



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:53 AM UTC

PDB ID : 4KWS / pdb_00004kws
Title : Crystal structure of d-mannonate dehydratase from chromohalobacter salexigens complexed with Mg and glycerol
Authors : Fedorov, A.A.; Fedorov, E.V.; Wichelecki, D.; Gerlt, J.A.; Almo, S.C.
Deposited on : 2013-05-24
Resolution : 1.64 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

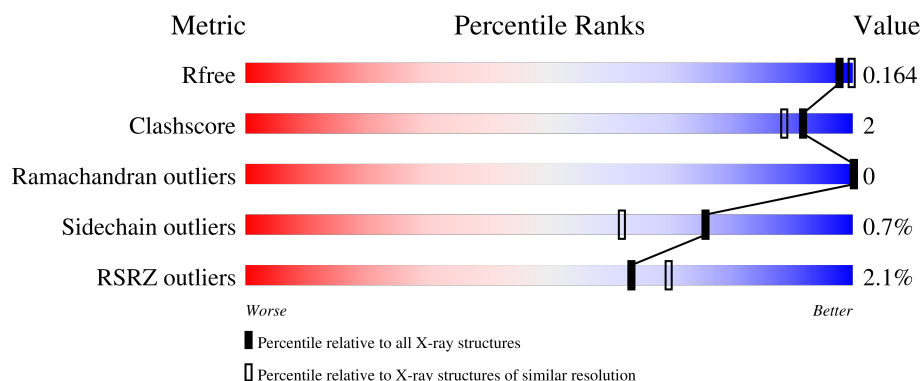
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.64 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	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

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	405	% 94% ..
1	B	405	2% 93% ..
1	C	405	% 92% 5% .
1	D	405	2% 93% ..
1	E	405	2% 94% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	405	
1	G	405	
1	H	405	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28246 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 D-mannonate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	3	0
			3174	2010	567	583	14			
1	B	393	Total	C	N	O	S	0	2	0
			3130	1984	556	575	15			
1	C	397	Total	C	N	O	S	0	2	0
			3159	2003	560	581	15			
1	D	395	Total	C	N	O	S	0	3	0
			3152	1995	564	578	15			
1	E	396	Total	C	N	O	S	0	2	0
			3146	1993	559	580	14			
1	F	395	Total	C	N	O	S	0	2	0
			3138	1989	558	576	15			
1	G	396	Total	C	N	O	S	0	3	0
			3159	2000	563	582	14			
1	H	395	Total	C	N	O	S	0	3	0
			3156	1998	565	578	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q1QT89
A	2	SER	-	expression tag	UNP Q1QT89
A	3	LEU	-	expression tag	UNP Q1QT89
B	1	MET	-	initiating methionine	UNP Q1QT89
B	2	SER	-	expression tag	UNP Q1QT89
B	3	LEU	-	expression tag	UNP Q1QT89
C	1	MET	-	initiating methionine	UNP Q1QT89
C	2	SER	-	expression tag	UNP Q1QT89
C	3	LEU	-	expression tag	UNP Q1QT89
D	1	MET	-	initiating methionine	UNP Q1QT89
D	2	SER	-	expression tag	UNP Q1QT89
D	3	LEU	-	expression tag	UNP Q1QT89
E	1	MET	-	initiating methionine	UNP Q1QT89

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	2	SER	-	expression tag	UNP Q1QT89
E	3	LEU	-	expression tag	UNP Q1QT89
F	1	MET	-	initiating methionine	UNP Q1QT89
F	2	SER	-	expression tag	UNP Q1QT89
F	3	LEU	-	expression tag	UNP Q1QT89
G	1	MET	-	initiating methionine	UNP Q1QT89
G	2	SER	-	expression tag	UNP Q1QT89
G	3	LEU	-	expression tag	UNP Q1QT89
H	1	MET	-	initiating methionine	UNP Q1QT89
H	2	SER	-	expression tag	UNP Q1QT89
H	3	LEU	-	expression tag	UNP Q1QT89

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0
2	B	2	Total Mg 2 2	0	0
2	C	2	Total Mg 2 2	0	0
2	D	3	Total Mg 3 3	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0
2	H	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	B	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		

- 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		
4	E	1	Total	Cl	0	0
			1	1		
4	F	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	374	Total 379	O 379	0	5
5	B	369	Total 370	O 370	0	1
5	C	389	Total 392	O 392	0	3
5	D	362	Total 362	O 362	0	0
5	E	381	Total 383	O 383	0	2
5	F	386	Total 387	O 387	0	1
5	G	356	Total 358	O 358	0	2
5	H	336	Total 336	O 336	0	0

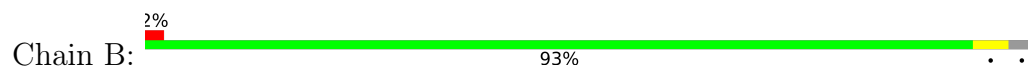
3 Residue-property plots [i](#)

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.

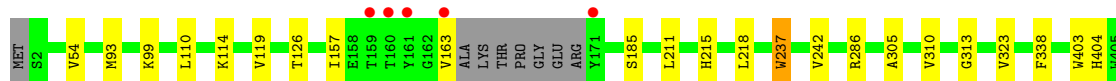
- Molecule 1: D-mannonate dehydratase



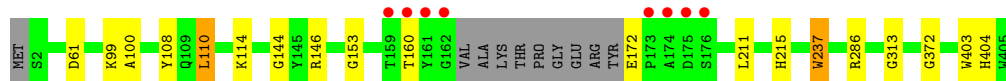
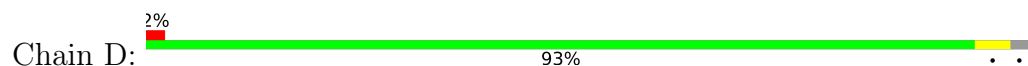
- Molecule 1: D-mannonate dehydratase



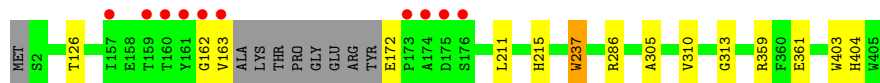
- Molecule 1: D-mannonate dehydratase



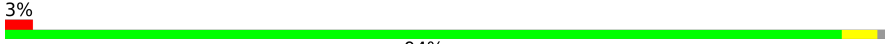
- Molecule 1: D-mannonate dehydratase

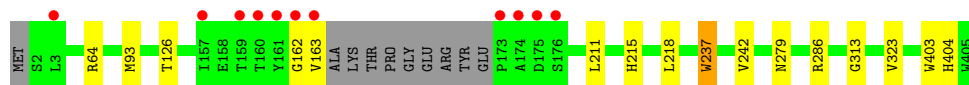


- Molecule 1: D-mannonate dehydratase

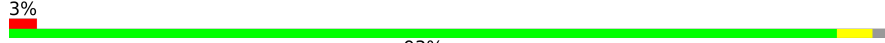


- Molecule 1: D-mannonate dehydratase

Chain F:  3% 94%

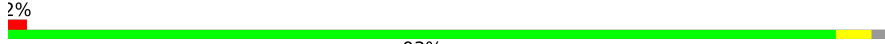


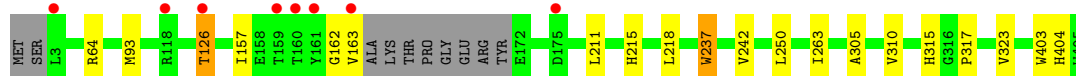
• Molecule 1: D-mannonate dehydratase

Chain G:  3% 93%



• Molecule 1: D-mannonate dehydratase

Chain H:  2% 93%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	195.27Å 85.76Å 195.10Å 90.00° 110.31° 90.00°	Depositor
Resolution (Å)	40.05 – 1.64 40.05 – 1.64	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.05-1.64) 99.8 (40.05-1.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 1.64Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.139 , 0.163 0.140 , 0.164	Depositor DCC
R_{free} test set	18484 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	17.9	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.1	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	0.98	EDS
Total number of atoms	28246	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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	0.42	0/3262	0.72	2/4442 (0.0%)
1	B	0.43	0/3217	0.73	2/4383 (0.0%)
1	C	0.42	1/3247 (0.0%)	0.72	0/4424
1	D	0.40	0/3242	0.72	2/4413 (0.0%)
1	E	0.42	0/3236	0.72	2/4407 (0.0%)
1	F	0.42	0/3225	0.72	0/4393
1	G	0.42	0/3246	0.72	2/4422 (0.0%)
1	H	0.40	0/3243	0.71	0/4415
All	All	0.41	1/25918 (0.0%)	0.72	10/35299 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	54	VAL	CA-CB	5.61	1.56	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	GLU	CA-C-N	6.86	126.37	119.24
1	A	172	GLU	C-N-CA	6.86	126.37	119.24
1	E	172	GLU	CA-C-N	6.07	125.56	119.24
1	E	172	GLU	C-N-CA	6.07	125.56	119.24
1	B	172	GLU	CA-C-N	5.99	126.15	119.32
1	B	172	GLU	C-N-CA	5.99	126.15	119.32
1	G	172	GLU	CA-C-N	5.42	126.62	119.84
1	G	172	GLU	C-N-CA	5.42	126.62	119.84
1	D	172	GLU	CA-C-N	5.31	126.47	119.84
1	D	172	GLU	C-N-CA	5.31	126.47	119.84

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	3174	0	3053	9	0
1	B	3130	0	3015	9	0
1	C	3159	0	3041	14	0
1	D	3152	0	3039	9	0
1	E	3146	0	3031	9	0
1	F	3138	0	3027	12	0
1	G	3159	0	3041	9	0
1	H	3156	0	3042	12	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	3	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	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	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	6	0	8	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	379	0	0	1	0
5	B	370	0	0	0	0
5	C	392	0	0	1	0
5	D	362	0	0	1	0
5	E	383	0	0	0	0
5	F	387	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	358	0	0	0	0
5	H	336	0	0	1	0
All	All	28246	0	24353	80	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (80) 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:E:126:THR:HG21	1:E:163:VAL:HA	1.76	0.67
1:F:126:THR:HG21	1:F:163:VAL:HA	1.77	0.66
1:G:359:ARG:NH2	1:G:361:GLU:OE2	2.31	0.64
1:G:286:ARG:HD2	1:G:313:GLY:O	2.05	0.56
1:F:218:LEU:O	1:F:242[A]:VAL:HG12	2.06	0.56
1:A:286:ARG:HD2	1:A:313:GLY:O	2.06	0.55
1:C:126:THR:HG21	1:C:163:VAL:HA	1.88	0.54
1:F:126:THR:HG21	1:F:162:GLY:O	2.08	0.54
1:B:215:HIS:ND1	1:B:405:TRP:OXT	2.26	0.53
1:D:144:GLY:O	1:D:146:ARG:NH1	2.41	0.53
1:C:286:ARG:HD2	1:C:313:GLY:O	2.09	0.52
1:G:4:LYS:HB2	1:G:27:GLU:HG3	1.91	0.52
1:D:108:TYR:CE1	1:D:114:LYS:HG3	2.45	0.52
1:C:99:LYS:HG2	1:C:110:LEU:HD21	1.92	0.51
1:E:126:THR:HG21	1:E:162:GLY:O	2.10	0.51
1:C:157:ILE:HD11	1:C:185:SER:HB3	1.92	0.51
1:D:286:ARG:HD2	1:D:313:GLY:O	2.11	0.50
1:C:157:ILE:HG13	5:C:986:HOH:O	2.12	0.50
1:D:61:ASP:OD2	5:D:757:HOH:O	2.19	0.50
1:G:218:LEU:O	1:G:242[A]:VAL:HG12	2.12	0.49
1:E:126:THR:CG2	1:E:163:VAL:HA	2.43	0.49
1:D:403:TRP:CG	1:D:404:HIS:H	2.31	0.49
1:G:403:TRP:CG	1:G:404:HIS:H	2.32	0.48
1:E:403:TRP:CG	1:E:404:HIS:H	2.31	0.48
1:F:126:THR:HG23	1:F:163:VAL:HG22	1.95	0.48
1:E:359:ARG:NH2	1:E:361:GLU:OE2	2.47	0.48
1:C:211:LEU:HD23	1:C:237:TRP:CE2	2.49	0.48
1:F:403:TRP:CG	1:F:404:HIS:H	2.32	0.48
1:A:403:TRP:CG	1:A:404:HIS:H	2.32	0.47
1:C:126:THR:HG23	1:C:163:VAL:HG22	1.96	0.47
1:F:93[B]:MET:HE1	1:F:323:VAL:HG12	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:403:TRP:CG	1:H:404:HIS:H	2.32	0.47
1:F:126:THR:CG2	1:F:163:VAL:HA	2.43	0.47
1:F:286:ARG:HD2	1:F:313:GLY:O	2.15	0.47
1:B:403:TRP:CG	1:B:404:HIS:H	2.33	0.46
1:B:211:LEU:HD23	1:B:237:TRP:CE2	2.50	0.46
1:C:403:TRP:CG	1:C:404:HIS:H	2.32	0.46
1:H:218:LEU:O	1:H:242:VAL:HG12	2.15	0.46
1:D:100:ALA:HB3	1:D:372:GLY:HA2	1.97	0.46
1:A:250:LEU:HD21	1:A:263:ILE:HD13	1.97	0.46
1:C:114:LYS:HZ3	1:H:64:ARG:HD2	1.81	0.46
1:F:211:LEU:HD23	1:F:237:TRP:CE2	2.51	0.46
1:B:218:LEU:O	1:B:242[A]:VAL:HG12	2.15	0.45
1:E:211:LEU:HD23	1:E:237:TRP:CE2	2.52	0.45
1:E:126:THR:HG23	1:E:163:VAL:HG22	1.97	0.45
1:A:211:LEU:HD23	1:A:237:TRP:CE2	2.51	0.45
1:F:93[B]:MET:CE	1:F:323:VAL:HG12	2.47	0.45
1:G:211:LEU:HD23	1:G:237:TRP:CE2	2.52	0.45
1:G:215:HIS:ND1	1:G:405:TRP:OXT	2.30	0.44
1:C:126:THR:CG2	1:C:163:VAL:HA	2.47	0.44
1:H:211:LEU:HD23	1:H:237:TRP:CE2	2.52	0.44
1:E:286:ARG:HD2	1:E:313:GLY:O	2.18	0.43
1:H:305:ALA:HB1	1:H:310:VAL:HB	1.99	0.43
1:C:218:LEU:O	1:C:242[A]:VAL:HG12	2.18	0.43
1:D:211:LEU:HD23	1:D:237:TRP:CE2	2.54	0.43
1:C:93[B]:MET:CE	1:C:323:VAL:HG12	2.49	0.43
1:D:99:LYS:HG2	1:D:110:LEU:HD21	2.01	0.42
1:B:114:LYS:HE3	1:F:64:ARG:NH1	2.34	0.42
1:H:126:THR:CG2	1:H:163:VAL:HA	2.49	0.42
1:H:315:HIS:CE1	1:H:317:PRO:HG3	2.54	0.42
1:D:153:GLY:HA2	1:D:160:THR:HG21	2.01	0.42
1:H:93[B]:MET:HE2	1:H:93[B]:MET:HB3	1.87	0.42
1:A:31:HIS:ND1	5:A:963:HOH:O	2.35	0.42
1:B:93[B]:MET:CE	1:B:323:VAL:HG12	2.50	0.42
1:H:126:THR:OG1	1:H:162:GLY:O	2.25	0.41
1:A:157:ILE:HD13	1:A:157:ILE:HA	1.89	0.41
1:A:251[A]:ARG:NH2	1:F:279:ASN:O	2.54	0.41
1:H:157:ILE:HG13	5:H:884:HOH:O	2.20	0.41
1:A:218:LEU:O	1:A:242:VAL:HG12	2.20	0.41
1:B:156:GLY:O	1:B:157:ILE:HD13	2.21	0.41
1:C:305:ALA:HB1	1:C:310:VAL:HB	2.03	0.41
1:E:305:ALA:HB1	1:E:310:VAL:HB	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:93[B]:MET:HE1	1:H:323:VAL:HG12	2.02	0.41
1:B:286:ARG:HD2	1:B:313:GLY:O	2.21	0.40
1:G:119:VAL:HG13	1:G:338:PHE:CZ	2.56	0.40
1:H:250:LEU:HD21	1:H:263:ILE:HD13	2.03	0.40
1:B:315:HIS:CE1	1:B:317:PRO:HG3	2.57	0.40
1:C:119:VAL:HG13	1:C:338:PHE:CZ	2.56	0.40
1:A:157:ILE:HD11	1:A:185:SER:HB3	2.03	0.40
1:G:96:TRP:CD1	1:G:295:ILE:HB	2.56	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	396/405 (98%)	385 (97%)	11 (3%)	0	100	100
1	B	391/405 (96%)	381 (97%)	10 (3%)	0	100	100
1	C	395/405 (98%)	385 (98%)	10 (2%)	0	100	100
1	D	394/405 (97%)	382 (97%)	12 (3%)	0	100	100
1	E	394/405 (97%)	383 (97%)	11 (3%)	0	100	100
1	F	393/405 (97%)	382 (97%)	11 (3%)	0	100	100
1	G	395/405 (98%)	384 (97%)	11 (3%)	0	100	100
1	H	394/405 (97%)	383 (97%)	11 (3%)	0	100	100
All	All	3152/3240 (97%)	3065 (97%)	87 (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	328/332 (99%)	326 (99%)	2 (1%)	78	66
1	B	325/332 (98%)	323 (99%)	2 (1%)	78	66
1	C	328/332 (99%)	326 (99%)	2 (1%)	78	66
1	D	327/332 (98%)	324 (99%)	3 (1%)	70	54
1	E	327/332 (98%)	325 (99%)	2 (1%)	78	66
1	F	326/332 (98%)	324 (99%)	2 (1%)	78	66
1	G	328/332 (99%)	326 (99%)	2 (1%)	78	66
1	H	327/332 (98%)	324 (99%)	3 (1%)	70	54
All	All	2616/2656 (98%)	2598 (99%)	18 (1%)	76	62

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	HIS
1	A	237	TRP
1	B	215	HIS
1	B	237	TRP
1	C	215	HIS
1	C	237	TRP
1	D	110	LEU
1	D	215	HIS
1	D	237	TRP
1	E	215	HIS
1	E	237	TRP
1	F	215	HIS
1	F	237	TRP
1	G	215	HIS
1	G	237	TRP
1	H	126	THR
1	H	215	HIS
1	H	237	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	B	192	HIS
1	B	278	GLN
1	B	280	GLN
1	C	192	HIS
1	C	280	GLN
1	D	192	HIS
1	G	31	HIS
1	G	192	HIS
1	H	31	HIS
1	H	128	GLN
1	H	192	HIS
1	H	280	GLN

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 25 ligands modelled in this entry, 17 are monoatomic - leaving 8 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	H	502	-	5,5,5	0.39	0	5,5,5	0.23	0
3	GOL	E	502	-	5,5,5	0.38	0	5,5,5	0.57	0
3	GOL	B	502	-	5,5,5	0.37	0	5,5,5	0.52	0
3	GOL	C	502	-	5,5,5	0.36	0	5,5,5	0.36	0
3	GOL	A	502	-	5,5,5	0.38	0	5,5,5	0.31	0
3	GOL	F	502	-	5,5,5	0.31	0	5,5,5	0.47	0
3	GOL	G	502	-	5,5,5	0.41	0	5,5,5	0.45	0
3	GOL	D	502	-	5,5,5	0.38	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	502	-	-	2/4/4/4	-
3	GOL	E	502	-	-	1/4/4/4	-
3	GOL	B	502	-	-	2/4/4/4	-
3	GOL	C	502	-	-	3/4/4/4	-
3	GOL	A	502	-	-	2/4/4/4	-
3	GOL	F	502	-	-	2/4/4/4	-
3	GOL	G	502	-	-	2/4/4/4	-
3	GOL	D	502	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	GOL	C1-C2-C3-O3
3	F	502	GOL	C1-C2-C3-O3
3	G	502	GOL	C1-C2-C3-O3
3	G	502	GOL	O2-C2-C3-O3
3	H	502	GOL	O1-C1-C2-C3
3	B	502	GOL	O1-C1-C2-C3
3	C	502	GOL	C1-C2-C3-O3
3	B	502	GOL	O1-C1-C2-O2
3	F	502	GOL	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	H	502	GOL	O1-C1-C2-O2
3	C	502	GOL	O2-C2-C3-O3
3	C	502	GOL	O1-C1-C2-O2
3	E	502	GOL	O1-C1-C2-O2
3	D	502	GOL	O2-C2-C3-O3
3	A	502	GOL	O2-C2-C3-O3

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	397/405 (98%)	-0.50	3 (0%) 82 86	8, 17, 33, 50	3 (0%)
1	B	393/405 (97%)	-0.51	10 (2%) 58 64	6, 15, 32, 79	2 (0%)
1	C	397/405 (98%)	-0.54	5 (1%) 75 80	6, 16, 32, 60	2 (0%)
1	D	395/405 (97%)	-0.40	8 (2%) 65 71	9, 19, 35, 80	3 (0%)
1	E	396/405 (97%)	-0.51	10 (2%) 58 64	11, 17, 32, 71	2 (0%)
1	F	395/405 (97%)	-0.44	11 (2%) 55 60	7, 16, 33, 63	2 (0%)
1	G	396/405 (97%)	-0.46	11 (2%) 55 60	7, 17, 35, 66	3 (0%)
1	H	395/405 (97%)	-0.37	8 (2%) 65 71	9, 19, 35, 51	3 (0%)
All	All	3164/3240 (97%)	-0.47	66 (2%) 63 70	6, 17, 33, 80	20 (0%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	174	ALA	6.7
1	F	174	ALA	5.9
1	G	174	ALA	5.5
1	H	163	VAL	5.1
1	D	174	ALA	5.0
1	B	161	TYR	5.0
1	D	161	TYR	4.9
1	F	173	PRO	4.8
1	G	175	ASP	4.7
1	E	174	ALA	4.6
1	D	162	GLY	4.4
1	F	163	VAL	4.3
1	D	175	ASP	4.2
1	G	162	GLY	4.2
1	G	159	THR	4.0
1	D	160	THR	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	175	ASP	3.9
1	F	176	SER	3.9
1	F	161	TYR	3.9
1	G	173	PRO	3.9
1	E	175	ASP	3.8
1	F	162	GLY	3.8
1	B	176	SER	3.7
1	G	161	TYR	3.6
1	E	161	TYR	3.5
1	D	176	SER	3.5
1	B	159	THR	3.5
1	F	175	ASP	3.5
1	G	157	ILE	3.5
1	H	159	THR	3.4
1	B	173	PRO	3.4
1	C	171	TYR	3.2
1	D	173	PRO	3.2
1	F	3	LEU	3.2
1	F	160	THR	3.2
1	A	3	LEU	3.2
1	B	157	ILE	3.1
1	G	176	SER	3.1
1	E	160	THR	3.1
1	E	176	SER	3.0
1	F	159	THR	3.0
1	H	3	LEU	2.9
1	C	159	THR	2.8
1	A	157	ILE	2.8
1	D	159	THR	2.8
1	E	159	THR	2.8
1	B	172	GLU	2.7
1	E	173	PRO	2.6
1	H	175	ASP	2.6
1	A	164	ALA	2.5
1	F	157	ILE	2.5
1	H	160	THR	2.5
1	B	160	THR	2.4
1	B	3	LEU	2.3
1	C	163	VAL	2.3
1	H	118[A]	ARG	2.3
1	H	161	TYR	2.2
1	E	163	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	163	VAL	2.2
1	C	161	TYR	2.2
1	E	157	ILE	2.1
1	E	162	GLY	2.1
1	G	160	THR	2.1
1	C	160	THR	2.1
1	G	172	GLU	2.0
1	H	126	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	C	502	6/6	0.88	0.14	22,33,37,44	0
3	GOL	E	502	6/6	0.89	0.12	22,27,36,37	0
3	GOL	H	502	6/6	0.89	0.14	23,37,50,50	0
4	CL	E	503	1/1	0.90	0.12	28,28,28,28	0
3	GOL	A	502	6/6	0.91	0.10	20,32,33,35	0
4	CL	F	503	1/1	0.91	0.09	22,22,22,22	0
3	GOL	B	502	6/6	0.93	0.12	21,26,43,48	0
3	GOL	D	502	6/6	0.94	0.09	21,27,33,40	0
4	CL	A	503	1/1	0.94	0.09	22,22,22,22	0
3	GOL	F	502	6/6	0.94	0.09	19,26,29,38	0
3	GOL	G	502	6/6	0.94	0.08	22,26,28,34	0
4	CL	C	503	1/1	0.95	0.08	21,21,21,21	0
2	MG	B	503	1/1	0.97	0.05	13,13,13,13	1
2	MG	D	504	1/1	0.98	0.05	24,24,24,24	1
2	MG	D	503	1/1	0.99	0.06	15,15,15,15	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	D	501	1/1	0.99	0.01	18,18,18,18	0
2	MG	E	501	1/1	0.99	0.02	13,13,13,13	0
2	MG	C	501	1/1	1.00	0.01	12,12,12,12	0
2	MG	F	501	1/1	1.00	0.01	14,14,14,14	0
2	MG	G	501	1/1	1.00	0.01	12,12,12,12	0
2	MG	H	501	1/1	1.00	0.01	16,16,16,16	0
2	MG	C	504	1/1	1.00	0.08	12,12,12,12	1
2	MG	A	504	1/1	1.00	0.07	12,12,12,12	1
2	MG	B	501	1/1	1.00	0.02	13,13,13,13	0
2	MG	A	501	1/1	1.00	0.01	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.