



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2022 – 12:24 pm GMT

PDB ID : 5EV8
Title : Crystal structure of the metallo-beta-lactamase IMP-1 in complex with the bithiazolidine inhibitor D-CS319
Authors : Hinchliffe, P.; Spencer, J.
Deposited on : 2015-11-19
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

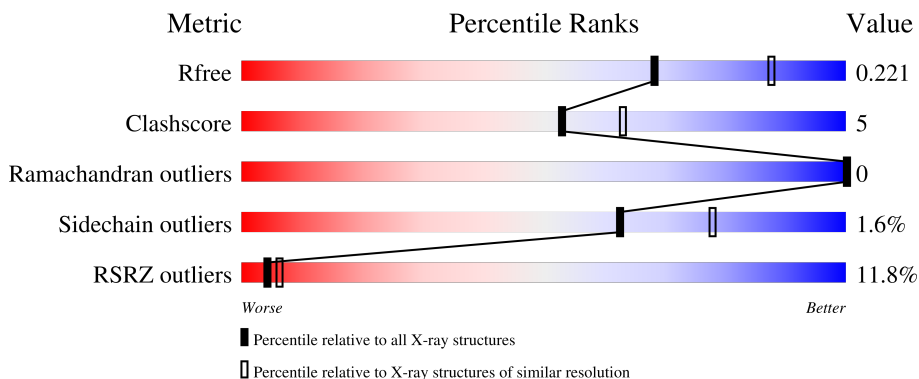
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	230	
1	B	230	
1	C	230	
1	D	230	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7320 atoms, of which 42 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 IMP-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	219	Total 1717	C 1113	N 282	O 321	S 1	0	1	0
1	B	219	Total 1717	C 1113	N 282	O 321	S 1	0	1	0
1	C	223	Total 1743	C 1130	N 288	O 324	S 1	0	0	0
1	D	218	Total 1711	C 1110	N 281	O 319	S 1	0	1	0

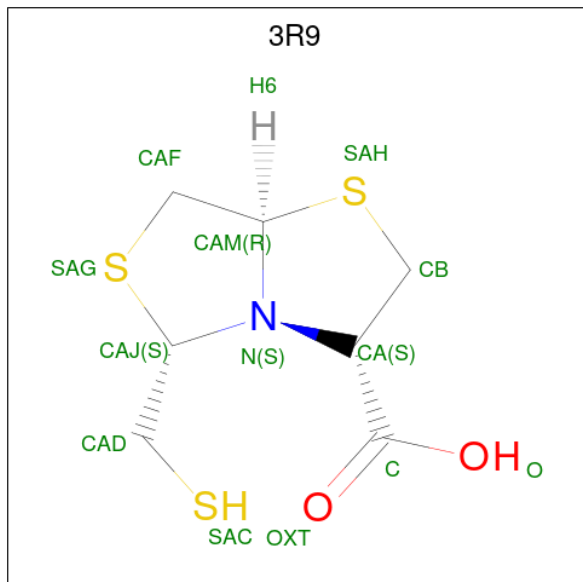
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P52699
A	0	PRO	-	expression tag	UNP P52699
B	-1	GLY	-	expression tag	UNP P52699
B	0	PRO	-	expression tag	UNP P52699
C	-1	GLY	-	expression tag	UNP P52699
C	0	PRO	-	expression tag	UNP P52699
D	-1	GLY	-	expression tag	UNP P52699
D	0	PRO	-	expression tag	UNP P52699

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Zn 2	0	0
2	B	2	Total 2	Zn 2	0	0
2	C	2	Total 2	Zn 2	0	0
2	D	2	Total 2	Zn 2	0	0

- Molecule 3 is (3S,5S,7aR)-5-(sulfanylmethyl)tetrahydro[1,3]thiazolo[4,3-b][1,3]thiazole-3-carboxylic acid (three-letter code: 3R9) (formula: $C_7H_{11}NO_2S_3$).



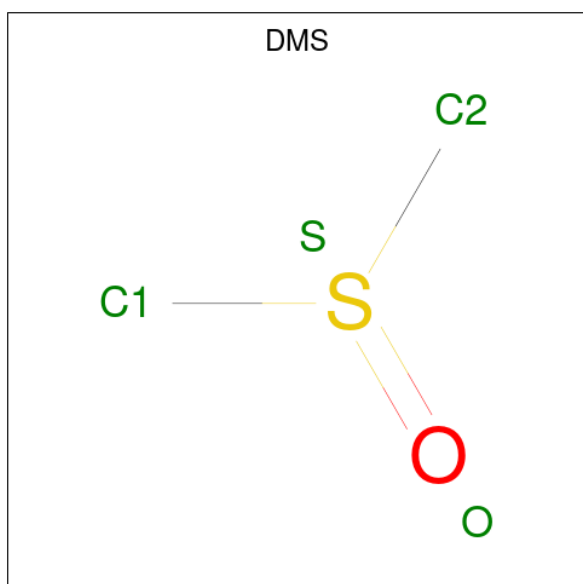
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			13	7	1	2	3		
3	A	1	Total	C	N	O	S	0	0
			13	7	1	2	3		
3	B	1	Total	C	N	O	S	0	0
			13	7	1	2	3		
3	C	1	Total	C	N	O	S	0	0
			13	7	1	2	3		
3	D	1	Total	C	N	O	S	0	0
			13	7	1	2	3		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



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

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Na	0	0
			1	1		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Cl	0	0
			1	1		

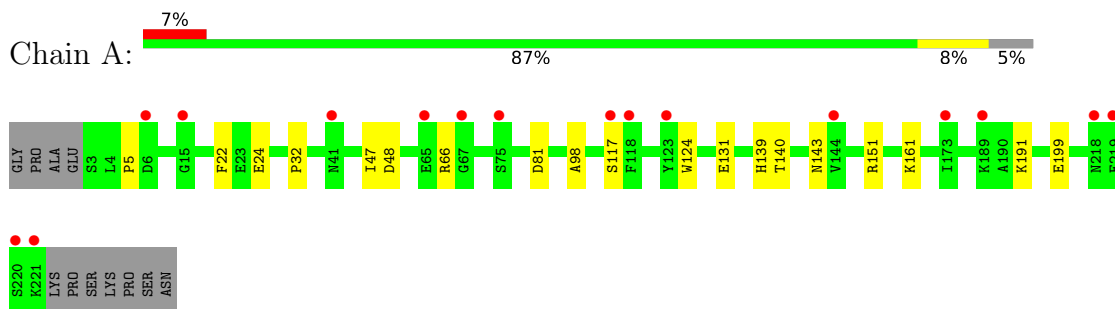
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	80	Total	O	0	0
			80	80		
8	B	87	Total	O	0	0
			87	87		
8	C	93	Total	O	0	0
			93	93		
8	D	27	Total	O	0	0
			27	27		

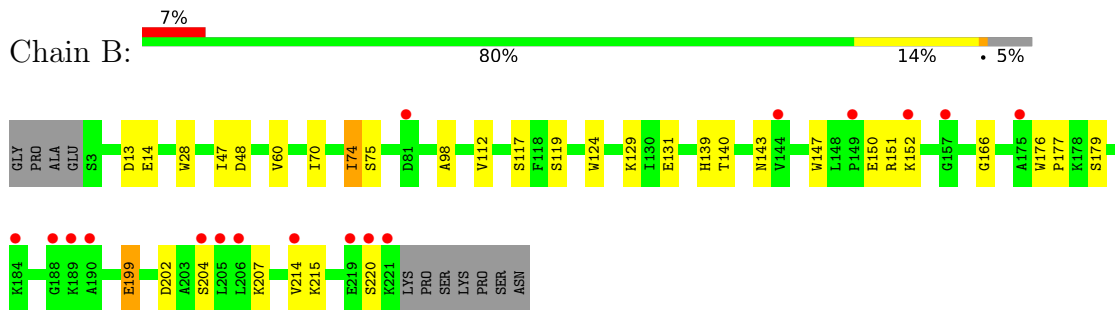
3 Residue-property plots

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.

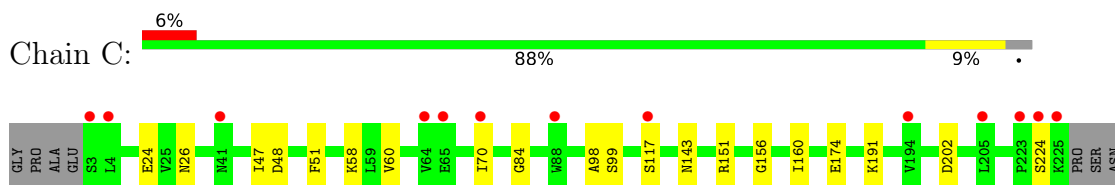
- Molecule 1: Beta-lactamase IMP-1



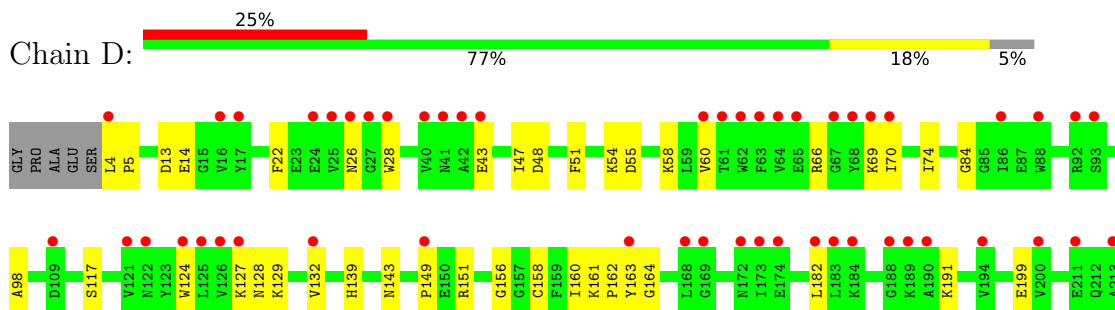
- Molecule 1: Beta-lactamase IMP-1



- Molecule 1: Beta-lactamase IMP-1



- Molecule 1: Beta-lactamase IMP-1



V214	LYS
K215	PRO
G216	SER
L217	LYS
N218	PRO
E219	SER
S220	ASN
K221	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.56Å 77.71Å 261.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.24 – 2.30 37.24 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (37.24-2.30) 99.9 (37.24-2.30)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.178 , 0.220 0.179 , 0.221	Depositor DCC
R_{free} test set	2206 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7320	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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: ZN, DMS, 3R9, NA, EDO, 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	0.47	0/1764	0.56	0/2394
1	B	0.49	0/1764	0.59	0/2394
1	C	0.46	0/1788	0.57	0/2425
1	D	0.40	0/1758	0.55	0/2386
All	All	0.45	0/7074	0.57	0/9599

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1717	0	1727	13	0
1	B	1717	0	1727	21	0
1	C	1743	0	1761	14	0
1	D	1711	0	1722	32	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	26	0	18	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	13	0	9	0	0
3	C	13	0	9	0	0
3	D	13	0	9	0	0
4	B	12	18	18	1	0
4	C	4	6	6	0	0
4	D	4	6	6	0	0
5	B	4	6	6	0	0
5	C	4	6	6	2	0
6	C	1	0	0	0	0
7	C	1	0	0	0	0
8	A	80	0	0	1	0
8	B	87	0	0	3	0
8	C	93	0	0	4	0
8	D	27	0	0	1	0
All	All	7278	42	7024	76	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 5.

All (76) 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:D:60:VAL:HG13	1:D:70:ILE:HG13	1.62	0.82
1:D:124:TRP:HZ3	1:D:127:LYS:HE3	1.46	0.81
1:D:124:TRP:CE3	1:D:127:LYS:HG3	2.17	0.79
1:C:174:GLU:OE1	8:C:401:HOH:O	2.00	0.79
1:B:124:TRP:CZ3	1:B:131:GLU:HB2	2.21	0.75
1:C:60:VAL:HG13	1:C:70:ILE:HG13	1.74	0.70
1:D:124:TRP:CZ3	1:D:127:LYS:HE3	2.29	0.67
1:A:124:TRP:CZ3	1:A:131:GLU:HB2	2.32	0.65
1:B:28:TRP:HH2	1:B:166:GLY:HA2	1.63	0.64
1:C:202:ASP:HB2	8:C:417:HOH:O	1.97	0.63
1:C:58:LYS:NZ	8:C:402:HOH:O	2.27	0.63
1:D:124:TRP:HE3	1:D:127:LYS:HG3	1.61	0.63
1:A:32:PRO:HG3	1:D:163:TYR:CZ	2.35	0.62
1:B:112:VAL:HB	4:B:304:EDO:H12	1.83	0.61
1:B:28:TRP:CH2	1:B:166:GLY:HA2	2.37	0.59
1:C:174:GLU:HG2	8:C:474:HOH:O	2.01	0.58
1:D:151:ARG:O	1:D:191:LYS:HE2	2.03	0.58
1:D:74:ILE:CD1	1:D:132:VAL:HG21	2.34	0.58
1:B:129:LYS:HE3	1:B:150:GLU:OE1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ARG:O	1:A:191:LYS:HE2	2.05	0.56
1:A:24:GLU:HG3	1:D:28:TRP:HE3	1.72	0.54
1:A:24:GLU:HG3	1:D:28:TRP:CE3	2.43	0.54
1:D:161:LYS:HB3	1:D:164:GLY:O	2.08	0.53
1:B:204:SER:O	1:B:207:LYS:HB3	2.09	0.52
1:A:47:ILE:O	1:A:48:ASP:HB2	2.10	0.52
1:C:99:SER:HB2	5:C:305:DMS:C2	2.40	0.51
1:D:55:ASP:HA	1:D:58:LYS:HD3	1.93	0.51
1:A:32:PRO:HG3	1:D:163:TYR:CE1	2.46	0.50
1:A:98:ALA:O	1:A:117:SER:HA	2.10	0.50
1:B:202:ASP:HB2	8:B:431:HOH:O	2.12	0.49
1:B:98:ALA:O	1:B:117:SER:HA	2.12	0.49
1:D:43:GLU:OE2	1:D:69:LYS:HD3	2.12	0.49
1:D:160:ILE:HG22	1:D:162:PRO:HD3	1.94	0.49
1:D:127:LYS:HG2	1:D:128:ASN:OD1	2.13	0.49
1:B:13:ASP:OD2	1:B:151:ARG:HD2	2.13	0.49
8:A:471:HOH:O	1:C:26:ASN:HB3	2.13	0.48
1:D:124:TRP:CZ3	1:D:127:LYS:HG3	2.47	0.48
1:C:156:GLY:HA3	1:C:160:ILE:CG1	2.44	0.48
1:B:14:GLU:HB2	1:B:151:ARG:HH21	1.79	0.48
1:B:47:ILE:O	1:B:48:ASP:HB2	2.13	0.48
1:A:139:HIS:CD2	1:A:140:THR:HG23	2.49	0.48
1:D:13:ASP:OD1	1:D:14:GLU:N	2.40	0.47
1:D:74:ILE:HD13	1:D:132:VAL:HG21	1.95	0.47
1:B:176:TRP:HB3	1:B:177:PRO:HD3	1.97	0.46
1:D:4:LEU:HA	1:D:5:PRO:HD3	1.81	0.46
1:B:139:HIS:CD2	1:B:140:THR:HG23	2.52	0.45
1:D:139:HIS:CD2	1:D:158:CYS:HB2	2.51	0.45
1:B:60:VAL:HG13	1:B:70:ILE:HG13	1.98	0.45
1:B:179:SER:N	8:B:403:HOH:O	2.49	0.45
1:D:47:ILE:O	1:D:48:ASP:HB2	2.16	0.45
1:D:51:PHE:O	1:D:84:GLY:HA3	2.17	0.45
1:C:51:PHE:O	1:C:84:GLY:HA3	2.18	0.44
1:C:98:ALA:O	1:C:117:SER:HA	2.17	0.44
1:B:199:GLU:H	1:B:199:GLU:CD	2.21	0.44
1:D:26:ASN:OD1	1:D:26:ASN:N	2.50	0.44
1:D:156:GLY:HA3	1:D:160:ILE:HG12	1.99	0.44
1:C:151:ARG:O	1:C:191:LYS:HE2	2.18	0.43
1:D:66:ARG:HH11	1:D:66:ARG:HG3	1.83	0.43
1:C:47:ILE:O	1:C:48:ASP:HB2	2.17	0.43
1:D:199:GLU:OE2	8:D:401:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ARG:HH11	1:A:66:ARG:HG3	1.83	0.43
1:B:119:SER:O	8:B:401:HOH:O	2.21	0.43
1:C:156:GLY:HA3	1:C:160:ILE:HG12	2.00	0.42
1:A:66:ARG:HG3	1:A:66:ARG:NH1	2.34	0.42
1:A:161:LYS:HZ3	3:A:303:3R9:C	2.27	0.42
1:D:54:LYS:O	1:D:58:LYS:HG3	2.21	0.41
1:D:98:ALA:O	1:D:117:SER:HA	2.20	0.41
1:B:74:ILE:HG13	1:B:75:SER:N	2.35	0.41
1:B:14:GLU:CB	1:B:151:ARG:HH21	2.34	0.41
1:B:214:VAL:HG23	1:B:215:LYS:N	2.36	0.41
1:C:99:SER:HB2	5:C:305:DMS:H22	2.03	0.41
1:D:156:GLY:HA3	1:D:160:ILE:CG1	2.51	0.40
1:D:4:LEU:HD13	1:D:22:PHE:O	2.21	0.40
1:D:129:LYS:O	1:D:149:PRO:HD2	2.21	0.40
1:B:147:TRP:CH2	1:B:152:LYS:HA	2.56	0.40
1:A:5:PRO:HB2	1:A:22:PHE:CD1	2.56	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	218/230 (95%)	212 (97%)	6 (3%)	0	100	100
1	B	218/230 (95%)	214 (98%)	4 (2%)	0	100	100
1	C	221/230 (96%)	216 (98%)	5 (2%)	0	100	100
1	D	217/230 (94%)	212 (98%)	5 (2%)	0	100	100
All	All	874/920 (95%)	854 (98%)	20 (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	189/197 (96%)	185 (98%)	4 (2%)	53	70
1	B	189/197 (96%)	185 (98%)	4 (2%)	53	70
1	C	192/197 (98%)	189 (98%)	3 (2%)	62	78
1	D	188/197 (95%)	186 (99%)	2 (1%)	73	86
All	All	758/788 (96%)	745 (98%)	13 (2%)	62	76

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81[A]	ASP
1	A	81[B]	ASP
1	A	143	ASN
1	A	199	GLU
1	B	74	ILE
1	B	143	ASN
1	B	199	GLU
1	B	220	SER
1	C	24	GLU
1	C	143	ASN
1	C	224	SER
1	D	143	ASN
1	D	182	LEU

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](#)

Of 22 ligands modelled in this entry, 10 are monoatomic - leaving 12 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
3	3R9	D	303	2	8,14,14	1.10	0	6,20,20	3.20	3 (50%)
3	3R9	A	304	-	8,14,14	2.16	4 (50%)	6,20,20	3.65	2 (33%)
4	EDO	B	305	-	3,3,3	0.51	0	2,2,2	0.33	0
5	DMS	C	305	-	3,3,3	0.65	0	3,3,3	0.74	0
4	EDO	B	304	-	3,3,3	0.47	0	2,2,2	0.33	0
4	EDO	B	306	-	3,3,3	1.25	0	2,2,2	0.46	0
5	DMS	B	307	-	3,3,3	0.61	0	3,3,3	0.91	0
3	3R9	A	303	2	8,14,14	1.06	0	6,20,20	3.23	2 (33%)
3	3R9	B	303	2	8,14,14	1.13	0	6,20,20	3.68	2 (33%)
3	3R9	C	303	2	8,14,14	2.47	2 (25%)	6,20,20	3.40	3 (50%)
4	EDO	D	304	-	3,3,3	0.50	0	2,2,2	0.26	0
4	EDO	C	304	-	3,3,3	0.50	0	2,2,2	0.22	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	3R9	D	303	2	-	0/0/28/28	0/2/2/2
3	3R9	A	304	-	-	0/0/28/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	305	-	-	1/1/1/1	-
4	EDO	B	304	-	-	1/1/1/1	-
4	EDO	B	306	-	-	1/1/1/1	-
3	3R9	A	303	2	-	0/0/28/28	0/2/2/2
3	3R9	B	303	2	-	0/0/28/28	0/2/2/2
3	3R9	C	303	2	-	0/0/28/28	0/2/2/2
4	EDO	D	304	-	-	0/1/1/1	-
4	EDO	C	304	-	-	1/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	303	3R9	CAJ-SAG	5.21	1.94	1.84
3	C	303	3R9	CAF-CAM	4.25	1.56	1.51
3	A	304	3R9	CA-N	-3.96	1.43	1.48
3	A	304	3R9	CAF-SAG	-2.78	1.72	1.81
3	A	304	3R9	CAD-SAC	2.40	1.86	1.81
3	A	304	3R9	CB-CA	-2.35	1.49	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	304	3R9	CAM-CAF-SAG	8.02	107.28	103.59
3	C	303	3R9	CAM-CAF-SAG	6.69	106.67	103.59
3	D	303	3R9	CAM-CAF-SAG	6.24	106.46	103.59
3	B	303	3R9	CAM-CAF-SAG	5.99	106.34	103.59
3	B	303	3R9	CAJ-CAD-SAC	-5.96	107.48	114.24
3	A	303	3R9	CAJ-CAD-SAC	-5.31	108.23	114.24
3	A	303	3R9	CAM-CAF-SAG	5.15	105.96	103.59
3	D	303	3R9	CAJ-CAD-SAC	-3.85	109.88	114.24
3	C	303	3R9	CAJ-CAD-SAC	-3.77	109.97	114.24
3	C	303	3R9	CA-CB-SAH	2.53	108.73	105.11
3	D	303	3R9	CB-SAH-CAM	2.36	94.67	90.61
3	A	304	3R9	CAF-SAG-CAJ	2.25	94.47	90.61

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	306	EDO	O1-C1-C2-O2
4	B	304	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	B	305	EDO	O1-C1-C2-O2
4	C	304	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	305	DMS	2	0
4	B	304	EDO	1	0
3	A	303	3R9	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	219/230 (95%)	0.64	16 (7%) 15 20	22, 37, 56, 81	0
1	B	219/230 (95%)	0.70	17 (7%) 13 17	18, 35, 63, 85	0
1	C	223/230 (96%)	0.50	13 (5%) 23 29	20, 36, 55, 79	0
1	D	218/230 (94%)	1.59	58 (26%) 0 0	38, 57, 82, 94	0
All	All	879/920 (95%)	0.85	104 (11%) 4 6	18, 41, 72, 94	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	26	ASN	8.2
1	C	3	SER	7.7
1	D	41	ASN	7.6
1	D	218	ASN	6.9
1	D	220	SER	6.6
1	C	225	LYS	6.5
1	D	70	ILE	6.4
1	D	221	LYS	6.2
1	D	217	LEU	6.1
1	D	189	LYS	5.9
1	D	188	GLY	5.2
1	D	60	VAL	4.9
1	C	223	PRO	4.6
1	D	4	LEU	4.6
1	D	200	VAL	4.5
1	B	221	LYS	4.4
1	D	43	GLU	4.3
1	D	173	ILE	4.3
1	D	86	ILE	4.2
1	D	124	TRP	4.2
1	D	28	TRP	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	41	ASN	4.1
1	D	172	ASN	4.1
1	D	64	VAL	4.0
1	D	65	GLU	3.9
1	B	188	GLY	3.8
1	D	68	TYR	3.7
1	C	64	VAL	3.7
1	B	189	LYS	3.6
1	D	62	TRP	3.6
1	D	215	LYS	3.6
1	B	204	SER	3.5
1	D	92	ARG	3.5
1	A	6	ASP	3.5
1	D	40	VAL	3.4
1	B	214	VAL	3.3
1	D	168	LEU	3.3
1	D	42	ALA	3.2
1	B	219	GLU	3.1
1	D	27	GLY	3.1
1	D	184	LYS	3.1
1	D	25	VAL	3.0
1	D	17	TYR	3.0
1	A	67	GLY	3.0
1	D	127	LYS	3.0
1	D	93	SER	3.0
1	D	88	TRP	2.9
1	A	218	ASN	2.9
1	C	4	LEU	2.9
1	A	15	GLY	2.9
1	D	69	LYS	2.8
1	D	174	GLU	2.8
1	D	149	PRO	2.7
1	A	189	LYS	2.7
1	D	67	GLY	2.7
1	C	88	TRP	2.7
1	D	211	GLU	2.7
1	D	219	GLU	2.7
1	B	152	LYS	2.7
1	A	173	ILE	2.7
1	D	213	ALA	2.7
1	D	194	VAL	2.6
1	C	70	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	122	ASN	2.6
1	D	125	LEU	2.6
1	D	214	VAL	2.6
1	B	81[A]	ASP	2.5
1	A	219	GLU	2.5
1	D	163	TYR	2.5
1	D	63	PHE	2.5
1	B	205	LEU	2.5
1	B	190	ALA	2.4
1	D	24	GLU	2.4
1	D	169	GLY	2.4
1	B	206	LEU	2.4
1	D	16	VAL	2.4
1	D	61	THR	2.4
1	D	182	LEU	2.4
1	B	149	PRO	2.4
1	B	220	SER	2.4
1	C	117	SER	2.3
1	D	126	VAL	2.3
1	B	175	ALA	2.3
1	A	220	SER	2.3
1	C	224	SER	2.3
1	A	123	TYR	2.3
1	A	118	PHE	2.3
1	D	132	VAL	2.2
1	D	183	LEU	2.2
1	B	157	GLY	2.2
1	A	75	SER	2.2
1	C	194	VAL	2.2
1	C	65	GLU	2.1
1	B	144	VAL	2.1
1	D	190	ALA	2.1
1	C	205	LEU	2.1
1	B	184	LYS	2.1
1	C	41	ASN	2.0
1	A	117	SER	2.0
1	D	109	ASP	2.0
1	A	144	VAL	2.0
1	D	121	VAL	2.0
1	A	65	GLU	2.0
1	A	221	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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(\AA^2)	Q<0.9
4	EDO	C	304	4/4	0.67	0.23	46,55,62,73	0
4	EDO	D	304	4/4	0.68	0.28	57,69,72,80	0
4	EDO	B	306	4/4	0.83	0.16	40,50,65,69	0
3	3R9	D	303	13/13	0.84	0.20	45,54,61,64	13
4	EDO	B	305	4/4	0.87	0.19	38,46,56,58	0
5	DMS	B	307	4/4	0.87	0.39	48,58,74,74	0
3	3R9	A	304	13/13	0.89	0.18	36,44,49,55	12
3	3R9	B	303	13/13	0.91	0.17	37,45,58,59	0
4	EDO	B	304	4/4	0.92	0.16	26,36,48,48	0
5	DMS	C	305	4/4	0.92	0.22	45,54,59,61	0
3	3R9	A	303	13/13	0.94	0.19	29,42,50,54	13
3	3R9	C	303	13/13	0.94	0.15	24,29,34,37	0
7	CL	C	307	1/1	0.94	0.18	53,53,53,53	0
6	NA	C	306	1/1	0.96	0.49	53,53,53,53	0
2	ZN	D	302	1/1	0.96	0.10	49,49,49,49	0
2	ZN	D	301	1/1	0.97	0.09	42,42,42,42	0
2	ZN	A	302	1/1	0.98	0.12	46,46,46,46	0
2	ZN	B	301	1/1	0.99	0.12	48,48,48,48	0
2	ZN	A	301	1/1	1.00	0.10	28,28,28,28	0
2	ZN	B	302	1/1	1.00	0.10	30,30,30,30	0
2	ZN	C	301	1/1	1.00	0.10	23,23,23,23	0
2	ZN	C	302	1/1	1.00	0.09	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.