Full wwPDB X-ray Structure Validation Report ⓘ

Sep 5, 2023 – 07:05 AM EDT

PDB ID	:	3TWA
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:

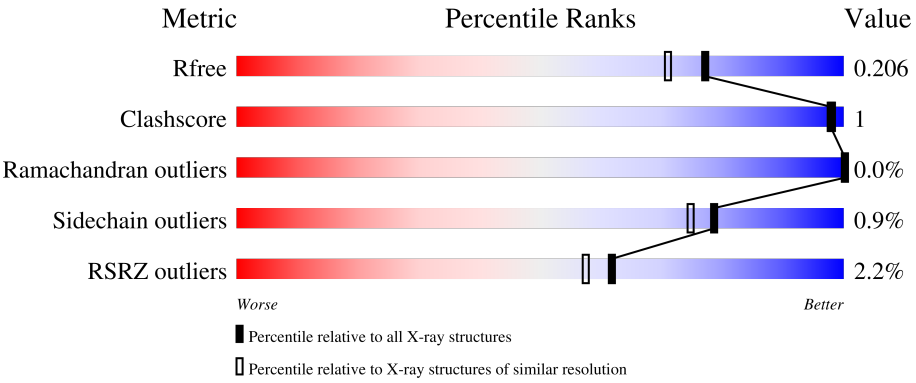
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

1 Overall quality at a glance (i)

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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (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 <=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	90% · 6%
1	B	442	% 93% · 6%
1	C	442	92% · 6%
1	D	442	91% · 6%

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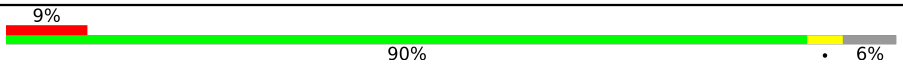
Mol	Chain	Length	Quality of chain
1	E	442	

2 Entry composition (i)

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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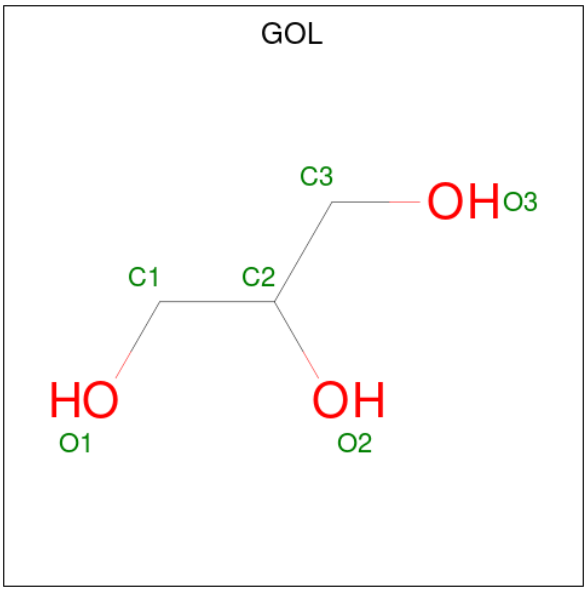
Chain	Residue	Modelled	Actual	Comment	Reference
E	-11	ASP	-	expression tag	UNP B5R541
E	-10	LEU	-	expression tag	UNP B5R541
E	-9	GLY	-	expression tag	UNP B5R541
E	-8	THR	-	expression tag	UNP B5R541
E	-7	GLU	-	expression tag	UNP B5R541
E	-6	ASN	-	expression tag	UNP B5R541
E	-5	LEU	-	expression tag	UNP 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 (three-letter code: 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 (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is water.

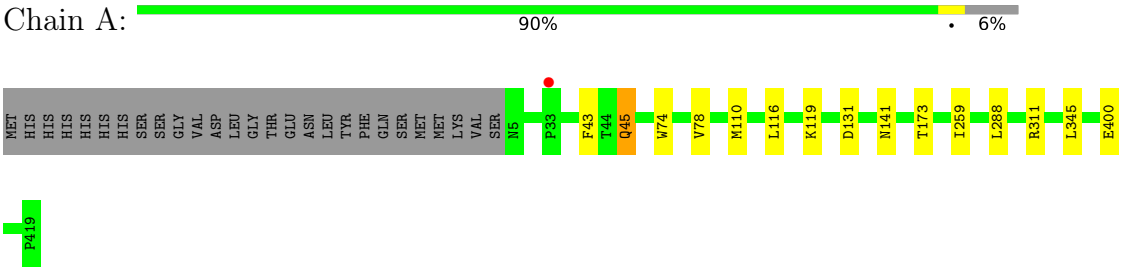
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	467	Total O 467 467	0	1
5	B	410	Total O 410 410	0	1
5	C	451	Total O 451 451	0	1
5	D	448	Total O 448 448	0	1
5	E	226	Total O 226 226	0	0

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.

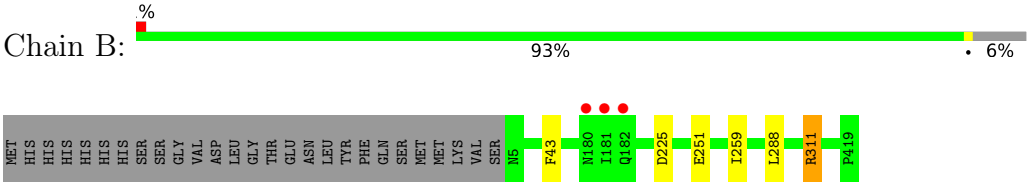
- Molecule 1: Putative dehydratase

Chain A:



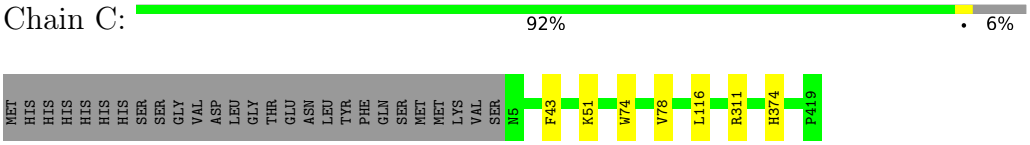
- Molecule 1: Putative dehydratase

Chain B:



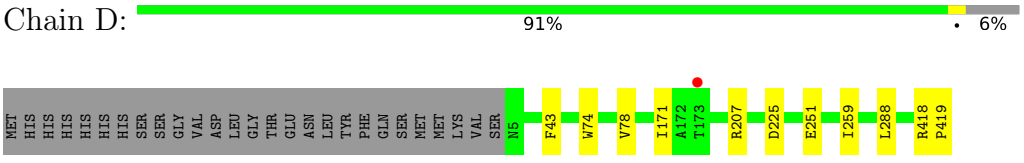
- Molecule 1: Putative dehydratase

Chain C:



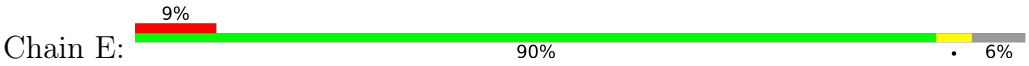
- Molecule 1: Putative dehydratase

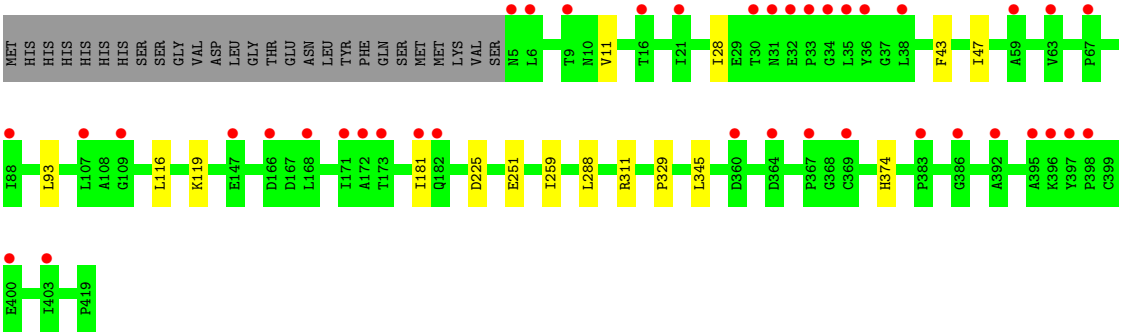
Chain D:



- Molecule 1: Putative dehydratase

Chain E:




MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET MET LYS VAL SER
N5 L6 T9 N10 V11 T16 I21 I28 E29 T30 N31 E32 P33 G34 L35 Y36 G37 L38 F43 I47 A59 V63 P67
I88 L93 L107 A108 G109 L116 K119 E147 D166 D167 L168 I171 A172 T173 I181 Q182 D225 E251 I259 L288 R311 P329 L345 D360 D364 P367 G368 C369 H374 P383 G386 A392 A396 K396 Y397 P398 C399
E400 I403 P419

4 Data and refinement statistics (i)

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 47.95 – 1.76	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-1.80) 99.2 (47.95-1.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$< I/\sigma(I) >$ [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 (3.01%)	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)	0.35 , 41.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	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.*

[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, MG, 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	0.48	0/3355	0.61	0/4561
1	B	0.48	1/3357 (0.0%)	0.62	1/4563 (0.0%)
1	C	0.49	0/3400	0.63	0/4617
1	D	0.47	0/3428	0.62	0/4652
1	E	0.42	0/3328	0.59	0/4522
All	All	0.47	1/16868 (0.0%)	0.61	1/22915 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	311	ARG	CB-CG	-6.34	1.35	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	311	ARG	NE-CZ-NH2	5.71	123.16	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	3256	0	3223	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3258	0	3222	2	0
1	C	3287	0	3288	3	0
1	D	3305	0	3318	5	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	23	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 (23) 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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	47	33
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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	351/370 (95%)	346 (99%)	5 (1%)	67	59
1	B	351/370 (95%)	349 (99%)	2 (1%)	86	84
1	C	356/370 (96%)	354 (99%)	2 (1%)	86	84
1	D	359/370 (97%)	357 (99%)	2 (1%)	86	84
1	E	348/370 (94%)	344 (99%)	4 (1%)	73	68
All	All	1765/1850 (95%)	1750 (99%)	15 (1%)	78	78

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

Mol	Chain	Res	Type
1	A	43	PHE
1	A	45	GLN
1	A	110	MET
1	A	173	THR
1	A	400	GLU
1	B	43	PHE
1	B	311	ARG
1	C	43	PHE
1	C	374	HIS
1	D	43	PHE
1	D	171	ILE
1	E	43	PHE
1	E	47	ILE
1	E	93	LEU
1	E	374	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

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

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Mol	Chain	Res	Type
1	C	91	ASN
1	D	85	ASN
1	D	91	ASN
1	E	75	GLN

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

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	B	421	-	5,5,5	0.39	0	5,5,5	0.51	0
3	GOL	B	422	-	5,5,5	0.35	0	5,5,5	0.42	0
3	GOL	C	422	-	5,5,5	0.36	0	5,5,5	0.40	0
3	GOL	E	420	-	5,5,5	0.41	0	5,5,5	0.27	0
3	GOL	A	422	-	5,5,5	0.40	0	5,5,5	0.52	0
3	GOL	D	421	-	5,5,5	0.36	0	5,5,5	0.47	0
3	GOL	D	422	-	5,5,5	0.35	0	5,5,5	0.36	0
3	GOL	A	421	-	5,5,5	0.41	0	5,5,5	0.35	0
3	GOL	C	421	-	5,5,5	0.54	0	5,5,5	0.47	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	B	421	-	-	0/4/4/4	-
3	GOL	B	422	-	-	0/4/4/4	-
3	GOL	C	422	-	-	0/4/4/4	-
3	GOL	E	420	-	-	0/4/4/4	-
3	GOL	A	422	-	-	0/4/4/4	-
3	GOL	D	421	-	-	0/4/4/4	-
3	GOL	D	422	-	-	0/4/4/4	-
3	GOL	A	421	-	-	0/4/4/4	-
3	GOL	C	421	-	-	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, 95^{th} 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%)	-0.54	1 (0%) 95 93	5, 12, 25, 41	0
1	B	415/442 (93%)	-0.48	3 (0%) 87 86	6, 13, 28, 49	0
1	C	415/442 (93%)	-0.65	0 100 100	5, 11, 22, 41	0
1	D	415/442 (93%)	-0.55	1 (0%) 95 93	5, 12, 23, 40	0
1	E	415/442 (93%)	0.64	40 (9%) 8 6	11, 29, 54, 71	0
All	All	2075/2210 (93%)	-0.32	45 (2%) 62 57	5, 13, 40, 71	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	392	ALA	4.8
1	E	109	GLY	4.0
1	E	36	TYR	3.7
1	E	16	THR	3.7
1	E	30	THR	3.6
1	E	364	ASP	3.5
1	E	35	LEU	3.3
1	E	33	PRO	3.3
1	E	6	LEU	3.3
1	E	31	ASN	3.0
1	B	181	ILE	2.9
1	E	63	VAL	2.9
1	E	171	ILE	2.9
1	E	400	GLU	2.9
1	E	396	LYS	2.9
1	E	181	ILE	2.9
1	E	397	TYR	2.8
1	E	383	PRO	2.8
1	E	5	ASN	2.7
1	E	32	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	398	PRO	2.7
1	E	172	ALA	2.6
1	E	173	THR	2.5
1	E	168	LEU	2.5
1	E	403	ILE	2.5
1	E	147	GLU	2.4
1	E	395	ALA	2.4
1	B	182	GLN	2.4
1	B	180	ASN	2.4
1	E	34	GLY	2.4
1	E	386	GLY	2.4
1	E	369	CYS	2.4
1	E	88	ILE	2.4
1	E	367	PRO	2.3
1	E	166	ASP	2.3
1	E	360	ASP	2.3
1	D	173	THR	2.3
1	E	9	THR	2.2
1	E	59	ALA	2.2
1	E	182	GLN	2.2
1	E	38	LEU	2.2
1	E	21	ILE	2.1
1	E	107	LEU	2.1
1	E	67	PRO	2.1
1	A	33	PRO	2.1

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, 95^{th} 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	0.88	0.20	25,34,42,47	0
3	GOL	B	422	6/6	0.91	0.15	16,23,27,27	0
3	GOL	C	422	6/6	0.93	0.12	14,17,20,21	0
3	GOL	A	422	6/6	0.93	0.13	10,16,22,24	0
3	GOL	D	422	6/6	0.94	0.08	14,17,21,21	0
4	CL	C	423	1/1	0.95	0.09	17,17,17,17	0
2	MG	E	421	1/1	0.96	0.06	28,28,28,28	0
3	GOL	B	421	6/6	0.96	0.08	11,13,17,22	0
3	GOL	A	421	6/6	0.96	0.07	14,14,18,20	0
4	CL	A	423	1/1	0.96	0.11	17,17,17,17	0
3	GOL	C	421	6/6	0.96	0.09	11,12,18,20	0
3	GOL	D	421	6/6	0.97	0.07	13,18,21,24	0
2	MG	A	420	1/1	0.99	0.02	12,12,12,12	0
2	MG	B	420	1/1	1.00	0.02	12,12,12,12	0
2	MG	C	420	1/1	1.00	0.02	10,10,10,10	0
2	MG	D	420	1/1	1.00	0.02	12,12,12,12	0

6.5 Other polymers (i)

There are no such residues in this entry.