



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:30 am BST

PDB ID : 3OW1
Title : Crystal structure of D-mannonate dehydratase from *Chromohalobacter salexigens* complexed with MG
Authors : Fedorov, A.A.; Fedorov, E.V.; Wichelecki, D.; Gerlt, J.A.; Almo, S.C.
Deposited on : 2010-09-17
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 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 : 2.11
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)
Validation Pipeline (wwPDB-VP) : 2.11

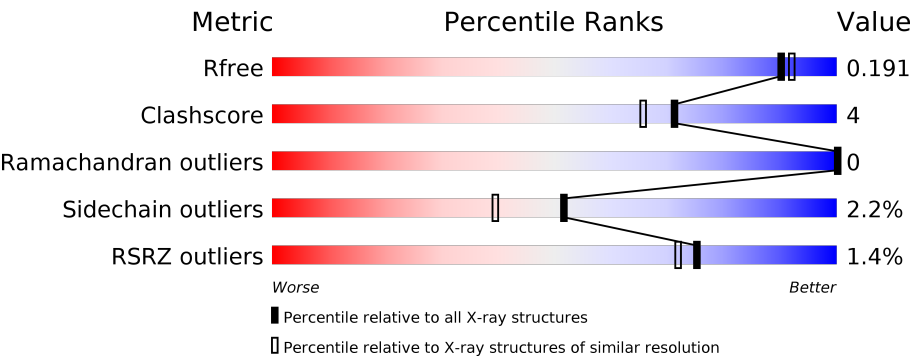
1 Overall quality at a glance i

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 on 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	405	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>85%9%5%</div></div>
1	B	405	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>89%6%</div></div>
1	C	405	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>87%8%</div></div>
1	D	405	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>87%8%</div></div>
1	E	405	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>89%7%</div></div>
1	F	405	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>87%8%</div></div>

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Mol	Chain	Length	Quality of chain
1	G	405	<div><div><div>%</div><div><div></div><div>87%</div><div>6%</div><div>5%</div></div></div></div>
1	H	405	<div><div><div>2%</div><div><div></div><div>87%</div><div>8%</div><div></div></div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26837 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 Mandelate racemase/muconate lactonizing enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	0	0
			3043	1929	545	555	14			
1	B	388	Total	C	N	O	S	0	0	0
			3072	1946	549	563	14			
1	C	387	Total	C	N	O	S	0	0	0
			3063	1941	548	560	14			
1	D	387	Total	C	N	O	S	0	0	0
			3063	1941	548	560	14			
1	E	389	Total	C	N	O	S	0	0	0
			3078	1949	550	565	14			
1	F	387	Total	C	N	O	S	0	1	0
			3074	1947	552	561	14			
1	G	383	Total	C	N	O	S	0	0	0
			3037	1926	544	553	14			
1	H	387	Total	C	N	O	S	0	0	0
			3063	1941	548	560	14			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP Q1QT89
A	2	SER	-	EXPRESSION TAG	UNP Q1QT89
A	3	LEU	-	EXPRESSION TAG	UNP Q1QT89
B	1	MET	-	EXPRESSION TAG	UNP Q1QT89
B	2	SER	-	EXPRESSION TAG	UNP Q1QT89
B	3	LEU	-	EXPRESSION TAG	UNP Q1QT89
C	1	MET	-	EXPRESSION TAG	UNP Q1QT89
C	2	SER	-	EXPRESSION TAG	UNP Q1QT89
C	3	LEU	-	EXPRESSION TAG	UNP Q1QT89
D	1	MET	-	EXPRESSION TAG	UNP Q1QT89
D	2	SER	-	EXPRESSION TAG	UNP Q1QT89
D	3	LEU	-	EXPRESSION TAG	UNP Q1QT89
E	1	MET	-	EXPRESSION TAG	UNP Q1QT89

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Chain	Residue	Modelled	Actual	Comment	Reference
E	2	SER	-	EXPRESSION TAG	UNP Q1QT89
E	3	LEU	-	EXPRESSION TAG	UNP Q1QT89
F	1	MET	-	EXPRESSION TAG	UNP Q1QT89
F	2	SER	-	EXPRESSION TAG	UNP Q1QT89
F	3	LEU	-	EXPRESSION TAG	UNP Q1QT89
G	1	MET	-	EXPRESSION TAG	UNP Q1QT89
G	2	SER	-	EXPRESSION TAG	UNP Q1QT89
G	3	LEU	-	EXPRESSION TAG	UNP Q1QT89
H	1	MET	-	EXPRESSION TAG	UNP Q1QT89
H	2	SER	-	EXPRESSION TAG	UNP Q1QT89
H	3	LEU	-	EXPRESSION TAG	UNP Q1QT89

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	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
2	H	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	A	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: 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	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	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	O	S	0	0
			5	4	1		

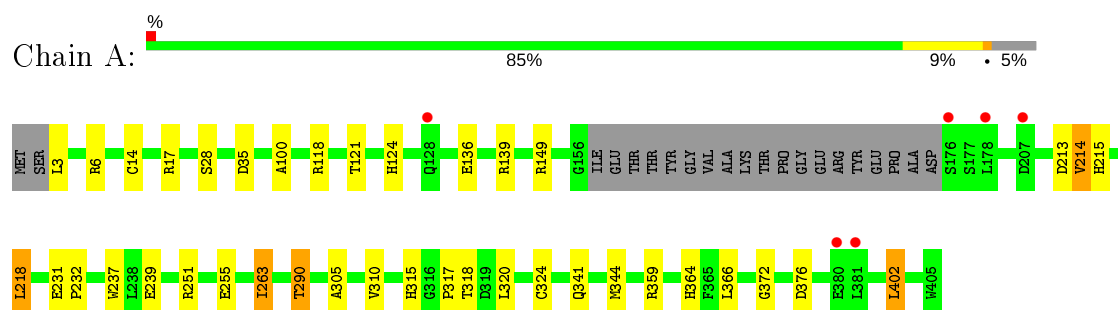
- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	265	Total	O		0	0
			265	265			
5	B	284	Total	O		0	0
			284	284			
5	C	284	Total	O		0	0
			284	284			
5	D	284	Total	O		0	0
			284	284			
5	E	274	Total	O		0	0
			274	274			
5	F	272	Total	O		0	0
			272	272			
5	G	249	Total	O		0	0
			249	249			
5	H	283	Total	O		0	0
			283	283			

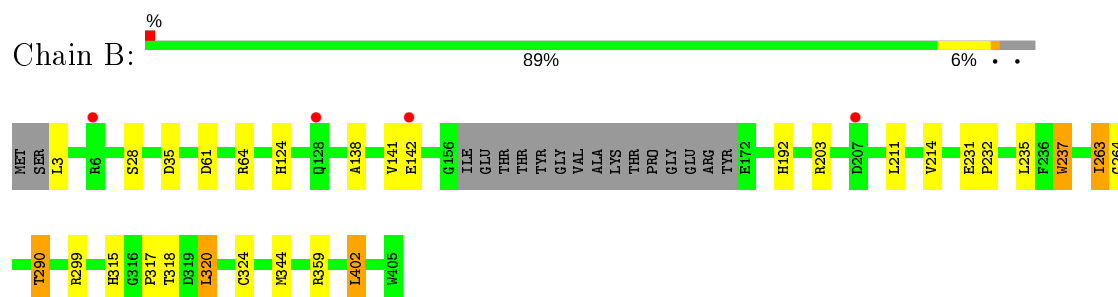
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

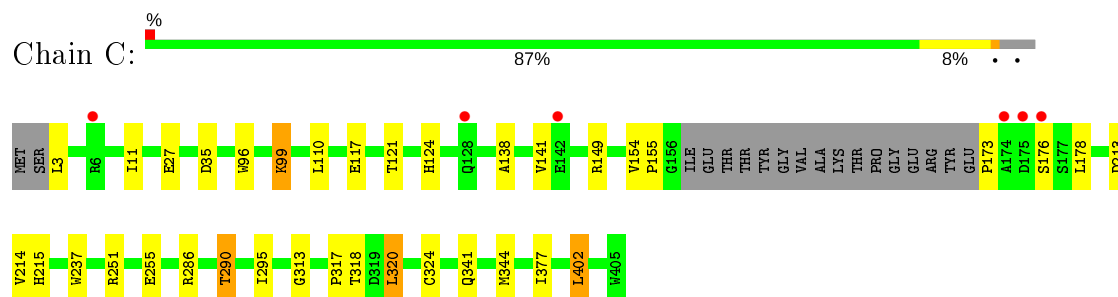
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



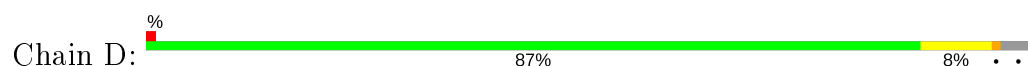
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

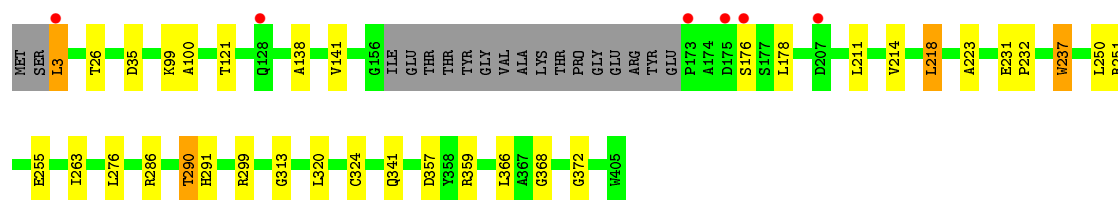


- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

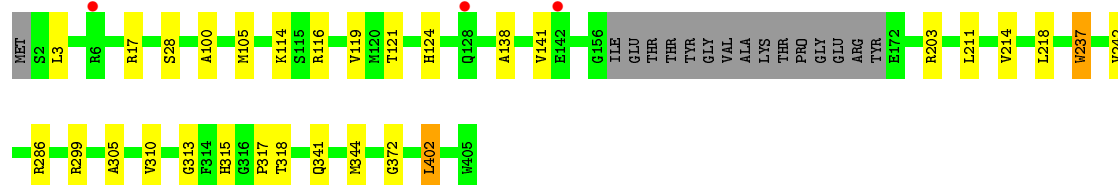
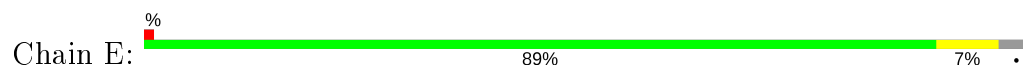


- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

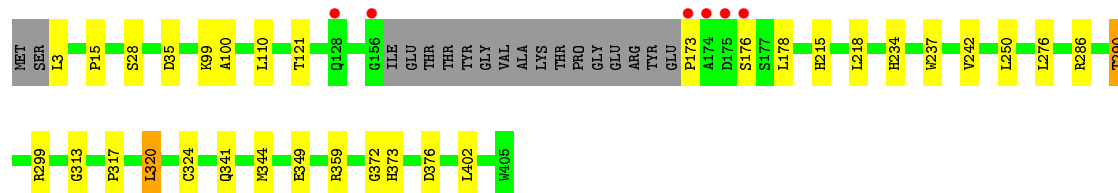
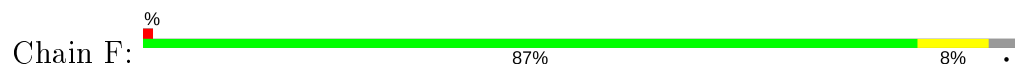




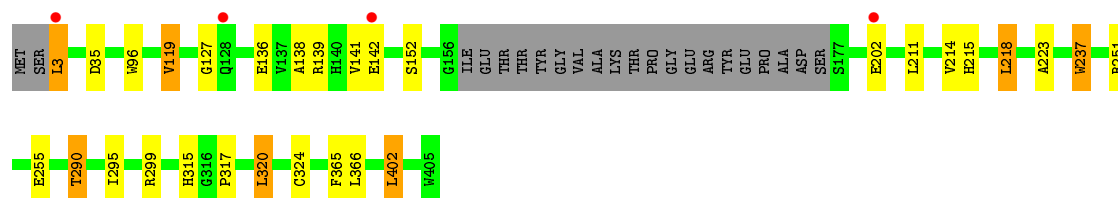
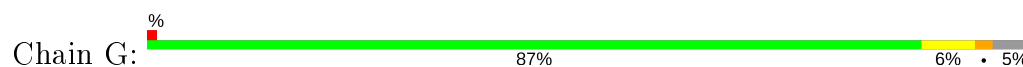
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



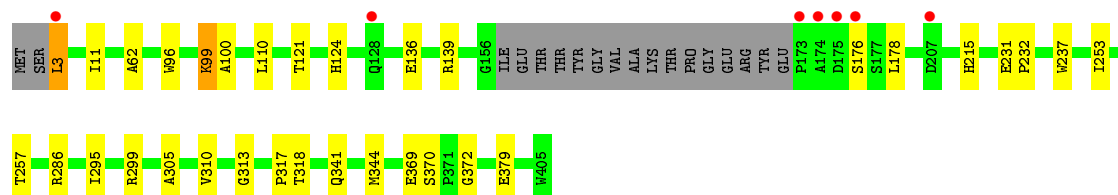
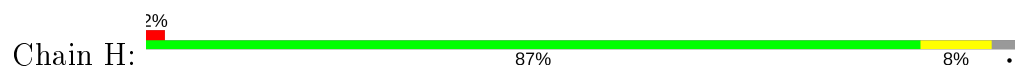
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.58 Å 177.79 Å 109.99 Å 90.00° 102.62° 90.00°	Depositor
Resolution (Å)	35.17 – 1.80 35.17 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.5 (35.17-1.80) 98.5 (35.17-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 1.79 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.161 , 0.194 0.159 , 0.191	Depositor DCC
R_{free} test set	14933 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	26837	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, SO4

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	0.35	0/3128	0.54	1/4259 (0.0%)
1	B	0.36	0/3158	0.55	1/4301 (0.0%)
1	C	0.36	0/3149	0.54	1/4288 (0.0%)
1	D	0.35	0/3149	0.53	0/4288
1	E	0.36	0/3164	0.55	1/4309 (0.0%)
1	F	0.35	0/3160	0.53	1/4302 (0.0%)
1	G	0.34	0/3122	0.53	1/4251 (0.0%)
1	H	0.38	0/3149	0.54	0/4288
All	All	0.36	0/25179	0.54	6/34286 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	402	LEU	CA-CB-CG	-7.46	98.15	115.30
1	E	402	LEU	CA-CB-CG	-7.17	98.82	115.30
1	A	402	LEU	CA-CB-CG	-6.02	101.45	115.30
1	G	402	LEU	CA-CB-CG	-5.61	102.39	115.30
1	C	402	LEU	CA-CB-CG	-5.47	102.71	115.30
1	F	402	LEU	CA-CB-CG	-5.16	103.42	115.30

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	3043	0	2936	29	0
1	B	3072	0	2958	23	0
1	C	3063	0	2953	19	0
1	D	3063	0	2953	26	0
1	E	3078	0	2963	15	0
1	F	3074	0	2965	19	0
1	G	3037	0	2931	22	0
1	H	3063	0	2953	20	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
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	12	0	16	0	0
3	B	6	0	8	0	0
3	C	12	0	16	0	0
3	D	6	0	8	0	0
3	E	6	0	8	0	0
3	F	6	0	8	0	0
3	G	6	0	8	0	0
3	H	12	0	16	3	0
4	A	10	0	0	0	0
4	B	5	0	0	0	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
4	E	5	0	0	0	0
4	F	10	0	0	0	0
4	G	15	0	0	0	0
4	H	10	0	0	0	0
5	A	265	0	0	4	0
5	B	284	0	0	5	0
5	C	284	0	0	1	0
5	D	284	0	0	2	0
5	E	274	0	0	1	0
5	F	272	0	0	3	0
5	G	249	0	0	1	0
5	H	283	0	0	1	0
All	All	26837	0	23700	171	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 4.

All (171) 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:250:LEU:HD22	1:D:276:LEU:HD22	1.52	0.89
1:G:290:THR:HG22	1:G:324:CYS:SG	2.14	0.88
1:A:290:THR:HG22	1:A:324:CYS:SG	2.18	0.83
1:B:263:ILE:HD11	5:B:2092:HOH:O	1.79	0.83
1:D:290:THR:HG22	1:D:324:CYS:SG	2.20	0.80
1:C:290:THR:HG22	1:C:324:CYS:SG	2.22	0.79
1:H:136:GLU:OE2	1:H:139:ARG:HD3	1.83	0.78
1:E:318:THR:H	1:E:344:MET:HE2	1.54	0.72
1:A:3:LEU:HD13	1:A:28:SER:HB3	1.70	0.72
1:E:3:LEU:HD13	1:E:28:SER:HB3	1.72	0.71
1:B:290:THR:HG22	1:B:324:CYS:SG	2.31	0.71
1:F:99:LYS:HG2	1:F:110:LEU:HD21	1.73	0.70
1:C:176:SER:HB2	1:C:178:LEU:O	1.95	0.66
1:H:3:LEU:HD13	1:H:62:ALA:HB3	1.78	0.66
1:C:3:LEU:HB3	1:C:27:GLU:HG2	1.79	0.65
1:F:290:THR:HG22	1:F:324:CYS:SG	2.38	0.64
3:H:408:GOL:H32	5:H:1059:HOH:O	1.98	0.63
1:B:124:HIS:CE1	1:B:344:MET:SD	2.93	0.62
1:B:138:ALA:O	1:B:142:GLU:HG2	2.00	0.61
1:B:3:LEU:HD13	1:B:28:SER:HB3	1.83	0.61
1:A:290:THR:HG23	1:A:320:LEU:HD22	1.82	0.61
1:A:118:ARG:HD2	1:A:364:HIS:CD2	2.36	0.60
1:A:359:ARG:NH2	5:A:2216:HOH:O	2.36	0.59
1:G:119:VAL:HG22	1:G:365:PHE:HB2	1.84	0.58
1:B:290:THR:CG2	1:B:324:CYS:SG	2.92	0.57
1:A:136:GLU:HA	1:A:139:ARG:HG2	1.86	0.57
1:A:214:VAL:HG21	1:A:218:LEU:HD22	1.86	0.57
1:C:290:THR:CG2	1:C:324:CYS:SG	2.92	0.57
1:B:317:PRO:HD2	1:B:320:LEU:HD22	1.86	0.57
1:A:318:THR:H	1:A:344:MET:HE2	1.70	0.56
1:G:214:VAL:HG11	1:G:218:LEU:HD22	1.87	0.56
1:C:11:ILE:HD12	1:C:377:ILE:HD13	1.87	0.56
1:F:3:LEU:HD13	1:F:28:SER:HB3	1.86	0.56
1:B:263:ILE:HD13	1:B:264:GLY:N	2.20	0.56
1:B:203:ARG:HD3	5:B:2303:HOH:O	2.05	0.56
1:C:318:THR:HG23	1:C:344:MET:HE2	1.86	0.56
1:D:290:THR:CG2	1:D:324:CYS:SG	2.93	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:THR:HG23	1:A:344:MET:HE2	1.89	0.55
1:H:136:GLU:HA	1:H:139:ARG:HG2	1.88	0.55
1:F:299:ARG:HD3	1:H:299:ARG:HD3	1.88	0.55
1:D:359:ARG:HG2	5:D:2228:HOH:O	2.07	0.54
1:E:124:HIS:CE1	1:E:344:MET:SD	3.00	0.54
1:H:124:HIS:CE1	1:H:344:MET:SD	3.01	0.54
1:G:142:GLU:HG2	5:G:859:HOH:O	2.07	0.54
1:E:114:LYS:HG2	1:E:116:ARG:O	2.08	0.54
1:B:359:ARG:NH2	5:B:662:HOH:O	2.41	0.54
1:E:203:ARG:HD3	5:E:1668:HOH:O	2.08	0.53
1:C:124:HIS:CE1	1:C:344:MET:SD	3.01	0.53
1:B:263:ILE:HD13	1:B:264:GLY:H	1.74	0.53
1:D:3:LEU:HD12	1:D:26:THR:HG21	1.88	0.53
1:A:136:GLU:OE2	1:A:139:ARG:HD3	2.09	0.53
1:C:35:ASP:OD2	1:C:290:THR:HG21	2.08	0.53
1:C:173:PRO:N	5:C:1383:HOH:O	2.42	0.52
1:D:251:ARG:NH1	1:D:255:GLU:OE2	2.43	0.52
1:H:286:ARG:HD2	1:H:313:GLY:O	2.09	0.52
1:A:359:ARG:HG2	5:A:2216:HOH:O	2.08	0.52
1:E:3:LEU:CD1	1:E:28:SER:HB3	2.38	0.52
1:B:138:ALA:O	1:B:141:VAL:HG22	2.09	0.52
1:G:136:GLU:OE2	1:G:139:ARG:HD3	2.10	0.51
1:C:121:THR:HA	1:C:341:GLN:O	2.10	0.51
1:D:290:THR:HG23	1:D:320:LEU:HD22	1.92	0.51
1:D:359:ARG:NH2	5:D:2228:HOH:O	2.44	0.51
1:G:317:PRO:HD2	1:G:320:LEU:HD22	1.92	0.51
1:G:290:THR:CG2	1:G:324:CYS:SG	2.94	0.51
1:A:35:ASP:OD2	1:A:290:THR:HG21	2.11	0.51
1:B:299:ARG:NH1	1:G:299:ARG:NH1	2.58	0.51
1:A:263:ILE:HD11	5:A:2125:HOH:O	2.10	0.51
1:F:317:PRO:HA	1:F:344:MET:SD	2.52	0.50
1:D:299:ARG:HD3	1:E:299:ARG:HD3	1.93	0.50
1:B:315:HIS:CE1	1:B:317:PRO:HG3	2.47	0.50
1:G:3:LEU:N	1:G:3:LEU:HD22	2.27	0.50
1:A:14:CYS:HA	1:A:17:ARG:O	2.12	0.49
1:B:35:ASP:OD2	1:B:290:THR:HG21	2.12	0.49
1:B:359:ARG:HG2	5:B:662:HOH:O	2.10	0.49
1:E:315:HIS:CE1	1:E:317:PRO:HG3	2.47	0.49
1:H:305:ALA:HB1	1:H:310:VAL:HB	1.94	0.49
1:A:318:THR:HG23	1:A:344:MET:CE	2.43	0.49
1:D:100:ALA:HB3	1:D:372:GLY:HA2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:317:PRO:HD2	1:F:320:LEU:HD22	1.94	0.49
1:C:286:ARG:HD2	1:C:313:GLY:O	2.13	0.48
1:D:35:ASP:OD2	1:D:290:THR:HG21	2.12	0.48
1:F:176:SER:HB2	1:F:178:LEU:O	2.13	0.48
1:A:3:LEU:CD1	1:A:28:SER:HB3	2.42	0.47
1:B:61:ASP:HB3	1:B:64:ARG:HG3	1.95	0.47
1:C:317:PRO:HD2	1:C:320:LEU:HD22	1.95	0.47
1:H:317:PRO:HA	1:H:344:MET:SD	2.55	0.47
1:F:35:ASP:OD2	1:F:290:THR:HG21	2.14	0.47
1:G:366:LEU:HD22	1:G:366:LEU:N	2.30	0.47
1:H:121:THR:HA	1:H:341:GLN:O	2.14	0.47
1:D:286:ARG:HD2	1:D:313:GLY:O	2.15	0.47
1:C:290:THR:HG23	1:C:320:LEU:HG	1.96	0.47
1:F:290:THR:CG2	1:F:324:CYS:SG	3.03	0.47
1:F:218:LEU:O	1:F:242:VAL:HG12	2.15	0.47
1:G:3:LEU:O	1:G:3:LEU:HD23	2.15	0.47
1:A:231:GLU:N	1:A:232:PRO:CD	2.78	0.46
1:D:218:LEU:HD23	1:D:223:ALA:HA	1.98	0.46
1:B:318:THR:H	1:B:344:MET:HE2	1.79	0.46
1:E:211:LEU:HD23	1:E:237:TRP:CE2	2.50	0.46
1:F:100:ALA:HB3	1:F:372:GLY:HA2	1.98	0.46
1:D:231:GLU:N	1:D:232:PRO:CD	2.79	0.45
1:F:121:THR:HA	1:F:341:GLN:O	2.17	0.45
1:G:35:ASP:OD2	1:G:290:THR:HG21	2.17	0.45
1:A:149:ARG:HD2	1:A:213:ASP:HB2	1.97	0.45
1:G:251:ARG:NH1	1:G:255:GLU:OE2	2.49	0.45
1:H:176:SER:HB2	1:H:178:LEU:O	2.16	0.45
1:F:234:HIS:HD2	5:F:2298:HOH:O	1.99	0.45
1:H:99:LYS:HG2	1:H:110:LEU:HD21	1.99	0.45
1:G:290:THR:HG23	1:G:320:LEU:HG	1.99	0.45
1:C:251:ARG:NH1	1:C:255:GLU:OE2	2.50	0.45
1:H:318:THR:H	1:H:344:MET:HE2	1.81	0.45
1:D:176:SER:HB2	1:D:178:LEU:O	2.17	0.45
1:A:100:ALA:HB3	1:A:372:GLY:HA2	1.98	0.45
1:F:15:PRO:O	1:F:349:GLU:HG2	2.17	0.45
1:H:253:ILE:O	1:H:257:THR:HG22	2.17	0.45
1:E:121:THR:HA	1:E:341:GLN:O	2.17	0.44
1:H:11:ILE:HD13	1:H:379:GLU:HG2	2.00	0.44
1:A:124:HIS:CE1	1:A:344:MET:SD	3.10	0.44
1:C:149:ARG:HD2	1:C:213:ASP:HB2	1.99	0.44
1:A:214:VAL:HG13	1:A:239:GLU:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:ALA:O	1:D:141:VAL:HG22	2.18	0.44
1:E:286:ARG:HD2	1:E:313:GLY:O	2.18	0.44
1:G:211:LEU:HD23	1:G:237:TRP:CE2	2.53	0.44
1:A:290:THR:CG2	1:A:324:CYS:SG	2.98	0.44
1:D:211:LEU:HD23	1:D:237:TRP:CE2	2.53	0.44
1:A:315:HIS:CE1	1:A:317:PRO:HG3	2.53	0.43
1:G:290:THR:CG2	1:G:320:LEU:HG	2.48	0.43
1:D:290:THR:HG22	1:D:324:CYS:CB	2.48	0.43
1:G:138:ALA:O	1:G:141:VAL:HG22	2.18	0.43
1:B:290:THR:HG23	1:B:320:LEU:HG	2.00	0.43
1:D:138:ALA:HA	1:D:141:VAL:HG22	2.00	0.43
1:G:315:HIS:CE1	1:G:317:PRO:HG3	2.53	0.43
1:A:366:LEU:N	1:A:366:LEU:HD22	2.33	0.43
1:D:290:THR:CG2	1:D:324:CYS:HB2	2.48	0.43
1:C:138:ALA:O	1:C:141:VAL:HG22	2.19	0.43
1:D:211:LEU:HD12	1:D:211:LEU:N	2.33	0.43
1:E:305:ALA:HB1	1:E:310:VAL:HB	2.01	0.43
1:A:251:ARG:NH1	1:A:255:GLU:OE2	2.52	0.43
1:D:121:THR:HA	1:D:341:GLN:O	2.19	0.43
1:G:127:GLY:O	1:G:152:SER:HA	2.19	0.43
1:H:96:TRP:CD1	1:H:295:ILE:HB	2.54	0.43
1:H:100:ALA:HB3	1:H:372:GLY:HA2	2.00	0.43
1:D:290:THR:HG22	1:D:324:CYS:HB2	2.00	0.43
1:F:286:ARG:HD2	1:F:313:GLY:O	2.19	0.42
1:A:290:THR:CG2	1:A:320:LEU:HD22	2.49	0.42
1:A:121:THR:HA	1:A:341:GLN:O	2.20	0.42
1:G:96:TRP:CD1	1:G:295:ILE:HB	2.55	0.42
1:F:173:PRO:HD2	5:F:1122:HOH:O	2.20	0.42
1:A:305:ALA:HB1	1:A:310:VAL:HB	2.01	0.41
1:A:6:ARG:NH2	5:A:2217:HOH:O	2.53	0.41
1:H:3:LEU:N	1:H:3:LEU:HD12	2.35	0.41
1:G:218:LEU:HD23	1:G:223:ALA:HA	2.03	0.41
1:C:99:LYS:HG2	1:C:110:LEU:HD21	2.03	0.41
1:D:357:ASP:OD2	1:D:368:GLY:HA3	2.21	0.41
1:H:370:SER:N	3:H:408:GOL:H31	2.36	0.41
1:B:192:HIS:HD2	5:B:2219:HOH:O	2.03	0.41
1:B:231:GLU:N	1:B:232:PRO:CD	2.83	0.41
1:E:100:ALA:HB3	1:E:372:GLY:HA2	2.02	0.41
1:F:290:THR:HG23	1:F:320:LEU:HG	2.03	0.41
1:H:231:GLU:N	1:H:232:PRO:CD	2.84	0.41
1:F:359:ARG:NH2	5:F:413:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:250:LEU:HG	1:F:276:LEU:HD22	2.03	0.41
1:H:369:GLU:HB2	3:H:408:GOL:H2	2.02	0.41
1:G:251:ARG:O	1:G:255:GLU:HG3	2.21	0.40
1:B:211:LEU:HD23	1:B:237:TRP:CE2	2.56	0.40
1:D:291:HIS:CE1	1:D:320:LEU:HD21	2.57	0.40
1:E:138:ALA:O	1:E:141:VAL:HG22	2.20	0.40
1:C:154:VAL:HA	1:C:155:PRO:HD3	1.92	0.40
1:C:96:TRP:CD1	1:C:295:ILE:HB	2.55	0.40
1:B:263:ILE:CD1	1:B:264:GLY:N	2.84	0.40
1:D:366:LEU:N	1:D:366:LEU:HD22	2.36	0.40
1:E:218:LEU:O	1:E:242:VAL:HG12	2.22	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	380/405 (94%)	368 (97%)	12 (3%)	0	100	100
1	B	384/405 (95%)	375 (98%)	9 (2%)	0	100	100
1	C	383/405 (95%)	368 (96%)	15 (4%)	0	100	100
1	D	383/405 (95%)	370 (97%)	13 (3%)	0	100	100
1	E	385/405 (95%)	376 (98%)	9 (2%)	0	100	100
1	F	384/405 (95%)	375 (98%)	9 (2%)	0	100	100
1	G	379/405 (94%)	368 (97%)	11 (3%)	0	100	100
1	H	383/405 (95%)	373 (97%)	10 (3%)	0	100	100
All	All	3061/3240 (94%)	2973 (97%)	88 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	315/332 (95%)	307 (98%)	8 (2%)	47	34
1	B	318/332 (96%)	311 (98%)	7 (2%)	52	39
1	C	317/332 (96%)	309 (98%)	8 (2%)	47	34
1	D	317/332 (96%)	310 (98%)	7 (2%)	52	39
1	E	319/332 (96%)	313 (98%)	6 (2%)	57	46
1	F	318/332 (96%)	312 (98%)	6 (2%)	57	46
1	G	314/332 (95%)	305 (97%)	9 (3%)	42	29
1	H	317/332 (96%)	313 (99%)	4 (1%)	69	62
All	All	2535/2656 (95%)	2480 (98%)	55 (2%)	52	39

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	VAL
1	A	215	HIS
1	A	218	LEU
1	A	237	TRP
1	A	263	ILE
1	A	290	THR
1	A	376	ASP
1	A	402	LEU
1	B	214	VAL
1	B	235	LEU
1	B	237	TRP
1	B	263	ILE
1	B	290	THR
1	B	320	LEU
1	B	402	LEU
1	C	99	LYS
1	C	117	GLU
1	C	214	VAL
1	C	215	HIS

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Mol	Chain	Res	Type
1	C	237	TRP
1	C	290	THR
1	C	320	LEU
1	C	402	LEU
1	D	3	LEU
1	D	99	LYS
1	D	214	VAL
1	D	218	LEU
1	D	237	TRP
1	D	263	ILE
1	D	290	THR
1	E	17	ARG
1	E	105	MET
1	E	119	VAL
1	E	214	VAL
1	E	237	TRP
1	E	402	LEU
1	F	215	HIS
1	F	237	TRP
1	F	290	THR
1	F	320	LEU
1	F	373	HIS
1	F	376	ASP
1	G	3	LEU
1	G	119	VAL
1	G	202	GLU
1	G	215	HIS
1	G	218	LEU
1	G	237	TRP
1	G	290	THR
1	G	320	LEU
1	G	402	LEU
1	H	3	LEU
1	H	99	LYS
1	H	215	HIS
1	H	237	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	341	GLN
1	F	234	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 34 ligands modelled in this entry, 8 are monoatomic - leaving 26 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	$\# Z > 2$
4	SO4	G	409	-	4,4,4	0.17	0	6,6,6	0.08	0
4	SO4	A	410	-	4,4,4	0.16	0	6,6,6	0.12	0
4	SO4	C	409	-	4,4,4	0.11	0	6,6,6	0.11	0
4	SO4	H	410	-	4,4,4	0.14	0	6,6,6	0.18	0
4	SO4	H	409	-	4,4,4	0.19	0	6,6,6	0.18	0
4	SO4	F	408	-	4,4,4	0.19	0	6,6,6	0.09	0
3	GOL	B	407	-	5,5,5	0.50	0	5,5,5	0.40	0
3	GOL	F	407	-	5,5,5	0.44	0	5,5,5	0.52	0
3	GOL	D	407	-	5,5,5	0.45	0	5,5,5	0.23	0
4	SO4	F	409	-	4,4,4	0.14	0	6,6,6	0.22	0
4	SO4	C	410	-	4,4,4	0.14	0	6,6,6	0.14	0
4	SO4	G	410	-	4,4,4	0.17	0	6,6,6	0.05	0
4	SO4	B	408	-	4,4,4	0.13	0	6,6,6	0.16	0
3	GOL	C	407	-	5,5,5	0.43	0	5,5,5	0.33	0
3	GOL	A	408	-	5,5,5	0.31	0	5,5,5	0.38	0
3	GOL	G	407	-	5,5,5	0.38	0	5,5,5	0.47	0
3	GOL	E	407	-	5,5,5	0.41	0	5,5,5	0.22	0
4	SO4	D	409	-	4,4,4	0.13	0	6,6,6	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	H	408	-	5,5,5	0.33	0	5,5,5	0.30	0
4	SO4	E	408	-	4,4,4	0.16	0	6,6,6	0.10	0
4	SO4	G	408	-	4,4,4	0.15	0	6,6,6	0.13	0
4	SO4	D	408	-	4,4,4	0.17	0	6,6,6	0.09	0
3	GOL	H	407	-	5,5,5	0.49	0	5,5,5	0.49	0
4	SO4	A	409	-	4,4,4	0.16	0	6,6,6	0.11	0
3	GOL	A	407	-	5,5,5	0.38	0	5,5,5	0.44	0
3	GOL	C	408	-	5,5,5	0.34	0	5,5,5	0.40	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	H	407	-	-	2/4/4/4	-
3	GOL	F	407	-	-	4/4/4/4	-
3	GOL	B	407	-	-	4/4/4/4	-
3	GOL	C	407	-	-	4/4/4/4	-
3	GOL	A	408	-	-	2/4/4/4	-
3	GOL	A	407	-	-	4/4/4/4	-
3	GOL	D	407	-	-	4/4/4/4	-
3	GOL	G	407	-	-	4/4/4/4	-
3	GOL	E	407	-	-	4/4/4/4	-
3	GOL	C	408	-	-	2/4/4/4	-
3	GOL	H	408	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	407	GOL	O1-C1-C2-C3
3	F	407	GOL	O1-C1-C2-C3
3	D	407	GOL	O1-C1-C2-C3
3	C	407	GOL	O1-C1-C2-C3
3	A	408	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	G	407	GOL	C1-C2-C3-O3
3	E	407	GOL	O1-C1-C2-C3
3	E	407	GOL	O2-C2-C3-O3
3	H	408	GOL	O1-C1-C2-C3
3	A	407	GOL	O1-C1-C2-C3
3	C	408	GOL	O1-C1-C2-C3
3	G	407	GOL	O1-C1-C2-O2
3	A	407	GOL	O2-C2-C3-O3
3	B	407	GOL	C1-C2-C3-O3
3	F	407	GOL	C1-C2-C3-O3
3	D	407	GOL	C1-C2-C3-O3
3	C	407	GOL	C1-C2-C3-O3
3	G	407	GOL	O1-C1-C2-C3
3	E	407	GOL	C1-C2-C3-O3
3	H	407	GOL	C1-C2-C3-O3
3	A	407	GOL	C1-C2-C3-O3
3	B	407	GOL	O1-C1-C2-O2
3	F	407	GOL	O1-C1-C2-O2
3	F	407	GOL	O2-C2-C3-O3
3	D	407	GOL	O1-C1-C2-O2
3	C	407	GOL	O2-C2-C3-O3
3	A	408	GOL	O1-C1-C2-O2
3	E	407	GOL	O1-C1-C2-O2
3	H	407	GOL	O2-C2-C3-O3
3	A	407	GOL	O1-C1-C2-O2
3	C	407	GOL	O1-C1-C2-O2
3	G	407	GOL	O2-C2-C3-O3
3	H	408	GOL	C1-C2-C3-O3
3	B	407	GOL	O2-C2-C3-O3
3	C	408	GOL	O1-C1-C2-O2
3	D	407	GOL	O2-C2-C3-O3
3	H	408	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	408	GOL	3	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	384/405 (94%)	-0.13	6 (1%) 72 68	14, 20, 34, 43	0
1	B	388/405 (95%)	-0.23	4 (1%) 82 80	13, 19, 31, 42	0
1	C	387/405 (95%)	-0.28	6 (1%) 72 68	13, 18, 31, 46	0
1	D	387/405 (95%)	-0.26	6 (1%) 72 68	13, 19, 32, 43	0
1	E	389/405 (96%)	-0.33	3 (0%) 86 84	13, 19, 32, 43	0
1	F	387/405 (95%)	-0.22	6 (1%) 72 68	14, 19, 32, 50	0
1	G	383/405 (94%)	-0.30	4 (1%) 82 80	14, 20, 33, 45	0
1	H	387/405 (95%)	-0.35	7 (1%) 68 64	13, 17, 29, 43	0
All	All	3092/3240 (95%)	-0.26	42 (1%) 75 72	13, 19, 32, 50	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	176	SER	8.6
1	A	176	SER	6.3
1	F	176	SER	5.9
1	H	175	ASP	5.7
1	C	175	ASP	5.3
1	F	175	ASP	5.1
1	H	176	SER	4.9
1	F	173	PRO	4.5
1	C	174	ALA	4.5
1	F	174	ALA	4.1
1	D	176	SER	4.0
1	E	142	GLU	3.6
1	D	207	ASP	3.5
1	H	173	PRO	3.5
1	H	3	LEU	3.4
1	D	175	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	178	LEU	3.0
1	E	128	GLN	3.0
1	A	128	GLN	3.0
1	C	128	GLN	3.0
1	A	380	GLU	2.9
1	D	173	PRO	2.8
1	G	3	LEU	2.8
1	B	6	ARG	2.7
1	D	3	LEU	2.7
1	G	128	GLN	2.6
1	A	381	LEU	2.6
1	B	128	GLN	2.4
1	B	142	GLU	2.4
1	G	142	GLU	2.4
1	F	156	GLY	2.4
1	C	6	ARG	2.3
1	D	128	GLN	2.3
1	B	207	ASP	2.3
1	A	207	ASP	2.2
1	G	202	GLU	2.2
1	C	142	GLU	2.2
1	H	174	ALA	2.2
1	H	128	GLN	2.1
1	H	207	ASP	2.1
1	E	6	ARG	2.1
1	F	128	GLN	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 carbohydrates 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(\AA^2)	Q<0.9
3	GOL	A	408	6/6	0.80	0.17	34,38,39,39	0
3	GOL	C	408	6/6	0.80	0.19	31,35,39,44	0
3	GOL	H	408	6/6	0.82	0.24	31,36,39,41	0
4	SO4	G	410	5/5	0.91	0.29	53,54,59,67	0
3	GOL	D	407	6/6	0.92	0.12	21,26,35,36	0
3	GOL	C	407	6/6	0.93	0.11	18,26,29,31	0
4	SO4	H	409	5/5	0.93	0.31	34,45,50,53	0
4	SO4	H	410	5/5	0.94	0.21	27,33,42,42	0
3	GOL	E	407	6/6	0.94	0.12	22,24,30,31	0
3	GOL	B	407	6/6	0.94	0.10	21,26,30,31	0
3	GOL	A	407	6/6	0.94	0.10	20,27,34,34	0
3	GOL	F	407	6/6	0.94	0.12	22,25,32,36	0
4	SO4	B	408	5/5	0.95	0.26	38,47,47,52	0
4	SO4	E	408	5/5	0.95	0.32	39,48,53,56	0
3	GOL	G	407	6/6	0.95	0.09	20,23,32,33	0
4	SO4	C	410	5/5	0.95	0.17	27,31,42,46	0
4	SO4	G	408	5/5	0.96	0.31	38,48,55,55	0
3	GOL	H	407	6/6	0.96	0.08	19,21,27,28	0
4	SO4	C	409	5/5	0.96	0.24	33,39,44,47	0
4	SO4	F	408	5/5	0.96	0.26	33,43,48,49	0
4	SO4	A	410	5/5	0.97	0.26	33,35,43,47	0
4	SO4	A	409	5/5	0.97	0.32	41,46,49,50	0
4	SO4	D	409	5/5	0.97	0.19	31,32,44,48	0
4	SO4	F	409	5/5	0.97	0.22	32,32,45,46	0
4	SO4	G	409	5/5	0.97	0.22	32,34,43,43	0
2	MG	E	406	1/1	0.98	0.05	27,27,27,27	0
4	SO4	D	408	5/5	0.98	0.27	34,44,46,53	0
2	MG	G	406	1/1	0.98	0.10	23,23,23,23	0
2	MG	B	406	1/1	0.98	0.07	25,25,25,25	0
2	MG	A	406	1/1	0.99	0.04	22,22,22,22	0
2	MG	C	406	1/1	0.99	0.05	19,19,19,19	0
2	MG	F	406	1/1	0.99	0.07	23,23,23,23	0
2	MG	H	406	1/1	0.99	0.06	18,18,18,18	0
2	MG	D	406	1/1	0.99	0.03	23,23,23,23	0

6.5 Other polymers ⓘ

There are no such residues in this entry.