Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:00 AM GMT

PDB ID	:	2OX4
Title	:	Crystal structure of putative dehydratase from Zymomonas mobilis ZM4
Authors	:	Patskovsky, Y.; Toro, R.; Sauder, J.M.; Freeman, J.C.; Bain, K.; Gheyi, T.; Wasserman, S.R.; Smith, D.; Gerlt, J.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2007-02-19
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

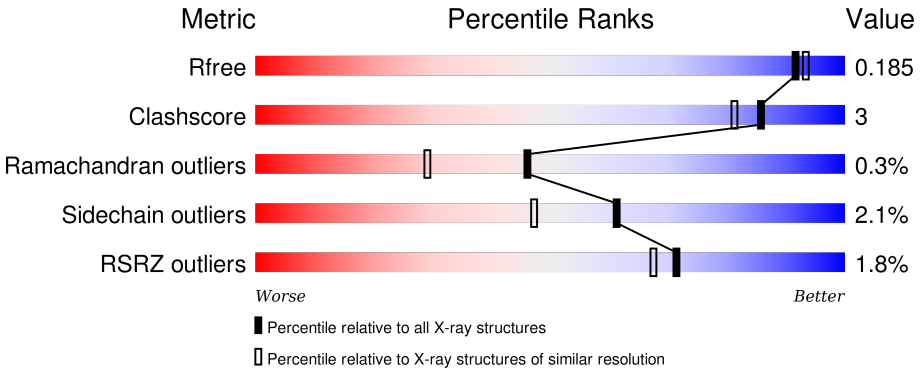
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (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. 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	403	2% 92% 6%
1	B	403	2% 90% 6%
1	C	403	% 93% 5%
1	D	403	2% 90% 8%
1	E	403	% 93%

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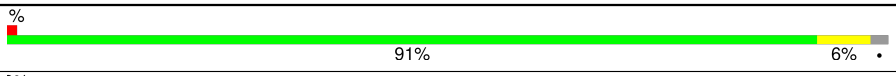
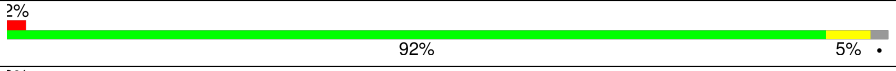
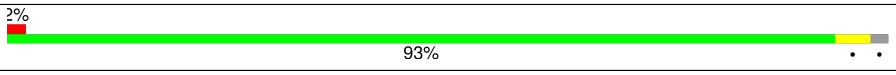
Mol	Chain	Length	Quality of chain
1	F	403	
1	G	403	
1	H	403	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	C	402	-	-	-	X
2	MG	G	502	-	-	-	X
2	MG	H	402	-	-	-	X
4	GOL	A	3414	-	-	-	X
4	GOL	B	3402	-	-	-	X
4	GOL	C	3403	-	-	-	X
4	GOL	D	3413	-	-	-	X
4	GOL	E	3407	-	-	-	X
4	GOL	G	3412	-	-	-	X
4	GOL	H	3410	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28439 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 mandelate racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	9	0
			3124	2014	523	582	5			
1	B	393	Total	C	N	O	S	0	11	0
			3141	2027	528	581	5			
1	C	397	Total	C	N	O	S	0	12	0
			3181	2054	538	584	5			
1	D	397	Total	C	N	O	S	0	11	0
			3170	2044	535	586	5			
1	E	393	Total	C	N	O	S	0	12	0
			3150	2032	530	583	5			
1	F	393	Total	C	N	O	S	0	10	0
			3135	2022	527	581	5			
1	G	393	Total	C	N	O	S	0	12	0
			3150	2034	525	586	5			
1	H	393	Total	C	N	O	S	0	10	0
			3132	2023	525	579	5			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP Q5NN22
A	0	SER	-	EXPRESSION TAG	UNP Q5NN22
A	1	LEU	-	EXPRESSION TAG	UNP Q5NN22
A	394	GLU	-	EXPRESSION TAG	UNP Q5NN22
A	395	GLY	-	EXPRESSION TAG	UNP Q5NN22
A	396	HIS	-	EXPRESSION TAG	UNP Q5NN22
A	397	HIS	-	EXPRESSION TAG	UNP Q5NN22
A	398	HIS	-	EXPRESSION TAG	UNP Q5NN22
A	399	HIS	-	EXPRESSION TAG	UNP Q5NN22
A	400	HIS	-	EXPRESSION TAG	UNP Q5NN22
A	401	HIS	-	EXPRESSION TAG	UNP Q5NN22
B	-1	MET	-	EXPRESSION TAG	UNP Q5NN22
B	0	SER	-	EXPRESSION TAG	UNP Q5NN22

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	LEU	-	EXPRESSION TAG	UNP Q5NN22
B	394	GLU	-	EXPRESSION TAG	UNP Q5NN22
B	395	GLY	-	EXPRESSION TAG	UNP Q5NN22
B	396	HIS	-	EXPRESSION TAG	UNP Q5NN22
B	397	HIS	-	EXPRESSION TAG	UNP Q5NN22
B	398	HIS	-	EXPRESSION TAG	UNP Q5NN22
B	399	HIS	-	EXPRESSION TAG	UNP Q5NN22
B	400	HIS	-	EXPRESSION TAG	UNP Q5NN22
B	401	HIS	-	EXPRESSION TAG	UNP Q5NN22
C	-1	MET	-	EXPRESSION TAG	UNP Q5NN22
C	0	SER	-	EXPRESSION TAG	UNP Q5NN22
C	1	LEU	-	EXPRESSION TAG	UNP Q5NN22
C	394	GLU	-	EXPRESSION TAG	UNP Q5NN22
C	395	GLY	-	EXPRESSION TAG	UNP Q5NN22
C	396	HIS	-	EXPRESSION TAG	UNP Q5NN22
C	397	HIS	-	EXPRESSION TAG	UNP Q5NN22
C	398	HIS	-	EXPRESSION TAG	UNP Q5NN22
C	399	HIS	-	EXPRESSION TAG	UNP Q5NN22
C	400	HIS	-	EXPRESSION TAG	UNP Q5NN22
C	401	HIS	-	EXPRESSION TAG	UNP Q5NN22
D	-1	MET	-	EXPRESSION TAG	UNP Q5NN22
D	0	SER	-	EXPRESSION TAG	UNP Q5NN22
D	1	LEU	-	EXPRESSION TAG	UNP Q5NN22
D	394	GLU	-	EXPRESSION TAG	UNP Q5NN22
D	395	GLY	-	EXPRESSION TAG	UNP Q5NN22
D	396	HIS	-	EXPRESSION TAG	UNP Q5NN22
D	397	HIS	-	EXPRESSION TAG	UNP Q5NN22
D	398	HIS	-	EXPRESSION TAG	UNP Q5NN22
D	399	HIS	-	EXPRESSION TAG	UNP Q5NN22
D	400	HIS	-	EXPRESSION TAG	UNP Q5NN22
D	401	HIS	-	EXPRESSION TAG	UNP Q5NN22
E	-1	MET	-	EXPRESSION TAG	UNP Q5NN22
E	0	SER	-	EXPRESSION TAG	UNP Q5NN22
E	1	LEU	-	EXPRESSION TAG	UNP Q5NN22
E	394	GLU	-	EXPRESSION TAG	UNP Q5NN22
E	395	GLY	-	EXPRESSION TAG	UNP Q5NN22
E	396	HIS	-	EXPRESSION TAG	UNP Q5NN22
E	397	HIS	-	EXPRESSION TAG	UNP Q5NN22
E	398	HIS	-	EXPRESSION TAG	UNP Q5NN22
E	399	HIS	-	EXPRESSION TAG	UNP Q5NN22
E	400	HIS	-	EXPRESSION TAG	UNP Q5NN22
E	401	HIS	-	EXPRESSION TAG	UNP Q5NN22

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	MET	-	EXPRESSION TAG	UNP Q5NN22
F	0	SER	-	EXPRESSION TAG	UNP Q5NN22
F	1	LEU	-	EXPRESSION TAG	UNP Q5NN22
F	394	GLU	-	EXPRESSION TAG	UNP Q5NN22
F	395	GLY	-	EXPRESSION TAG	UNP Q5NN22
F	396	HIS	-	EXPRESSION TAG	UNP Q5NN22
F	397	HIS	-	EXPRESSION TAG	UNP Q5NN22
F	398	HIS	-	EXPRESSION TAG	UNP Q5NN22
F	399	HIS	-	EXPRESSION TAG	UNP Q5NN22
F	400	HIS	-	EXPRESSION TAG	UNP Q5NN22
F	401	HIS	-	EXPRESSION TAG	UNP Q5NN22
G	-1	MET	-	EXPRESSION TAG	UNP Q5NN22
G	0	SER	-	EXPRESSION TAG	UNP Q5NN22
G	1	LEU	-	EXPRESSION TAG	UNP Q5NN22
G	394	GLU	-	EXPRESSION TAG	UNP Q5NN22
G	395	GLY	-	EXPRESSION TAG	UNP Q5NN22
G	396	HIS	-	EXPRESSION TAG	UNP Q5NN22
G	397	HIS	-	EXPRESSION TAG	UNP Q5NN22
G	398	HIS	-	EXPRESSION TAG	UNP Q5NN22
G	399	HIS	-	EXPRESSION TAG	UNP Q5NN22
G	400	HIS	-	EXPRESSION TAG	UNP Q5NN22
G	401	HIS	-	EXPRESSION TAG	UNP Q5NN22
H	-1	MET	-	EXPRESSION TAG	UNP Q5NN22
H	0	SER	-	EXPRESSION TAG	UNP Q5NN22
H	1	LEU	-	EXPRESSION TAG	UNP Q5NN22
H	394	GLU	-	EXPRESSION TAG	UNP Q5NN22
H	395	GLY	-	EXPRESSION TAG	UNP Q5NN22
H	396	HIS	-	EXPRESSION TAG	UNP Q5NN22
H	397	HIS	-	EXPRESSION TAG	UNP Q5NN22
H	398	HIS	-	EXPRESSION TAG	UNP Q5NN22
H	399	HIS	-	EXPRESSION TAG	UNP Q5NN22
H	400	HIS	-	EXPRESSION TAG	UNP Q5NN22
H	401	HIS	-	EXPRESSION TAG	UNP Q5NN22

- 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

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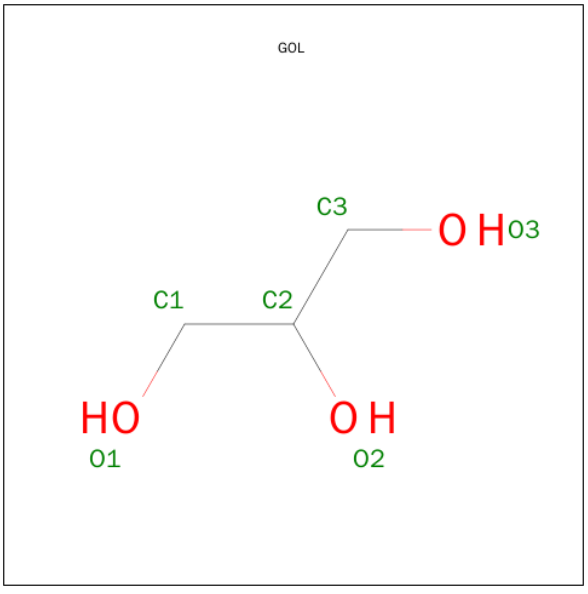
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0
3	F	1	Total Cl 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	384	Total O 384 384	0	0
5	B	400	Total O 400 400	0	0
5	C	387	Total O 387 387	0	0
5	D	397	Total O 397 397	0	0
5	E	413	Total O 413 413	0	0
5	F	394	Total O 394 394	0	0

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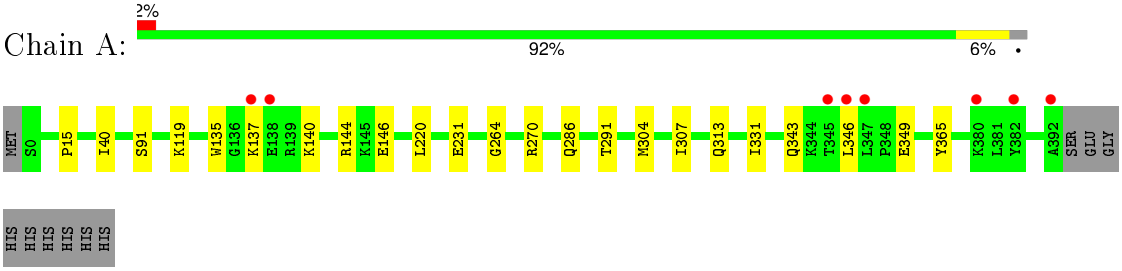
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	392	Total O 392 392	0	0
5	H	393	Total O 393 393	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

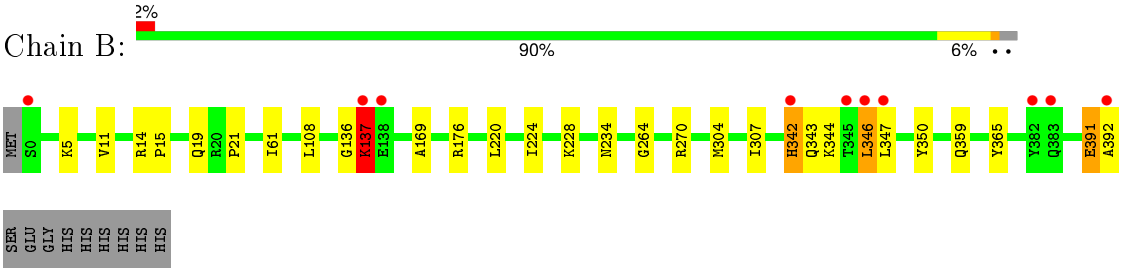
- Molecule 1: Putative mandelate racemase

Chain A:



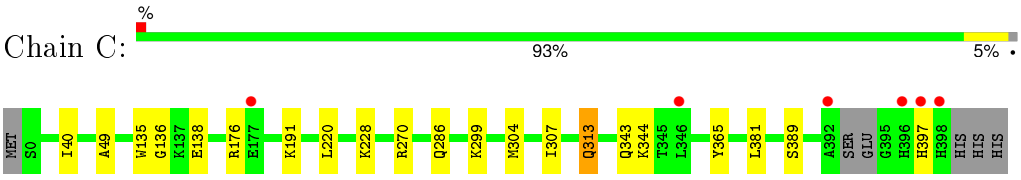
- Molecule 1: Putative mandelate racemase

Chain B:



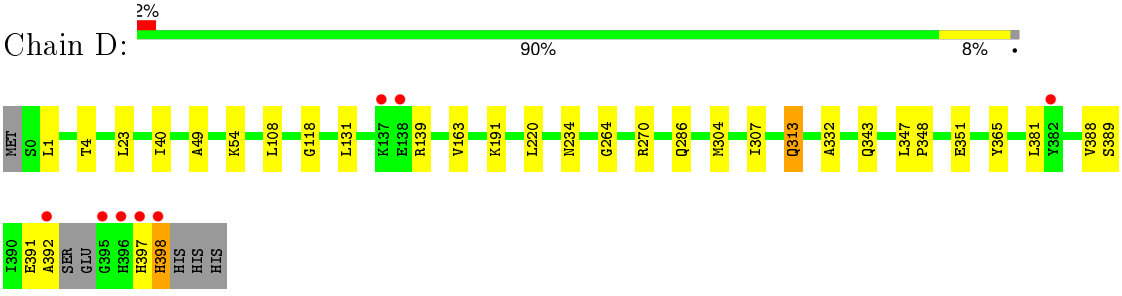
- Molecule 1: Putative mandelate racemase

Chain C:



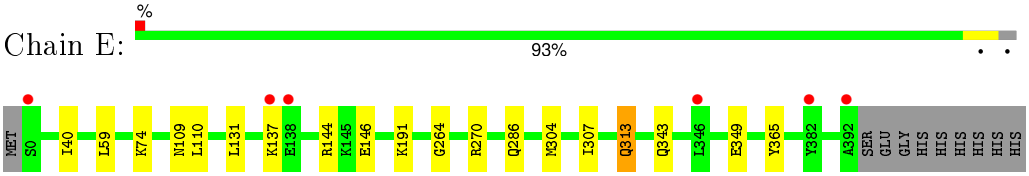
- Molecule 1: Putative mandelate racemase

Chain D:



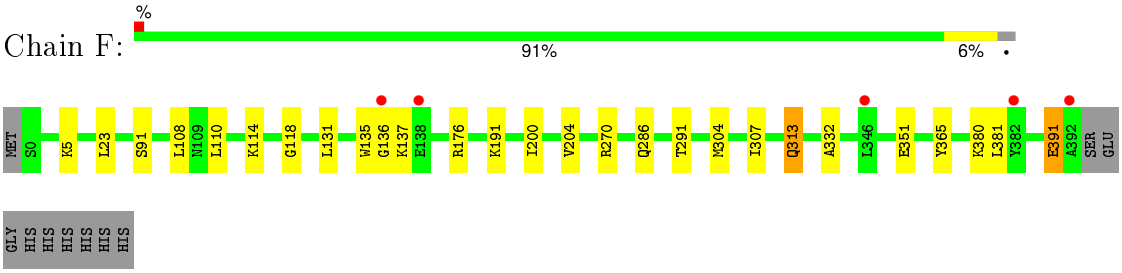
- Molecule 1: Putative mandelate racemase

Chain E:



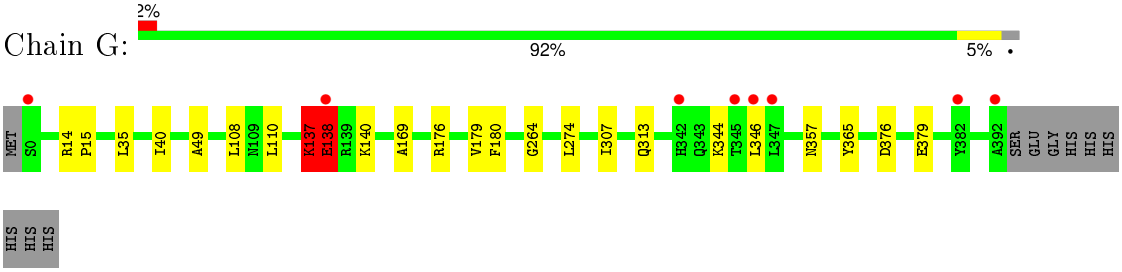
• Molecule 1: Putative mandelate racemase

Chain F:



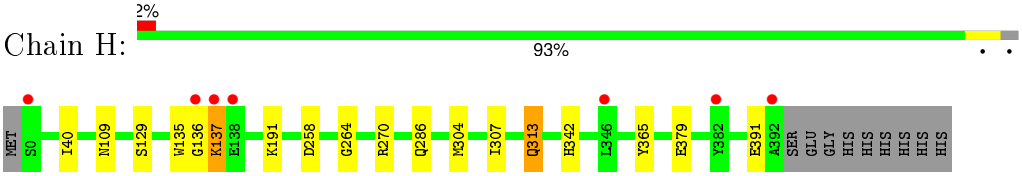
• Molecule 1: Putative mandelate racemase

Chain G:



• Molecule 1: Putative mandelate racemase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	190.18Å 190.41Å 85.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 34.21 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-1.80) 99.6 (34.21-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.3.0028	Depositor
R, R_{free}	0.144 , 0.186 0.144 , 0.185	Depositor DCC
R_{free} test set	8741 reflections (3.14%)	DCC
Wilson B-factor (Å^2)	15.6	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 61.1	EDS
Estimated twinning fraction	0.003 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	2 of 287916 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	28439	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 2.97% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.47	0/3219	0.58	0/4354
1	B	0.50	0/3242	0.59	0/4382
1	C	0.47	0/3284	0.57	0/4436
1	D	0.49	0/3273	0.58	0/4423
1	E	0.52	0/3255	0.59	0/4401
1	F	0.49	0/3233	0.58	0/4371
1	G	0.50	0/3245	0.59	1/4389 (0.0%)
1	H	0.48	0/3230	0.57	0/4367
All	All	0.49	0/25981	0.58	1/35123 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
1	C	0	1
1	D	0	1
1	F	0	2
1	G	0	2
1	H	0	1
All	All	0	11

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	138	GLU	N-CA-C	-5.03	97.43	111.00

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	135	TRP	Peptide
1	B	137	LYS	Peptide
1	B	346	LEU	Peptide
1	B	391	GLU	Peptide
1	C	135	TRP	Peptide
1	D	391	GLU	Peptide
1	F	135	TRP	Peptide
1	F	391	GLU	Peptide
1	G	137	LYS	Peptide
1	G	138	GLU	Peptide
1	H	135	TRP	Peptide

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	3124	0	3137	24	0
1	B	3141	0	3169	39	0
1	C	3181	0	3209	24	0
1	D	3170	0	3184	23	0
1	E	3150	0	3170	23	0
1	F	3135	0	3156	26	0
1	G	3150	0	3170	20	0
1	H	3132	0	3161	22	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	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1	0	0	0	0
4	A	12	0	16	0	0
4	B	6	0	8	0	0
4	C	12	0	16	1	0
4	D	12	0	16	1	0
4	E	6	0	8	0	0
4	F	12	0	16	0	0
4	G	18	0	24	2	0
4	H	6	0	8	0	0
5	A	384	0	0	0	0
5	B	400	0	0	1	0
5	C	387	0	0	1	0
5	D	397	0	0	1	0
5	E	413	0	0	2	0
5	F	394	0	0	3	0
5	G	392	0	0	0	0
5	H	393	0	0	0	0
All	All	28439	0	25468	142	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 3.

All (142) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304[B]:MET:CE	1:C:304[B]:MET:HG3	1.82	1.09
1:B:307[B]:ILE:CD1	1:C:304[B]:MET:HE1	1.93	0.97
1:A:307[B]:ILE:CD1	1:H:304[B]:MET:HE1	1.96	0.95
1:C:299:LYS:HE2	4:C:3403:GOL:H31	1.48	0.95
1:B:304[B]:MET:HE1	1:C:304[B]:MET:HG3	1.46	0.94
1:B:304[B]:MET:HE2	1:C:304[B]:MET:HG3	1.52	0.92
1:B:137:LYS:HB2	1:B:347:LEU:HD23	1.51	0.90
1:B:304[B]:MET:HE3	1:C:307[B]:ILE:HD11	1.54	0.89
1:A:304[B]:MET:HE1	1:H:307[B]:ILE:CD1	2.04	0.87
1:A:307[B]:ILE:HD12	1:H:304[B]:MET:HE1	1.56	0.86
1:B:304[B]:MET:HE3	1:C:307[B]:ILE:CD1	2.06	0.85
1:B:307[B]:ILE:HD11	1:C:304[B]:MET:HE1	1.58	0.85
1:D:270:ARG:HD2	1:G:307[A]:ILE:HD11	1.58	0.85
1:A:307[B]:ILE:CD1	1:H:304[B]:MET:CE	2.59	0.80
1:E:307[B]:ILE:HD11	1:F:304[B]:MET:CE	2.12	0.80
1:A:270:ARG:HD2	1:H:307[A]:ILE:HD11	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307[A]:ILE:HD11	1:H:270:ARG:HD2	1.63	0.79
1:E:270:ARG:HD2	1:F:307[A]:ILE:HD11	1.64	0.79
1:B:307[B]:ILE:CD1	1:C:304[B]:MET:CE	2.61	0.78
1:B:307[B]:ILE:HD11	1:C:304[B]:MET:CE	2.14	0.78
1:B:270:ARG:HD2	1:C:307[A]:ILE:HD11	1.67	0.76
1:A:307[B]:ILE:HD11	1:H:304[B]:MET:CE	2.16	0.76
1:B:304[B]:MET:CE	1:C:307[B]:ILE:CD1	2.64	0.75
1:E:307[A]:ILE:HD11	1:F:270:ARG:HD2	1.67	0.74
1:E:304[B]:MET:CE	1:F:307[B]:ILE:HD11	2.19	0.73
1:E:307[B]:ILE:HD11	1:F:304[B]:MET:HE3	1.70	0.73
1:D:4:THR:O	1:D:392:ALA:HB2	1.87	0.73
1:B:136:GLY:HA2	1:B:343:GLN:NE2	2.05	0.72
1:A:304[B]:MET:CE	1:H:307[B]:ILE:CD1	2.67	0.72
1:B:307[A]:ILE:HD11	1:C:270:ARG:HD2	1.71	0.72
1:D:304[B]:MET:HE1	1:G:307[B]:ILE:CD1	2.21	0.71
1:B:307[B]:ILE:HD13	1:C:304[B]:MET:HE1	1.72	0.70
1:B:137:LYS:HG3	1:B:137:LYS:O	1.92	0.69
1:A:304[B]:MET:HE1	1:H:307[B]:ILE:HD11	1.75	0.69
1:A:15:PRO:HD2	1:A:349:GLU:HG2	1.74	0.69
1:A:304[B]:MET:CE	1:H:307[B]:ILE:HD11	2.23	0.68
1:E:304[B]:MET:HE3	1:F:307[B]:ILE:HD11	1.75	0.68
1:B:137:LYS:O	1:B:137:LYS:CG	2.39	0.66
1:A:304[B]:MET:HE1	1:H:307[B]:ILE:HD12	1.75	0.66
1:B:137:LYS:HB2	1:B:347:LEU:CD2	2.24	0.66
1:E:307[B]:ILE:CD1	1:F:304[B]:MET:CE	2.73	0.66
1:B:19:GLN:NE2	1:B:350:TYR:OH	2.30	0.65
1:D:307[B]:ILE:HD11	1:G:274:LEU:HD22	1.79	0.65
1:B:61:ILE:HG21	1:B:392:ALA:HA	1.79	0.64
1:B:304[B]:MET:HE1	1:C:307[B]:ILE:HD12	1.78	0.64
1:A:307[B]:ILE:HD11	1:H:304[B]:MET:HE3	1.79	0.63
1:F:304[B]:MET:HE2	5:F:3563:HOH:O	1.98	0.62
1:D:304[B]:MET:HE1	1:G:307[B]:ILE:HD11	1.80	0.62
1:B:304[B]:MET:CE	1:C:307[B]:ILE:HD12	2.29	0.62
1:E:307[B]:ILE:CD1	1:F:304[B]:MET:HE1	2.30	0.61
1:E:144:ARG:NH2	1:E:146[B]:GLU:OE1	2.32	0.61
1:G:137:LYS:HB3	1:G:137:LYS:HZ2	1.66	0.61
1:F:304[B]:MET:CE	5:F:3563:HOH:O	2.47	0.61
1:E:304[B]:MET:CE	1:F:307[B]:ILE:CD1	2.80	0.60
1:E:307[B]:ILE:HD11	1:F:304[B]:MET:HE1	1.82	0.59
1:B:234:ASN:ND2	5:B:3737:HOH:O	2.37	0.57
1:D:304[B]:MET:CE	1:G:307[B]:ILE:CD1	2.84	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:304[B]:MET:HE2	5:E:3576:HOH:O	2.06	0.55
1:E:304[B]:MET:HE1	1:F:307[B]:ILE:HD11	1.88	0.55
1:B:136:GLY:HA2	1:B:343:GLN:HE21	1.71	0.54
1:E:304[B]:MET:CE	5:E:3576:HOH:O	2.55	0.54
1:F:176[B]:ARG:NH2	5:F:3575:HOH:O	2.34	0.53
1:D:304[B]:MET:CE	1:G:307[B]:ILE:HD11	2.39	0.53
1:C:228[B]:LYS:HG3	5:C:3552:HOH:O	2.10	0.52
1:B:5:LYS:HG3	1:B:391:GLU:HG2	1.92	0.51
1:C:389:SER:HB3	1:C:397:HIS:HB2	1.92	0.51
1:E:304[B]:MET:HE1	1:F:307[B]:ILE:CD1	2.39	0.51
1:D:398:HIS:CD2	1:D:398:HIS:N	2.79	0.51
1:D:23:LEU:HD12	1:D:381:LEU:HD21	1.92	0.51
1:E:270:ARG:CD	1:F:307[A]:ILE:HD11	2.37	0.50
1:A:270:ARG:CD	1:H:307[A]:ILE:HD11	2.39	0.50
1:B:304[B]:MET:HE2	1:C:304[B]:MET:CG	2.34	0.49
1:D:389:SER:HB3	1:D:397:HIS:HB3	1.94	0.49
1:D:234:ASN:ND2	5:D:3805:HOH:O	2.45	0.49
1:D:139:ARG:HH22	4:D:3413:GOL:C1	2.26	0.49
1:B:220:LEU:HD23	1:B:220:LEU:C	2.34	0.48
1:E:307[A]:ILE:HD11	1:F:270:ARG:CD	2.41	0.48
1:C:40[A]:ILE:HD12	1:C:49:ALA:HB2	1.95	0.48
1:A:304[B]:MET:HE3	1:H:307[B]:ILE:HD11	1.96	0.48
1:G:35[B]:LEU:CD1	1:G:376:ASP:HA	2.43	0.48
1:G:180:PHE:H	4:G:3412:GOL:H2	1.78	0.48
1:C:220:LEU:HD23	1:C:220:LEU:C	2.34	0.48
1:B:270:ARG:CD	1:C:307[A]:ILE:HD11	2.39	0.47
1:G:179:VAL:HA	4:G:3412:GOL:H2	1.96	0.47
1:A:91[A]:SER:OG	1:A:291:THR:HG22	2.14	0.47
1:B:346:LEU:HD23	1:B:359:GLN:CD	2.35	0.47
1:A:119:LYS:HG2	1:A:331:ILE:HG12	1.98	0.46
1:F:304[B]:MET:HE2	1:F:304[B]:MET:HB2	1.55	0.46
1:D:270:ARG:CD	1:G:307[A]:ILE:HD11	2.37	0.46
1:A:304[B]:MET:HB2	1:A:304[B]:MET:HE2	1.66	0.46
1:G:40[A]:ILE:HD12	1:G:49:ALA:HB2	1.98	0.46
1:B:307[A]:ILE:HD11	1:C:270:ARG:CD	2.44	0.45
1:F:110:LEU:HD22	1:F:114[B]:LYS:HD2	1.98	0.45
1:B:342:HIS:N	1:B:342:HIS:CD2	2.84	0.44
1:D:304[B]:MET:HE1	1:G:307[B]:ILE:HD13	1.96	0.44
1:B:220:LEU:CD2	1:B:224:ILE:HD12	2.48	0.44
1:H:286:GLN:HA	1:H:313:GLN:O	2.18	0.44
1:G:346:LEU:CD2	1:G:357:ASN:HD21	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:14:ARG:HA	1:G:15:PRO:HD3	1.89	0.44
1:G:35[B]:LEU:HD12	1:G:376:ASP:HA	1.98	0.44
1:F:200:ILE:O	1:F:204:VAL:HG22	2.18	0.44
1:G:138:GLU:O	1:G:138:GLU:CG	2.66	0.44
1:B:137:LYS:CB	1:B:347:LEU:HD23	2.37	0.43
1:A:343:GLN:HA	1:A:346:LEU:HD13	2.00	0.43
1:A:286:GLN:HA	1:A:313:GLN:O	2.19	0.43
1:B:342:HIS:CD2	1:B:342:HIS:H	2.37	0.43
1:D:40[A]:ILE:HD12	1:D:49:ALA:HB2	2.01	0.43
1:B:11:VAL:HB	1:B:21:PRO:HD2	2.00	0.43
1:D:54:LYS:HD3	1:D:388:VAL:HG11	2.01	0.42
1:E:304[B]:MET:HB2	1:E:304[B]:MET:HE2	1.45	0.42
1:B:169:ALA:O	1:B:176[A]:ARG:HD2	2.19	0.42
1:E:349:GLU:HG2	1:E:349:GLU:H	1.69	0.42
1:E:110:LEU:HD11	1:F:108:LEU:HD21	2.01	0.42
1:A:307[A]:ILE:HD11	1:H:270:ARG:CD	2.41	0.42
1:F:5:LYS:HG3	1:F:391:GLU:HG2	2.01	0.42
1:A:146:GLU:CD	1:A:146:GLU:H	2.22	0.42
1:F:23:LEU:HD12	1:F:381:LEU:HD21	2.00	0.42
1:C:286:GLN:HA	1:C:313:GLN:O	2.20	0.41
1:B:220:LEU:HD23	1:B:224:ILE:HD12	2.02	0.41
1:H:129:SER:HB3	1:H:342:HIS:HA	2.02	0.41
1:B:14:ARG:HA	1:B:15:PRO:HD3	1.92	0.41
1:E:59:LEU:HB3	1:E:74:LYS:HE2	2.01	0.41
1:B:228:LYS:NZ	1:H:258[B]:ASP:O	2.54	0.41
1:F:91[A]:SER:OG	1:F:291:THR:HG22	2.21	0.41
1:E:286:GLN:HA	1:E:313:GLN:O	2.20	0.41
1:D:131:LEU:HD11	1:D:163:VAL:HB	2.02	0.41
1:H:137:LYS:HB2	1:H:137:LYS:HE3	1.66	0.41
1:D:108:LEU:HD21	1:G:110:LEU:HD11	2.03	0.41
1:A:304[B]:MET:HG3	1:H:304[B]:MET:HE1	2.03	0.40
1:G:169:ALA:O	1:G:176:ARG:HD2	2.22	0.40
1:F:286:GLN:HA	1:F:313:GLN:O	2.22	0.40
1:D:118:GLY:O	1:D:332:ALA:HA	2.20	0.40
1:D:286:GLN:HA	1:D:313:GLN:O	2.21	0.40
1:D:347:LEU:HA	1:D:348:PRO:HD3	1.95	0.40
1:F:118:GLY:O	1:F:332:ALA:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	399/403 (99%)	379 (95%)	19 (5%)	1 (0%)	46	29
1	B	402/403 (100%)	381 (95%)	19 (5%)	2 (0%)	34	17
1	C	405/403 (100%)	386 (95%)	18 (4%)	1 (0%)	52	35
1	D	404/403 (100%)	390 (96%)	13 (3%)	1 (0%)	52	35
1	E	403/403 (100%)	385 (96%)	17 (4%)	1 (0%)	52	35
1	F	401/403 (100%)	384 (96%)	16 (4%)	1 (0%)	52	35
1	G	403/403 (100%)	386 (96%)	16 (4%)	1 (0%)	52	35
1	H	401/403 (100%)	384 (96%)	15 (4%)	2 (0%)	34	17
All	All	3218/3224 (100%)	3075 (96%)	133 (4%)	10 (0%)	46	29

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	344	LYS
1	C	136	GLY
1	D	264	GLY
1	E	264	GLY
1	H	136	GLY
1	A	264	GLY
1	G	264	GLY
1	H	264	GLY
1	B	264	GLY
1	F	136	GLY

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	329/329 (100%)	323 (98%)	6 (2%)	66	54
1	B	331/329 (101%)	327 (99%)	4 (1%)	78	71
1	C	335/329 (102%)	326 (97%)	9 (3%)	52	36
1	D	334/329 (102%)	326 (98%)	8 (2%)	57	41
1	E	332/329 (101%)	325 (98%)	7 (2%)	61	47
1	F	330/329 (100%)	323 (98%)	7 (2%)	61	47
1	G	332/329 (101%)	325 (98%)	7 (2%)	61	47
1	H	330/329 (100%)	323 (98%)	7 (2%)	61	47
All	All	2653/2632 (101%)	2598 (98%)	55 (2%)	61	47

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

Mol	Chain	Res	Type
1	A	137	LYS
1	A	140	LYS
1	A	144	ARG
1	A	220	LEU
1	A	231	GLU
1	A	365	TYR
1	B	108	LEU
1	B	137	LYS
1	B	342	HIS
1	B	365	TYR
1	C	138	GLU
1	C	176[A]	ARG
1	C	176[B]	ARG
1	C	191	LYS
1	C	313	GLN
1	C	343	GLN
1	C	344	LYS
1	C	365	TYR
1	C	381	LEU
1	D	1	LEU
1	D	191	LYS
1	D	220	LEU
1	D	313	GLN
1	D	343	GLN

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Mol	Chain	Res	Type
1	D	351	GLU
1	D	365	TYR
1	D	398	HIS
1	E	109	ASN
1	E	131	LEU
1	E	137	LYS
1	E	191	LYS
1	E	313	GLN
1	E	343	GLN
1	E	365	TYR
1	F	131	LEU
1	F	137	LYS
1	F	191	LYS
1	F	313	GLN
1	F	351	GLU
1	F	365	TYR
1	F	380	LYS
1	G	108	LEU
1	G	137	LYS
1	G	140	LYS
1	G	313	GLN
1	G	344	LYS
1	G	365	TYR
1	G	379	GLU
1	H	109	ASN
1	H	137	LYS
1	H	191	LYS
1	H	313	GLN
1	H	365	TYR
1	H	379	GLU
1	H	391	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	ASN
1	A	234	ASN
1	B	19	GLN
1	B	120	ASN
1	B	173	ASN
1	B	342	HIS
1	B	343	GLN

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Mol	Chain	Res	Type
1	C	120	ASN
1	C	214	ASN
1	C	234	ASN
1	D	109	ASN
1	D	120	ASN
1	D	214	ASN
1	D	234	ASN
1	D	398	HIS
1	E	120	ASN
1	E	214	ASN
1	E	234	ASN
1	F	109	ASN
1	F	214	ASN
1	F	234	ASN
1	F	343	GLN
1	G	214	ASN
1	G	234	ASN
1	H	173	ASN
1	H	214	ASN
1	H	234	ASN
1	H	343	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 26 ligands modelled in this entry, 12 are monoatomic - leaving 14 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	GOL	A	3401	-	5,5,5	0.33	0	5,5,5	0.32	0
4	GOL	A	3414	-	5,5,5	0.33	0	5,5,5	0.52	0
4	GOL	B	3402	-	5,5,5	0.34	0	5,5,5	0.42	0
4	GOL	C	3403	-	5,5,5	0.39	0	5,5,5	0.26	0
4	GOL	C	3404	-	5,5,5	0.44	0	5,5,5	0.38	0
4	GOL	D	3406	-	5,5,5	0.36	0	5,5,5	0.42	0
4	GOL	D	3413	-	5,5,5	0.35	0	5,5,5	0.63	0
4	GOL	E	3407	-	5,5,5	0.38	0	5,5,5	0.48	0
4	GOL	F	3409	-	5,5,5	0.33	0	5,5,5	0.56	0
4	GOL	F	3411	-	5,5,5	0.36	0	5,5,5	0.43	0
4	GOL	G	3405	-	5,5,5	0.35	0	5,5,5	0.52	0
4	GOL	G	3408	-	5,5,5	0.33	0	5,5,5	0.39	0
4	GOL	G	3412	-	5,5,5	0.42	0	5,5,5	0.70	0
4	GOL	H	3410	-	5,5,5	0.33	0	5,5,5	0.39	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
4	GOL	A	3401	-	-	0/4/4/4	0/0/0/0
4	GOL	A	3414	-	-	0/4/4/4	0/0/0/0
4	GOL	B	3402	-	-	0/4/4/4	0/0/0/0
4	GOL	C	3403	-	-	0/4/4/4	0/0/0/0
4	GOL	C	3404	-	-	0/4/4/4	0/0/0/0
4	GOL	D	3406	-	-	0/4/4/4	0/0/0/0
4	GOL	D	3413	-	-	0/4/4/4	0/0/0/0
4	GOL	E	3407	-	-	0/4/4/4	0/0/0/0
4	GOL	F	3409	-	-	0/4/4/4	0/0/0/0
4	GOL	F	3411	-	-	0/4/4/4	0/0/0/0
4	GOL	G	3405	-	-	0/4/4/4	0/0/0/0
4	GOL	G	3408	-	-	0/4/4/4	0/0/0/0
4	GOL	G	3412	-	-	0/4/4/4	0/0/0/0
4	GOL	H	3410	-	-	0/4/4/4	0/0/0/0

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.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	3403	GOL	1	0
4	D	3413	GOL	1	0
4	G	3412	GOL	2	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, 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	393/403 (97%)	-0.41	8 (2%)	68	64	8, 15, 38, 71	0
1	B	393/403 (97%)	-0.47	10 (2%)	61	56	7, 14, 40, 70	0
1	C	397/403 (98%)	-0.39	6 (1%)	76	72	8, 14, 35, 74	0
1	D	397/403 (98%)	-0.43	8 (2%)	68	64	7, 14, 37, 73	0
1	E	393/403 (97%)	-0.53	6 (1%)	76	72	6, 12, 32, 68	0
1	F	393/403 (97%)	-0.51	5 (1%)	79	76	7, 14, 32, 58	0
1	G	393/403 (97%)	-0.50	8 (2%)	68	64	7, 13, 40, 65	0
1	H	393/403 (97%)	-0.49	7 (1%)	71	67	7, 13, 32, 65	0
All	All	3152/3224 (97%)	-0.47	58 (1%)	71	67	6, 14, 36, 74	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	346	LEU	6.6
1	A	346	LEU	6.5
1	B	392	ALA	5.9
1	B	347	LEU	5.2
1	D	397	HIS	5.1
1	A	392	ALA	5.1
1	C	398	HIS	4.9
1	D	398	HIS	4.8
1	C	396	HIS	4.7
1	B	345	THR	4.4
1	F	392	ALA	4.3
1	D	396	HIS	4.2
1	C	397	HIS	3.8
1	E	392	ALA	3.7
1	G	346	LEU	3.7
1	E	138	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	345	THR	3.5
1	A	380	LYS	3.4
1	A	347	LEU	3.4
1	F	346	LEU	3.3
1	H	392	ALA	3.3
1	D	395	GLY	3.2
1	E	137	LYS	3.2
1	B	0	SER	3.1
1	H	137	LYS	3.1
1	A	382	TYR	3.1
1	D	392	ALA	3.0
1	G	382	TYR	2.9
1	H	136	GLY	2.9
1	B	138	GLU	2.8
1	H	382	TYR	2.8
1	A	345	THR	2.7
1	H	346	LEU	2.6
1	G	392	ALA	2.6
1	B	382	TYR	2.5
1	G	0	SER	2.5
1	D	382	TYR	2.5
1	A	138	GLU	2.4
1	E	0	SER	2.4
1	G	138	GLU	2.4
1	E	382	TYR	2.4
1	F	382	TYR	2.3
1	G	347	LEU	2.3
1	C	346	LEU	2.3
1	A	137	LYS	2.3
1	F	138	GLU	2.2
1	E	346	LEU	2.2
1	B	137	LYS	2.2
1	D	138	GLU	2.2
1	C	177	GLU	2.2
1	C	392	ALA	2.1
1	G	342	HIS	2.1
1	B	383	GLN	2.1
1	D	137	LYS	2.1
1	H	0	SER	2.1
1	B	342	HIS	2.1
1	F	136	GLY	2.0
1	H	138	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
4	GOL	G	3412	6/6	0.95	0.16	14.46	23,30,34,42	0
4	GOL	H	3410	6/6	0.93	0.13	10.02	19,24,26,31	0
4	GOL	A	3414	6/6	0.82	0.21	7.08	27,45,48,50	0
4	GOL	C	3403	6/6	0.89	0.20	5.66	29,33,60,62	0
4	GOL	D	3413	6/6	0.86	0.20	4.57	37,38,50,55	0
4	GOL	B	3402	6/6	0.94	0.10	3.99	21,29,31,34	0
4	GOL	E	3407	6/6	0.93	0.14	3.10	21,25,28,30	0
2	MG	G	502	1/1	1.00	0.11	2.57	8,8,8,8	0
2	MG	H	402	1/1	1.00	0.11	2.42	8,8,8,8	0
2	MG	C	402	1/1	1.00	0.11	2.29	8,8,8,8	0
4	GOL	G	3408	6/6	0.87	0.19	1.54	29,38,41,49	0
4	GOL	G	3405	6/6	0.94	0.10	1.53	20,25,33,35	0
4	GOL	C	3404	6/6	0.96	0.09	1.31	14,19,25,25	0
2	MG	E	402	1/1	1.00	0.10	1.14	6,6,6,6	0
4	GOL	F	3409	6/6	0.96	0.08	1.10	18,22,25,33	0
4	GOL	F	3411	6/6	0.91	0.16	0.95	22,35,46,51	0
2	MG	F	402	1/1	1.00	0.10	0.43	8,8,8,8	0
4	GOL	D	3406	6/6	0.95	0.09	0.39	14,20,25,25	0
4	GOL	A	3401	6/6	0.94	0.09	0.26	16,18,24,24	0
2	MG	A	402	1/1	1.00	0.07	-0.81	10,10,10,10	0
3	CL	D	501	1/1	1.00	0.06	-0.83	12,12,12,12	0
2	MG	D	402	1/1	0.99	0.07	-0.90	8,8,8,8	0
2	MG	B	502	1/1	1.00	0.06	-1.02	9,9,9,9	0
3	CL	B	501	1/1	0.99	0.06	-1.37	12,12,12,12	0
3	CL	G	501	1/1	0.99	0.04	-2.29	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	CL	F	501	1/1	1.00	0.04	-3.34	11,11,11,11	0

6.5 Other polymers (i)

There are no such residues in this entry.