



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:50 PM UTC

PDB ID : 3TWA / pdb_00003twa
Title : Crystal structure of gluconate dehydratase (TARGET EFI-501679) from Salmonella enterica subsp. enterica serovar Enteritidis str. P125109 complexed with magnesium and glycerol
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 : 1.80 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)

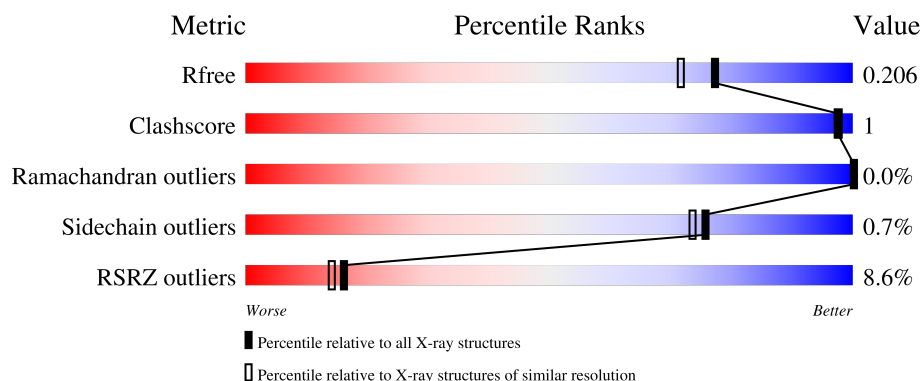
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	
1	B	442	
1	C	442	
1	D	442	

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Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	E	442	39% 90% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18409 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	415	Total	C	N	O	S	0	6	0
			3256	2072	555	609	20			
1	B	415	Total	C	N	O	S	0	6	0
			3258	2072	556	610	20			
1	C	415	Total	C	N	O	S	0	11	0
			3287	2096	561	609	21			
1	D	415	Total	C	N	O	S	0	14	0
			3305	2110	564	610	21			
1	E	415	Total	C	N	O	S	0	3	0
			3240	2060	554	606	20			

There are 115 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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	PHE	-	expression tag	UNP B5R541
A	-2	GLN	-	expression tag	UNP B5R541
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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	GLU	-	expression tag	UNP B5R541
C	-6	ASN	-	expression tag	UNP B5R541
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
E	-22	MET	-	expression tag	UNP B5R541
E	-21	HIS	-	expression tag	UNP B5R541
E	-20	HIS	-	expression tag	UNP B5R541
E	-19	HIS	-	expression tag	UNP B5R541
E	-18	HIS	-	expression tag	UNP B5R541
E	-17	HIS	-	expression tag	UNP B5R541
E	-16	HIS	-	expression tag	UNP B5R541
E	-15	SER	-	expression tag	UNP B5R541
E	-14	SER	-	expression tag	UNP B5R541
E	-13	GLY	-	expression tag	UNP B5R541
E	-12	VAL	-	expression tag	UNP B5R541

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-11	ASP	-	expression tag	UNP B5R541
E	-10	LEU	-	expression tag	UNP B5R541
E	-9	GLY	-	expression tag	UNP B5R541
E	-8	THR	-	expression tag	UNP B5R541
E	-7	GLU	-	expression tag	UNP B5R541
E	-6	ASN	-	expression tag	UNP B5R541
E	-5	LEU	-	expression tag	UNP B5R541
E	-4	TYR	-	expression tag	UNP B5R541
E	-3	PHE	-	expression tag	UNP B5R541
E	-2	GLN	-	expression tag	UNP B5R541
E	-1	SER	-	expression tag	UNP B5R541
E	0	MET	-	expression tag	UNP B5R541

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		

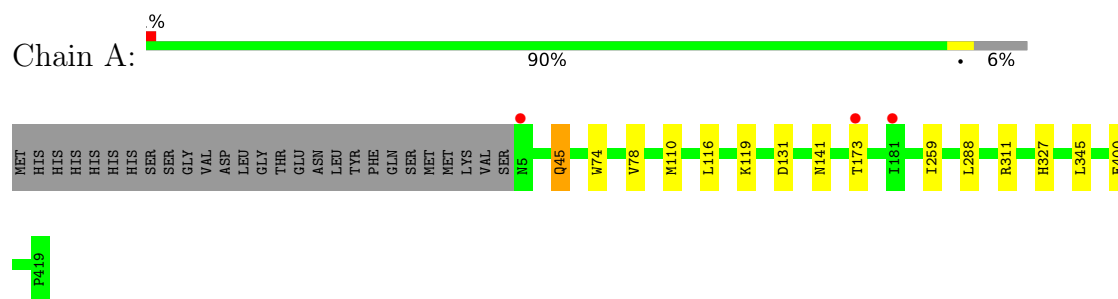
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	467	Total 467	O 467	0	1
5	B	410	Total 410	O 410	0	1
5	C	451	Total 451	O 451	0	1
5	D	448	Total 448	O 448	0	1
5	E	226	Total 226	O 226	0	0

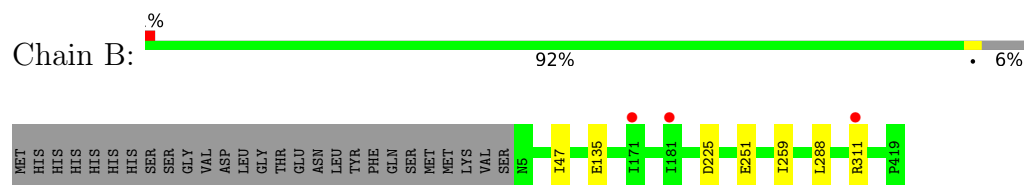
3 Residue-property plots [i](#)

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.

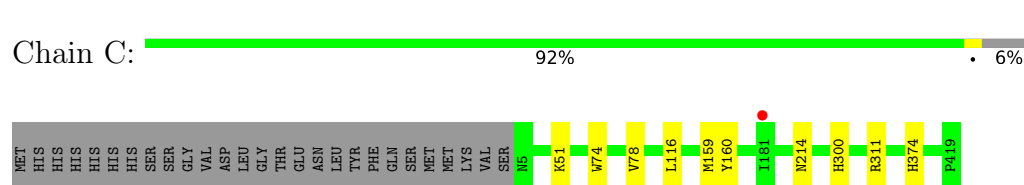
- Molecule 1: Putative dehydratase



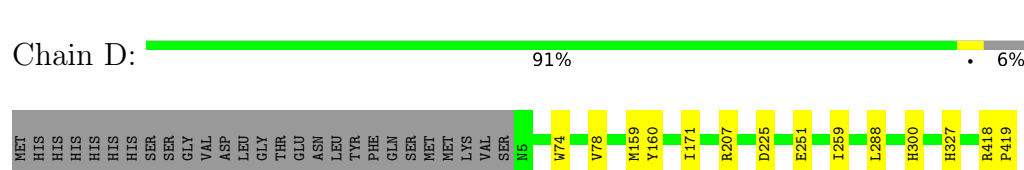
- Molecule 1: Putative dehydratase



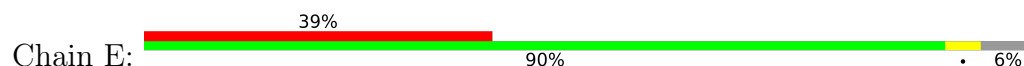
- Molecule 1: Putative dehydratase

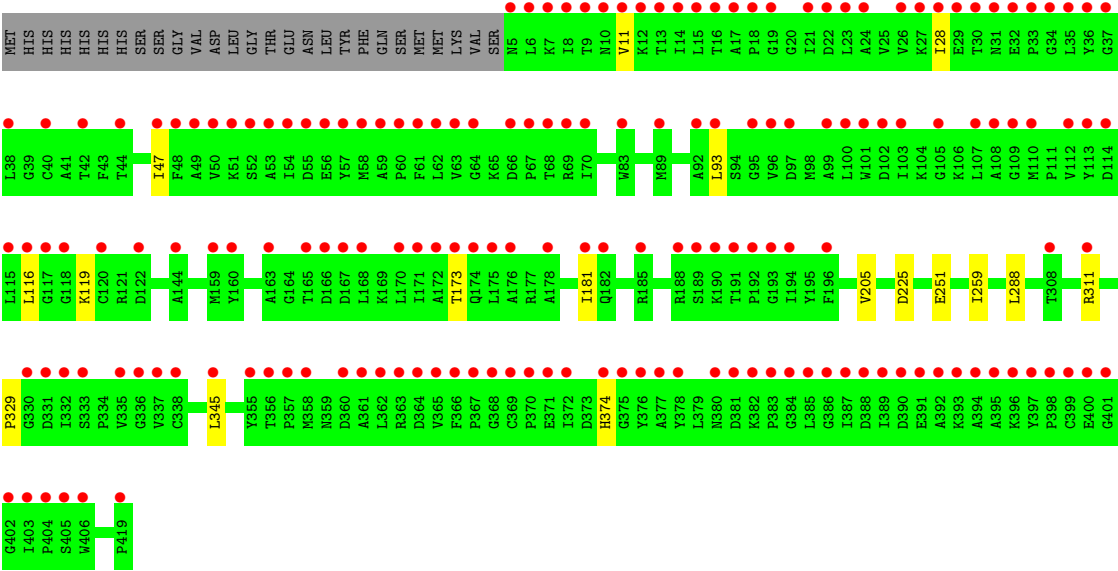


- Molecule 1: Putative dehydratase



- Molecule 1: Putative dehydratase





4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	144.68Å 144.68Å 446.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 50.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-1.80) 100.0 (50.00-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.167 , 0.206 0.168 , 0.206	Depositor DCC
R_{free} test set	6959 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	14.0	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.5	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	18409	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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: CL, GOL, MG

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	0.63	1/3355 (0.0%)	0.81	0/4561
1	B	0.62	1/3357 (0.0%)	0.82	0/4563
1	C	0.63	3/3400 (0.1%)	0.80	0/4617
1	D	0.62	2/3428 (0.1%)	0.82	0/4652
1	E	0.58	1/3328 (0.0%)	0.86	0/4522
All	All	0.62	8/16868 (0.0%)	0.82	0/22915

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	327	HIS	C-O	-5.93	1.16	1.23
1	B	311	ARG	CB-CG	-5.67	1.35	1.52
1	D	300	HIS	C-O	-5.67	1.17	1.24
1	E	205	VAL	CA-CB	5.55	1.57	1.54
1	C	300	HIS	C-O	-5.53	1.17	1.24
1	A	327	HIS	C-O	-5.29	1.17	1.23
1	C	214[A]	ASN	C-O	-5.04	1.18	1.24
1	C	214[B]	ASN	C-O	-5.04	1.18	1.24

There are no bond angle outliers.

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	3256	0	3223	7	0
1	B	3258	0	3222	2	0
1	C	3287	0	3288	4	0
1	D	3305	0	3318	6	0
1	E	3240	0	3210	6	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	12	0	16	0	0
3	B	12	0	16	0	0
3	C	12	0	16	0	0
3	D	12	0	16	0	0
3	E	6	0	8	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	467	0	0	0	0
5	B	410	0	0	0	0
5	C	451	0	0	1	0
5	D	448	0	0	1	0
5	E	226	0	0	1	0
All	All	18409	0	16333	25	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 (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:159[A]:MET:HE3	1:C:160[A]:TYR:CZ	2.37	0.59
1:D:159[A]:MET:HE3	1:D:160[A]:TYR:CE2	2.41	0.56
1:C:116:LEU:HD22	1:C:311[A]:ARG:HD3	1.89	0.54
1:A:131:ASP:H	1:A:141[A]:ASN:HD22	1.59	0.51
1:E:259:ILE:HB	1:E:288:LEU:HD21	1.93	0.50
1:E:181:ILE:HD11	5:E:434:HOH:O	2.12	0.49
1:E:116:LEU:HD22	1:E:311:ARG:HD3	1.94	0.49
1:A:116:LEU:HD22	1:A:311:ARG:HD3	1.95	0.49
1:A:119:LYS:HE2	1:A:345:LEU:HD21	1.98	0.46
1:B:225:ASP:HA	1:B:251:GLU:HB3	1.98	0.46
1:C:74:TRP:CH2	1:C:78[B]:VAL:HG21	2.51	0.46
1:D:259:ILE:HB	1:D:288:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:ILE:HB	1:B:288:LEU:HD21	1.99	0.44
1:A:74:TRP:CH2	1:A:78[B]:VAL:HG21	2.53	0.43
1:E:225:ASP:HA	1:E:251:GLU:HB3	2.01	0.43
1:E:11:VAL:HG22	1:E:28:ILE:HG12	2.01	0.42
1:A:45:GLN:HE21	1:A:45:GLN:H	1.66	0.42
1:D:74:TRP:CH2	1:D:78[B]:VAL:HG21	2.54	0.42
1:A:45:GLN:H	1:A:45:GLN:NE2	2.18	0.41
1:D:418:ARG:HA	1:D:419:PRO:HD3	1.97	0.41
1:D:225:ASP:HA	1:D:251:GLU:HB3	2.02	0.41
1:A:259:ILE:HB	1:A:288:LEU:HD21	2.02	0.41
1:C:51:LYS:HE2	5:C:1343:HOH:O	2.20	0.40
1:E:119:LYS:HE2	1:E:345:LEU:HD21	2.02	0.40
1:D:207:ARG:NH1	5:D:1196:HOH:O	2.38	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	419/442 (95%)	408 (97%)	11 (3%)	0	100	100
1	B	419/442 (95%)	410 (98%)	9 (2%)	0	100	100
1	C	424/442 (96%)	411 (97%)	13 (3%)	0	100	100
1	D	427/442 (97%)	418 (98%)	9 (2%)	0	100	100
1	E	416/442 (94%)	403 (97%)	12 (3%)	1 (0%)	43	31
All	All	2105/2210 (95%)	2050 (97%)	54 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	329	PRO

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	351/370 (95%)	347 (99%)	4 (1%)	65	60
1	B	351/370 (95%)	349 (99%)	2 (1%)	78	77
1	C	356/370 (96%)	355 (100%)	1 (0%)	86	86
1	D	359/370 (97%)	358 (100%)	1 (0%)	86	86
1	E	348/370 (94%)	344 (99%)	4 (1%)	65	60
All	All	1765/1850 (95%)	1753 (99%)	12 (1%)	76	73

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	110	MET
1	A	173	THR
1	A	400	GLU
1	B	47	ILE
1	B	135	GLU
1	C	374	HIS
1	D	171	ILE
1	E	47	ILE
1	E	93	LEU
1	E	173	THR
1	E	374	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	85	ASN
1	A	91	ASN
1	A	244	GLN
1	A	291	ASN
1	B	5	ASN

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Mol	Chain	Res	Type
1	B	237	ASN
1	C	91	ASN
1	C	246	GLN
1	C	291	ASN
1	D	85	ASN
1	D	291	ASN
1	E	5	ASN
1	E	75	GLN
1	E	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 16 ligands modelled in this entry, 7 are monoatomic - leaving 9 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	GOL	D	421	-	5,5,5	0.37	0	5,5,5	0.50	0
3	GOL	B	422	-	5,5,5	0.37	0	5,5,5	0.43	0
3	GOL	C	421	-	5,5,5	0.55	0	5,5,5	0.51	0
3	GOL	C	422	-	5,5,5	0.38	0	5,5,5	0.40	0
3	GOL	B	421	-	5,5,5	0.39	0	5,5,5	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	A	421	-	5,5,5	0.42	0	5,5,5	0.37	0
3	GOL	A	422	-	5,5,5	0.42	0	5,5,5	0.53	0
3	GOL	D	422	-	5,5,5	0.37	0	5,5,5	0.37	0
3	GOL	E	420	-	5,5,5	0.41	0	5,5,5	0.31	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	421	-	-	0/4/4/4	-
3	GOL	B	422	-	-	0/4/4/4	-
3	GOL	C	421	-	-	0/4/4/4	-
3	GOL	C	422	-	-	0/4/4/4	-
3	GOL	B	421	-	-	0/4/4/4	-
3	GOL	A	421	-	-	0/4/4/4	-
3	GOL	A	422	-	-	0/4/4/4	-
3	GOL	D	422	-	-	0/4/4/4	-
3	GOL	E	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	415/442 (93%)	-0.57	3 (0%) 84 85	5, 11, 25, 41	6 (1%)
1	B	415/442 (93%)	-0.51	3 (0%) 84 85	6, 13, 28, 49	6 (1%)
1	C	415/442 (93%)	-0.68	1 (0%) 91 91	5, 10, 21, 41	11 (2%)
1	D	415/442 (93%)	-0.63	0 100 100	4, 11, 23, 40	14 (3%)
1	E	415/442 (93%)	1.57	172 (41%) 0 0	9, 29, 54, 71	3 (0%)
All	All	2075/2210 (93%)	-0.17	179 (8%) 16 14	4, 13, 40, 71	40 (1%)

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	35	LEU	6.1
1	E	36	TYR	5.3
1	E	392	ALA	4.9
1	E	34	GLY	4.9
1	E	63	VAL	4.9
1	E	394	ALA	4.9
1	E	109	GLY	4.8
1	E	107	LEU	4.7
1	E	30	THR	4.6
1	E	6	LEU	4.5
1	E	365	VAL	4.5
1	E	16	THR	4.5
1	E	21	ILE	4.4
1	E	54	ILE	4.4
1	E	28	ILE	4.3
1	E	23	LEU	4.2
1	E	367	PRO	4.2
1	E	395	ALA	4.2
1	E	386	GLY	4.1
1	E	61	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	397	TYR	4.1
1	E	389	ILE	4.1
1	E	53	ALA	4.0
1	E	364	ASP	4.0
1	E	5	ASN	4.0
1	E	59	ALA	3.9
1	E	383	PRO	3.9
1	E	99	ALA	3.8
1	E	168	LEU	3.8
1	E	335	VAL	3.8
1	E	100	LEU	3.8
1	E	108	ALA	3.7
1	E	362	LEU	3.6
1	E	13	THR	3.6
1	E	38	LEU	3.6
1	E	369	CYS	3.6
1	E	48	PHE	3.6
1	E	33	PRO	3.5
1	E	372	ILE	3.5
1	E	15	LEU	3.5
1	E	49	ALA	3.5
1	E	67	PRO	3.5
1	E	68	THR	3.5
1	E	399	CYS	3.4
1	E	103	ILE	3.4
1	E	92	ALA	3.4
1	E	419	PRO	3.4
1	E	403	ILE	3.4
1	E	96	VAL	3.4
1	E	64	GLY	3.4
1	E	24	ALA	3.4
1	E	401	GLY	3.4
1	E	171	ILE	3.3
1	E	393	LYS	3.3
1	E	52	SER	3.3
1	E	382	LYS	3.3
1	E	31	ASN	3.3
1	E	167	ASP	3.3
1	E	387	ILE	3.2
1	E	11	VAL	3.2
1	E	27	LYS	3.2
1	E	172	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	159	MET	3.2
1	E	388	ASP	3.2
1	E	9	THR	3.1
1	E	398	PRO	3.1
1	E	19	GLY	3.1
1	E	366	PHE	3.1
1	E	7	LYS	3.1
1	E	396	LYS	3.1
1	E	58	MET	3.1
1	E	384	GLY	3.1
1	E	110	MET	3.0
1	E	165	THR	3.0
1	E	14	ILE	3.0
1	E	361	ALA	3.0
1	E	12	LYS	3.0
1	E	93	LEU	2.9
1	E	44	THR	2.9
1	E	363	ARG	2.9
1	E	32	GLU	2.9
1	E	62	LEU	2.9
1	E	175	LEU	2.9
1	E	189	SER	2.9
1	E	10	ASN	2.9
1	E	51	LYS	2.9
1	E	181	ILE	2.9
1	E	112	VAL	2.9
1	E	118	GLY	2.9
1	E	368	GLY	2.9
1	E	122	ASP	2.9
1	E	170	LEU	2.9
1	E	380	ASN	2.8
1	E	360	ASP	2.8
1	E	402	GLY	2.8
1	E	173	THR	2.8
1	E	26	VAL	2.8
1	E	66	ASP	2.8
1	E	113	TYR	2.7
1	E	378	TYR	2.7
1	B	181	ILE	2.7
1	C	181	ILE	2.7
1	E	391	GLU	2.7
1	E	56	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	160	TYR	2.7
1	E	114	ASP	2.6
1	E	390	ASP	2.6
1	B	311	ARG	2.6
1	E	116	LEU	2.6
1	E	400	GLU	2.6
1	E	70	ILE	2.6
1	E	355	TYR	2.5
1	E	371	GLU	2.5
1	E	331	ASP	2.5
1	E	105	GLY	2.5
1	E	377	ALA	2.5
1	E	18	PRO	2.5
1	E	358	MET	2.5
1	E	404	PRO	2.5
1	A	5	ASN	2.5
1	E	374	HIS	2.5
1	E	337	VAL	2.5
1	E	376	TYR	2.5
1	E	330	GLY	2.5
1	E	385	LEU	2.5
1	E	406	TRP	2.5
1	E	405	SER	2.4
1	B	171	ILE	2.4
1	E	60	PRO	2.4
1	E	311	ARG	2.4
1	E	47	ILE	2.4
1	E	97	ASP	2.4
1	A	173	THR	2.4
1	E	42	THR	2.4
1	E	356	THR	2.4
1	E	50	VAL	2.4
1	E	40	CYS	2.4
1	E	102	ASP	2.3
1	E	166	ASP	2.3
1	E	101	TRP	2.3
1	E	89	MET	2.3
1	E	192	PRO	2.3
1	E	174	GLN	2.3
1	E	338	CYS	2.3
1	E	191	THR	2.3
1	E	336	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	375	GLY	2.3
1	E	22	ASP	2.3
1	E	69	ARG	2.2
1	E	37	GLY	2.2
1	E	185	ARG	2.2
1	E	29	GLU	2.2
1	E	95	GLY	2.2
1	E	182	GLN	2.2
1	E	178	ALA	2.2
1	E	115	LEU	2.2
1	E	345	LEU	2.2
1	E	117	GLY	2.2
1	E	333	SER	2.2
1	E	163	ALA	2.2
1	E	176	ALA	2.2
1	E	196	PHE	2.2
1	E	83	TRP	2.2
1	E	190	LYS	2.2
1	A	181	ILE	2.1
1	E	194	ILE	2.1
1	E	55	ASP	2.1
1	E	188	ARG	2.1
1	E	370	PRO	2.1
1	E	8	ILE	2.1
1	E	120	CYS	2.1
1	E	17	ALA	2.1
1	E	144	ALA	2.1
1	E	57	TYR	2.1
1	E	332	ILE	2.1
1	E	357	PRO	2.0
1	E	381	ASP	2.0
1	E	193	GLY	2.0
1	E	308	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	E	420	6/6	0.84	0.17	25,34,42,47	0
3	GOL	B	422	6/6	0.92	0.11	16,23,27,27	0
3	GOL	C	422	6/6	0.93	0.11	14,17,20,21	0
3	GOL	D	422	6/6	0.94	0.07	14,17,21,21	0
3	GOL	A	422	6/6	0.94	0.10	10,16,22,24	0
4	CL	A	423	1/1	0.94	0.06	17,17,17,17	0
2	MG	E	421	1/1	0.95	0.05	28,28,28,28	0
3	GOL	A	421	6/6	0.95	0.07	14,14,18,20	0
4	CL	C	423	1/1	0.95	0.07	17,17,17,17	0
3	GOL	C	421	6/6	0.96	0.06	11,12,18,20	0
3	GOL	B	421	6/6	0.96	0.06	11,13,17,22	0
3	GOL	D	421	6/6	0.97	0.05	13,18,21,24	0
2	MG	A	420	1/1	0.99	0.03	12,12,12,12	0
2	MG	B	420	1/1	0.99	0.03	12,12,12,12	0
2	MG	C	420	1/1	0.99	0.03	10,10,10,10	0
2	MG	D	420	1/1	0.99	0.03	12,12,12,12	0

6.5 Other polymers

There are no such residues in this entry.