WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Sep 11, 2023 – 02:53 AM EDT

|		
PDB ID	:	4KZP
Title	:	Crystal Structure of a Putative Short Chain Dehydrogenase from Mycobacterium smegmatis
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2013-05-30
Resolution	:	1.68 Å(reported)

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 1.68 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	Percentile Ranks	Value
Rfree		0.204
Clashscore		2
Ramachandran outliers		0.1%
Sidechain outliers		0.6%
RSRZ outliers		3.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

❚ Percentile relative to X-ray structures of similar resolution
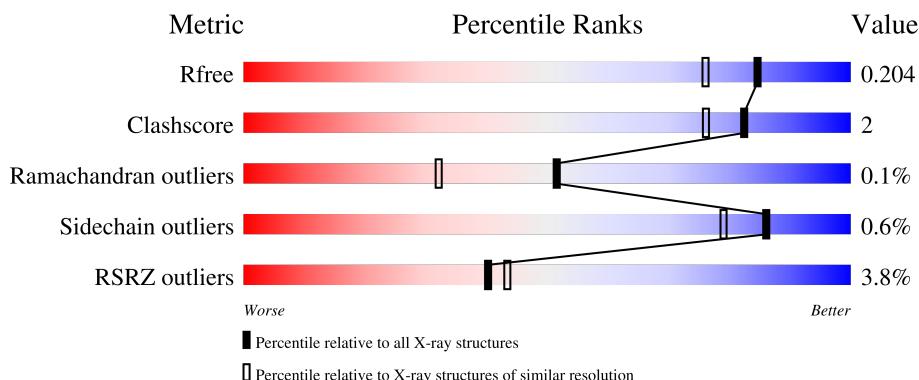
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6780 (1.70-1.66)
Clashscore	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)
RSRZ outliers	127900	6661 (1.70-1.66)

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 <=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	320	4% 87% • 9%
1	B	320	2% 86% • 12%
1	C	320	5% 87% 5% 8%
1	D	320	3% 85% 6% 9%
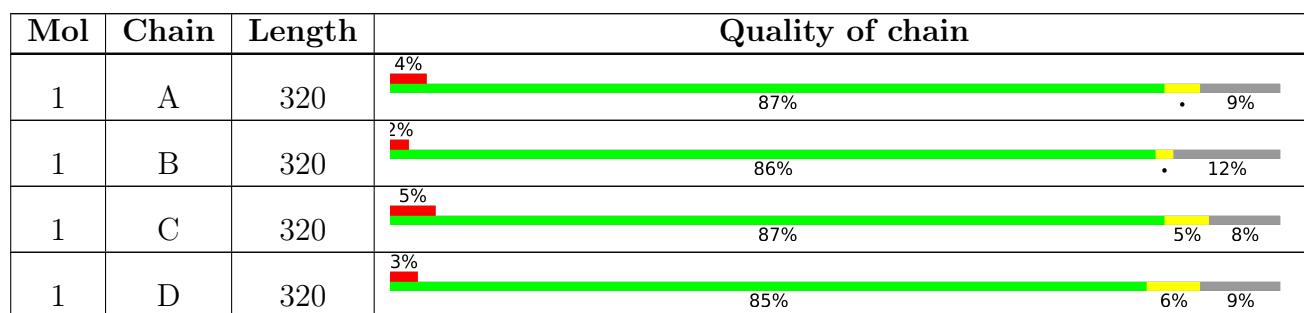
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	C	401	-	-	-	X
2	EDO	D	401	-	-	X	-
3	GOL	A	407	-	-	X	-
3	GOL	C	406	-	-	X	-

2 Entity composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9616 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 Oxidoreductase, short chain dehydrogenase/reductase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	7	0
			2108	1318	373	415	2			
1	B	283	Total	C	N	O	S	0	6	0
			2066	1296	365	403	2			
1	C	295	Total	C	N	O	S	0	7	0
			2129	1332	377	417	3			
1	D	292	Total	C	N	O	S	0	7	0
			2114	1326	371	413	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP A0R4P1
A	-2	PRO	-	expression tag	UNP A0R4P1
A	-1	GLY	-	expression tag	UNP A0R4P1
A	0	SER	-	expression tag	UNP A0R4P1
B	-3	GLY	-	expression tag	UNP A0R4P1
B	-2	PRO	-	expression tag	UNP A0R4P1
B	-1	GLY	-	expression tag	UNP A0R4P1
B	0	SER	-	expression tag	UNP A0R4P1
C	-3	GLY	-	expression tag	UNP A0R4P1
C	-2	PRO	-	expression tag	UNP A0R4P1
C	-1	GLY	-	expression tag	UNP A0R4P1
C	0	SER	-	expression tag	UNP A0R4P1
D	-3	GLY	-	expression tag	UNP A0R4P1
D	-2	PRO	-	expression tag	UNP A0R4P1
D	-1	GLY	-	expression tag	UNP A0R4P1
D	0	SER	-	expression tag	UNP A0R4P1

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

EDO

O2
OH

C1

C2

HO

O1
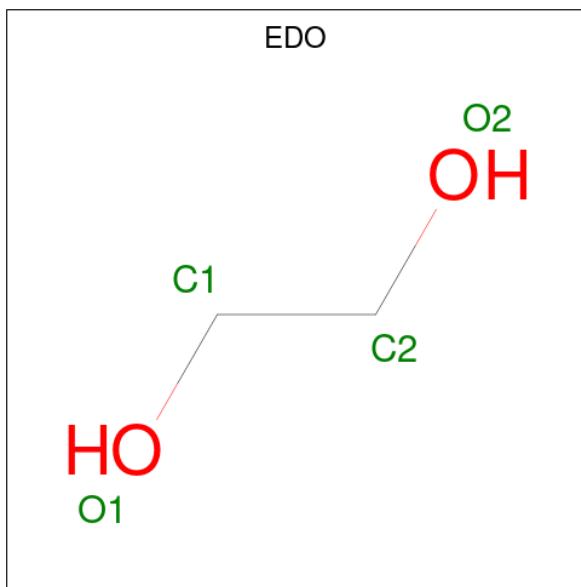
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	C	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0
2	D	1	Total 4	C 2	O 2	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

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GOL
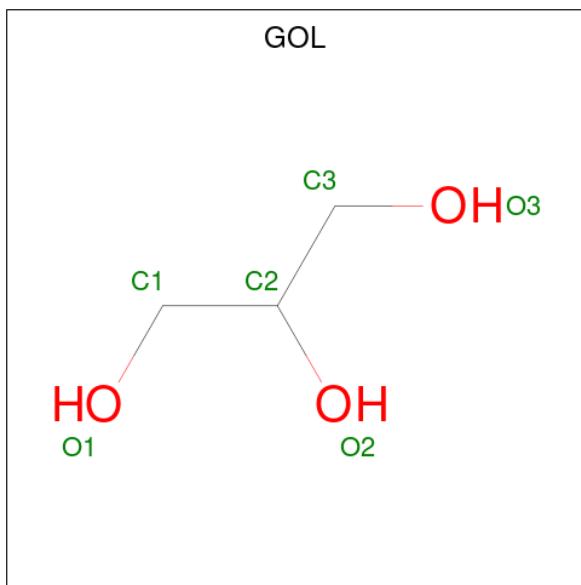
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	274	Total 274	O 274	0	0
4	B	269	Total 269	O 269	0	0
4	C	286	Total 286	O 286	0	0
4	D	294	Total 294	O 294	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family protein
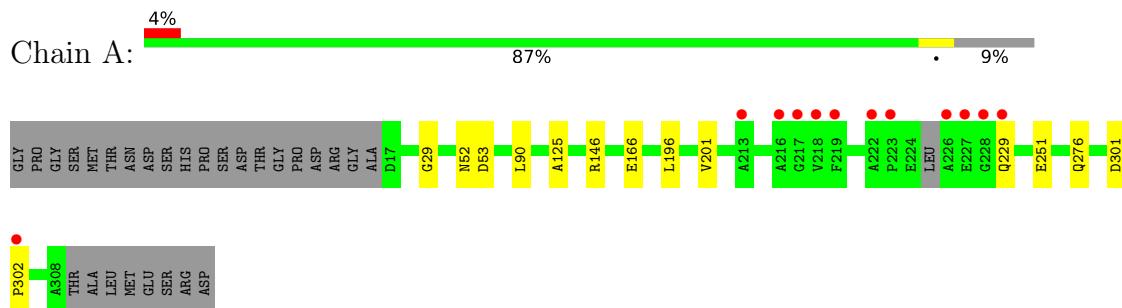
• Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family protein

• Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family protein

• Molecule 1: Oxidoreductase, short chain dehydrogenase/reductase family protein

ALA GLU GLY Q229 T266 K275 Q276 F277 D299 E313 SER ARG ASP
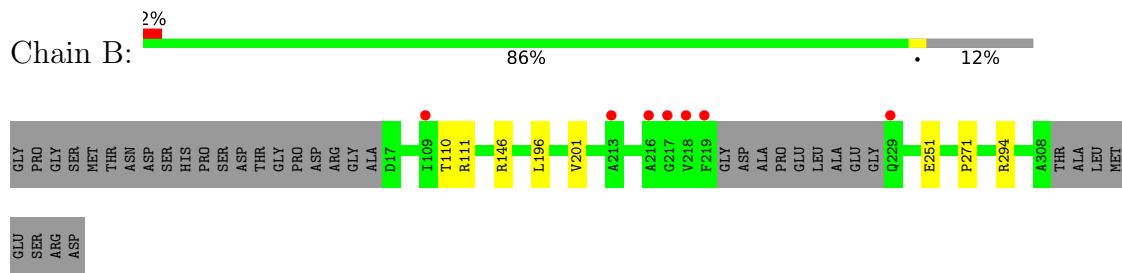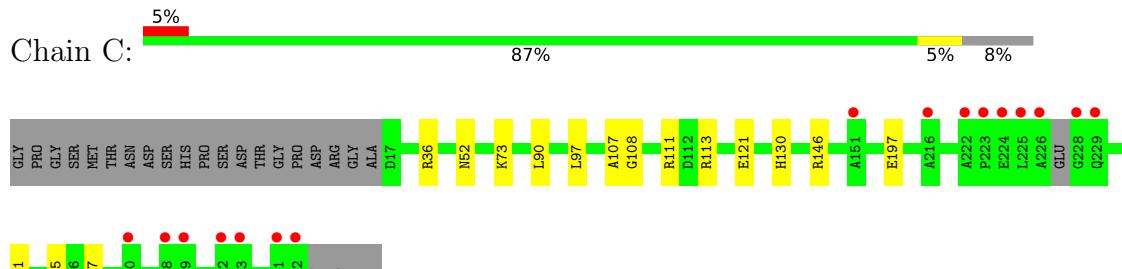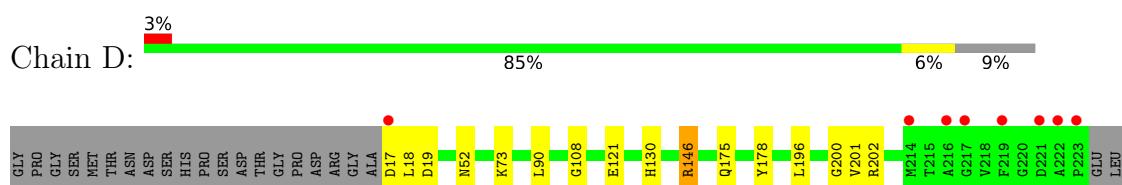
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.70Å 86.07Å 92.33Å 90.00° 103.40° 90.00°	Depositor
Resolution (Å)	46.43 – 1.68 46.39 – 1.68	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.43-1.68) 98.5 (46.39-1.68)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.05 (at 1.68Å)	Xtriage
Refinement program	REFMAC 5.7.0032, PHENIX	Depositor
R, R_{free}	0.176 , 0.205 0.175 , 0.204	Depositor DCC
R_{free} test set	7331 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	16.3	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.3	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9616	wwPDB-VP
Average B, all atoms (Å^2)	22.0	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 36.35 % 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 5.0679e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, EDO

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	0.49	0/2160	0.64	0/2942
1	B	0.49	0/2114	0.65	1/2877 (0.0%)
1	C	0.51	0/2184	0.66	1/2973 (0.0%)
1	D	0.52	0/2168	0.67	0/2950
All	All	0.50	0/8626	0.65	2/11742 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	36	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	B	294	ARG	NE-CZ-NH1	5.05	122.82	120.30

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	2108	0	2073	11	0
1	B	2066	0	2063	4	0
1	C	2129	0	2102	13	0
1	D	2114	0	2098	14	0
2	A	24	0	36	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4	0	6	0	0
2	C	16	0	24	0	0
2	D	8	0	12	4	0
3	A	6	0	8	5	0
3	C	12	0	16	5	0
3	D	6	0	8	2	0
4	A	274	0	0	4	0
4	B	269	0	0	1	0
4	C	286	0	0	1	0
4	D	294	0	0	2	0
All	All	9616	0	8446	42	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 (42) 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:146:ARG:HD2	2:D:401:EDO:H22	1.54	0.89
1:C:108:GLY:H	3:C:406:GOL:H11	1.39	0.87
1:D:200:GLY:HA2	3:D:403:GOL:H32	1.67	0.76
1:D:17:ASP:O	1:D:19:ASP:N	2.15	0.76
1:C:197[B]:GLU:OE1	3:C:405:GOL:H2	1.91	0.70
3:A:407:GOL:H11	4:A:547:HOH:O	1.93	0.67
1:C:113:ARG:HD2	4:C:580:HOH:O	1.93	0.67
1:D:146:ARG:HD2	2:D:401:EDO:C2	2.23	0.67
1:C:111[B]:ARG:NH2	1:C:121:GLU:OE2	2.30	0.64
1:A:125:ALA:HA	2:A:406:EDO:H21	1.85	0.59
1:D:146:ARG:HB3	2:D:401:EDO:H22	1.85	0.58
1:A:276:GLN:OE1	1:D:266:THR:OG1	2.20	0.57
1:C:108:GLY:H	3:C:406:GOL:C1	2.15	0.56
1:A:251:GLU:HG2	4:A:605:HOH:O	2.07	0.54
1:D:121[A]:GLU:HG2	4:D:700:HOH:O	2.07	0.54
1:A:29:GLY:CA	3:A:407:GOL:H2	2.40	0.52
1:B:271:PRO:HG3	1:C:271:PRO:HG3	1.90	0.52
1:C:107:ALA:HA	3:C:406:GOL:H12	1.91	0.52
1:C:108:GLY:N	3:C:406:GOL:H11	2.16	0.51
1:C:73:LYS:HE3	1:C:97:LEU:HD22	1.92	0.51
1:A:196:LEU:HB3	1:A:201:VAL:HB	1.92	0.51
1:C:73:LYS:HE3	1:C:97:LEU:CD2	2.41	0.51
1:D:275[B]:LYS:HG2	1:D:277:PHE:CZ	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:LEU:HB3	1:B:201:VAL:HB	1.94	0.49
1:C:275:LYS:HG2	1:C:277:PHE:CZ	2.46	0.49
1:A:52:ASN:HB2	1:A:90:LEU:HD21	1.94	0.48
4:A:769:HOH:O	2:D:401:EDO:H11	2.14	0.48
1:B:110:THR:O	1:B:111[B]:ARG:HD3	2.15	0.46
1:D:202:ARG:HH22	3:D:403:GOL:C3	2.30	0.44
1:D:196:LEU:HB3	1:D:201:VAL:HB	1.98	0.44
1:A:53:ASP:OD1	3:A:407:GOL:H31	2.17	0.44
1:A:166[B]:GLU:HG3	4:A:538:HOH:O	2.18	0.44
1:C:108:GLY:HA3	1:C:130:HIS:CE1	2.53	0.44
1:A:29:GLY:HA2	3:A:407:GOL:H2	2.01	0.43
1:B:251:GLU:HG2	4:B:623:HOH:O	2.20	0.42
1:D:108:GLY:HA3	1:D:130:HIS:CE1	2.54	0.41
1:A:29:GLY:HA3	3:A:407:GOL:H2	2.02	0.41
1:A:301:ASP:HA	1:A:302:PRO:HD3	1.86	0.41
1:C:52:ASN:HB2	1:C:90:LEU:HD21	2.03	0.41
1:D:52:ASN:HB2	1:D:90:LEU:HD21	2.03	0.41
1:D:175:GLN:HB3	1:D:178:TYR:HB3	2.03	0.41
1:D:73:LYS:HE3	4:D:758:HOH:O	2.20	0.40

There are no symmetry-related clashes.

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	295/320 (92%)	286 (97%)	9 (3%)	0	100	100
1	B	285/320 (89%)	277 (97%)	8 (3%)	0	100	100
1	C	299/320 (93%)	292 (98%)	7 (2%)	0	100	100
1	D	296/320 (92%)	287 (97%)	8 (3%)	1 (0%)	41	23
All	All	1175/1280 (92%)	1142 (97%)	32 (3%)	1 (0%)	51	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	18	LEU

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	204/229 (89%)	202 (99%)	2 (1%)	76	65
1	B	204/229 (89%)	203 (100%)	1 (0%)	88	83
1	C	206/229 (90%)	205 (100%)	1 (0%)	88	83
1	D	206/229 (90%)	205 (100%)	1 (0%)	88	83
All	All	820/916 (90%)	815 (99%)	5 (1%)	86	79

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	ARG
1	A	229	GLN
1	B	146	ARG
1	C	146	ARG
1	D	146	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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)

17 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	$\#|Z| > 2$
2	EDO	B	401	-	3,3,3	0.46	0	2,2,2	0.29	0
2	EDO	C	404	-	3,3,3	0.44	0	2,2,2	0.43	0
2	EDO	D	402	-	3,3,3	0.46	0	2,2,2	0.42	0
3	GOL	D	403	-	5,5,5	0.41	0	5,5,5	0.34	0
2	EDO	C	402	-	3,3,3	0.48	0	2,2,2	0.31	0
2	EDO	A	402	-	3,3,3	0.50	0	2,2,2	0.30	0
2	EDO	A	404	-	3,3,3	0.46	0	2,2,2	0.50	0
3	GOL	A	407	-	5,5,5	0.39	0	5,5,5	0.40	0
2	EDO	A	406	-	3,3,3	0.51	0	2,2,2	0.23	0
2	EDO	A	401	-	3,3,3	0.49	0	2,2,2	0.50	0
2	EDO	C	401	-	3,3,3	0.51	0	2,2,2	0.19	0
3	GOL	C	406	-	5,5,5	0.48	0	5,5,5	0.88	0
3	GOL	C	405	-	5,5,5	0.56	0	5,5,5	0.59	0
2	EDO	A	403	-	3,3,3	0.50	0	2,2,2	0.19	0
2	EDO	D	401	-	3,3,3	0.42	0	2,2,2	0.29	0
2	EDO	C	403	-	3,3,3	0.41	0	2,2,2	0.55	0
2	EDO	A	405	-	3,3,3	0.51	0	2,2,2	0.36	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
2	EDO	B	401	-	-	0/1/1/1	-
2	EDO	C	404	-	-	0/1/1/1	-
2	EDO	D	402	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	403	-	-	2/4/4/4	-
2	EDO	C	402	-	-	0/1/1/1	-
2	EDO	A	402	-	-	1/1/1/1	-
2	EDO	A	404	-	-	1/1/1/1	-
3	GOL	A	407	-	-	0/4/4/4	-
2	EDO	A	406	-	-	0/1/1/1	-
2	EDO	A	401	-	-	1/1/1/1	-
2	EDO	C	401	-	-	1/1/1/1	-
3	GOL	C	406	-	-	4/4/4/4	-
3	GOL	C	405	-	-	0/4/4/4	-
2	EDO	A	403	-	-	1/1/1/1	-
2	EDO	D	401	-	-	1/1/1/1	-
2	EDO	C	403	-	-	0/1/1/1	-
2	EDO	A	405	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	406	GOL	O1-C1-C2-C3
3	C	406	GOL	C1-C2-C3-O3
3	D	403	GOL	C1-C2-C3-O3
3	C	406	GOL	O1-C1-C2-O2
3	C	406	GOL	O2-C2-C3-O3
2	C	401	EDO	O1-C1-C2-O2
3	D	403	GOL	O2-C2-C3-O3
2	A	404	EDO	O1-C1-C2-O2
2	A	405	EDO	O1-C1-C2-O2
2	A	403	EDO	O1-C1-C2-O2
2	A	402	EDO	O1-C1-C2-O2
2	D	402	EDO	O1-C1-C2-O2
2	A	401	EDO	O1-C1-C2-O2
2	D	401	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	403	GOL	2	0
3	A	407	GOL	5	0
2	A	406	EDO	1	0
3	C	406	GOL	4	0
3	C	405	GOL	1	0
2	D	401	EDO	4	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	291/320 (90%)	0.08	12 (4%)	37	39	11, 19, 46, 64	0
1	B	283/320 (88%)	0.04	7 (2%)	57	60	11, 20, 38, 61	0
1	C	295/320 (92%)	0.20	16 (5%)	25	27	10, 17, 47, 56	0
1	D	292/320 (91%)	0.03	9 (3%)	49	51	10, 17, 40, 60	0
All	All	1161/1280 (90%)	0.09	44 (3%)	40	43	10, 18, 44, 64	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	222	ALA	8.2
1	B	216	ALA	8.1
1	A	228	GLY	6.6
1	C	223	PRO	5.4
1	D	217	GLY	5.3
1	D	299	ASP	4.9
1	A	223	PRO	4.9
1	C	298	ALA	4.5
1	A	216	ALA	4.2
1	C	302	PRO	4.2
1	C	216	ALA	3.9
1	B	218	VAL	3.8
1	D	216	ALA	3.8
1	C	299	ASP	3.7
1	C	228	GLY	3.6
1	D	222	ALA	3.5
1	D	17	ASP	3.4
1	A	213	ALA	3.4
1	D	223	PRO	3.3
1	C	222	ALA	3.3
1	A	229	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	312	MET	3.1
1	D	214	MET	3.1
1	C	224	GLU	3.1
1	B	213	ALA	3.0
1	C	151	ALA	2.9
1	A	217	GLY	2.8
1	C	226	ALA	2.7
1	C	229	GLN	2.7
1	C	303	GLU	2.6
1	A	219	PHE	2.6
1	B	229	GLN	2.6
1	D	219	PHE	2.5
1	C	311	LEU	2.5
1	B	217	GLY	2.4
1	C	225	LEU	2.3
1	A	226	ALA	2.3
1	A	218	VAL	2.2
1	D	221	ASP	2.2
1	A	302	PRO	2.2
1	A	227	GLU	2.1
1	C	280	ASP	2.0
1	B	109[A]	ILE	2.0
1	B	219	PHE	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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
2	EDO	C	401	4/4	0.24	0.43	73,75,76,77	0
2	EDO	A	402	4/4	0.68	0.19	42,45,46,47	0
2	EDO	C	404	4/4	0.71	0.26	52,55,55,59	0
3	GOL	A	407	6/6	0.72	0.27	40,41,44,46	0
3	GOL	C	406	6/6	0.72	0.19	33,36,38,40	0
2	EDO	A	406	4/4	0.73	0.22	42,46,46,48	0
3	GOL	D	403	6/6	0.76	0.20	30,35,36,37	0
2	EDO	A	401	4/4	0.77	0.21	44,45,46,47	0
2	EDO	A	405	4/4	0.78	0.23	44,45,46,51	0
3	GOL	C	405	6/6	0.79	0.17	29,32,34,38	0
2	EDO	D	402	4/4	0.80	0.27	40,43,45,51	0
2	EDO	C	403	4/4	0.82	0.23	41,42,45,46	0
2	EDO	A	403	4/4	0.86	0.28	40,40,41,42	0
2	EDO	A	404	4/4	0.86	0.18	37,41,42,43	0
2	EDO	D	401	4/4	0.89	0.36	32,34,34,36	0
2	EDO	C	402	4/4	0.92	0.18	34,37,41,46	0
2	EDO	B	401	4/4	0.93	0.12	34,39,40,43	0

6.5 Other polymers (i)

There are no such residues in this entry.