



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 07:51 AM EDT

PDB ID : 6OGO / pdb_00006ogo
Title : Crystal structure of NDM-9 metallo-beta-lactamase
Authors : Raczynska, J.E.; Imiolczyk, B.; Jaskolski, M.
Deposited on : 2019-04-03
Resolution : 1.43 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

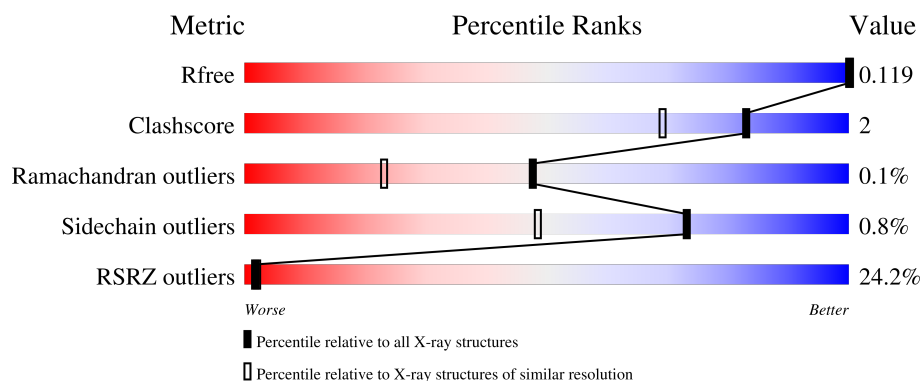
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.43 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	3234 (1.46-1.42)
Clashscore	190562	3289 (1.46-1.42)
Ramachandran outliers	187476	3248 (1.46-1.42)
Sidechain outliers	187428	3248 (1.46-1.42)
RSRZ outliers	180081	3234 (1.46-1.42)

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	243	16% 87% 7% 6%
1	B	243	26% 90% • 6%
1	C	243	26% 86% 7% 7%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6046 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 SUBCLASS B1 METALLO-BETA-LACTAMASE NDM-9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	9	0
			1746	1104	308	325	9			
1	B	229	Total	C	N	O	S	0	3	0
			1717	1084	304	321	8			
1	C	227	Total	C	N	O	S	0	5	0
			1706	1078	299	320	9			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	GLY	-	expression tag	UNP A0A1M2CSI6
B	28	GLY	-	expression tag	UNP A0A1M2CSI6
C	28	GLY	-	expression tag	UNP A0A1M2CSI6

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

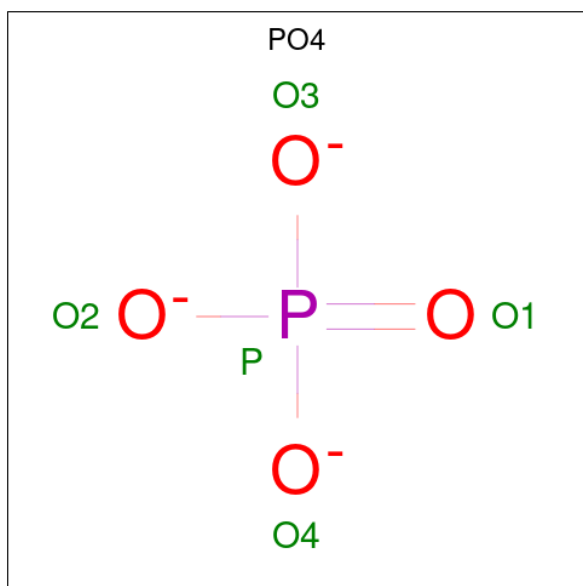
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Cl	0	0
			3	3		
3	B	3	Total	Cl	0	0
			3	3		

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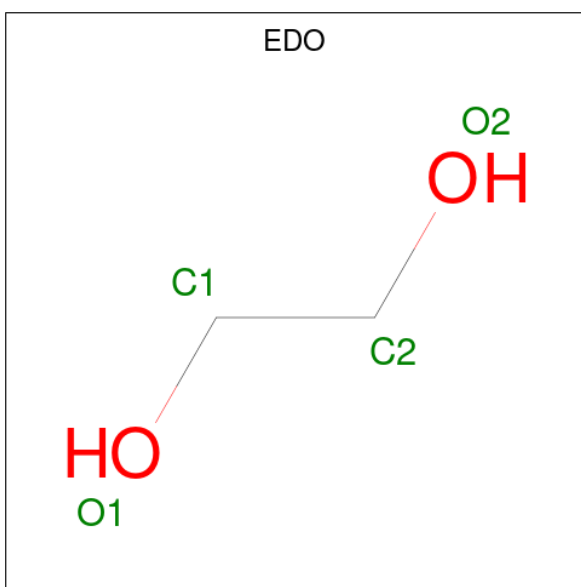
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	3	Total	Cl	0	0
			3	3		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



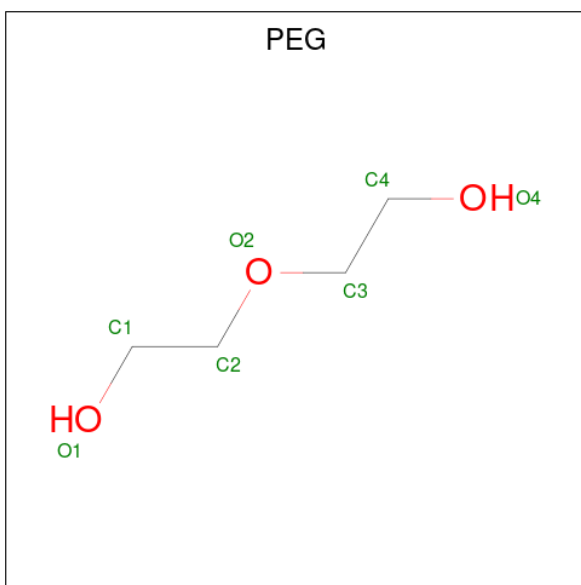
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



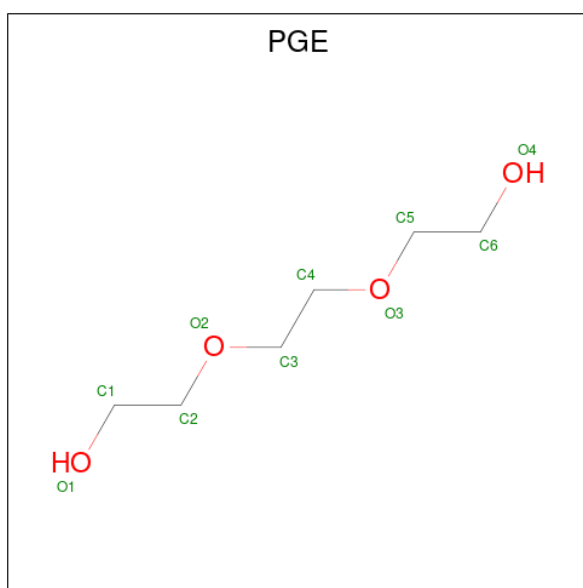
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



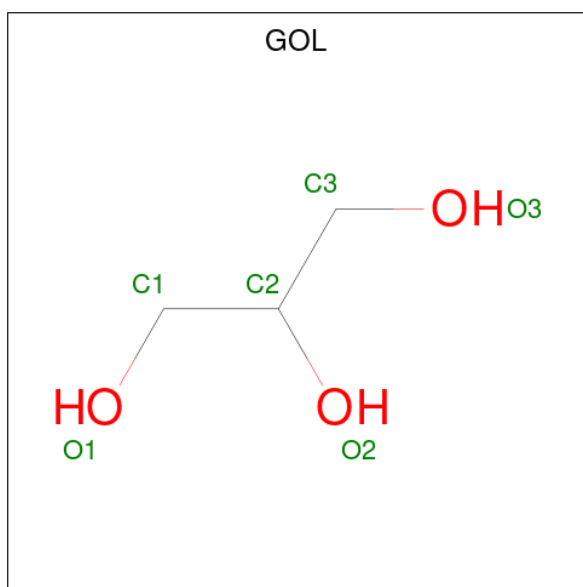
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			6	4	2		
6	B	1	Total	C	O	0	0
			6	4	2		
6	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			10	6	4		
7	C	1	Total	C	O	0	0
			5	3	2		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		

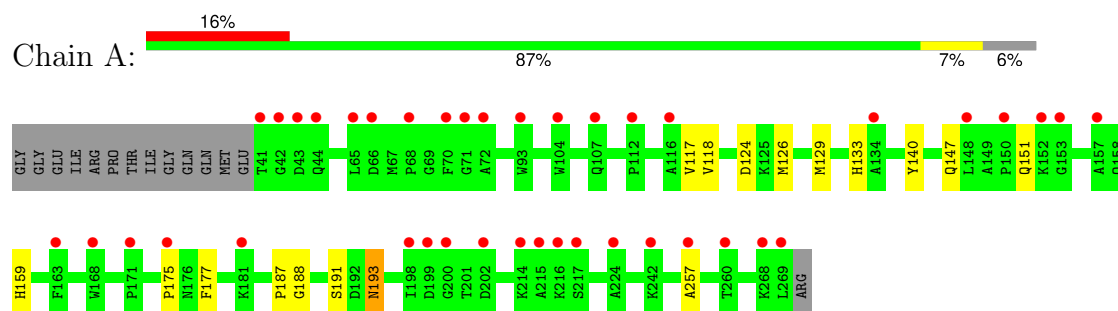
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	272	Total	O	0	3
			272	272		
9	B	273	Total	O	0	0
			273	273		
9	C	233	Total	O	0	0
			233	233		

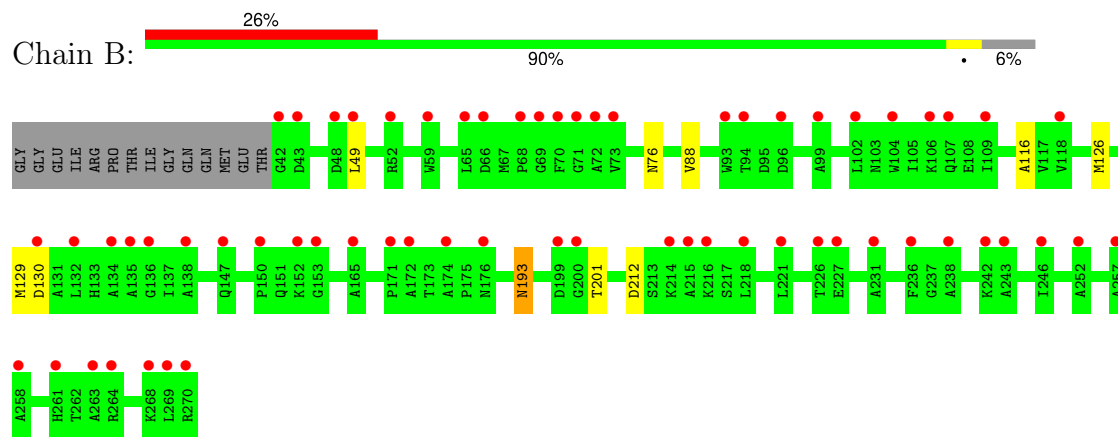
3 Residue-property plots [i](#)

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.

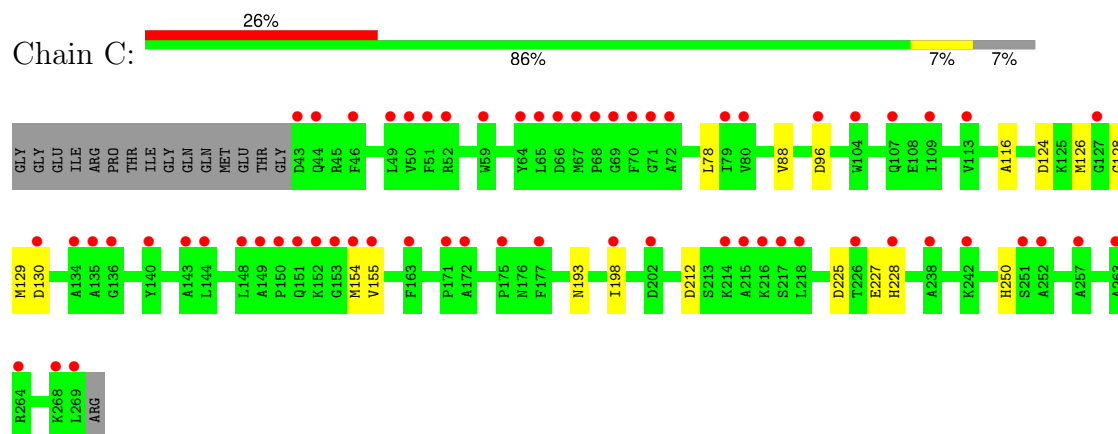
• Molecule 1: SUBCLASS B1 METALLO-BETA-LACTAMASE NDM-9



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4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	122.93Å 122.93Å 38.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	61.46 – 1.43 61.46 – 1.43	Depositor EDS
% Data completeness (in resolution range)	99.8 (61.46-1.43) 99.9 (61.46-1.43)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 1.43Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.074 , 0.116 0.079 , 0.119	Depositor DCC
R_{free} test set	3004 reflections (2.49%)	wwPDB-VP
Wilson B-factor (Å ²)	14.7	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	0.437 for -h,-k,l 0.185 for h,-h-k,-l 0.177 for -k,-h,-l	Xtriage
Reported twinning fraction	0.398 for H, K, L 0.010 for K, H, -L 0.500 for -h,-k,l 0.091 for -K, -H, -L	Depositor
Outliers	0 of 120214 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	6046	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PEG, EDO, CL, ZN, PGE, PO4

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	1.05	1/1814 (0.1%)	1.10	2/2468 (0.1%)
1	B	1.05	0/1766	1.15	3/2405 (0.1%)
1	C	1.10	3/1761 (0.2%)	1.14	1/2399 (0.0%)
All	All	1.07	4/5341 (0.1%)	1.13	6/7272 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	175	PRO	C-O	5.79	1.30	1.23
1	C	96	ASP	CG-OD2	5.50	1.35	1.25
1	C	128	GLY	C-O	-5.32	1.20	1.24
1	C	250	HIS	CE1-NE2	5.12	1.37	1.32

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	ASN	CA-CB-CG	6.75	119.36	112.60
1	C	124	ASP	CA-CB-CG	6.45	119.05	112.60
1	A	124	ASP	CA-CB-CG	6.22	118.82	112.60
1	B	193	ASN	CA-CB-CG	5.77	118.37	112.60
1	B	212	ASP	CA-CB-CG	5.32	117.92	112.60
1	B	130	ASP	CA-CB-CG	5.23	117.83	112.60

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	1746	0	1728	8	1
1	B	1717	0	1685	7	0
1	C	1706	0	1672	7	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
5	A	8	0	12	2	0
5	B	4	0	6	0	0
5	C	4	0	6	0	0
6	A	13	0	17	1	0
6	B	6	0	7	1	0
6	C	7	0	10	1	0
7	A	10	0	14	1	0
7	C	5	0	5	0	0
8	B	6	0	8	1	0
8	C	6	0	8	0	0
9	A	272	0	0	2	1
9	B	273	0	0	0	1
9	C	233	0	0	2	0
All	All	6046	0	5178	25	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (25) 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:C:126:MET:O	1:C:129:MET:HG2	2.01	0.61
6:C:308:PEG:H32	9:C:445:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:MET:O	1:A:129[A]:MET:HG2	2.06	0.55
1:B:126:MET:O	1:B:129:MET:HG2	2.07	0.55
1:C:212:ASP:OD1	9:C:401:HOH:O	2.18	0.53
1:A:129[B]:MET:HG3	1:A:133:HIS:CE1	2.43	0.53
5:A:308:EDO:C1	9:A:402:HOH:O	2.57	0.52
1:C:78:LEU:HD13	1:C:198:ILE:HD11	1.95	0.49
1:A:117[A]:VAL:HG21	1:A:177:PHE:CE2	2.48	0.48
1:A:187:PRO:HB3	1:A:191:SER:HA	1.97	0.47
5:A:308:EDO:H11	9:A:402:HOH:O	2.16	0.46
1:C:227[B]:GLU:HG3	1:C:228:HIS:CE1	2.50	0.46
1:B:76:ASN:OD1	6:B:308:PEG:H22	2.16	0.46
1:A:257:ALA:HA	7:A:311:PGE:H6	1.98	0.44
1:A:118:VAL:HG11	1:A:129[B]:MET:HE1	2.00	0.44
1:A:147:GLN:HG2	6:A:310:PEG:H41	1.99	0.44
1:B:201:THR:CG2	8:B:309:GOL:H31	2.48	0.43
1:C:88:VAL:O	1:C:116:ALA:HA	2.18	0.43
1:C:225:ASP:OD1	1:C:227[B]:GLU:HG2	2.18	0.43
1:B:88:VAL:O	1:B:116:ALA:HA	2.19	0.43
1:C:130:ASP:OD1	1:C:155:VAL:HG21	2.20	0.41
1:A:140:TYR:CD2	1:A:159:HIS:HB2	2.57	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:539:HOH:O	9:B:652:HOH:O[1_556]	2.16	0.04
1:A:151[B]:GLN:NE2	9:A:428:HOH:O[1_556]	2.18	0.02

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	236/243 (97%)	232 (98%)	3 (1%)	1 (0%)	30	11
1	B	230/243 (95%)	228 (99%)	2 (1%)	0	100	100
1	C	230/243 (95%)	227 (99%)	3 (1%)	0	100	100
All	All	696/729 (96%)	687 (99%)	8 (1%)	1 (0%)	48	23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	GLY

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	180/182 (99%)	179 (99%)	1 (1%)	78	57
1	B	174/182 (96%)	173 (99%)	1 (1%)	78	57
1	C	174/182 (96%)	172 (99%)	2 (1%)	65	35
All	All	528/546 (97%)	524 (99%)	4 (1%)	73	48

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

Mol	Chain	Res	Type
1	A	193	ASN
1	B	193	ASN
1	C	154	MET
1	C	193	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	60	GLN

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](#)

Of 30 ligands modelled in this entry, 15 are monoatomic - leaving 15 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	$\# Z > 2$
8	GOL	C	310	-	5,5,5	0.32	0	5,5,5	0.69	0
8	GOL	B	309	-	5,5,5	0.17	0	5,5,5	0.19	0
5	EDO	A	308	-	3,3,3	0.08	0	2,2,2	0.16	0
6	PEG	A	309	-	6,6,6	0.43	0	5,5,5	0.76	0
4	PO4	C	306	2	4,4,4	1.76	1 (25%)	6,6,6	1.02	0
5	EDO	B	307	-	3,3,3	0.76	0	2,2,2	0.65	0
4	PO4	A	306	2	4,4,4	0.90	0	6,6,6	0.76	0
6	PEG	B	308	-	5,5,6	0.22	0	4,4,5	0.93	0
6	PEG	C	308	-	6,6,6	0.17	0	5,5,5	0.26	0
4	PO4	B	306	2	4,4,4	1.21	1 (25%)	6,6,6	0.74	0
7	PGE	C	309	-	4,4,9	0.44	0	3,3,8	0.20	0
7	PGE	A	311	-	9,9,9	0.38	0	8,8,8	0.28	0
5	EDO	A	307	-	3,3,3	0.48	0	2,2,2	0.42	0
5	EDO	C	307	-	3,3,3	0.27	0	2,2,2	0.30	0
6	PEG	A	310	-	5,5,6	0.47	0	4,4,5	0.51	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
8	GOL	C	310	-	-	0/4/4/4	-
8	GOL	B	309	-	-	2/4/4/4	-
5	EDO	A	308	-	-	0/1/1/1	-
6	PEG	A	309	-	-	2/4/4/4	-
5	EDO	B	307	-	-	1/1/1/1	-
6	PEG	B	308	-	-	2/3/3/4	-
6	PEG	C	308	-	-	2/4/4/4	-
7	PGE	C	309	-	-	1/2/2/7	-
7	PGE	A	311	-	-	5/7/7/7	-
5	EDO	A	307	-	-	0/1/1/1	-
5	EDO	C	307	-	-	1/1/1/1	-
6	PEG	A	310	-	-	1/3/3/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	306	PO4	P-O1	3.00	1.57	1.50
4	B	306	PO4	P-O1	-2.32	1.45	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	309	GOL	O1-C1-C2-C3
6	B	308	PEG	O2-C3-C4-O4
6	A	310	PEG	C1-C2-O2-C3
8	B	309	GOL	O1-C1-C2-O2
7	A	311	PGE	O2-C3-C4-O3
5	B	307	EDO	O1-C1-C2-O2
6	C	308	PEG	O1-C1-C2-O2
7	C	309	PGE	C1-C2-O2-C3
6	A	309	PEG	O2-C3-C4-O4
7	A	311	PGE	C4-C3-O2-C2
7	A	311	PGE	C3-C4-O3-C5
7	A	311	PGE	C6-C5-O3-C4
7	A	311	PGE	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
6	A	309	PEG	C1-C2-O2-C3
6	C	308	PEG	C1-C2-O2-C3
6	B	308	PEG	C1-C2-O2-C3
5	C	307	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	309	GOL	1	0
5	A	308	EDO	2	0
6	B	308	PEG	1	0
6	C	308	PEG	1	0
7	A	311	PGE	1	0
6	A	310	PEG	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	229/243 (94%)	1.34	40 (17%) 4 4	8, 15, 34, 84	9 (3%)
1	B	229/243 (94%)	1.65	63 (27%) 1 1	8, 17, 36, 104	3 (1%)
1	C	227/243 (93%)	1.70	63 (27%) 1 1	9, 18, 42, 71	5 (2%)
All	All	685/729 (93%)	1.56	166 (24%) 2 2	8, 17, 40, 104	17 (2%)

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	42	GLY	10.1
1	A	41	THR	7.1
1	B	71	GLY	6.8
1	A	216	LYS	6.7
1	C	153	GLY	6.3
1	A	70	PHE	6.3
1	C	151	GLN	6.2
1	B	270	ARG	6.1
1	C	269	LEU	6.0
1	B	216	LYS	5.6
1	C	70	PHE	5.6
1	A	42	GLY	5.5
1	C	242	LYS	5.3
1	C	71	GLY	5.3
1	A	71	GLY	5.1
1	A	268	LYS	5.0
1	A	214	LYS	4.9
1	C	148	LEU	4.7
1	B	136	GLY	4.7
1	C	155	VAL	4.7
1	C	109	ILE	4.7
1	A	181	LYS	4.5
1	B	72	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	268	LYS	4.3
1	B	269	LEU	4.2
1	C	152	LYS	4.2
1	B	66	ASP	4.2
1	C	96	ASP	4.1
1	C	107	GLN	4.1
1	C	214	LYS	4.1
1	C	268	LYS	4.1
1	B	214	LYS	4.0
1	C	130	ASP	4.0
1	A	93	TRP	3.9
1	A	153	GLY	3.9
1	C	149	ALA	3.9
1	B	48	ASP	3.9
1	A	202	ASP	3.8
1	B	43	ASP	3.8
1	A	152	LYS	3.8
1	C	135	ALA	3.8
1	C	134	ALA	3.7
1	C	216	LYS	3.7
1	A	269	LEU	3.7
1	B	68	PRO	3.6
1	C	43	ASP	3.6
1	B	242	LYS	3.6
1	C	175	PRO	3.6
1	B	70	PHE	3.6
1	B	227	GLU	3.5
1	B	221	LEU	3.5
1	B	73	VAL	3.5
1	A	66	ASP	3.4
1	B	49[A]	LEU	3.4
1	B	102	LEU	3.4
1	B	153	GLY	3.3
1	C	150	PRO	3.3
1	C	257	ALA	3.3
1	C	113	VAL	3.3
1	B	264	ARG	3.3
1	B	263	ALA	3.2
1	C	44	GLN	3.2
1	A	68	PRO	3.2
1	B	59	TRP	3.1
1	C	264	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	200	GLY	3.1
1	B	69	GLY	3.1
1	C	198	ILE	3.1
1	C	59	TRP	3.1
1	B	171	PRO	3.1
1	C	68	PRO	3.1
1	C	252	ALA	3.1
1	C	67[A]	MET	3.0
1	B	107	GLN	3.0
1	B	152	LYS	3.0
1	C	72	ALA	3.0
1	A	72	ALA	2.9
1	C	172	ALA	2.9
1	C	69	GLY	2.9
1	A	175	PRO	2.9
1	A	148	LEU	2.9
1	C	50	VAL	2.9
1	B	130	ASP	2.8
1	B	134	ALA	2.8
1	A	242	LYS	2.8
1	B	172	ALA	2.7
1	B	226	THR	2.7
1	C	79	ILE	2.7
1	B	215	ALA	2.7
1	B	243	ALA	2.7
1	B	118	VAL	2.7
1	B	93	TRP	2.7
1	B	150	PRO	2.7
1	C	215	ALA	2.6
1	B	258	ALA	2.6
1	C	154	MET	2.6
1	C	218	LEU	2.6
1	A	215	ALA	2.5
1	B	176	ASN	2.5
1	A	43	ASP	2.5
1	B	147	GLN	2.5
1	B	65	LEU	2.5
1	C	52	ARG	2.5
1	B	104	TRP	2.5
1	C	171	PRO	2.5
1	C	177	PHE	2.5
1	B	135	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	238	ALA	2.4
1	C	202	ASP	2.4
1	C	80	VAL	2.4
1	B	199	ASP	2.4
1	A	65	LEU	2.4
1	C	65	LEU	2.4
1	C	226	THR	2.4
1	C	163	PHE	2.4
1	B	96	ASP	2.4
1	A	198[A]	ILE	2.4
1	A	163	PHE	2.4
1	A	157	ALA	2.3
1	B	257	ALA	2.3
1	A	107[A]	GLN	2.3
1	B	109	ILE	2.3
1	C	144	LEU	2.3
1	B	200	GLY	2.3
1	A	224	ALA	2.3
1	B	236	PHE	2.3
1	C	217	SER	2.3
1	C	104	TRP	2.3
1	B	231	ALA	2.3
1	A	217	SER	2.3
1	B	252	ALA	2.2
1	B	52	ARG	2.2
1	C	127	GLY	2.2
1	B	246	ILE	2.2
1	A	257	ALA	2.2
1	A	150	PRO	2.2
1	A	44	GLN	2.2
1	A	199	ASP	2.2
1	A	134	ALA	2.2
1	B	99	ALA	2.2
1	B	165	ALA	2.2
1	C	143	ALA	2.2
1	C	263	ALA	2.2
1	B	261	HIS	2.2
1	B	94	THR	2.2
1	C	251	SER	2.2
1	B	138	ALA	2.1
1	A	168	TRP	2.1
1	C	66	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	238	ALA	2.1
1	B	106	LYS	2.1
1	C	51	PHE	2.1
1	C	136	GLY	2.1
1	A	112	PRO	2.1
1	A	116	ALA	2.1
1	B	174	ALA	2.1
1	A	104	TRP	2.1
1	A	171	PRO	2.1
1	C	46	PHE	2.0
1	B	132	LEU	2.0
1	C	228	HIS	2.0
1	C	64	TYR	2.0
1	A	260	THR	2.0
1	B	218	LEU	2.0
1	C	49	LEU	2.0
1	C	140	TYR	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 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
5	EDO	B	307	4/4	0.59	0.23	27,32,36,42	0
5	EDO	A	308	4/4	0.61	0.25	28,37,43,49	0
7	PGE	C	309	5/10	0.62	0.20	18,28,32,40	0
7	PGE	A	311	10/10	0.66	0.25	28,42,67,88	0
6	PEG	C	308	7/7	0.68	0.34	33,44,81,96	0
8	GOL	B	309	6/6	0.70	0.20	28,35,53,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	PEG	B	308	6/7	0.76	0.17	19,25,29,35	0
6	PEG	A	310	6/7	0.78	0.28	35,53,73,90	0
5	EDO	C	307	4/4	0.81	0.15	28,32,36,45	0
8	GOL	C	310	6/6	0.83	0.23	24,51,56,59	0
6	PEG	A	309	7/7	0.88	0.20	21,26,40,42	0
3	CL	B	304	1/1	0.88	0.17	30,30,30,30	0
5	EDO	A	307	4/4	0.91	0.13	22,24,28,39	0
3	CL	C	304	1/1	0.93	0.12	27,27,27,27	0
4	PO4	B	306	5/5	0.94	0.08	13,14,16,17	0
3	CL	C	303	1/1	0.95	0.07	19,19,19,19	0
3	CL	C	305	1/1	0.96	0.09	30,30,30,30	0
3	CL	B	305	1/1	0.96	0.10	33,33,33,33	0
4	PO4	C	306	5/5	0.96	0.07	15,15,18,19	0
4	PO4	A	306	5/5	0.98	0.05	11,11,12,13	0
3	CL	A	305	1/1	0.98	0.09	17,17,17,17	1
3	CL	A	303	1/1	0.98	0.05	13,13,13,13	0
2	ZN	C	302	1/1	0.99	0.02	16,16,16,16	0
2	ZN	B	301	1/1	0.99	0.02	14,14,14,14	0
3	CL	A	304	1/1	0.99	0.10	27,27,27,27	0
2	ZN	B	302	1/1	0.99	0.02	16,16,16,16	0
3	CL	B	303	1/1	0.99	0.05	17,17,17,17	0
2	ZN	A	302	1/1	1.00	0.01	12,12,12,12	0
2	ZN	C	301	1/1	1.00	0.03	15,15,15,15	0
2	ZN	A	301	1/1	1.00	0.02	12,12,12,12	0

6.5 Other polymers

There are no such residues in this entry.