



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:02 am GMT

PDB ID : 2O56  
Title : Crystal Structure of a Member of the Enolase Superfamily from Salmonella Typhimurium  
Authors : Patskovsky, Y.; Sauder, J.M.; Dickey, M.; Adams, J.M.; Ozyurt, S.; Wasserman, S.R.; Gerlt, J.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2006-12-05  
Resolution : 2.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

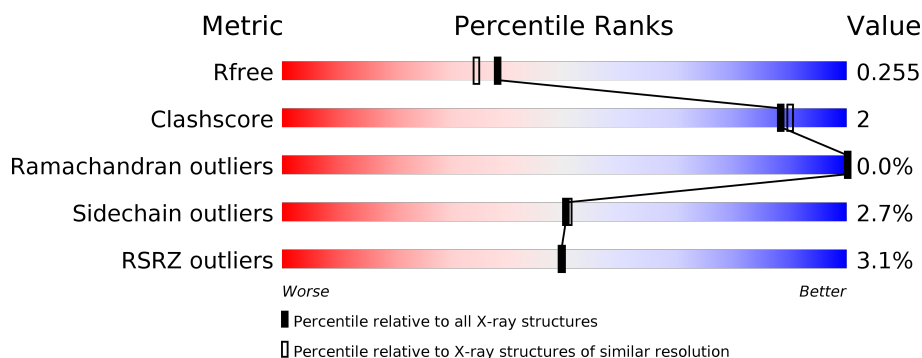
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	407	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>5%</div> <div>.</div> </div> </div>
1	B	407	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div>.</div> </div> </div>
1	C	407	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div>.</div> </div> </div>
1	D	407	<div> <div>4%</div> <div> <div></div> <div>92%</div> <div>.</div> <div>.</div> </div> </div>
1	E	407	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div>.</div> </div> </div>
1	F	407	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	407	
1	H	407	

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	F	2006	-	-	-	X
2	MG	H	2008	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26214 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	392	Total	C	N	O	S	0	4	0
			3054	1953	508	569	24			
1	B	392	Total	C	N	O	S	0	8	0
			3075	1968	510	573	24			
1	C	392	Total	C	N	O	S	0	2	0
			3042	1944	505	569	24			
1	D	392	Total	C	N	O	S	0	3	0
			3046	1948	505	569	24			
1	E	392	Total	C	N	O	S	0	6	0
			3063	1959	508	572	24			
1	F	392	Total	C	N	O	S	0	3	0
			3046	1948	505	569	24			
1	G	391	Total	C	N	O	S	0	4	0
			3045	1947	506	568	24			
1	H	389	Total	C	N	O	S	0	4	0
			3027	1936	504	563	24			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	CLONING ARTIFACT	UNP Q8ZKY6
A	0	SER	-	CLONING ARTIFACT	UNP Q8ZKY6
A	1	LEU	-	CLONING ARTIFACT	UNP Q8ZKY6
A	398	GLU	-	CLONING ARTIFACT	UNP Q8ZKY6
A	399	GLY	-	CLONING ARTIFACT	UNP Q8ZKY6
A	400	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
A	401	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
A	402	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
A	403	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
A	404	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
A	405	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
B	-1	MET	-	CLONING ARTIFACT	UNP Q8ZKY6
B	0	SER	-	CLONING ARTIFACT	UNP Q8ZKY6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	LEU	-	CLONING ARTIFACT	UNP Q8ZKY6
B	398	GLU	-	CLONING ARTIFACT	UNP Q8ZKY6
B	399	GLY	-	CLONING ARTIFACT	UNP Q8ZKY6
B	400	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
B	401	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
B	402	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
B	403	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
B	404	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
B	405	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
C	-1	MET	-	CLONING ARTIFACT	UNP Q8ZKY6
C	0	SER	-	CLONING ARTIFACT	UNP Q8ZKY6
C	1	LEU	-	CLONING ARTIFACT	UNP Q8ZKY6
C	398	GLU	-	CLONING ARTIFACT	UNP Q8ZKY6
C	399	GLY	-	CLONING ARTIFACT	UNP Q8ZKY6
C	400	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
C	401	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
C	402	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
C	403	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
C	404	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
C	405	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
D	-1	MET	-	CLONING ARTIFACT	UNP Q8ZKY6
D	0	SER	-	CLONING ARTIFACT	UNP Q8ZKY6
D	1	LEU	-	CLONING ARTIFACT	UNP Q8ZKY6
D	398	GLU	-	CLONING ARTIFACT	UNP Q8ZKY6
D	399	GLY	-	CLONING ARTIFACT	UNP Q8ZKY6
D	400	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
D	401	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
D	402	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
D	403	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
D	404	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
D	405	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
E	-1	MET	-	CLONING ARTIFACT	UNP Q8ZKY6
E	0	SER	-	CLONING ARTIFACT	UNP Q8ZKY6
E	1	LEU	-	CLONING ARTIFACT	UNP Q8ZKY6
E	398	GLU	-	CLONING ARTIFACT	UNP Q8ZKY6
E	399	GLY	-	CLONING ARTIFACT	UNP Q8ZKY6
E	400	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
E	401	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
E	402	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
E	403	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
E	404	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
E	405	HIS	-	EXPRESSION TAG	UNP Q8ZKY6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	MET	-	CLONING ARTIFACT	UNP Q8ZKY6
F	0	SER	-	CLONING ARTIFACT	UNP Q8ZKY6
F	1	LEU	-	CLONING ARTIFACT	UNP Q8ZKY6
F	398	GLU	-	CLONING ARTIFACT	UNP Q8ZKY6
F	399	GLY	-	CLONING ARTIFACT	UNP Q8ZKY6
F	400	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
F	401	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
F	402	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
F	403	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
F	404	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
F	405	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
G	-1	MET	-	CLONING ARTIFACT	UNP Q8ZKY6
G	0	SER	-	CLONING ARTIFACT	UNP Q8ZKY6
G	1	LEU	-	CLONING ARTIFACT	UNP Q8ZKY6
G	398	GLU	-	CLONING ARTIFACT	UNP Q8ZKY6
G	399	GLY	-	CLONING ARTIFACT	UNP Q8ZKY6
G	400	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
G	401	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
G	402	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
G	403	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
G	404	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
G	405	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
H	-1	MET	-	CLONING ARTIFACT	UNP Q8ZKY6
H	0	SER	-	CLONING ARTIFACT	UNP Q8ZKY6
H	1	LEU	-	CLONING ARTIFACT	UNP Q8ZKY6
H	398	GLU	-	CLONING ARTIFACT	UNP Q8ZKY6
H	399	GLY	-	CLONING ARTIFACT	UNP Q8ZKY6
H	400	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
H	401	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
H	402	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
H	403	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
H	404	HIS	-	EXPRESSION TAG	UNP Q8ZKY6
H	405	HIS	-	EXPRESSION TAG	UNP Q8ZKY6

- 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 1	Mg 1	0	0
2	B	1	Total 1	Mg 1	0	0
2	C	1	Total 1	Mg 1	0	0
2	A	1	Total 1	Mg 1	0	0
2	F	1	Total 1	Mg 1	0	0

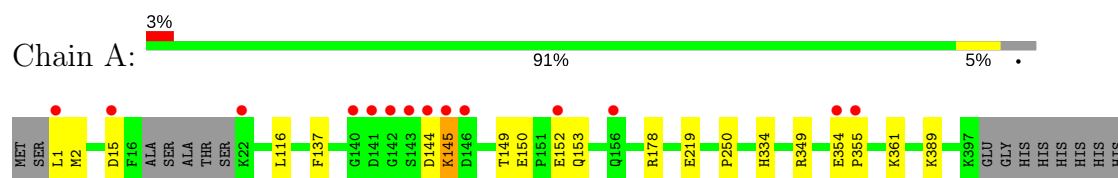
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	208	Total 208	O 208	0	0
3	B	242	Total 242	O 242	0	0
3	C	214	Total 214	O 214	0	0
3	D	212	Total 212	O 212	0	0
3	E	234	Total 234	O 234	0	0
3	F	227	Total 227	O 227	0	0
3	G	236	Total 236	O 236	0	0
3	H	235	Total 235	O 235	0	0

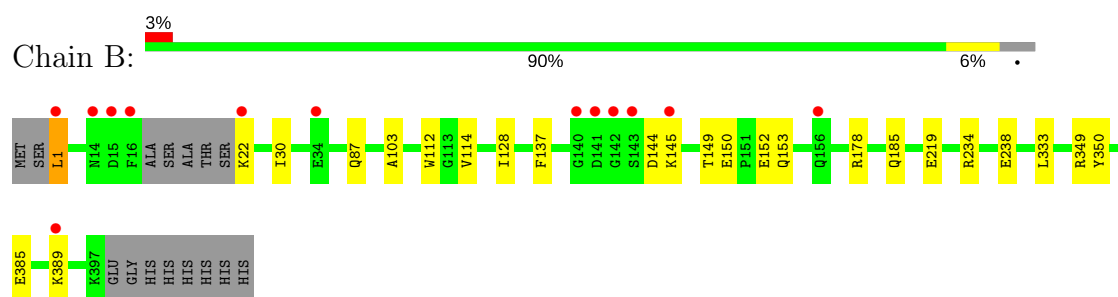
### 3 Residue-property plots [i](#)

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.

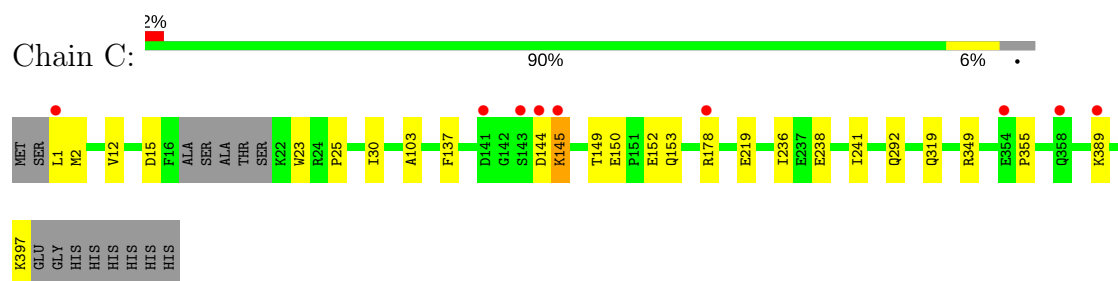
- Molecule 1: Putative mandelate racemase



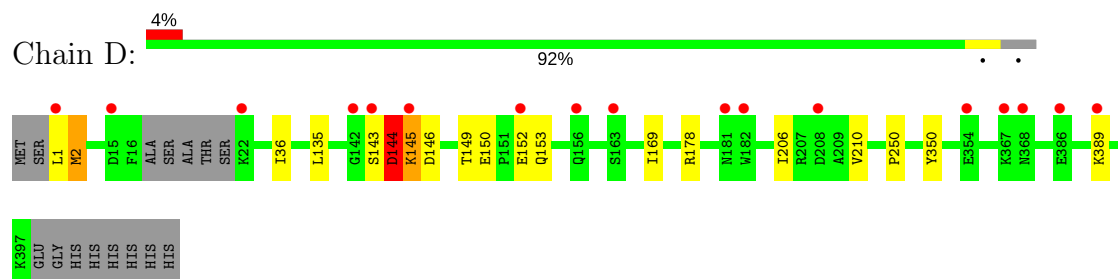
- Molecule 1: Putative mandelate racemase



- Molecule 1: Putative mandelate racemase

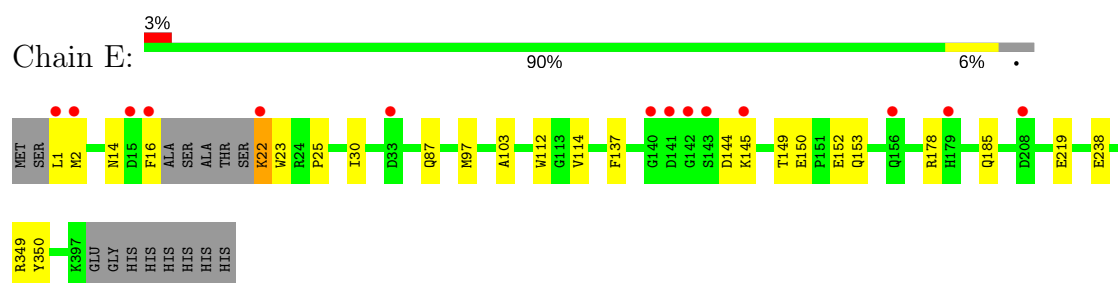


- Molecule 1: Putative mandelate racemase

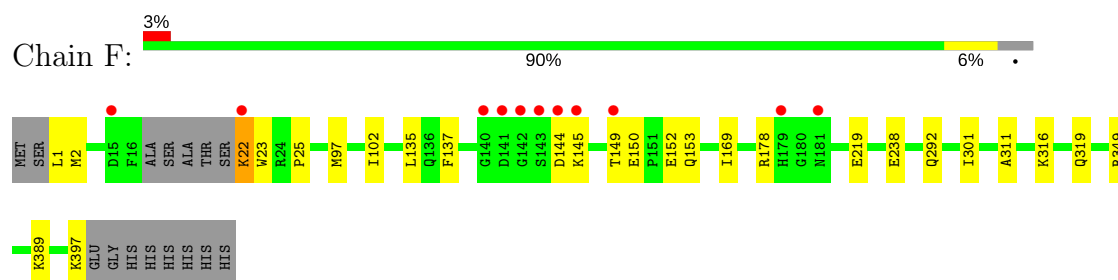


- Molecule 1: Putative mandelate racemase

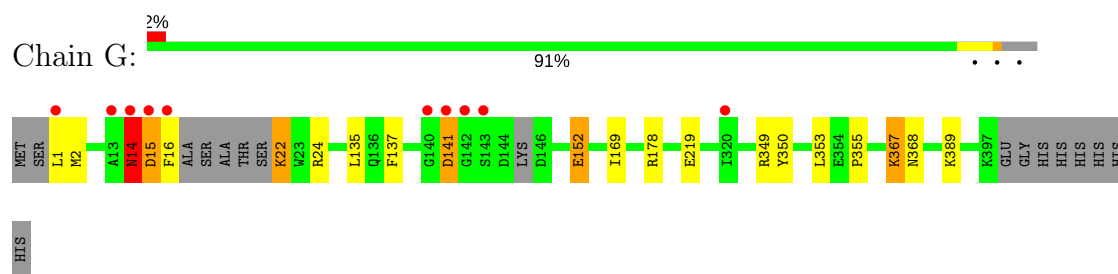




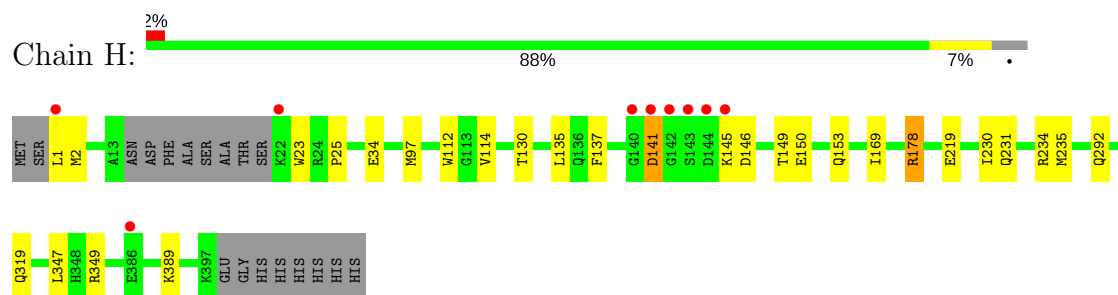
- Molecule 1: Putative mandelate racemase



- Molecule 1: Putative mandelate racemase



- Molecule 1: Putative mandelate racemase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.66Å 140.82Å 126.84Å 90.00° 105.94° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 37.03 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.8 (20.00-2.00) 96.6 (37.03-2.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.209 , 0.255 0.209 , 0.255	Depositor DCC
$R_{free}$ test set	4760 reflections (2.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.9	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 63.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	26214	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.19% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	0.51	0/3133	0.60	0/4245
1	B	0.50	0/3166	0.60	0/4288
1	C	0.49	0/3115	0.60	0/4220
1	D	0.49	0/3122	0.60	0/4231
1	E	0.50	0/3148	0.60	0/4265
1	F	0.49	0/3122	0.60	0/4231
1	G	0.51	0/3123	0.61	1/4231 (0.0%)
1	H	0.52	0/3105	0.62	0/4207
All	All	0.50	0/25034	0.60	1/33918 (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	D	0	1
1	G	0	2
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	14	ASN	N-CA-C	-5.67	95.68	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	144	ASP	Peptide
1	G	14	ASN	Peptide
1	G	15	ASP	Peptide

## 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	3054	0	3057	8	0
1	B	3075	0	3089	21	0
1	C	3042	0	3035	12	0
1	D	3046	0	3044	14	0
1	E	3063	0	3068	13	0
1	F	3046	0	3044	12	0
1	G	3045	0	3043	18	0
1	H	3027	0	3038	17	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	208	0	0	1	0
3	B	242	0	0	2	0
3	C	214	0	0	0	0
3	D	212	0	0	0	0
3	E	234	0	0	1	0
3	F	227	0	0	1	0
3	G	236	0	0	2	0
3	H	235	0	0	1	0
All	All	26214	0	24418	113	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 (113) 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:G:15:ASP:OD2	1:G:16:PHE:CA	1.73	1.37
1:D:145:LYS:HG2	1:D:146:ASP:OD1	1.45	1.17
1:B:234[B]:ARG:HG2	1:B:234[B]:ARG:HH11	1.28	0.98
1:G:15:ASP:OD2	1:G:16:PHE:HA	0.81	0.97
1:G:367:LYS:HD2	1:G:368:ASN:ND2	1.81	0.96
1:B:1:LEU:HD12	1:B:1:LEU:N	1.85	0.91
1:G:152:GLU:HG2	3:G:2154:HOH:O	1.76	0.84
1:D:144:ASP:N	1:D:145:LYS:HB3	1.96	0.80
1:C:150:GLU:H	1:C:153:GLN:HE21	1.31	0.78
1:H:150:GLU:H	1:H:153:GLN:HE21	1.30	0.78
1:D:150:GLU:H	1:D:153:GLN:HE21	1.31	0.78
1:B:150:GLU:H	1:B:153:GLN:HE21	1.33	0.76
1:D:145:LYS:CG	1:D:146:ASP:OD1	2.30	0.76
1:A:150:GLU:H	1:A:153:GLN:HE21	1.31	0.75
1:B:1:LEU:H3	1:B:1:LEU:HD12	1.51	0.74
1:B:1:LEU:CD1	1:B:1:LEU:N	2.51	0.73
1:E:150:GLU:H	1:E:153:GLN:HE21	1.36	0.73
1:D:143:SER:O	1:D:145:LYS:N	2.21	0.72
1:B:1:LEU:O	1:B:1:LEU:HD13	1.90	0.72
1:B:385:GLU:O	1:B:389:LYS:HG2	1.91	0.70
1:G:137:PHE:O	1:G:349:ARG:NH1	2.25	0.69
1:C:137:PHE:O	1:C:349:ARG:NH1	2.25	0.69
1:F:150:GLU:H	1:F:153:GLN:HE21	1.40	0.69
1:H:137:PHE:O	1:H:349:ARG:NH1	2.26	0.67
1:G:367:LYS:O	1:G:367:LYS:HG3	1.95	0.66
1:G:141:ASP:OD1	1:G:141:ASP:N	2.30	0.65
1:G:15:ASP:OD1	1:G:355:PRO:HB3	1.98	0.64
1:F:349:ARG:HD3	3:F:2056:HOH:O	1.96	0.64
1:H:141:ASP:OD1	1:H:141:ASP:N	2.30	0.63
1:B:234[B]:ARG:CG	1:B:234[B]:ARG:HH11	2.07	0.63
1:B:1:LEU:HD12	1:B:1:LEU:H1	1.64	0.62
1:H:150:GLU:H	1:H:153:GLN:NE2	1.98	0.62
1:F:137:PHE:O	1:F:349:ARG:NH1	2.33	0.62
1:G:367:LYS:HD2	1:G:368:ASN:HD22	1.64	0.60
1:B:185:GLN:HG2	3:B:2154:HOH:O	2.02	0.59
1:D:143:SER:C	1:D:145:LYS:HB3	2.24	0.58
1:B:238[B]:GLU:HG3	3:B:2150:HOH:O	2.04	0.57
1:D:143:SER:C	1:D:145:LYS:N	2.58	0.55
1:C:149:THR:H	1:C:153:GLN:NE2	2.06	0.54
1:B:234[B]:ARG:HG2	1:B:234[B]:ARG:NH1	2.07	0.54
1:D:2:MET:HE1	1:D:36:ILE:HD12	1.91	0.52
1:A:149:THR:H	1:A:153:GLN:NE2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:15:ASP:OD2	1:G:16:PHE:CB	2.55	0.51
1:A:137:PHE:O	1:A:349:ARG:NH1	2.43	0.51
1:H:230:ILE:O	1:H:234[B]:ARG:HG3	2.11	0.51
1:B:1:LEU:H3	1:B:1:LEU:CD1	2.17	0.50
1:A:145:LYS:HG2	1:A:145:LYS:O	2.11	0.50
1:C:150:GLU:H	1:C:153:GLN:NE2	2.05	0.50
1:H:149:THR:H	1:H:153:GLN:NE2	2.10	0.50
1:H:2:MET:HE3	1:H:34:GLU:HB2	1.93	0.49
1:G:14:ASN:OD1	1:G:16:PHE:HB2	2.13	0.49
1:H:234[B]:ARG:NH2	3:H:2164:HOH:O	2.45	0.49
1:A:349:ARG:HD3	3:A:2101:HOH:O	2.13	0.48
1:B:137:PHE:O	1:B:349:ARG:NH1	2.46	0.48
1:E:30:ILE:HD12	1:E:103:ALA:HB3	1.95	0.48
1:D:135:LEU:HD22	1:D:169:ILE:HD13	1.95	0.47
1:D:149:THR:H	1:D:153:GLN:NE2	2.13	0.47
1:G:135:LEU:HD22	1:G:169:ILE:HD13	1.97	0.47
1:E:185:GLN:HG2	3:E:2142:HOH:O	2.13	0.47
1:H:135:LEU:HD22	1:H:169:ILE:HD13	1.96	0.47
1:C:145:LYS:O	1:C:145:LYS:HG2	2.15	0.47
1:C:30:ILE:HD12	1:C:103:ALA:HB3	1.97	0.46
1:D:250:PRO:HD2	1:E:87:GLN:O	2.15	0.46
1:E:97[B]:MET:HB2	1:E:97[B]:MET:HE2	1.79	0.46
1:E:112:TRP:HB2	1:E:114[A]:VAL:HG22	1.98	0.46
1:G:367:LYS:CD	1:G:368:ASN:ND2	2.68	0.46
1:E:22:LYS:HB3	1:E:23:TRP:H	1.51	0.45
1:A:354:GLU:HB2	1:A:355:PRO:HD3	1.98	0.45
1:B:149:THR:H	1:B:153:GLN:NE2	2.14	0.45
1:B:150:GLU:H	1:B:153:GLN:NE2	2.08	0.44
1:C:12:VAL:HB	1:C:25:PRO:HG2	2.00	0.44
1:H:23:TRP:CD1	1:H:25:PRO:HD3	2.53	0.44
1:B:30:ILE:HD12	1:B:103:ALA:HB3	2.00	0.44
1:H:130:THR:HG21	1:H:347:LEU:HB2	2.00	0.44
1:E:150:GLU:H	1:E:153:GLN:NE2	2.10	0.44
1:F:149:THR:H	1:F:153:GLN:NE2	2.14	0.44
1:C:236:ILE:HD12	1:C:241:ILE:HG13	2.00	0.44
1:C:15:ASP:HB2	1:C:355:PRO:HB3	1.98	0.44
1:D:150:GLU:H	1:D:153:GLN:NE2	2.06	0.44
1:E:149:THR:H	1:E:153:GLN:NE2	2.16	0.43
1:E:137:PHE:O	1:E:349:ARG:NH1	2.51	0.43
1:B:112:TRP:HB2	1:B:114[A]:VAL:HG22	1.99	0.43
1:B:128[A]:ILE:HD13	1:B:333:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:ILE:O	1:D:210:VAL:HG22	2.18	0.43
1:E:14:ASN:HD22	1:E:16:PHE:H	1.67	0.43
1:A:116:LEU:HB3	1:A:334:HIS:CG	2.54	0.43
1:C:292:GLN:HA	1:C:319:GLN:O	2.19	0.43
1:G:15:ASP:OD1	1:G:355:PRO:CB	2.65	0.43
1:G:22:LYS:HZ2	1:G:24:ARG:HG3	1.84	0.43
1:C:149:THR:H	1:C:153:GLN:HE22	1.67	0.42
1:C:23:TRP:CD1	1:C:25:PRO:HD3	2.54	0.42
1:F:22:LYS:HA	1:F:22:LYS:HD2	1.47	0.42
1:G:353:LEU:HB2	3:G:2052:HOH:O	2.18	0.42
1:F:292:GLN:HA	1:F:319:GLN:O	2.19	0.42
1:H:178:ARG:HG3	1:H:178:ARG:H	1.68	0.42
1:E:23:TRP:CD1	1:E:25:PRO:HD3	2.55	0.42
1:H:97[B]:MET:HE3	1:H:97[B]:MET:HB3	1.81	0.42
1:H:149:THR:H	1:H:153:GLN:HE22	1.68	0.42
1:H:292:GLN:HA	1:H:319:GLN:O	2.20	0.41
1:F:135:LEU:HD22	1:F:169:ILE:HD13	2.02	0.41
1:G:350:TYR:C	1:G:350:TYR:CD1	2.93	0.41
1:F:97[B]:MET:HE3	1:F:97[B]:MET:HB3	1.89	0.41
1:H:112:TRP:HB2	1:H:114[A]:VAL:HG22	2.02	0.41
1:B:350:TYR:C	1:B:350:TYR:CD1	2.93	0.41
1:E:350:TYR:C	1:E:350:TYR:CD1	2.94	0.41
1:G:15:ASP:OD2	1:G:16:PHE:N	2.47	0.41
1:H:231:GLN:O	1:H:235:MET:HG3	2.20	0.41
1:D:350:TYR:C	1:D:350:TYR:CD1	2.94	0.41
1:F:23:TRP:CD1	1:F:25:PRO:HD3	2.56	0.41
1:F:97[B]:MET:HE2	1:F:97[B]:MET:HB2	1.89	0.41
1:F:102:ILE:HA	1:F:301:ILE:HD12	2.03	0.40
1:F:311:ALA:HB1	1:F:316:LYS:HB2	2.02	0.40
1:A:250:PRO:HD2	1:B:87:GLN:O	2.21	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	392/407 (96%)	382 (97%)	10 (3%)	0	100	100
1	B	396/407 (97%)	387 (98%)	9 (2%)	0	100	100
1	C	390/407 (96%)	381 (98%)	9 (2%)	0	100	100
1	D	391/407 (96%)	380 (97%)	11 (3%)	0	100	100
1	E	394/407 (97%)	385 (98%)	9 (2%)	0	100	100
1	F	391/407 (96%)	381 (97%)	10 (3%)	0	100	100
1	G	389/407 (96%)	380 (98%)	9 (2%)	0	100	100
1	H	389/407 (96%)	380 (98%)	8 (2%)	1 (0%)	44	40
All	All	3132/3256 (96%)	3056 (98%)	75 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	146	ASP

### 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	324/332 (98%)	314 (97%)	10 (3%)	45	44
1	B	328/332 (99%)	321 (98%)	7 (2%)	59	62
1	C	322/332 (97%)	312 (97%)	10 (3%)	45	44
1	D	323/332 (97%)	316 (98%)	7 (2%)	57	60
1	E	326/332 (98%)	316 (97%)	10 (3%)	45	44
1	F	323/332 (97%)	312 (97%)	11 (3%)	42	40
1	G	323/332 (97%)	314 (97%)	9 (3%)	49	49
1	H	321/332 (97%)	315 (98%)	6 (2%)	62	66
All	All	2590/2656 (98%)	2520 (97%)	70 (3%)	50	51



All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LEU
1	A	2	MET
1	A	15	ASP
1	A	144	ASP
1	A	145	LYS
1	A	152	GLU
1	A	178	ARG
1	A	219	GLU
1	A	361	LYS
1	A	389	LYS
1	B	1	LEU
1	B	22	LYS
1	B	144	ASP
1	B	145	LYS
1	B	152	GLU
1	B	178	ARG
1	B	219	GLU
1	C	1	LEU
1	C	2	MET
1	C	144	ASP
1	C	145	LYS
1	C	152	GLU
1	C	178	ARG
1	C	219	GLU
1	C	238	GLU
1	C	389	LYS
1	C	397	LYS
1	D	1	LEU
1	D	2	MET
1	D	144	ASP
1	D	145	LYS
1	D	152	GLU
1	D	178	ARG
1	D	389	LYS
1	E	1	LEU
1	E	2	MET
1	E	22	LYS
1	E	144	ASP
1	E	145	LYS
1	E	152	GLU
1	E	178	ARG
1	E	219	GLU

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Mol	Chain	Res	Type
1	E	238[A]	GLU
1	E	238[B]	GLU
1	F	1	LEU
1	F	2	MET
1	F	22	LYS
1	F	144	ASP
1	F	145	LYS
1	F	152	GLU
1	F	178	ARG
1	F	219	GLU
1	F	238	GLU
1	F	389	LYS
1	F	397	LYS
1	G	1	LEU
1	G	2	MET
1	G	22	LYS
1	G	141	ASP
1	G	152	GLU
1	G	178	ARG
1	G	219	GLU
1	G	367	LYS
1	G	389	LYS
1	H	1	LEU
1	H	141	ASP
1	H	145	LYS
1	H	178	ARG
1	H	219	GLU
1	H	389	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	153	GLN
1	B	153	GLN
1	C	153	GLN
1	D	153	GLN
1	E	14	ASN
1	E	153	GLN
1	F	153	GLN
1	G	368	ASN
1	H	153	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	392/407 (96%)	-0.10	14 (3%) 43 44	21, 30, 54, 79	0
1	B	392/407 (96%)	0.00	13 (3%) 47 47	20, 30, 54, 79	0
1	C	392/407 (96%)	-0.18	9 (2%) 61 60	20, 30, 54, 79	0
1	D	392/407 (96%)	-0.07	17 (4%) 36 36	20, 30, 55, 79	0
1	E	392/407 (96%)	-0.05	14 (3%) 43 44	21, 30, 54, 79	0
1	F	392/407 (96%)	-0.12	11 (2%) 53 53	21, 30, 54, 79	0
1	G	391/407 (96%)	-0.01	10 (2%) 56 56	20, 29, 53, 97	0
1	H	389/407 (95%)	-0.10	9 (2%) 61 60	19, 29, 52, 79	0
All	All	3132/3256 (96%)	-0.08	97 (3%) 49 49	19, 30, 54, 97	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	143	SER	7.7
1	H	140	GLY	7.3
1	G	140	GLY	7.1
1	D	142	GLY	6.6
1	G	14	ASN	6.5
1	A	142	GLY	6.5
1	D	143	SER	6.2
1	H	143	SER	5.9
1	E	143	SER	5.3
1	G	142	GLY	5.2
1	H	141	ASP	5.0
1	G	1	LEU	5.0
1	D	22	LYS	4.9
1	G	141	ASP	4.9
1	F	145	LYS	4.9
1	G	16	PHE	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	141	ASP	4.8
1	H	142	GLY	4.5
1	B	142	GLY	4.3
1	A	145	LYS	4.3
1	A	143	SER	4.1
1	E	1	LEU	4.0
1	G	13	ALA	4.0
1	C	145	LYS	4.0
1	E	142	GLY	3.9
1	F	142	GLY	3.9
1	H	145	LYS	3.7
1	A	1	LEU	3.6
1	H	22	LYS	3.6
1	A	144	ASP	3.5
1	G	320	ILE	3.5
1	B	143	SER	3.4
1	D	15	ASP	3.2
1	D	181	ASN	3.2
1	E	22	LYS	3.2
1	E	141	ASP	3.1
1	B	16	PHE	3.1
1	G	15	ASP	3.1
1	A	15	ASP	3.1
1	B	140	GLY	3.0
1	E	140	GLY	3.0
1	B	1	LEU	2.9
1	D	156	GLN	2.8
1	H	1	LEU	2.8
1	B	389	LYS	2.8
1	F	141	ASP	2.8
1	D	386	GLU	2.8
1	E	145	LYS	2.8
1	F	143	SER	2.8
1	A	156	GLN	2.7
1	A	354	GLU	2.7
1	D	145	LYS	2.6
1	B	15	ASP	2.6
1	F	144	ASP	2.6
1	A	22	LYS	2.5
1	D	152	GLU	2.5
1	F	22	LYS	2.5
1	D	1	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	145	LYS	2.5
1	B	34	GLU	2.4
1	D	354	GLU	2.4
1	B	14	ASN	2.4
1	F	149	THR	2.4
1	A	141	ASP	2.4
1	C	358	GLN	2.3
1	C	389	LYS	2.3
1	E	33	ASP	2.3
1	D	367	LYS	2.3
1	E	16	PHE	2.3
1	C	178	ARG	2.3
1	F	140	GLY	2.2
1	E	179	HIS	2.2
1	C	144	ASP	2.2
1	E	15	ASP	2.2
1	F	15	ASP	2.2
1	E	2	MET	2.2
1	F	179	HIS	2.2
1	A	355	PRO	2.2
1	C	141	ASP	2.2
1	A	140	GLY	2.2
1	H	144	ASP	2.2
1	H	386	GLU	2.1
1	C	143	SER	2.1
1	A	152	GLU	2.1
1	D	368	ASN	2.1
1	B	22	LYS	2.1
1	B	156	GLN	2.1
1	C	354	GLU	2.1
1	D	389	LYS	2.1
1	D	163	SER	2.1
1	F	181	ASN	2.1
1	A	146	ASP	2.1
1	E	156	GLN	2.0
1	D	182	TRP	2.0
1	D	208	ASP	2.0
1	E	208	ASP	2.0
1	C	1	LEU	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	MG	F	2006	1/1	0.94	0.16	5.94	37,37,37,37	0
2	MG	H	2008	1/1	0.97	0.19	4.50	30,30,30,30	0
2	MG	G	2007	1/1	0.96	0.13	0.33	27,27,27,27	0
2	MG	D	2004	1/1	0.93	0.07	-1.13	36,36,36,36	0
2	MG	A	2001	1/1	0.95	0.07	-1.54	38,38,38,38	0
2	MG	C	2003	1/1	0.97	0.07	-1.67	34,34,34,34	0
2	MG	B	2002	1/1	0.92	0.05	-2.88	37,37,37,37	0
2	MG	E	2005	1/1	0.96	0.06	-5.34	37,37,37,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.