



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:51 PM UTC

PDB ID : 6HB8 / pdb_00006hb8
Title : Crystal structure of OXA-517 beta-lactamase
Authors : Raczyńska, J.E.; Dabos, L.; Zavala, A.; Retailleau, P.; Iorga, B.; Jaskolski, M.; Naas, T.
Deposited on : 2018-08-09
Resolution : 1.86 Å(reported)

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

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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

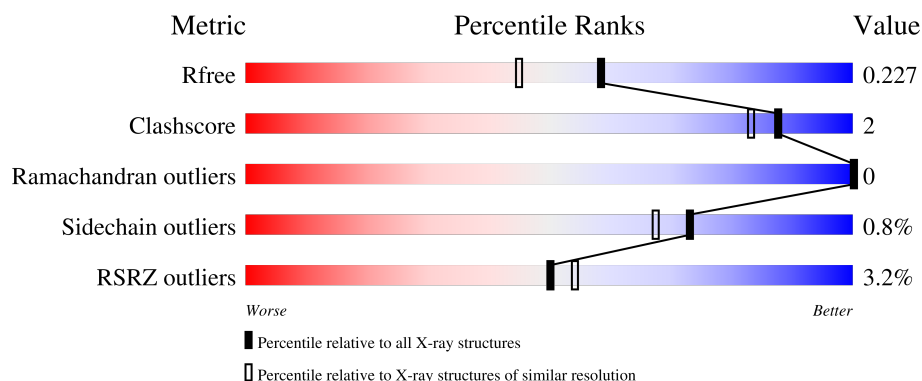
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	254	6% 89% 7% .
1	B	254	2% 89% 7% .
1	C	254	2% 88% 8% .
1	D	254	2% 87% 7% 5%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8981 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	C	N	O	S	0	4	0
			2012	1289	350	365	8			
1	B	243	Total	C	N	O	S	0	9	0
			2041	1307	360	366	8			
1	C	244	Total	C	N	O	S	0	8	0
			2043	1309	359	367	8			
1	D	241	Total	C	N	O	S	0	7	0
			2010	1287	351	364	8			

There are 44 discrepancies between the modelled and reference sequences:

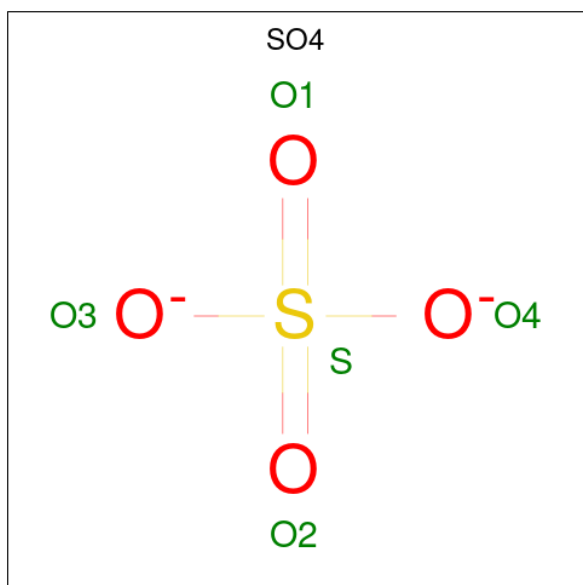
Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	initiating methionine	UNP A0A1U8YI81
A	266	PHE	-	expression tag	UNP A0A1U8YI81
A	267	GLU	-	expression tag	UNP A0A1U8YI81
A	268	HIS	-	expression tag	UNP A0A1U8YI81
A	269	HIS	-	expression tag	UNP A0A1U8YI81
A	270	HIS	-	expression tag	UNP A0A1U8YI81
A	271	HIS	-	expression tag	UNP A0A1U8YI81
A	272	HIS	-	expression tag	UNP A0A1U8YI81
A	273	HIS	-	expression tag	UNP A0A1U8YI81
A	274	HIS	-	expression tag	UNP A0A1U8YI81
A	275	HIS	-	expression tag	UNP A0A1U8YI81
B	20	MET	-	initiating methionine	UNP A0A1U8YI81
B	266	PHE	-	expression tag	UNP A0A1U8YI81
B	267	GLU	-	expression tag	UNP A0A1U8YI81
B	268	HIS	-	expression tag	UNP A0A1U8YI81
B	269	HIS	-	expression tag	UNP A0A1U8YI81
B	270	HIS	-	expression tag	UNP A0A1U8YI81
B	271	HIS	-	expression tag	UNP A0A1U8YI81
B	272	HIS	-	expression tag	UNP A0A1U8YI81
B	273	HIS	-	expression tag	UNP A0A1U8YI81
B	274	HIS	-	expression tag	UNP A0A1U8YI81

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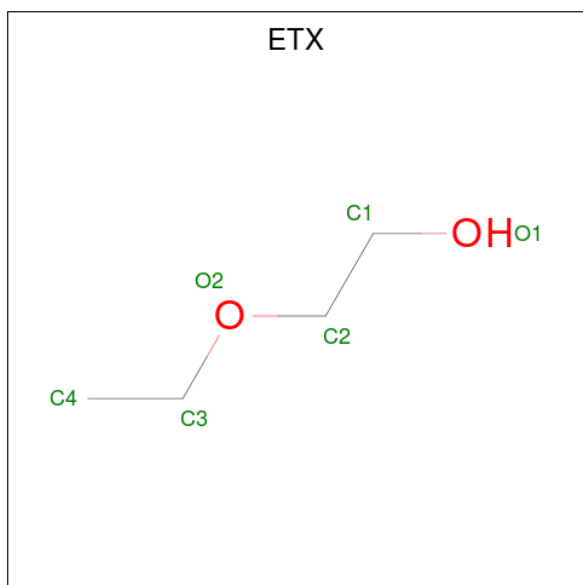
Chain	Residue	Modelled	Actual	Comment	Reference
B	275	HIS	-	expression tag	UNP A0A1U8YI81
C	20	MET	-	initiating methionine	UNP A0A1U8YI81
C	266	PHE	-	expression tag	UNP A0A1U8YI81
C	267	GLU	-	expression tag	UNP A0A1U8YI81
C	268	HIS	-	expression tag	UNP A0A1U8YI81
C	269	HIS	-	expression tag	UNP A0A1U8YI81
C	270	HIS	-	expression tag	UNP A0A1U8YI81
C	271	HIS	-	expression tag	UNP A0A1U8YI81
C	272	HIS	-	expression tag	UNP A0A1U8YI81
C	273	HIS	-	expression tag	UNP A0A1U8YI81
C	274	HIS	-	expression tag	UNP A0A1U8YI81
C	275	HIS	-	expression tag	UNP A0A1U8YI81
D	20	MET	-	initiating methionine	UNP A0A1U8YI81
D	266	PHE	-	expression tag	UNP A0A1U8YI81
D	267	GLU	-	expression tag	UNP A0A1U8YI81
D	268	HIS	-	expression tag	UNP A0A1U8YI81
D	269	HIS	-	expression tag	UNP A0A1U8YI81
D	270	HIS	-	expression tag	UNP A0A1U8YI81
D	271	HIS	-	expression tag	UNP A0A1U8YI81
D	272	HIS	-	expression tag	UNP A0A1U8YI81
D	273	HIS	-	expression tag	UNP A0A1U8YI81
D	274	HIS	-	expression tag	UNP A0A1U8YI81
D	275	HIS	-	expression tag	UNP A0A1U8YI81

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



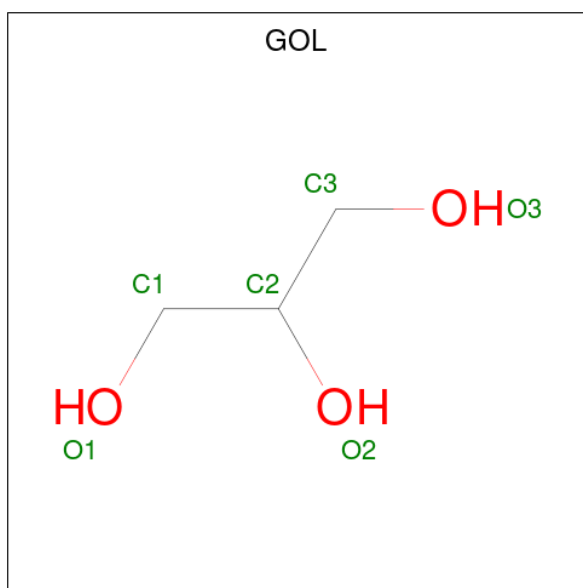
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	1
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	1
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0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

- Molecule 3 is 2-ETHOXYETHANOL (CCD ID: ETX) (formula: C₄H₁₀O₂).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	1
			12	6	6		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

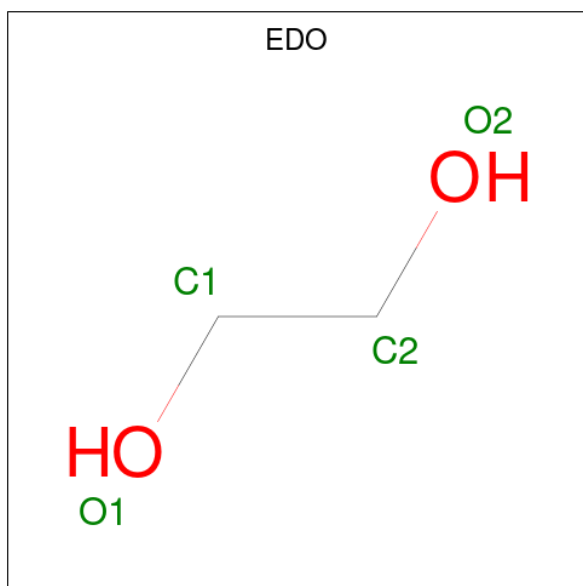
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	1
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	1
			1	1		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

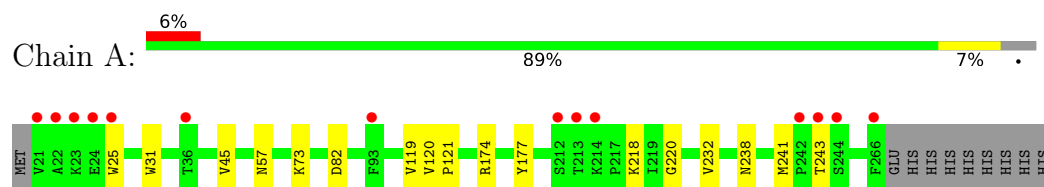
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	175	Total	O	0	0
			175	175		
7	B	199	Total	O	0	2
			200	200		
7	C	179	Total	O	0	4
			180	180		
7	D	182	Total	O	0	2
			183	183		

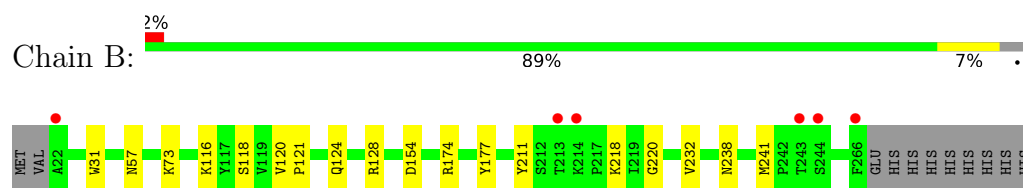
3 Residue-property plots [i](#)

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.

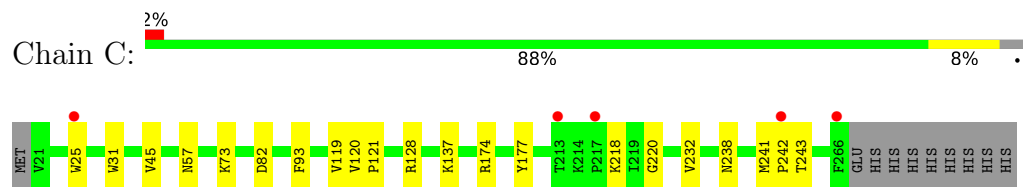
- Molecule 1: Beta-lactamase



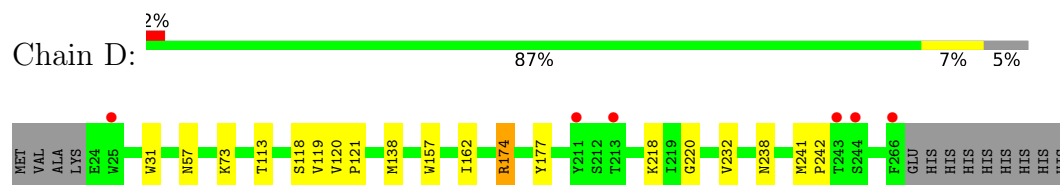
- Molecule 1: Beta-lactamase



- Molecule 1: Beta-lactamase



- Molecule 1: Beta-lactamase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.80Å 125.05Å 82.66Å 90.00° 94.65° 90.00°	Depositor
Resolution (Å)	46.18 – 1.86 46.18 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.18-1.86) 99.7 (46.18-1.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.170 , 0.219 0.181 , 0.227	Depositor DCC
R_{free} test set	4278 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8981	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 63.73 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.2488e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL, EDO, ETX, KCX, CL

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	0.93	0/2065	0.93	2/2792 (0.1%)
1	B	0.93	2/2109 (0.1%)	0.90	0/2848
1	C	0.92	0/2107	0.91	2/2846 (0.1%)
1	D	0.91	1/2073 (0.0%)	0.90	2/2802 (0.1%)
All	All	0.92	3/8354 (0.0%)	0.91	6/11288 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	4
1	C	0	2
1	D	0	1
All	All	0	8

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	138	MET	C-O	-5.29	1.17	1.24
1	B	116	LYS	C-O	-5.24	1.18	1.24
1	B	211	TYR	C-O	-5.13	1.17	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	VAL	CA-C-N	5.66	124.85	120.33
1	A	119	VAL	C-N-CA	5.66	124.85	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	119	VAL	CA-C-N	5.31	124.58	120.33
1	C	119	VAL	C-N-CA	5.31	124.58	120.33
1	D	119	VAL	CA-C-N	5.17	124.46	120.33
1	D	119	VAL	C-N-CA	5.17	124.46	120.33

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	174	ARG	Sidechain
1	B	128[A]	ARG	Sidechain
1	B	128[B]	ARG	Sidechain
1	B	174[A]	ARG	Sidechain
1	B	174[B]	ARG	Sidechain
1	C	174[A]	ARG	Sidechain
1	C	174[B]	ARG	Sidechain
1	D	174	ARG	Sidechain

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	2012	0	1971	7	0
1	B	2041	0	2017	6	0
1	C	2043	0	2020	10	0
1	D	2010	0	1969	9	0
2	A	10	0	0	0	0
2	B	15	0	0	0	0
2	C	20	0	0	0	0
2	D	10	0	0	0	0
3	A	6	0	10	0	0
4	A	6	0	8	0	0
4	B	6	0	8	1	0
4	C	30	0	40	0	0
4	D	24	0	32	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	4	0	6	0	0
6	D	4	0	6	0	0
7	A	175	0	0	0	0
7	B	200	0	0	0	0
7	C	180	0	0	2	0
7	D	183	0	0	1	0
All	All	8981	0	8087	33	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 2.

All (33) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:305:GOL:O1	4:B:305:GOL:O3	2.14	0.64
1:C:137:LYS:HG3	7:C:479:HOH:O	1.96	0.64
1:C:218:LYS:HB3	1:C:241:MET:O	2.00	0.61
1:A:218:LYS:HB3	1:A:241:MET:O	2.01	0.59
1:D:218:LYS:HB3	1:D:241:MET:O	2.02	0.59
1:B:218:LYS:HB3	1:B:241:MET:O	2.02	0.59
1:D:113:THR:HG21	4:D:305[A]:GOL:O2	2.06	0.56
1:D:177:TYR:CZ	1:D:232[B]:VAL:HG21	2.40	0.56
1:C:25:TRP:CZ3	1:C:45:VAL:CG1	2.90	0.54
1:D:220:GLY:O	1:D:238:ASN:HA	2.08	0.54
1:D:174:ARG:NH2	4:D:306:GOL:O1	2.32	0.54
1:A:31:TRP:HB2	1:A:57:ASN:HB3	1.90	0.54
1:B:220:GLY:O	1:B:238:ASN:HA	2.08	0.53
1:D:31:TRP:HB2	1:D:57:ASN:HB3	1.91	0.52
1:A:220:GLY:O	1:A:238:ASN:HA	2.10	0.52
1:B:31:TRP:HB2	1:B:57:ASN:HB3	1.91	0.51
1:C:220:GLY:O	1:C:238:ASN:HA	2.10	0.51
1:C:31:TRP:HB2	1:C:57:ASN:HB3	1.93	0.51
1:B:177:TYR:CZ	1:B:232[B]:VAL:HG21	2.48	0.49
1:C:218:LYS:HD2	1:C:242:PRO:HA	1.96	0.48
1:D:242:PRO:HD2	7:D:554:HOH:O	2.14	0.48
1:D:120:VAL:N	1:D:121:PRO:HD2	2.31	0.45
1:A:25:TRP:CZ3	1:A:45:VAL:CG1	3.00	0.45
1:B:120:VAL:N	1:B:121:PRO:HD2	2.32	0.44
1:C:25:TRP:CZ3	1:C:45:VAL:HG13	2.52	0.44
1:C:177:TYR:CZ	1:C:232[B]:VAL:HG21	2.53	0.44
1:A:25:TRP:CZ3	1:A:45:VAL:HG13	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:TYR:CZ	1:A:232[B]:VAL:HG21	2.55	0.41
1:A:120:VAL:N	1:A:121:PRO:HD2	2.36	0.41
1:B:124:GLN:HG2	1:B:154:ASP:O	2.20	0.41
1:C:128[B]:ARG:NH1	7:C:404:HOH:O	2.40	0.41
1:C:120:VAL:N	1:C:121:PRO:HD2	2.35	0.41
1:D:157:TRP:HA	1:D:162:ILE:CG2	2.51	0.41

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	245/254 (96%)	240 (98%)	5 (2%)	0	100	100
1	B	249/254 (98%)	244 (98%)	5 (2%)	0	100	100
1	C	249/254 (98%)	243 (98%)	6 (2%)	0	100	100
1	D	245/254 (96%)	240 (98%)	5 (2%)	0	100	100
All	All	988/1016 (97%)	967 (98%)	21 (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	215/221 (97%)	213 (99%)	2 (1%)	70	64
1	B	219/221 (99%)	218 (100%)	1 (0%)	81	77
1	C	219/221 (99%)	215 (98%)	4 (2%)	51	40
1	D	216/221 (98%)	215 (100%)	1 (0%)	81	77
All	All	869/884 (98%)	861 (99%)	8 (1%)	73	64

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ASP
1	A	243	THR
1	B	118	SER
1	C	82	ASP
1	C	93[A]	PHE
1	C	93[B]	PHE
1	C	243	THR
1	D	118	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	B	26	GLN
1	B	64	GLN
1	D	26	GLN
1	D	193	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	A	73	1	10,11,12	3.58	1 (10%)	6,12,14	2.04	1 (16%)
1	KCX	D	73	1	10,11,12	2.87	1 (10%)	6,12,14	2.45	1 (16%)
1	KCX	B	73	1	10,11,12	2.48	1 (10%)	6,12,14	2.41	1 (16%)
1	KCX	C	73	1	10,11,12	3.33	1 (10%)	6,12,14	2.06	1 (16%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	KCX	OQ1-CX	10.97	1.41	1.21
1	C	73	KCX	OQ1-CX	10.19	1.40	1.21
1	D	73	KCX	OQ1-CX	8.85	1.37	1.21
1	B	73	KCX	OQ1-CX	7.62	1.35	1.21

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	73	KCX	OQ1-CX-NZ	-5.96	115.87	124.92
1	B	73	KCX	OQ1-CX-NZ	-5.87	116.00	124.92
1	A	73	KCX	OQ1-CX-NZ	-4.93	117.43	124.92
1	C	73	KCX	OQ1-CX-NZ	-4.93	117.44	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 27 ligands modelled in this entry, 2 are monoatomic - leaving 25 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	B	302	-	4,4,4	0.42	0	6,6,6	0.35	0
2	SO4	C	303	-	4,4,4	0.51	0	6,6,6	0.75	0
2	SO4	D	302	-	4,4,4	0.52	0	6,6,6	0.50	0
4	GOL	D	304	-	5,5,5	0.22	0	5,5,5	0.73	0
4	GOL	C	307	-	5,5,5	0.95	0	5,5,5	1.55	1 (20%)
4	GOL	C	308	-	5,5,5	0.63	0	5,5,5	0.86	0
2	SO4	D	303[B]	-	4,4,4	0.35	0	6,6,6	0.85	0
2	SO4	A	302	-	4,4,4	0.50	0	6,6,6	0.31	0
4	GOL	C	306	-	5,5,5	0.26	0	5,5,5	0.64	0
3	ETX	A	303	-	5,5,5	0.73	0	4,4,4	0.29	0
2	SO4	C	301	-	4,4,4	0.48	0	6,6,6	0.63	0
6	EDO	D	301	-	3,3,3	0.66	0	2,2,2	0.17	0
4	GOL	C	305	-	5,5,5	0.34	0	5,5,5	0.47	0
4	GOL	B	305	-	5,5,5	0.37	0	5,5,5	1.05	0
2	SO4	C	304	-	4,4,4	0.79	0	6,6,6	0.60	0
2	SO4	C	302[B]	-	4,4,4	0.43	0	6,6,6	0.43	0
2	SO4	A	301	-	4,4,4	0.56	0	6,6,6	0.28	0
2	SO4	B	303[B]	-	4,4,4	0.29	0	6,6,6	0.86	0
6	EDO	B	301	-	3,3,3	1.17	0	2,2,2	0.60	0
4	GOL	A	304	-	5,5,5	0.40	0	5,5,5	0.58	0
4	GOL	C	309	-	5,5,5	0.53	0	5,5,5	0.92	0
4	GOL	D	306	-	5,5,5	0.65	0	5,5,5	0.97	0
4	GOL	D	305[A]	-	5,5,5	0.77	0	5,5,5	0.56	0
4	GOL	D	305[B]	-	5,5,5	0.66	0	5,5,5	1.05	0
2	SO4	B	304	-	4,4,4	0.49	0	6,6,6	0.32	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	GOL	D	305[B]	-	-	2/4/4/4	-
4	GOL	D	306	-	-	2/4/4/4	-
6	EDO	B	301	-	-	0/1/1/1	-
6	EDO	D	301	-	-	1/1/1/1	-
4	GOL	D	304	-	-	2/4/4/4	-
4	GOL	C	307	-	-	2/4/4/4	-
4	GOL	C	305	-	-	2/4/4/4	-
4	GOL	B	305	-	-	0/4/4/4	-
4	GOL	C	308	-	-	2/4/4/4	-
4	GOL	A	304	-	-	2/4/4/4	-
4	GOL	D	305[A]	-	-	4/4/4/4	-
4	GOL	C	306	-	-	0/4/4/4	-
4	GOL	C	309	-	-	0/4/4/4	-
3	ETX	A	303	-	-	2/3/3/3	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	307	GOL	C3-C2-C1	2.78	122.01	111.80

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	304	GOL	C1-C2-C3-O3
4	C	305	GOL	O1-C1-C2-O2
4	C	305	GOL	O1-C1-C2-C3
4	D	305[A]	GOL	O1-C1-C2-C3
4	D	305[A]	GOL	C1-C2-C3-O3
4	D	305[B]	GOL	O1-C1-C2-C3
4	C	307	GOL	O1-C1-C2-C3
4	D	304	GOL	C1-C2-C3-O3
4	D	306	GOL	C1-C2-C3-O3
4	A	304	GOL	O2-C2-C3-O3
4	C	307	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	303	ETX	O1-C1-C2-O2
4	D	305[A]	GOL	O1-C1-C2-O2
4	D	305[A]	GOL	O2-C2-C3-O3
4	D	305[B]	GOL	O1-C1-C2-O2
4	D	306	GOL	O2-C2-C3-O3
6	D	301	EDO	O1-C1-C2-O2
4	C	308	GOL	O2-C2-C3-O3
4	D	304	GOL	O2-C2-C3-O3
3	A	303	ETX	C1-C2-O2-C3
4	C	308	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	305	GOL	1	0
4	D	306	GOL	1	0
4	D	305[A]	GOL	1	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

6.1 Protein, DNA and RNA chains

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	243/254 (95%)	0.36	14 (5%) 29 31	22, 37, 73, 97	4 (1%)
1	B	242/254 (95%)	0.18	6 (2%) 58 62	20, 35, 59, 91	9 (3%)
1	C	243/254 (95%)	0.32	5 (2%) 63 67	20, 37, 64, 95	8 (3%)
1	D	240/254 (94%)	0.23	6 (2%) 58 62	21, 36, 59, 89	7 (2%)
All	All	968/1016 (95%)	0.27	31 (3%) 50 54	20, 36, 64, 97	28 (2%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	22	ALA	3.8
1	A	21	VAL	3.4
1	D	25	TRP	3.3
1	C	266	PHE	3.2
1	A	25	TRP	3.1
1	B	266	PHE	3.0
1	D	266	PHE	3.0
1	C	25	TRP	2.8
1	A	266	PHE	2.8
1	C	213	THR	2.7
1	B	22	ALA	2.6
1	D	213	THR	2.6
1	D	211	TYR	2.5
1	A	23	LYS	2.5
1	A	214	LYS	2.5
1	A	244	SER	2.4
1	C	242	PRO	2.4
1	A	213	THR	2.4
1	A	212	SER	2.4
1	A	243	THR	2.3
1	D	243	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	24	GLU	2.3
1	B	214	LYS	2.2
1	A	242	PRO	2.2
1	C	217	PRO	2.2
1	A	36	THR	2.1
1	B	243	THR	2.1
1	B	213	THR	2.1
1	B	244	SER	2.1
1	D	244	SER	2.0
1	A	93[A]	PHE	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(Å ²)	Q<0.9
1	KCX	B	73	12/13	0.94	0.09	28,31,37,37	0
1	KCX	C	73	12/13	0.94	0.09	29,32,44,48	0
1	KCX	A	73	12/13	0.95	0.08	27,37,41,43	0
1	KCX	D	73	12/13	0.96	0.08	27,30,39,42	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(Å ²)	Q<0.9
4	GOL	B	305	6/6	0.77	0.18	58,71,72,81	0
2	SO4	C	303	5/5	0.79	0.17	39,52,56,62	5
2	SO4	C	304	5/5	0.81	0.16	65,77,100,105	0
4	GOL	C	306	6/6	0.81	0.14	75,80,82,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	D	305[A]	6/6	0.82	0.17	38,47,50,53	6
4	GOL	D	305[B]	6/6	0.82	0.17	53,65,70,70	6
2	SO4	B	304	5/5	0.83	0.17	52,58,69,73	5
2	SO4	A	302	5/5	0.85	0.17	46,48,52,65	5
4	GOL	C	309	6/6	0.85	0.13	52,58,64,65	0
6	EDO	D	301	4/4	0.86	0.16	52,57,60,68	0
4	GOL	C	305	6/6	0.88	0.11	61,72,77,77	0
4	GOL	D	306	6/6	0.88	0.13	59,65,67,79	0
3	ETX	A	303	6/6	0.88	0.20	60,66,75,76	0
2	SO4	A	301	5/5	0.89	0.10	47,72,78,81	0
4	GOL	C	308	6/6	0.90	0.14	42,64,69,72	0
4	GOL	D	304	6/6	0.90	0.14	42,58,60,73	0
2	SO4	C	302[B]	5/5	0.91	0.13	50,51,66,66	5
4	GOL	C	307	6/6	0.91	0.13	35,48,55,56	0
2	SO4	B	302	5/5	0.91	0.11	59,60,81,81	0
6	EDO	B	301	4/4	0.92	0.17	39,43,52,53	0
4	GOL	A	304	6/6	0.93	0.12	42,64,70,71	0
2	SO4	D	302	5/5	0.94	0.09	54,57,73,77	0
2	SO4	C	301	5/5	0.95	0.08	55,58,75,77	0
2	SO4	D	303[B]	5/5	0.96	0.09	30,33,34,35	5
2	SO4	B	303[B]	5/5	0.97	0.09	34,34,39,40	5
5	CL	A	305[A]	1/1	0.99	0.08	37,37,37,37	1
5	CL	B	306[A]	1/1	0.99	0.07	33,33,33,33	1

6.5 Other polymers [i](#)

There are no such residues in this entry.