



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:24 AM UTC

PDB ID : 3TW9 / pdb_00003tw9
Title : Crystal structure of gluconate dehydratase (TARGET EFI-501679) from Salmonella enterica subsp. enterica serovar Enteritidis str. P125109
Authors : Patskovsky, Y.; Toro, R.; Bhosle, R.; Hillerich, B.; Seidel, R.D.; Washington, E.; Scott Glenn, A.; Chowdhury, S.; Evans, B.; Hammonds, J.; Zencheck, W.D.; Imker, H.J.; Gerlt, J.A.; Almo, S.C.; Enzyme Function Initiative (EFI)
Deposited on : 2011-09-21
Resolution : 1.70 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

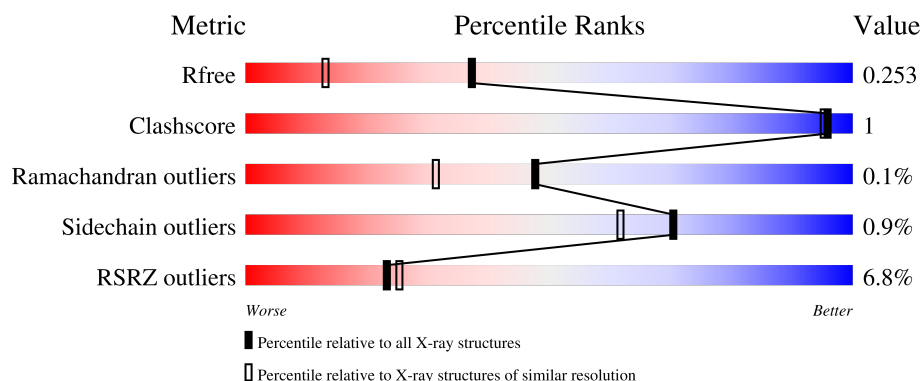
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	442	4% 86% • 11%
1	B	442	9% 89% • 7%
1	C	442	5% 87% • 11%
1	D	442	7% 89% • 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13901 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 Putative dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	7	0
			3110	1981	531	577	21			
1	B	410	Total	C	N	O	S	0	9	0
			3244	2070	552	601	21			
1	C	395	Total	C	N	O	S	0	7	0
			3115	1986	527	581	21			
1	D	408	Total	C	N	O	S	0	9	0
			3226	2056	550	599	21			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP B5R541
A	-21	HIS	-	expression tag	UNP B5R541
A	-20	HIS	-	expression tag	UNP B5R541
A	-19	HIS	-	expression tag	UNP B5R541
A	-18	HIS	-	expression tag	UNP B5R541
A	-17	HIS	-	expression tag	UNP B5R541
A	-16	HIS	-	expression tag	UNP B5R541
A	-15	SER	-	expression tag	UNP B5R541
A	-14	SER	-	expression tag	UNP B5R541
A	-13	GLY	-	expression tag	UNP B5R541
A	-12	VAL	-	expression tag	UNP B5R541
A	-11	ASP	-	expression tag	UNP B5R541
A	-10	LEU	-	expression tag	UNP B5R541
A	-9	GLY	-	expression tag	UNP B5R541
A	-8	THR	-	expression tag	UNP B5R541
A	-7	GLU	-	expression tag	UNP B5R541
A	-6	ASN	-	expression tag	UNP B5R541
A	-5	LEU	-	expression tag	UNP B5R541
A	-4	TYR	-	expression tag	UNP B5R541
A	-3	PHE	-	expression tag	UNP B5R541
A	-2	GLN	-	expression tag	UNP B5R541

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP B5R541
A	0	MET	-	expression tag	UNP B5R541
B	-22	MET	-	expression tag	UNP B5R541
B	-21	HIS	-	expression tag	UNP B5R541
B	-20	HIS	-	expression tag	UNP B5R541
B	-19	HIS	-	expression tag	UNP B5R541
B	-18	HIS	-	expression tag	UNP B5R541
B	-17	HIS	-	expression tag	UNP B5R541
B	-16	HIS	-	expression tag	UNP B5R541
B	-15	SER	-	expression tag	UNP B5R541
B	-14	SER	-	expression tag	UNP B5R541
B	-13	GLY	-	expression tag	UNP B5R541
B	-12	VAL	-	expression tag	UNP B5R541
B	-11	ASP	-	expression tag	UNP B5R541
B	-10	LEU	-	expression tag	UNP B5R541
B	-9	GLY	-	expression tag	UNP B5R541
B	-8	THR	-	expression tag	UNP B5R541
B	-7	GLU	-	expression tag	UNP B5R541
B	-6	ASN	-	expression tag	UNP B5R541
B	-5	LEU	-	expression tag	UNP B5R541
B	-4	TYR	-	expression tag	UNP B5R541
B	-3	PHE	-	expression tag	UNP B5R541
B	-2	GLN	-	expression tag	UNP B5R541
B	-1	SER	-	expression tag	UNP B5R541
B	0	MET	-	expression tag	UNP B5R541
C	-22	MET	-	expression tag	UNP B5R541
C	-21	HIS	-	expression tag	UNP B5R541
C	-20	HIS	-	expression tag	UNP B5R541
C	-19	HIS	-	expression tag	UNP B5R541
C	-18	HIS	-	expression tag	UNP B5R541
C	-17	HIS	-	expression tag	UNP B5R541
C	-16	HIS	-	expression tag	UNP B5R541
C	-15	SER	-	expression tag	UNP B5R541
C	-14	SER	-	expression tag	UNP B5R541
C	-13	GLY	-	expression tag	UNP B5R541
C	-12	VAL	-	expression tag	UNP B5R541
C	-11	ASP	-	expression tag	UNP B5R541
C	-10	LEU	-	expression tag	UNP B5R541
C	-9	GLY	-	expression tag	UNP B5R541
C	-8	THR	-	expression tag	UNP B5R541
C	-7	GLU	-	expression tag	UNP B5R541
C	-6	ASN	-	expression tag	UNP B5R541

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	LEU	-	expression tag	UNP B5R541
C	-4	TYR	-	expression tag	UNP B5R541
C	-3	PHE	-	expression tag	UNP B5R541
C	-2	GLN	-	expression tag	UNP B5R541
C	-1	SER	-	expression tag	UNP B5R541
C	0	MET	-	expression tag	UNP B5R541
D	-22	MET	-	expression tag	UNP B5R541
D	-21	HIS	-	expression tag	UNP B5R541
D	-20	HIS	-	expression tag	UNP B5R541
D	-19	HIS	-	expression tag	UNP B5R541
D	-18	HIS	-	expression tag	UNP B5R541
D	-17	HIS	-	expression tag	UNP B5R541
D	-16	HIS	-	expression tag	UNP B5R541
D	-15	SER	-	expression tag	UNP B5R541
D	-14	SER	-	expression tag	UNP B5R541
D	-13	GLY	-	expression tag	UNP B5R541
D	-12	VAL	-	expression tag	UNP B5R541
D	-11	ASP	-	expression tag	UNP B5R541
D	-10	LEU	-	expression tag	UNP B5R541
D	-9	GLY	-	expression tag	UNP B5R541
D	-8	THR	-	expression tag	UNP B5R541
D	-7	GLU	-	expression tag	UNP B5R541
D	-6	ASN	-	expression tag	UNP B5R541
D	-5	LEU	-	expression tag	UNP B5R541
D	-4	TYR	-	expression tag	UNP B5R541
D	-3	PHE	-	expression tag	UNP B5R541
D	-2	GLN	-	expression tag	UNP B5R541
D	-1	SER	-	expression tag	UNP B5R541
D	0	MET	-	expression tag	UNP B5R541

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- 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	2	Total	Cl	0	0
			2	2		
3	C	4	Total	Cl	0	0
			4	4		
3	D	2	Total	Cl	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	298	Total	O	0	0
			298	298		

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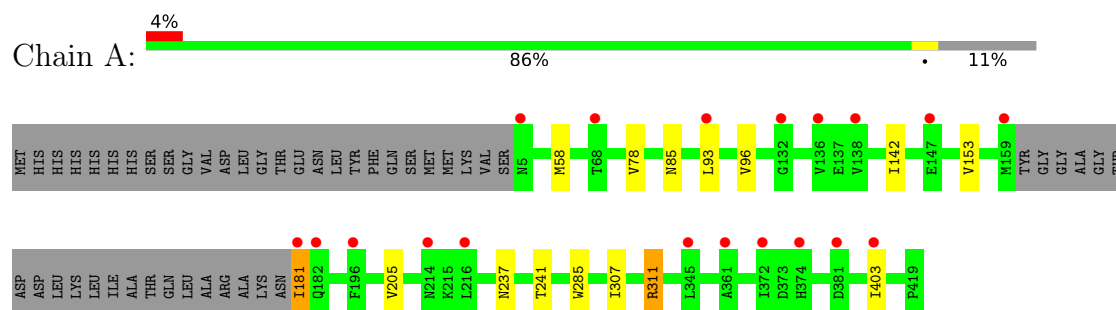
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	279	Total 279	O 279	0	0
4	C	297	Total 297	O 297	0	0
4	D	297	Total 297	O 297	0	0

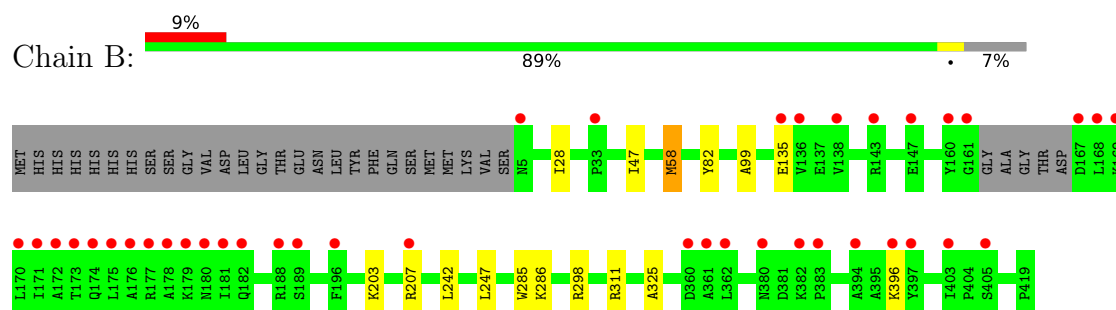
3 Residue-property plots [i](#)

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.

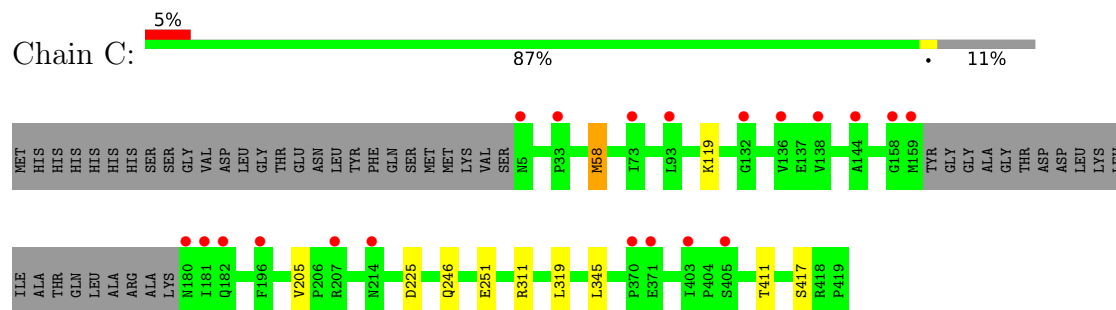
- Molecule 1: Putative dehydratase



- Molecule 1: Putative dehydratase

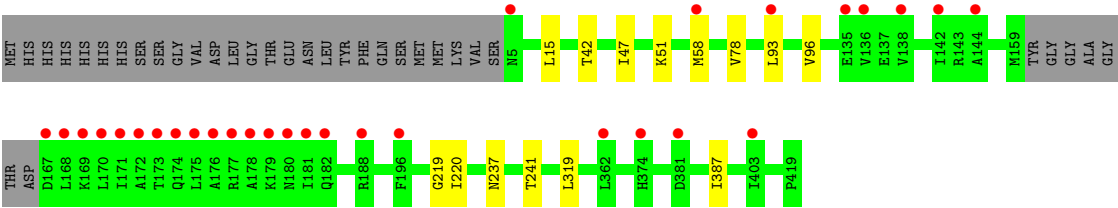


- Molecule 1: Putative dehydratase



- Molecule 1: Putative dehydratase





4 Data and refinement statistics

Property	Value	Source
Space group	P 4 ₂ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	177.53Å 177.53Å 110.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.70 50.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-1.70) 99.9 (50.00-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.211 , 0.252 0.213 , 0.253	Depositor DCC
R_{free} test set	6320 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13901	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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 44.89 % 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 1.4295e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	0.79	2/3208 (0.1%)	0.91	0/4358
1	B	0.78	0/3349	0.94	2/4546 (0.0%)
1	C	0.81	1/3213 (0.0%)	0.91	0/4366
1	D	0.77	1/3330 (0.0%)	0.92	1/4523 (0.0%)
All	All	0.79	4/13100 (0.0%)	0.92	3/17793 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	205	VAL	CA-CB	7.21	1.58	1.54
1	A	205	VAL	CA-CB	6.51	1.57	1.54
1	A	403	ILE	CA-CB	5.43	1.58	1.54
1	D	220	ILE	CA-CB	5.01	1.59	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	42	THR	N-CA-C	5.18	117.14	108.23
1	B	286	LYS	CA-C-N	-5.15	113.73	119.19
1	B	286	LYS	C-N-CA	-5.15	113.73	119.19

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	3110	0	3088	10	0
1	B	3244	0	3245	8	0
1	C	3115	0	3089	7	0
1	D	3226	0	3218	7	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
2	C	6	0	8	0	0
2	D	6	0	8	0	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
3	C	4	0	0	0	0
3	D	2	0	0	0	0
4	A	298	0	0	1	0
4	B	279	0	0	0	0
4	C	297	0	0	0	0
4	D	297	0	0	0	0
All	All	13901	0	12672	28	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 1.

All (28) 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:B:58[B]:MET:HA	1:B:58[B]:MET:HE2	1.61	0.82
1:B:58[B]:MET:HA	1:B:58[B]:MET:CE	2.28	0.64
1:D:58[B]:MET:HE2	1:D:96:VAL:HG21	1.80	0.62
1:A:58[A]:MET:HA	1:A:58[A]:MET:HE2	1.83	0.61
1:A:285:TRP:HH2	1:C:319[A]:LEU:HD13	1.67	0.58
1:B:203[B]:LYS:HG2	1:C:246[B]:GLN:OE1	2.04	0.57
1:D:58[A]:MET:HA	1:D:58[A]:MET:HE2	1.91	0.52
1:A:58[B]:MET:HE2	1:A:96:VAL:HG21	1.93	0.51
1:D:78:VAL:HG23	1:D:93:LEU:HD11	1.94	0.49
1:A:181:ILE:HD13	1:D:219:GLY:HA2	1.95	0.48
1:C:58[A]:MET:HE2	1:C:58[A]:MET:HB3	1.62	0.47
1:A:78:VAL:HG23	1:A:93:LEU:HD11	1.96	0.46
1:C:411:THR:HG23	1:C:417[B]:SER:OG	2.16	0.44
1:C:58[A]:MET:HE3	1:C:58[A]:MET:HA	1.99	0.44
1:A:307:ILE:O	1:A:311[B]:ARG:HB2	2.18	0.44
1:B:28:ILE:HD12	1:B:99:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:TRP:HH2	1:D:319[B]:LEU:HD13	1.83	0.43
1:A:58[B]:MET:CA	1:A:58[B]:MET:HE3	2.49	0.43
1:C:225:ASP:HA	1:C:251:GLU:HB3	2.01	0.43
1:A:142:ILE:HG12	1:A:153[B]:VAL:HG11	2.01	0.42
1:D:15:LEU:HD11	1:D:51:LYS:HD2	2.01	0.42
1:D:237:ASN:O	1:D:241:THR:HG23	2.19	0.41
1:A:85:ASN:ND2	4:A:1042:HOH:O	2.53	0.41
1:B:298:ARG:HA	1:B:325:ALA:O	2.21	0.41
1:B:203[B]:LYS:HB2	1:B:203[B]:LYS:HE2	1.81	0.40
1:C:119:LYS:HG2	1:C:345:LEU:HG	2.03	0.40
1:A:237:ASN:O	1:A:241:THR:HG23	2.22	0.40
1:B:242:LEU:HD13	1:B:247[A]:LEU:HD11	2.03	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	397/442 (90%)	388 (98%)	9 (2%)	0	100	100
1	B	415/442 (94%)	407 (98%)	7 (2%)	1 (0%)	43	28
1	C	398/442 (90%)	389 (98%)	9 (2%)	0	100	100
1	D	413/442 (93%)	405 (98%)	8 (2%)	0	100	100
All	All	1623/1768 (92%)	1589 (98%)	33 (2%)	1 (0%)	48	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	82	TYR

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	338/370 (91%)	335 (99%)	3 (1%)	70	62
1	B	352/370 (95%)	345 (98%)	7 (2%)	48	32
1	C	339/370 (92%)	336 (99%)	3 (1%)	70	62
1	D	350/370 (95%)	348 (99%)	2 (1%)	78	72
All	All	1379/1480 (93%)	1364 (99%)	15 (1%)	70	54

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	181	ILE
1	A	311[A]	ARG
1	A	311[B]	ARG
1	B	47	ILE
1	B	58[A]	MET
1	B	58[B]	MET
1	B	135	GLU
1	B	207	ARG
1	B	311	ARG
1	B	396	LYS
1	C	58[A]	MET
1	C	58[B]	MET
1	C	311	ARG
1	D	47	ILE
1	D	387	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	75	GLN
1	A	85	ASN
1	A	244	GLN

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Mol	Chain	Res	Type
1	A	267	GLN
1	B	5	ASN
1	B	10	ASN
1	B	85	ASN
1	B	91	ASN
1	B	237	ASN
1	B	246	GLN
1	B	258	ASN
1	B	267	GLN
1	C	85	ASN
1	C	180	ASN
1	C	340	ASN
1	D	5	ASN
1	D	174	GLN
1	D	267	GLN
1	D	291	ASN

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 15 ligands modelled in this entry, 11 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	B	420	-	5,5,5	0.58	0	5,5,5	0.41	0
2	GOL	A	420	-	5,5,5	0.63	0	5,5,5	0.41	0
2	GOL	D	420	-	5,5,5	0.61	0	5,5,5	0.57	0
2	GOL	C	420	-	5,5,5	0.51	0	5,5,5	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	GOL	B	420	-	-	0/4/4/4	-
2	GOL	A	420	-	-	0/4/4/4	-
2	GOL	D	420	-	-	0/4/4/4	-
2	GOL	C	420	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	394/442 (89%)	0.65	19 (4%)	35 39	16, 25, 45, 74	7 (1%)
1	B	410/442 (92%)	0.90	40 (9%)	13 13	11, 26, 53, 94	9 (2%)
1	C	395/442 (89%)	0.65	20 (5%)	33 37	10, 25, 44, 79	7 (1%)
1	D	408/442 (92%)	0.85	30 (7%)	20 22	11, 26, 53, 95	9 (2%)
All	All	1607/1768 (90%)	0.76	109 (6%)	23 25	10, 25, 50, 95	32 (1%)

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	171	ILE	8.5
1	D	178	ALA	6.8
1	B	171	ILE	6.7
1	B	178	ALA	6.5
1	A	181	ILE	6.1
1	D	175	LEU	5.9
1	D	172	ALA	5.5
1	B	170	LEU	5.1
1	C	136	VAL	5.0
1	B	160	TYR	5.0
1	B	168	LEU	4.9
1	D	167	ASP	4.9
1	D	170	LEU	4.8
1	C	138	VAL	4.7
1	B	173	THR	4.5
1	B	172	ALA	4.4
1	B	138	VAL	4.3
1	B	161	GLY	4.2
1	D	168	LEU	4.2
1	B	136	VAL	4.2
1	B	175	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	196	PHE	4.1
1	C	181	ILE	4.1
1	B	176	ALA	4.0
1	A	136	VAL	3.9
1	D	176	ALA	3.8
1	B	167	ASP	3.8
1	B	180	ASN	3.6
1	D	173	THR	3.6
1	B	179	LYS	3.6
1	D	180	ASN	3.5
1	B	188[A]	ARG	3.5
1	D	174	GLN	3.5
1	B	181	ILE	3.4
1	D	136	VAL	3.4
1	C	196	PHE	3.3
1	D	169	LYS	3.3
1	A	159	MET	3.3
1	A	196	PHE	3.2
1	A	182	GLN	3.2
1	B	362	LEU	3.2
1	B	169	LYS	3.1
1	A	403	ILE	3.1
1	A	138	VAL	3.1
1	B	405	SER	3.1
1	D	179	LYS	3.0
1	D	196	PHE	3.0
1	C	159	MET	2.9
1	C	403	ILE	2.9
1	C	180	ASN	2.9
1	A	214	ASN	2.9
1	B	174	GLN	2.9
1	D	374	HIS	2.9
1	C	371	GLU	2.8
1	D	181	ILE	2.8
1	D	403	ILE	2.7
1	C	158	GLY	2.7
1	C	144	ALA	2.7
1	A	374	HIS	2.7
1	B	403	ILE	2.7
1	C	182	GLN	2.6
1	C	405	SER	2.6
1	A	345	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	93	LEU	2.6
1	B	394	ALA	2.6
1	B	383	PRO	2.6
1	C	132	GLY	2.5
1	B	207	ARG	2.5
1	D	144	ALA	2.5
1	A	132	GLY	2.5
1	B	382	LYS	2.5
1	B	147	GLU	2.5
1	C	73	ILE	2.5
1	C	214	ASN	2.4
1	D	142	ILE	2.4
1	B	5	ASN	2.4
1	D	5	ASN	2.4
1	D	182	GLN	2.4
1	A	5	ASN	2.4
1	A	372	ILE	2.3
1	B	361	ALA	2.3
1	C	93	LEU	2.3
1	B	177	ARG	2.3
1	B	143	ARG	2.3
1	D	138	VAL	2.3
1	A	93	LEU	2.2
1	C	370	PRO	2.2
1	A	381	ASP	2.2
1	D	177	ARG	2.2
1	B	189	SER	2.2
1	A	361	ALA	2.2
1	B	360	ASP	2.2
1	C	207	ARG	2.2
1	A	147	GLU	2.1
1	D	188[A]	ARG	2.1
1	A	216	LEU	2.1
1	D	362	LEU	2.1
1	D	58[A]	MET	2.1
1	B	380	ASN	2.1
1	C	5	ASN	2.1
1	B	135	GLU	2.1
1	D	381	ASP	2.1
1	A	68	THR	2.1
1	C	33	PRO	2.1
1	B	397	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	33	PRO	2.0
1	D	135	GLU	2.0
1	B	182	GLN	2.0
1	B	396	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 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($\text{\AA}^2$)	Q<0.9
3	CL	B	422	1/1	0.92	0.15	42,42,42,42	0
3	CL	A	423	1/1	0.93	0.22	43,43,43,43	0
2	GOL	C	420	6/6	0.95	0.08	22,25,25,27	0
3	CL	B	421	1/1	0.95	0.09	31,31,31,31	0
2	GOL	D	420	6/6	0.95	0.09	21,24,26,28	0
2	GOL	B	420	6/6	0.96	0.08	24,26,27,36	0
3	CL	C	423	1/1	0.96	0.13	45,45,45,45	0
3	CL	C	424	1/1	0.96	0.16	45,45,45,45	0
3	CL	D	421	1/1	0.96	0.10	34,34,34,34	0
3	CL	D	422	1/1	0.96	0.14	32,32,32,32	1
2	GOL	A	420	6/6	0.97	0.07	19,24,27,30	0
3	CL	C	422	1/1	0.97	0.07	31,31,31,31	0
3	CL	A	421	1/1	0.98	0.04	23,23,23,23	0
3	CL	A	422	1/1	0.98	0.05	34,34,34,34	0
3	CL	C	421	1/1	0.99	0.04	21,21,21,21	1

6.5 Other polymers [i](#)

There are no such residues in this entry.