



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:56 PM UTC

PDB ID : 6J8Q / pdb_00006j8q
Title : Serine Beta-Lactamase KPC-2 in Complex with Dual MBL/SBL Inhibitor WL-001
Authors : Li, G.-B.; Liu, S.
Deposited on : 2019-01-21
Resolution : 1.79 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

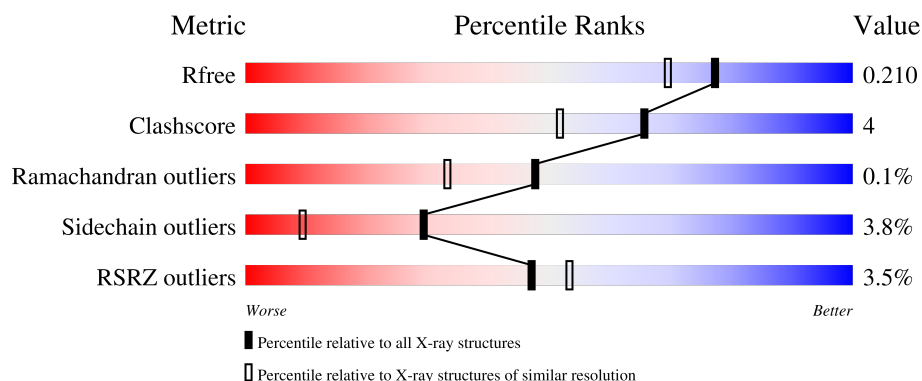
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	265	
1	B	265	
1	C	265	
1	D	265	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8838 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.

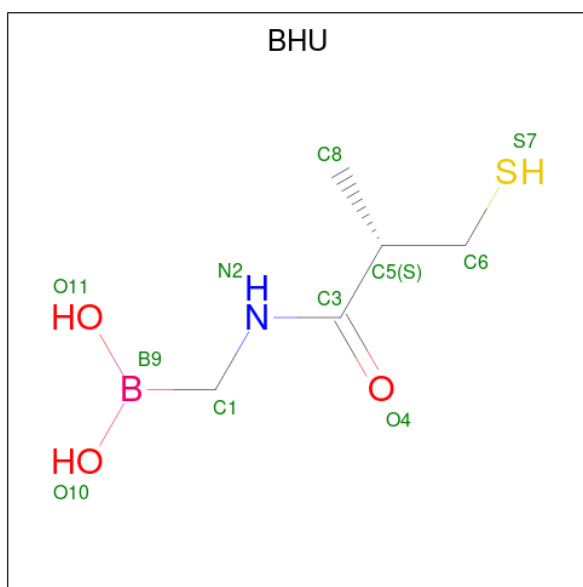
- Molecule 1 is a protein called Serine Beta-Lactamase KPC-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	1
			1973	1242	347	379	5			
1	B	263	Total	C	N	O	S	0	0	1
			1961	1235	345	376	5			
1	C	265	Total	C	N	O	S	0	0	1
			1974	1242	347	380	5			
1	D	259	Total	C	N	O	S	0	0	1
			1929	1214	339	371	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	SER	-	expression tag	UNP Q93LQ9
B	25	SER	-	expression tag	UNP Q93LQ9
C	25	SER	-	expression tag	UNP Q93LQ9
D	25	SER	-	expression tag	UNP Q93LQ9

- Molecule 2 is [[(2S)-2-methyl-3-sulfanyl-propanoyl]amino]methylboronic acid (CCD ID: BHU) (formula: C₅H₁₂BNO₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	B	C	N	O	S	0	0
			11	1	5	1	3	1		
2	B	1	Total	B	C	N	O	S	0	0
			11	1	5	1	3	1		
2	C	1	Total	B	C	N	O	S	0	0
			11	1	5	1	3	1		
2	D	1	Total	B	C	N	O	S	0	0
			11	1	5	1	3	1		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 4 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	246	Total	O	0	0
			246	246		
6	B	234	Total	O	0	1
			235	235		
6	C	152	Total	O	0	1
			153	153		
6	D	176	Total	O	0	1
			177	177		

3 Residue-property plots [i](#)

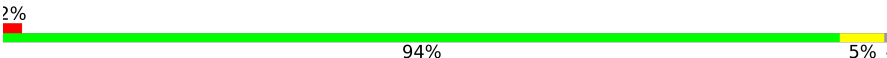
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Serine Beta-Lactamase KPC-2

Chain A: 

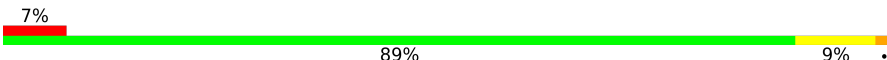


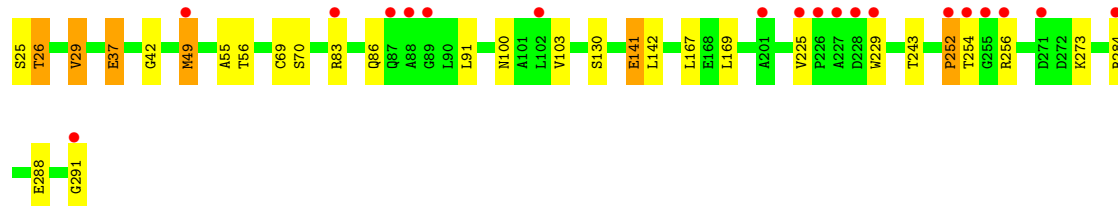
• Molecule 1: Serine Beta-Lactamase KPC-2

Chain B: 

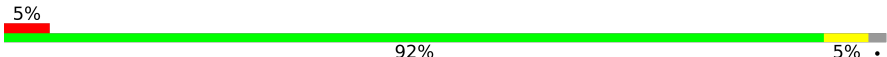


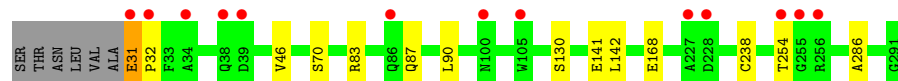
• Molecule 1: Serine Beta-Lactamase KPC-2

Chain C: 



• Molecule 1: Serine Beta-Lactamase KPC-2

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	165.16Å 165.16Å 94.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.68 – 1.79 47.68 – 1.79	Depositor EDS
% Data completeness (in resolution range)	77.0 (47.68-1.79) 71.9 (47.68-1.79)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 1.78Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.170 , 0.205 0.180 , 0.210	Depositor DCC
R_{free} test set	1983 reflections (1.83%)	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8838	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% 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: SO4, BHU, ACY, PEG

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	0/2013	0.63	0/2743
1	B	0.56	0/2001	0.64	0/2726
1	C	0.49	1/2014 (0.0%)	0.63	2/2744 (0.1%)
1	D	0.51	0/1969	0.63	0/2683
All	All	0.52	1/7997 (0.0%)	0.63	2/10896 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	25	SER	CB-OG	5.86	1.53	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	254	THR	N-CA-C	-5.71	95.01	111.00
1	C	252	PRO	CA-C-O	-5.37	115.52	122.13

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	1973	0	1951	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1961	0	1941	12	0
1	C	1974	0	1953	15	0
1	D	1929	0	1900	15	0
2	A	11	0	0	2	0
2	B	11	0	0	3	0
2	C	11	0	0	2	0
2	D	11	0	0	2	0
3	A	49	0	70	2	0
3	B	28	0	40	3	0
3	C	14	0	20	1	0
3	D	21	0	30	2	0
4	A	8	0	6	0	0
4	B	8	0	6	0	0
4	C	4	0	3	0	0
4	D	4	0	3	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
6	A	246	0	0	5	1
6	B	235	0	0	10	3
6	C	153	0	0	2	0
6	D	177	0	0	4	1
All	All	8838	0	7923	61	4

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 (61) 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)
3:B:302:PEG:O1	6:B:401:HOH:O	1.82	0.94
1:B:224:ALA:O	6:B:402:HOH:O	2.02	0.76
1:B:225:VAL:O	6:B:403:HOH:O	2.09	0.71
1:D:254:THR:O	6:D:401:HOH:O	2.08	0.70
1:A:110:GLU:OE2	6:A:401:HOH:O	2.10	0.69
1:D:31:GLU:N	1:D:31:GLU:OE1	2.27	0.67
1:D:168:GLU:OE1	6:D:402:HOH:O	2.13	0.67
1:C:26:THR:CG2	1:C:56:THR:H	2.08	0.66
1:C:49:MET:HG2	1:C:56:THR:HG22	1.81	0.62
3:B:303:PEG:O4	6:B:401:HOH:O	1.73	0.62
1:A:25:SER:N	6:A:405:HOH:O	2.32	0.61
1:B:290:LEU:O	6:B:405:HOH:O	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:GLU:HB2	1:D:32:PRO:HD2	1.81	0.60
3:B:303:PEG:O2	6:B:404:HOH:O	2.16	0.59
1:D:70:SER:OG	2:D:301:BHU:C1	2.52	0.57
1:B:70:SER:OG	2:B:301:BHU:C1	2.52	0.56
1:C:284:ARG:O	1:C:288:GLU:HG2	2.04	0.56
1:D:70:SER:HG	2:D:301:BHU:C1	2.18	0.56
1:A:70:SER:OG	2:A:301:BHU:C1	2.54	0.56
1:C:26:THR:HG23	1:C:56:THR:H	1.71	0.55
1:D:31:GLU:CB	1:D:32:PRO:HD2	2.37	0.55
1:B:27:ASN:N	6:B:407:HOH:O	2.40	0.54
1:B:204:ARG:HD3	6:B:506:HOH:O	2.08	0.54
1:A:70:SER:HG	2:A:301:BHU:C1	2.20	0.54
1:C:37:GLU:HG2	1:C:42:GLY:O	2.08	0.54
1:C:70:SER:OG	2:C:301:BHU:O11	2.26	0.53
1:A:212:LYS:NZ	3:A:306:PEG:O2	2.23	0.53
1:C:26:THR:HG21	1:C:55:ALA:HA	1.91	0.52
1:B:83:ARG:NH1	6:B:408:HOH:O	2.43	0.52
1:A:29:VAL:HG22	6:A:477:HOH:O	2.10	0.52
1:C:70:SER:OG	2:C:301:BHU:C1	2.58	0.52
1:C:291:GLY:N	6:C:405:HOH:O	2.44	0.51
1:A:26:THR:HG22	1:A:27:ASN:H	1.76	0.50
3:D:303:PEG:H31	6:D:545:HOH:O	2.11	0.50
1:A:229:TRP:HZ2	1:D:168:GLU:HG2	1.77	0.48
1:B:70:SER:OG	2:B:301:BHU:O11	2.32	0.48
1:C:229:TRP:CD2	1:C:252:PRO:HB3	2.48	0.48
3:C:302:PEG:H21	6:C:510:HOH:O	2.13	0.48
1:D:31:GLU:HG2	1:D:32:PRO:HD2	1.97	0.47
1:A:29:VAL:HG22	1:A:29:VAL:O	2.15	0.46
1:D:46:VAL:HG11	1:D:286:ALA:HB2	1.97	0.46
1:B:70:SER:OG	2:B:301:BHU:O10	2.35	0.45
1:C:229:TRP:CE3	1:C:252:PRO:HB3	2.50	0.45
1:D:31:GLU:CG	1:D:32:PRO:HD2	2.46	0.45
1:D:31:GLU:HG2	1:D:32:PRO:CD	2.47	0.45
1:D:238:CYS:O	3:D:303:PEG:H22	2.17	0.44
1:A:92:ASP:OD1	6:A:402:HOH:O	2.21	0.44
1:D:87:GLN:HG3	1:D:90:LEU:HB2	2.00	0.44
1:A:111:LYS:NZ	6:A:409:HOH:O	2.43	0.43
1:A:266:ARG:CZ	1:A:266:ARG:HB2	2.48	0.43
1:B:229:TRP:HE3	1:B:250:VAL:CG1	2.32	0.42
1:D:83:ARG:NE	6:D:404:HOH:O	2.27	0.42
1:C:69:CYS:SG	1:C:243:THR:HG22	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:VAL:HG13	1:C:229:TRP:CE3	2.55	0.42
3:A:307:PEG:H11	6:B:424:HOH:O	2.18	0.41
1:C:83:ARG:NH2	1:C:141:GLU:O	2.44	0.41
1:A:169:LEU:HD12	1:A:169:LEU:C	2.46	0.41
1:B:225:VAL:CG1	1:B:229:TRP:HB2	2.50	0.41
1:C:169:LEU:HD12	1:C:169:LEU:C	2.46	0.40
1:B:104:PRO:HB2	1:B:105:TRP:CE3	2.56	0.40
1:A:69:CYS:SG	1:A:243:THR:HG22	2.61	0.40

All (4) 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)
6:B:587:HOH:O	6:B:587:HOH:O[2_545]	1.92	0.28
6:A:417:HOH:O	6:D:474:HOH:O[4_647]	2.07	0.13
6:B:512:HOH:O	6:B:618:HOH:O[3_655]	2.14	0.06
6:B:406:HOH:O	6:B:513:HOH:O[3_655]	2.15	0.05

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	263/265 (99%)	258 (98%)	5 (2%)	0	100	100
1	B	261/265 (98%)	259 (99%)	2 (1%)	0	100	100
1	C	263/265 (99%)	258 (98%)	4 (2%)	1 (0%)	30	16
1	D	257/265 (97%)	254 (99%)	3 (1%)	0	100	100
All	All	1044/1060 (98%)	1029 (99%)	14 (1%)	1 (0%)	48	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	29	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	199/200 (100%)	189 (95%)	10 (5%)	22	5
1	B	198/200 (99%)	196 (99%)	2 (1%)	68	55
1	C	200/200 (100%)	186 (93%)	14 (7%)	14	2
1	D	194/200 (97%)	190 (98%)	4 (2%)	47	27
All	All	791/800 (99%)	761 (96%)	30 (4%)	29	9

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	THR
1	A	29	VAL
1	A	63	GLU
1	A	83	ARG
1	A	86	GLN
1	A	91	LEU
1	A	130	SER
1	A	141	GLU
1	A	142	LEU
1	A	167	LEU
1	B	130	SER
1	B	142	LEU
1	C	26	THR
1	C	29	VAL
1	C	37	GLU
1	C	49	MET
1	C	86	GLN
1	C	91	LEU
1	C	100	ASN
1	C	103	VAL
1	C	130	SER

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Mol	Chain	Res	Type
1	C	141	GLU
1	C	142	LEU
1	C	167	LEU
1	C	256	ARG
1	C	273	LYS
1	D	31	GLU
1	D	130	SER
1	D	141	GLU
1	D	142	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	87	GLN
1	C	27	ASN
1	D	206	GLN
1	D	219	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

28 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	PEG	D	302	-	6,6,6	0.55	0	5,5,5	0.35	0
3	PEG	A	302	-	6,6,6	0.60	0	5,5,5	0.47	0
3	PEG	A	304	-	6,6,6	0.63	0	5,5,5	0.83	0
3	PEG	D	306	-	6,6,6	0.59	0	5,5,5	0.62	0
3	PEG	A	306	-	6,6,6	0.52	0	5,5,5	0.29	0
4	ACY	B	307	-	3,3,3	1.18	0	3,3,3	0.65	0
3	PEG	A	308	-	6,6,6	0.52	0	5,5,5	0.55	0
3	PEG	A	303	-	6,6,6	0.55	0	5,5,5	0.75	0
3	PEG	C	302	-	6,6,6	0.53	0	5,5,5	0.63	0
3	PEG	B	304	-	6,6,6	0.51	0	5,5,5	0.45	0
4	ACY	B	306	-	3,3,3	1.01	0	3,3,3	0.55	0
2	BHU	B	301	-	10,10,10	1.78	2 (20%)	7,12,12	1.68	1 (14%)
3	PEG	A	305	-	6,6,6	0.50	0	5,5,5	0.19	0
3	PEG	C	303	-	6,6,6	0.61	0	5,5,5	1.02	0
4	ACY	A	310	-	3,3,3	0.73	0	3,3,3	1.90	1 (33%)
3	PEG	D	303	-	6,6,6	0.56	0	5,5,5	0.55	0
2	BHU	D	301	-	10,10,10	1.81	2 (20%)	7,12,12	1.91	3 (42%)
2	BHU	A	301	-	10,10,10	1.73	1 (10%)	7,12,12	1.78	1 (14%)
4	ACY	A	309	-	3,3,3	1.33	1 (33%)	3,3,3	0.20	0
3	PEG	B	305	-	6,6,6	0.45	0	5,5,5	0.46	0
2	BHU	C	301	-	10,10,10	1.68	2 (20%)	7,12,12	1.26	1 (14%)
3	PEG	B	302	-	6,6,6	0.45	0	5,5,5	0.61	0
3	PEG	A	307	-	6,6,6	0.45	0	5,5,5	0.63	0
4	ACY	C	305	-	3,3,3	1.01	0	3,3,3	0.51	0
5	SO4	C	304	-	4,4,4	0.29	0	6,6,6	0.41	0
5	SO4	D	304	-	4,4,4	0.14	0	6,6,6	0.41	0
3	PEG	B	303	-	6,6,6	0.52	0	5,5,5	0.42	0
4	ACY	D	305	-	3,3,3	0.85	0	3,3,3	1.29	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
3	PEG	D	302	-	-	3/4/4/4	-
3	PEG	A	302	-	-	1/4/4/4	-
3	PEG	A	304	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	D	306	-	-	2/4/4/4	-
3	PEG	A	306	-	-	2/4/4/4	-
3	PEG	A	308	-	-	0/4/4/4	-
3	PEG	A	303	-	-	1/4/4/4	-
3	PEG	C	302	-	-	0/4/4/4	-
3	PEG	B	304	-	-	1/4/4/4	-
2	BHU	B	301	-	-	2/8/11/11	-
3	PEG	A	305	-	-	1/4/4/4	-
3	PEG	C	303	-	-	2/4/4/4	-
3	PEG	D	303	-	-	0/4/4/4	-
2	BHU	D	301	-	-	0/8/11/11	-
2	BHU	A	301	-	-	0/8/11/11	-
3	PEG	B	305	-	-	2/4/4/4	-
2	BHU	C	301	-	-	2/8/11/11	-
3	PEG	B	302	-	-	1/4/4/4	-
3	PEG	A	307	-	-	2/4/4/4	-
3	PEG	B	303	-	-	1/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	BHU	C3-N2	4.79	1.44	1.33
2	C	301	BHU	C3-N2	4.54	1.44	1.33
2	B	301	BHU	C3-N2	4.34	1.43	1.33
2	D	301	BHU	C3-N2	4.27	1.43	1.33
2	B	301	BHU	O4-C3	-3.12	1.17	1.23
2	D	301	BHU	C1-N2	-2.35	1.42	1.45
2	C	301	BHU	O4-C3	-2.29	1.19	1.23
4	A	309	ACY	OXT-C	-2.25	1.20	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	BHU	C8-C5-C3	-3.88	102.51	109.64
2	A	301	BHU	C5-C6-S7	-3.63	109.34	114.04
2	D	301	BHU	C5-C3-N2	-3.39	112.29	116.68
2	D	301	BHU	O4-C3-C5	2.66	126.41	121.51
4	A	310	ACY	O-C-CH3	-2.61	111.83	122.53
2	C	301	BHU	C8-C5-C3	-2.29	105.42	109.64
2	D	301	BHU	C8-C5-C3	-2.13	105.72	109.64

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	BHU	C3-C5-C6-S7
2	B	301	BHU	C8-C5-C6-S7
2	C	301	BHU	C3-C5-C6-S7
3	A	305	PEG	O2-C3-C4-O4
3	D	302	PEG	O1-C1-C2-O2
3	D	302	PEG	O2-C3-C4-O4
3	B	304	PEG	O2-C3-C4-O4
3	A	306	PEG	O2-C3-C4-O4
3	B	303	PEG	O2-C3-C4-O4
3	B	305	PEG	O2-C3-C4-O4
3	A	302	PEG	O1-C1-C2-O2
3	B	305	PEG	O1-C1-C2-O2
3	C	303	PEG	O1-C1-C2-O2
3	B	302	PEG	O2-C3-C4-O4
3	D	306	PEG	O1-C1-C2-O2
3	A	304	PEG	C4-C3-O2-C2
3	C	303	PEG	C1-C2-O2-C3
3	A	307	PEG	C1-C2-O2-C3
3	D	302	PEG	C1-C2-O2-C3
3	A	304	PEG	O1-C1-C2-O2
3	A	307	PEG	C4-C3-O2-C2
3	A	303	PEG	O1-C1-C2-O2
3	D	306	PEG	C1-C2-O2-C3
2	C	301	BHU	C8-C5-C6-S7
3	A	306	PEG	C1-C2-O2-C3

There are no ring outliers.

10 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	306	PEG	1	0
3	C	302	PEG	1	0
2	B	301	BHU	3	0
3	D	303	PEG	2	0
2	D	301	BHU	2	0
2	A	301	BHU	2	0
2	C	301	BHU	2	0
3	B	302	PEG	1	0
3	A	307	PEG	1	0
3	B	303	PEG	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 ⓘ

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	265/265 (100%)	-0.25	1 (0%) 88 92	10, 16, 33, 52	0
1	B	263/265 (99%)	-0.37	4 (1%) 72 78	8, 14, 33, 48	0
1	C	265/265 (100%)	0.56	19 (7%) 21 26	16, 26, 51, 85	0
1	D	259/265 (97%)	0.05	13 (5%) 34 40	11, 18, 47, 96	0
All	All	1052/1060 (99%)	-0.00	37 (3%) 47 53	8, 19, 44, 96	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	254	THR	7.9
1	C	229	TRP	5.9
1	C	252	PRO	5.8
1	D	31	GLU	5.1
1	C	227	ALA	5.1
1	B	291	GLY	4.9
1	C	255	GLY	4.2
1	C	228	ASP	4.2
1	D	32	PRO	4.1
1	C	225	VAL	4.0
1	D	255	GLY	4.0
1	D	34	ALA	3.9
1	C	226	PRO	3.8
1	C	256	ARG	3.5
1	D	254	THR	3.5
1	D	105	TRP	3.2
1	D	100	ASN	3.0
1	A	26	THR	3.0
1	C	49	MET	3.0
1	D	39	ASP	2.9
1	C	89	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	88	ALA	2.7
1	C	284	ARG	2.7
1	D	256	ARG	2.6
1	D	227	ALA	2.6
1	C	271	ASP	2.5
1	D	86	GLN	2.4
1	C	83	ARG	2.4
1	C	291	GLY	2.3
1	C	201	ALA	2.3
1	C	102	LEU	2.3
1	D	228	ASP	2.3
1	B	254	THR	2.2
1	D	38	GLN	2.2
1	C	87	GLN	2.2
1	B	228	ASP	2.1
1	B	227	ALA	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 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
3	PEG	C	303	7/7	0.76	0.21	31,34,42,46	0
3	PEG	D	303	7/7	0.77	0.15	33,39,47,48	0
3	PEG	A	308	7/7	0.78	0.15	36,36,43,45	0
3	PEG	B	305	7/7	0.79	0.15	37,40,44,46	0
3	PEG	C	302	7/7	0.80	0.13	38,39,41,42	0
3	PEG	D	306	7/7	0.81	0.15	29,37,43,45	0
4	ACY	A	310	4/4	0.81	0.19	13,25,25,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PEG	A	306	7/7	0.83	0.14	36,39,46,49	0
3	PEG	B	304	7/7	0.84	0.13	34,35,45,46	0
3	PEG	D	302	7/7	0.85	0.15	32,37,50,52	0
2	BHU	D	301	11/11	0.85	0.14	15,31,45,45	0
3	PEG	A	305	7/7	0.86	0.12	36,39,45,48	0
2	BHU	B	301	11/11	0.86	0.12	16,22,36,46	0
3	PEG	A	307	7/7	0.86	0.13	31,34,44,46	0
3	PEG	A	304	7/7	0.86	0.12	24,30,33,42	0
4	ACY	B	307	4/4	0.86	0.16	16,22,25,27	0
3	PEG	B	303	7/7	0.87	0.12	31,39,40,44	0
2	BHU	A	301	11/11	0.87	0.12	14,24,33,55	0
2	BHU	C	301	11/11	0.88	0.12	24,32,41,52	0
3	PEG	A	303	7/7	0.89	0.09	16,19,22,27	0
3	PEG	B	302	7/7	0.90	0.10	25,39,41,41	0
3	PEG	A	302	7/7	0.91	0.10	16,18,25,27	0
4	ACY	D	305	4/4	0.91	0.12	14,27,29,30	0
4	ACY	B	306	4/4	0.93	0.15	9,16,26,36	0
5	SO4	D	304	5/5	0.93	0.07	36,37,51,56	0
4	ACY	A	309	4/4	0.94	0.08	18,21,22,28	0
4	ACY	C	305	4/4	0.95	0.09	19,27,29,31	0
5	SO4	C	304	5/5	0.96	0.10	26,33,35,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.