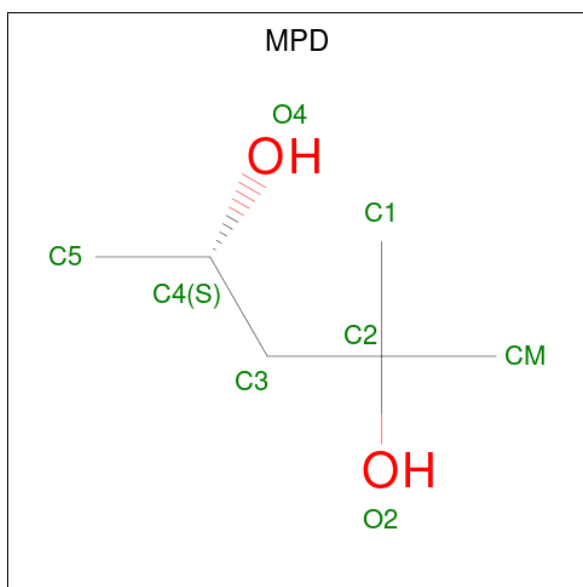
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0
5	B	1	Total Na 1 1	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



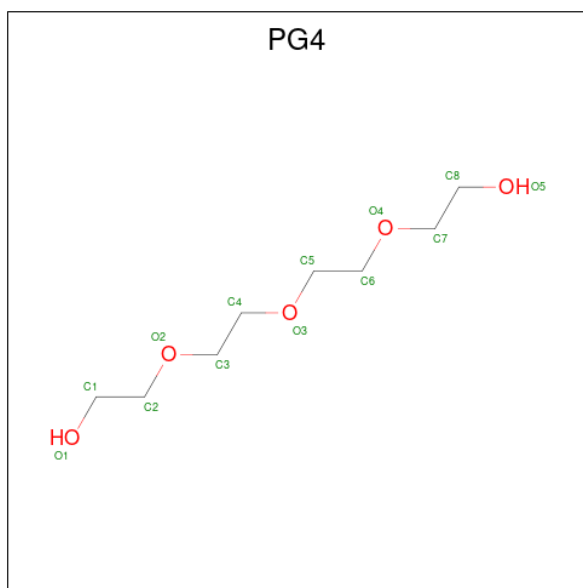
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	A	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0
6	B	1	Total C O 7 4 3	0	0

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 8 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

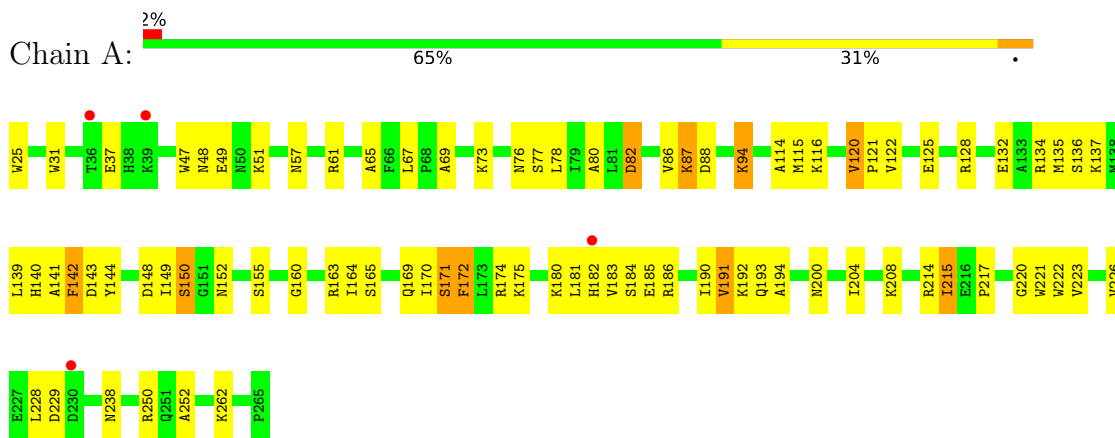
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	155	Total O 155 155	0	0
10	B	122	Total O 122 122	0	0

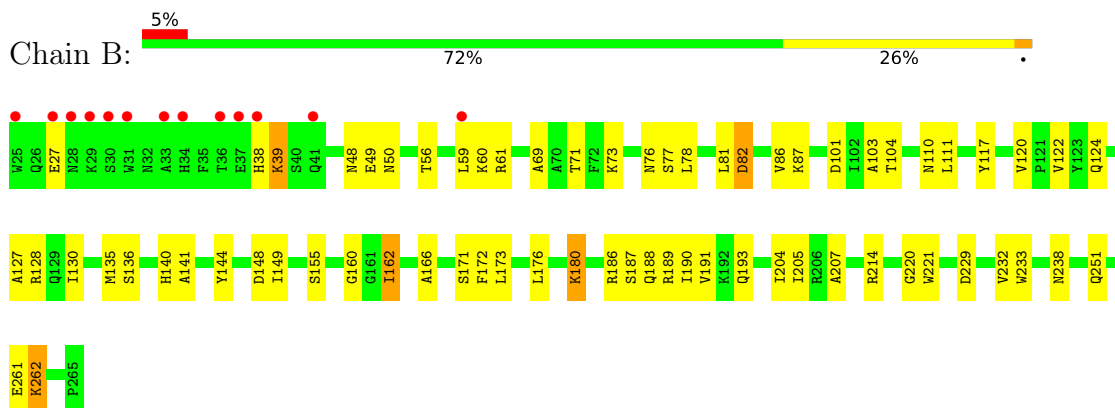
3 Residue-property plots

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: Beta-lactamase



- Molecule 1: Beta-lactamase



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	121.90Å 121.90Å 161.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	57.02 – 1.89 57.02 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.9 (57.02-1.89) 99.9 (57.02-1.89)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 1.71Å)	Xtrriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.191 , 0.226 0.204 , 0.200	Depositor DCC
R_{free} test set	3780 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	21.6	Xtrriage
Anisotropy	0.398	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4371	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CL, KCX, MPD, PEG, NA, EDO, PG4, PGE, 1PE

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	2.10	63/2032 (3.1%)	1.08	11/2748 (0.4%)
1	B	1.85	49/2009 (2.4%)	1.05	8/2717 (0.3%)
All	All	1.98	112/4041 (2.8%)	1.07	19/5465 (0.3%)

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	171[A]	SER	N-CA	16.05	1.65	1.46
1	A	171[B]	SER	N-CA	16.05	1.65	1.46
1	A	150[A]	SER	N-CA	14.79	1.65	1.46
1	A	150[B]	SER	N-CA	14.79	1.65	1.46
1	A	150[A]	SER	CA-C	14.33	1.70	1.52
1	A	150[B]	SER	CA-C	14.33	1.70	1.52
1	A	171[A]	SER	CA-C	14.09	1.71	1.52
1	A	171[B]	SER	CA-C	14.09	1.71	1.52
1	A	120	VAL	C-O	-8.80	1.17	1.24
1	B	120	VAL	C-O	-7.17	1.18	1.24
1	A	86	VAL	C-O	-7.13	1.16	1.24
1	A	114	ALA	C-O	-6.62	1.16	1.24
1	B	135	MET	C-O	-6.62	1.16	1.24
1	A	116	LYS	C-O	-6.61	1.16	1.24
1	B	148	ASP	C-O	-6.51	1.16	1.24
1	A	134	ARG	C-O	-6.43	1.16	1.24
1	B	232	VAL	C-O	-6.42	1.17	1.24
1	A	137	LYS	C-O	-6.42	1.16	1.24
1	A	140	HIS	C-O	-6.34	1.16	1.24
1	A	94	LYS	C-O	-6.29	1.16	1.23
1	A	135	MET	C-O	-6.27	1.16	1.24
1	A	193	GLN	C-O	-6.27	1.16	1.24
1	A	165	SER	C-O	-6.26	1.15	1.23
1	A	204	ILE	C-O	-6.21	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	49	GLU	C-O	-6.19	1.16	1.24
1	B	127	ALA	C-O	-6.19	1.16	1.24
1	A	128	ARG	C-O	-6.17	1.17	1.24
1	B	76	ASN	C-O	-6.14	1.17	1.24
1	B	191	VAL	C-O	-6.13	1.17	1.24
1	B	204	ILE	C-O	-6.11	1.17	1.24
1	B	140	HIS	C-O	-6.10	1.17	1.24
1	A	250	ARG	C-O	-6.09	1.17	1.24
1	A	69	ALA	C-O	-6.06	1.16	1.24
1	B	193	GLN	C-O	-6.03	1.17	1.24
1	A	88	ASP	C-O	-5.99	1.17	1.23
1	B	172	PHE	C-O	-5.98	1.17	1.24
1	A	160	GLY	C-O	-5.91	1.18	1.24
1	A	252	ALA	C-O	-5.91	1.17	1.24
1	B	82	ASP	C-O	-5.90	1.16	1.24
1	B	111	LEU	C-O	-5.88	1.17	1.24
1	B	205	ILE	C-O	-5.87	1.17	1.24
1	B	176	LEU	C-O	-5.86	1.17	1.24
1	B	69	ALA	C-O	-5.83	1.16	1.24
1	A	136	SER	C-O	-5.80	1.17	1.24
1	B	48	ASN	C-O	-5.80	1.16	1.24
1	B	188	GLN	C-O	-5.80	1.17	1.24
1	A	47	TRP	C-O	-5.74	1.17	1.24
1	A	223	VAL	C-O	-5.72	1.18	1.24
1	B	160	GLY	C-O	-5.71	1.18	1.24
1	A	82	ASP	C-O	-5.70	1.17	1.24
1	A	152	ASN	C-O	-5.65	1.17	1.23
1	B	155	SER	C-O	-5.64	1.17	1.24
1	B	103	ALA	C-O	-5.62	1.17	1.24
1	B	124	GLN	C-O	-5.61	1.17	1.24
1	A	122	VAL	C-O	-5.59	1.17	1.24
1	A	183	VAL	C-O	-5.57	1.17	1.24
1	B	136	SER	C-O	-5.56	1.17	1.24
1	B	122	VAL	C-O	-5.49	1.18	1.24
1	A	139	LEU	C-O	-5.49	1.17	1.24
1	A	149	ILE	C-O	-5.49	1.16	1.23
1	B	61	ARG	C-O	-5.48	1.17	1.24
1	B	189	ARG	C-O	-5.46	1.17	1.24
1	A	169	GLN	C-O	-5.46	1.17	1.24
1	B	86	VAL	C-O	-5.45	1.18	1.24
1	B	171	SER	C-O	-5.45	1.17	1.24
1	A	185	GLU	C-O	-5.43	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	LYS	C-O	-5.43	1.17	1.23
1	A	141	ALA	C-O	-5.42	1.17	1.24
1	A	144	TYR	C-O	-5.41	1.17	1.24
1	A	148	ASP	C-O	-5.41	1.17	1.24
1	A	87	LYS	C-O	-5.40	1.17	1.24
1	B	173	LEU	C-O	-5.35	1.17	1.24
1	B	190	ILE	C-O	-5.35	1.18	1.24
1	A	164	ILE	C-O	-5.35	1.18	1.23
1	A	125	GLU	C-O	-5.33	1.17	1.24
1	A	115	MET	C-O	-5.30	1.18	1.24
1	A	194	ALA	C-O	-5.30	1.17	1.24
1	A	76	ASN	C-O	-5.30	1.18	1.24
1	A	155	SER	C-O	-5.29	1.18	1.24
1	A	174	ARG	C-O	-5.26	1.18	1.24
1	B	162	ILE	C-O	-5.24	1.18	1.24
1	B	251	GLN	C-O	-5.23	1.17	1.24
1	B	81	LEU	C-O	-5.23	1.18	1.24
1	A	77	SER	C-O	-5.22	1.18	1.24
1	B	71	THR	C-O	-5.20	1.17	1.24
1	A	172	PHE	C-O	-5.20	1.18	1.24
1	B	77	SER	C-O	-5.18	1.18	1.24
1	B	233	TRP	C-O	-5.18	1.18	1.24
1	B	187	SER	C-O	-5.17	1.18	1.24
1	A	192	LYS	C-O	-5.17	1.18	1.24
1	B	166	ALA	C-O	-5.16	1.18	1.24
1	B	186	ARG	C-O	-5.14	1.18	1.24
1	B	229	ASP	C-O	-5.14	1.18	1.24
1	A	226	VAL	C-O	-5.13	1.18	1.24
1	B	117	TYR	C-O	-5.12	1.17	1.24
1	A	200	ASN	C-O	-5.10	1.19	1.24
1	B	50	ASN	C-O	-5.10	1.18	1.24
1	B	141	ALA	C-O	-5.10	1.18	1.24
1	B	104	THR	C-O	-5.08	1.17	1.24
1	A	215	ILE	C-O	-5.08	1.18	1.24
1	A	186	ARG	C-O	-5.08	1.18	1.24
1	B	78	LEU	C-O	-5.06	1.18	1.24
1	B	130	ILE	C-O	-5.06	1.18	1.24
1	B	87	LYS	C-O	-5.05	1.18	1.24
1	A	80	ALA	C-O	-5.04	1.18	1.24
1	A	142	PHE	C-O	-5.04	1.17	1.24
1	A	190	ILE	C-O	-5.03	1.18	1.24
1	A	191	VAL	C-O	-5.03	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	49	GLU	C-O	-5.03	1.18	1.24
1	B	128	ARG	C-O	-5.02	1.18	1.24
1	A	222	TRP	C-O	-5.01	1.18	1.23
1	A	61	ARG	C-O	-5.00	1.17	1.24

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	ARG	N-CA-C	7.03	121.09	112.23
1	A	181	LEU	O-C-N	-6.97	114.24	122.81
1	A	221	TRP	CA-CB-CG	6.72	126.37	113.60
1	B	120	VAL	O-C-N	6.43	124.53	120.42
1	B	214	ARG	N-CA-C	5.93	117.82	111.36
1	B	144	TYR	N-CA-C	5.88	117.88	108.41
1	B	149	ILE	N-CA-C	5.40	117.39	111.77
1	A	149	ILE	CA-C-N	5.38	129.95	121.56
1	A	149	ILE	C-N-CA	5.38	129.95	121.56
1	A	132	GLU	N-CA-C	5.33	117.08	111.28
1	B	207	ALA	N-CA-C	5.26	116.28	108.60
1	B	101	ASP	N-CA-C	5.20	118.88	112.54
1	B	221	TRP	CA-CB-CG	5.16	123.39	113.60
1	A	171[A]	SER	N-CA-C	-5.12	104.77	111.02
1	A	171[B]	SER	N-CA-C	-5.12	104.77	111.02
1	A	144	TYR	N-CA-C	5.05	116.53	108.41
1	B	39	LYS	N-CA-C	-5.04	104.47	111.28
1	A	150[A]	SER	CA-C-O	-5.03	115.48	120.96
1	A	150[B]	SER	CA-C-O	-5.03	115.48	120.96

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	1989	0	1942	23	0
1	B	1973	0	1926	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
3	A	16	0	22	1	0
4	A	20	0	28	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	28	0	40	7	0
6	B	28	0	40	0	0
7	A	8	0	14	0	0
8	B	13	0	18	0	0
9	B	16	0	24	0	0
10	A	155	0	0	1	0
10	B	122	0	0	0	0
All	All	4371	0	4054	31	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 (31) 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:171[B]:SER:CA	1:A:172:PHE:N	2.53	0.65
6:A:309:PEG:H41	1:B:110:ASN:HD21	1.67	0.59
1:B:261:GLU:O	1:B:262:LYS:HB2	2.05	0.57
6:A:309:PEG:C4	1:B:110:ASN:HD21	2.18	0.56
1:A:25:TRP:N	10:A:401:HOH:O	2.39	0.55
1:A:67:LEU:HD11	1:A:215:ILE:HD12	1.90	0.52
1:A:228:LEU:C	6:A:309:PEG:H22	2.35	0.52
1:A:228:LEU:O	6:A:309:PEG:H22	2.10	0.52
1:A:229:ASP:OD1	6:A:309:PEG:H11	2.10	0.51
1:A:78:LEU:HD23	1:A:191:VAL:HG21	1.93	0.49
1:A:175:LYS:HG2	4:A:304:PGE:H62	1.94	0.49
1:A:31:TRP:HB2	1:A:57:ASN:HB3	1.94	0.49
1:A:180:LYS:HD2	4:A:304:PGE:H2	1.96	0.47
1:A:48:ASN:ND2	1:A:51:LYS:HD2	2.30	0.47
1:A:142:PHE:CE1	1:A:182[A]:HIS:CD2	3.02	0.47
1:A:170:ILE:C	1:A:171[A]:SER:CA	2.73	0.47
1:A:65:ALA:HB1	1:A:163:ARG:HB3	2.00	0.44
1:A:217:PRO:HD3	3:A:302:1PE:H142	2.00	0.43
1:A:184:SER:OG	6:A:307:PEG:H32	2.19	0.42
1:B:27:GLU:HA	1:B:56:THR:O	2.18	0.42
1:B:180:LYS:HD2	1:B:180:LYS:HA	1.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:VAL:N	1:A:121:PRO:HD2	2.35	0.42
1:A:220:GLY:O	1:A:238:ASN:HA	2.19	0.42
1:B:38:HIS:O	1:B:39:LYS:C	2.61	0.42
1:B:220:GLY:O	1:B:238:ASN:HA	2.20	0.41
1:A:94:LYS:HE3	1:A:94:LYS:HB3	1.85	0.41
1:A:262:LYS:HA	1:A:262:LYS:HD2	1.83	0.40
6:A:307:PEG:H41	6:A:307:PEG:H22	1.79	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	241/241 (100%)	237 (98%)	4 (2%)	0	100	100
1	B	238/241 (99%)	233 (98%)	5 (2%)	0	100	100
All	All	479/482 (99%)	470 (98%)	9 (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	211/208 (101%)	207 (98%)	4 (2%)	50	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	208/208 (100%)	202 (97%)	6 (3%)	37	31
All	All	419/416 (101%)	409 (98%)	10 (2%)	43	38

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

Mol	Chain	Res	Type
1	A	37	GLU
1	A	82	ASP
1	A	87	LYS
1	A	143	ASP
1	B	59	LEU
1	B	60	LYS
1	B	82	ASP
1	B	162	ILE
1	B	180	LYS
1	B	262	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	124	GLN
1	B	90	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](#)

2 non-standard protein/DNA/RNA residues 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
1	KCX	B	73	1	10,11,12	1.72	1 (10%)	6,12,14	1.41	2 (33%)
1	KCX	A	73	1	10,11,12	1.41	1 (10%)	6,12,14	1.83	2 (33%)

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
1	KCX	B	73	1	-	0/9/10/12	-
1	KCX	A	73	1	-	0/9/10/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	73	KCX	OQ1-CX	4.59	1.30	1.21
1	A	73	KCX	OQ1-CX	2.93	1.27	1.21

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	KCX	OQ1-CX-NZ	-3.72	119.27	124.92
1	B	73	KCX	CD-CE-NZ	2.20	118.36	112.20
1	A	73	KCX	CE-NZ-CX	2.17	125.67	121.98
1	B	73	KCX	OQ1-CX-NZ	-2.17	121.62	124.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 3 are monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PEG	B	305	-	6,6,6	0.47	0	5,5,5	0.30	0
9	EDO	B	309	-	3,3,3	0.31	0	2,2,2	0.16	0
6	PEG	A	307	-	6,6,6	0.30	0	5,5,5	0.55	0
6	PEG	B	302	-	6,6,6	0.43	0	5,5,5	0.48	0
6	PEG	A	309	-	6,6,6	0.43	0	5,5,5	0.84	0
6	PEG	B	303	-	6,6,6	0.45	0	5,5,5	0.55	0
6	PEG	B	304	-	6,6,6	0.46	0	5,5,5	0.27	0
9	EDO	B	307	-	3,3,3	0.50	0	2,2,2	0.19	0
9	EDO	B	308	-	3,3,3	0.36	0	2,2,2	0.06	0
3	1PE	A	302	-	15,15,15	0.55	0	14,14,14	0.37	0
6	PEG	A	306	-	6,6,6	0.53	0	5,5,5	0.37	0
8	PG4	B	306	-	12,12,12	0.45	0	11,11,11	0.45	0
4	PGE	A	304	-	9,9,9	0.41	0	8,8,8	0.54	0
6	PEG	A	308	-	6,6,6	0.52	0	5,5,5	0.25	0
9	EDO	B	310	-	3,3,3	0.44	0	2,2,2	0.42	0
4	PGE	A	303	-	9,9,9	0.49	0	8,8,8	0.37	0
7	MPD	A	310	-	7,7,7	0.38	0	9,10,10	0.55	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PEG	B	305	-	-	2/4/4/4	-
9	EDO	B	309	-	-	1/1/1/1	-
6	PEG	A	307	-	-	3/4/4/4	-
6	PEG	B	302	-	-	1/4/4/4	-
6	PEG	A	309	-	-	3/4/4/4	-
6	PEG	B	303	-	-	2/4/4/4	-
6	PEG	B	304	-	-	0/4/4/4	-
9	EDO	B	307	-	-	0/1/1/1	-
9	EDO	B	308	-	-	0/1/1/1	-
3	1PE	A	302	-	-	7/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PEG	A	306	-	-	2/4/4/4	-
8	PG4	B	306	-	-	7/10/10/10	-
4	PGE	A	304	-	-	4/7/7/7	-
6	PEG	A	308	-	-	3/4/4/4	-
9	EDO	B	310	-	-	1/1/1/1	-
4	PGE	A	303	-	-	5/7/7/7	-
7	MPD	A	310	-	-	0/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	306	PG4	O3-C5-C6-O4
6	A	307	PEG	O1-C1-C2-O2
3	A	302	1PE	OH5-C14-C24-OH4
6	A	309	PEG	O2-C3-C4-O4
6	B	305	PEG	O2-C3-C4-O4
4	A	303	PGE	O2-C3-C4-O3
3	A	302	1PE	OH7-C16-C26-OH6
4	A	303	PGE	O1-C1-C2-O2
6	A	308	PEG	O1-C1-C2-O2
4	A	303	PGE	O3-C5-C6-O4
9	B	309	EDO	O1-C1-C2-O2
6	A	309	PEG	O1-C1-C2-O2
4	A	304	PGE	O2-C3-C4-O3
4	A	304	PGE	C6-C5-O3-C4
4	A	303	PGE	C6-C5-O3-C4
8	B	306	PG4	C6-C5-O3-C4
4	A	304	PGE	C1-C2-O2-C3
6	A	306	PEG	C1-C2-O2-C3
6	A	307	PEG	C4-C3-O2-C2
8	B	306	PG4	C8-C7-O4-C6
4	A	303	PGE	C4-C3-O2-C2
8	B	306	PG4	C4-C3-O2-C2
3	A	302	1PE	OH6-C15-C25-OH5
8	B	306	PG4	O2-C3-C4-O3
6	B	302	PEG	C4-C3-O2-C2
6	A	307	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
6	A	306	PEG	O2-C3-C4-O4
3	A	302	1PE	C15-C25-OH5-C14
6	A	308	PEG	C1-C2-O2-C3
6	A	308	PEG	C4-C3-O2-C2
3	A	302	1PE	C25-C15-OH6-C26
3	A	302	1PE	C14-C24-OH4-C13
6	B	303	PEG	O1-C1-C2-O2
3	A	302	1PE	C23-C13-OH4-C24
9	B	310	EDO	O1-C1-C2-O2
6	B	303	PEG	C1-C2-O2-C3
6	B	305	PEG	C1-C2-O2-C3
6	A	309	PEG	C1-C2-O2-C3
8	B	306	PG4	C1-C2-O2-C3
4	A	304	PGE	O1-C1-C2-O2
8	B	306	PG4	C5-C6-O4-C7

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	307	PEG	2	0
6	A	309	PEG	5	0
3	A	302	1PE	1	0
4	A	304	PGE	2	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	240/241 (99%)	0.02	4 (1%) 69 72	13, 21, 39, 60	3 (1%)
1	B	240/241 (99%)	0.25	13 (5%) 31 33	14, 24, 48, 72	0
All	All	480/482 (99%)	0.14	17 (3%) 47 50	13, 23, 43, 72	3 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	182[A]	HIS	4.0
1	B	25	TRP	3.3
1	B	36	THR	3.1
1	B	33	ALA	2.9
1	B	59	LEU	2.9
1	B	34	HIS	2.7
1	A	36	THR	2.7
1	B	38	HIS	2.7
1	B	37	GLU	2.5
1	B	31	TRP	2.5
1	B	30	SER	2.4
1	B	28	ASN	2.3
1	B	29	LYS	2.3
1	A	230	ASP	2.2
1	B	41	GLN	2.1
1	B	27	GLU	2.0
1	A	39	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(\AA^2)	Q<0.9
1	KCX	A	73	12/13	0.96	0.05	8,13,15,17	0
1	KCX	B	73	12/13	0.97	0.06	11,15,20,21	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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(\AA^2)	Q<0.9
6	PEG	A	307	7/7	0.59	0.24	34,47,50,50	0
7	MPD	A	310	8/8	0.72	0.25	39,48,55,58	0
9	EDO	B	307	4/4	0.72	0.19	44,44,48,48	0
9	EDO	B	309	4/4	0.75	0.20	47,56,57,60	0
6	PEG	A	308	7/7	0.77	0.19	37,45,49,58	0
6	PEG	A	306	7/7	0.77	0.18	31,39,44,49	0
9	EDO	B	310	4/4	0.78	0.15	43,48,48,49	0
3	1PE	A	302	16/16	0.79	0.17	37,41,48,55	0
9	EDO	B	308	4/4	0.79	0.21	31,40,41,53	0
6	PEG	B	303	7/7	0.80	0.16	29,36,48,49	0
4	PGE	A	303	10/10	0.80	0.17	39,44,50,51	0
4	PGE	A	304	10/10	0.83	0.17	39,49,57,61	0
6	PEG	A	309	7/7	0.84	0.15	29,33,40,52	0
8	PG4	B	306	13/13	0.84	0.16	36,50,56,58	0
6	PEG	B	304	7/7	0.84	0.15	40,45,48,49	0
6	PEG	B	302	7/7	0.87	0.14	39,43,45,48	0
6	PEG	B	305	7/7	0.87	0.13	40,42,46,52	0
5	NA	A	305	1/1	0.89	0.13	41,41,41,41	0
5	NA	B	301	1/1	0.92	0.24	41,41,41,41	0
2	CL	A	301	1/1	0.99	0.04	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.