



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 03:49 PM EDT

PDB ID : 3FCP  
Title : Crystal structure of Muconate lactonizing enzyme from *Klebsiella pneumoniae*  
Authors : Fedorov, A.A.; Fedorov, E.V.; Sauder, J.M.; Burley, S.K.; Gerlt, J.A.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2008-11-22  
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](mailto: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>.

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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)	:	1.20.1
EDS	:	2.36.2
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)	:	2.36.2

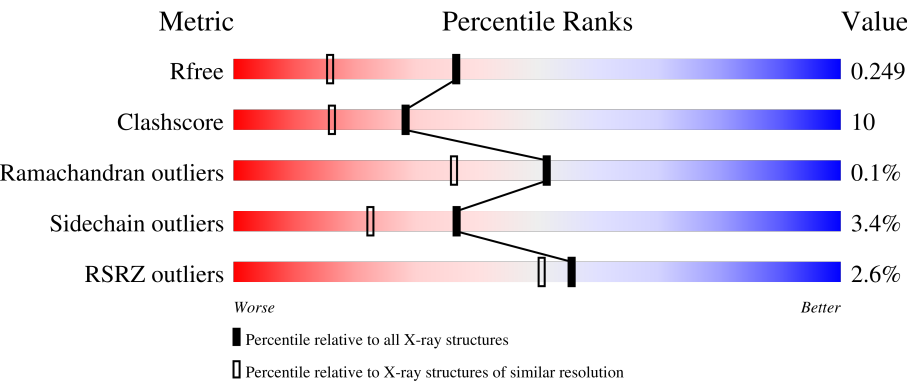
# 1 Overall quality at a glance i

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 <sub>free</sub>	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	381	<div><div>2%</div><div><div></div><div>78%</div><div>14%</div><div>7%</div></div></div>
1	B	381	<div><div>2%</div><div><div></div><div>75%</div><div>17%</div><div>7%</div></div></div>
1	C	381	<div><div>4%</div><div><div></div><div>77%</div><div>15%</div><div>7%</div></div></div>
1	D	381	<div><div>3%</div><div><div></div><div>78%</div><div>14%</div><div>7%</div></div></div>
1	E	381	<div><div>3%</div><div><div></div><div>75%</div><div>16%</div><div>7%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	381	
1	G	381	
1	H	381	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21638 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 L-Ala-D/L-Glu epimerase, a muconate lactonizing enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	0	0
			2611	1651	447	506	7			
1	B	354	Total	C	N	O	S	0	0	0
			2596	1641	445	503	7			
1	C	354	Total	C	N	O	S	0	0	0
			2596	1641	445	503	7			
1	D	354	Total	C	N	O	S	0	0	0
			2596	1641	445	503	7			
1	E	355	Total	C	N	O	S	0	0	0
			2603	1645	446	505	7			
1	F	354	Total	C	N	O	S	0	0	0
			2596	1641	445	503	7			
1	G	354	Total	C	N	O	S	0	0	0
			2596	1641	445	503	7			
1	H	356	Total	C	N	O	S	0	0	0
			2611	1651	447	506	7			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP A6T9N5
A	2	SER	-	expression tag	UNP A6T9N5
A	3	LEU	-	expression tag	UNP A6T9N5
A	374	GLU	-	expression tag	UNP A6T9N5
A	375	GLY	-	expression tag	UNP A6T9N5
A	376	HIS	-	expression tag	UNP A6T9N5
A	377	HIS	-	expression tag	UNP A6T9N5
A	378	HIS	-	expression tag	UNP A6T9N5
A	379	HIS	-	expression tag	UNP A6T9N5
A	380	HIS	-	expression tag	UNP A6T9N5
A	381	HIS	-	expression tag	UNP A6T9N5
B	1	MET	-	expression tag	UNP A6T9N5
B	2	SER	-	expression tag	UNP A6T9N5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	3	LEU	-	expression tag	UNP A6T9N5
B	374	GLU	-	expression tag	UNP A6T9N5
B	375	GLY	-	expression tag	UNP A6T9N5
B	376	HIS	-	expression tag	UNP A6T9N5
B	377	HIS	-	expression tag	UNP A6T9N5
B	378	HIS	-	expression tag	UNP A6T9N5
B	379	HIS	-	expression tag	UNP A6T9N5
B	380	HIS	-	expression tag	UNP A6T9N5
B	381	HIS	-	expression tag	UNP A6T9N5
C	1	MET	-	expression tag	UNP A6T9N5
C	2	SER	-	expression tag	UNP A6T9N5
C	3	LEU	-	expression tag	UNP A6T9N5
C	374	GLU	-	expression tag	UNP A6T9N5
C	375	GLY	-	expression tag	UNP A6T9N5
C	376	HIS	-	expression tag	UNP A6T9N5
C	377	HIS	-	expression tag	UNP A6T9N5
C	378	HIS	-	expression tag	UNP A6T9N5
C	379	HIS	-	expression tag	UNP A6T9N5
C	380	HIS	-	expression tag	UNP A6T9N5
C	381	HIS	-	expression tag	UNP A6T9N5
D	1	MET	-	expression tag	UNP A6T9N5
D	2	SER	-	expression tag	UNP A6T9N5
D	3	LEU	-	expression tag	UNP A6T9N5
D	374	GLU	-	expression tag	UNP A6T9N5
D	375	GLY	-	expression tag	UNP A6T9N5
D	376	HIS	-	expression tag	UNP A6T9N5
D	377	HIS	-	expression tag	UNP A6T9N5
D	378	HIS	-	expression tag	UNP A6T9N5
D	379	HIS	-	expression tag	UNP A6T9N5
D	380	HIS	-	expression tag	UNP A6T9N5
D	381	HIS	-	expression tag	UNP A6T9N5
E	1	MET	-	expression tag	UNP A6T9N5
E	2	SER	-	expression tag	UNP A6T9N5
E	3	LEU	-	expression tag	UNP A6T9N5
E	374	GLU	-	expression tag	UNP A6T9N5
E	375	GLY	-	expression tag	UNP A6T9N5
E	376	HIS	-	expression tag	UNP A6T9N5
E	377	HIS	-	expression tag	UNP A6T9N5
E	378	HIS	-	expression tag	UNP A6T9N5
E	379	HIS	-	expression tag	UNP A6T9N5
E	380	HIS	-	expression tag	UNP A6T9N5
E	381	HIS	-	expression tag	UNP A6T9N5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1	MET	-	expression tag	UNP A6T9N5
F	2	SER	-	expression tag	UNP A6T9N5
F	3	LEU	-	expression tag	UNP A6T9N5
F	374	GLU	-	expression tag	UNP A6T9N5
F	375	GLY	-	expression tag	UNP A6T9N5
F	376	HIS	-	expression tag	UNP A6T9N5
F	377	HIS	-	expression tag	UNP A6T9N5
F	378	HIS	-	expression tag	UNP A6T9N5
F	379	HIS	-	expression tag	UNP A6T9N5
F	380	HIS	-	expression tag	UNP A6T9N5
F	381	HIS	-	expression tag	UNP A6T9N5
G	1	MET	-	expression tag	UNP A6T9N5
G	2	SER	-	expression tag	UNP A6T9N5
G	3	LEU	-	expression tag	UNP A6T9N5
G	374	GLU	-	expression tag	UNP A6T9N5
G	375	GLY	-	expression tag	UNP A6T9N5
G	376	HIS	-	expression tag	UNP A6T9N5
G	377	HIS	-	expression tag	UNP A6T9N5
G	378	HIS	-	expression tag	UNP A6T9N5
G	379	HIS	-	expression tag	UNP A6T9N5
G	380	HIS	-	expression tag	UNP A6T9N5
G	381	HIS	-	expression tag	UNP A6T9N5
H	1	MET	-	expression tag	UNP A6T9N5
H	2	SER	-	expression tag	UNP A6T9N5
H	3	LEU	-	expression tag	UNP A6T9N5
H	374	GLU	-	expression tag	UNP A6T9N5
H	375	GLY	-	expression tag	UNP A6T9N5
H	376	HIS	-	expression tag	UNP A6T9N5
H	377	HIS	-	expression tag	UNP A6T9N5
H	378	HIS	-	expression tag	UNP A6T9N5
H	379	HIS	-	expression tag	UNP A6T9N5
H	380	HIS	-	expression tag	UNP A6T9N5
H	381	HIS	-	expression tag	UNP A6T9N5

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

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

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

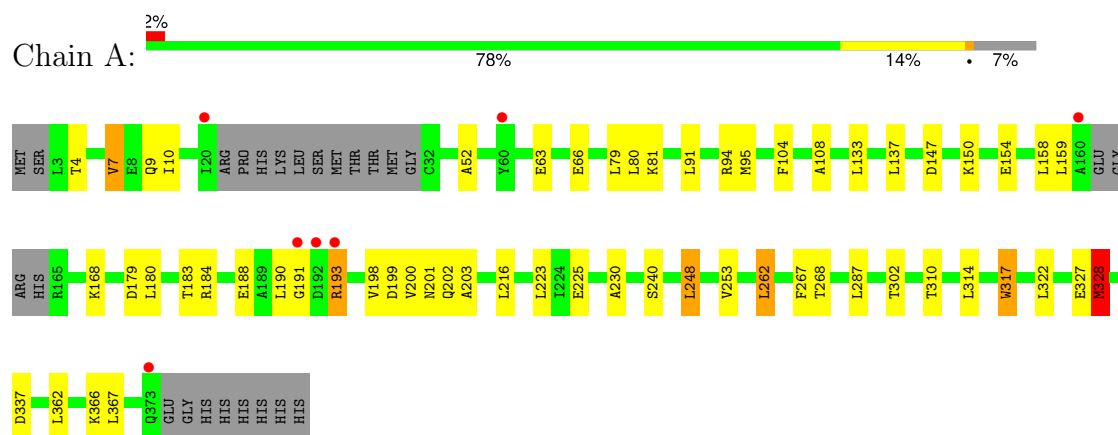
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	114	Total 114	O 114	0	0
3	B	116	Total 116	O 116	0	0
3	C	94	Total 94	O 94	0	0
3	D	91	Total 91	O 91	0	0
3	E	97	Total 97	O 97	0	0
3	F	121	Total 121	O 121	0	0
3	G	89	Total 89	O 89	0	0
3	H	103	Total 103	O 103	0	0

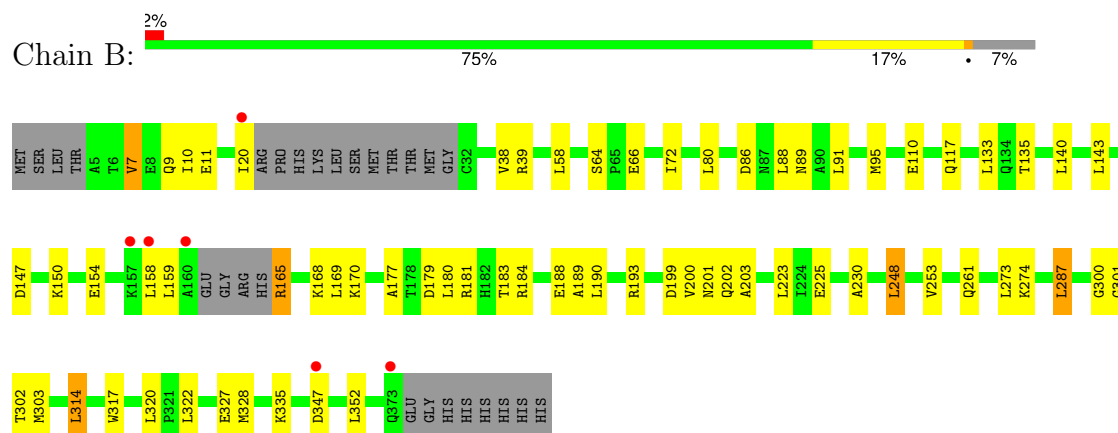
### 3 Residue-property plots [i](#)

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.

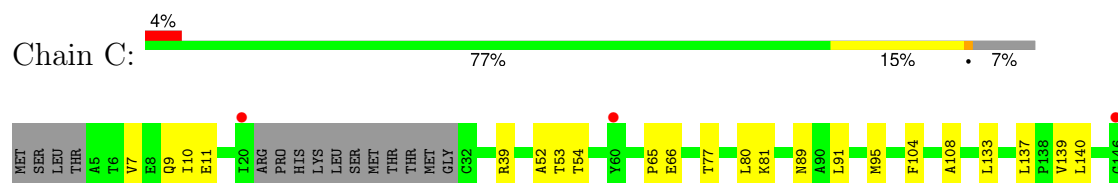
- Molecule 1: L-Ala-D/L-Glu epimerase, a muconate lactonizing enzyme

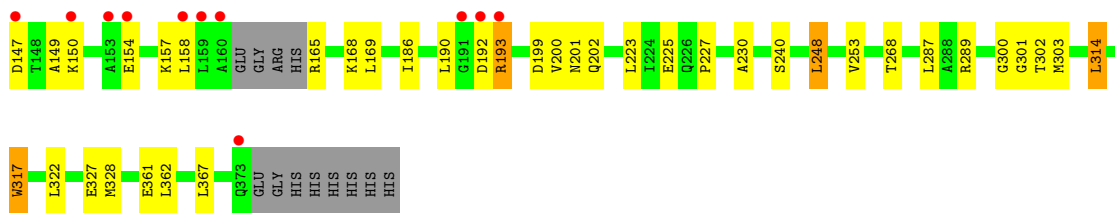


- Molecule 1: L-Ala-D/L-Glu epimerase, a muconate lactonizing enzyme

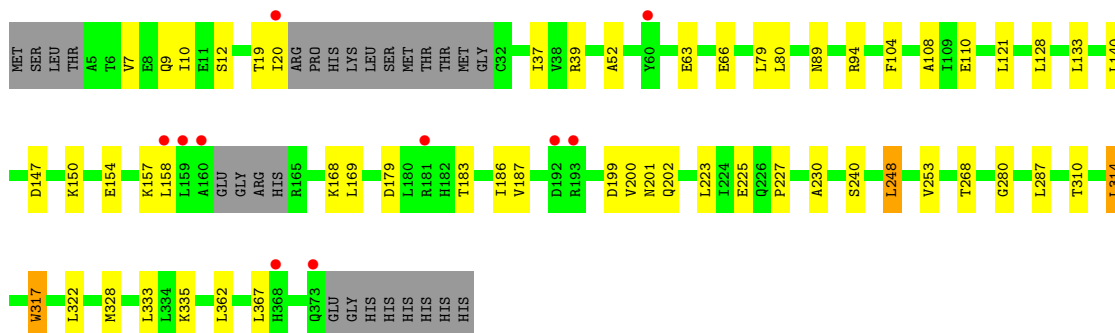
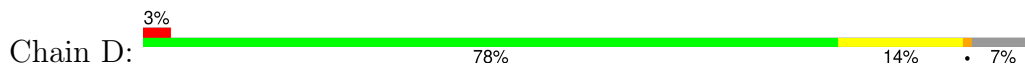


- Molecule 1: L-Ala-D/L-Glu epimerase, a muconate lactonizing enzyme

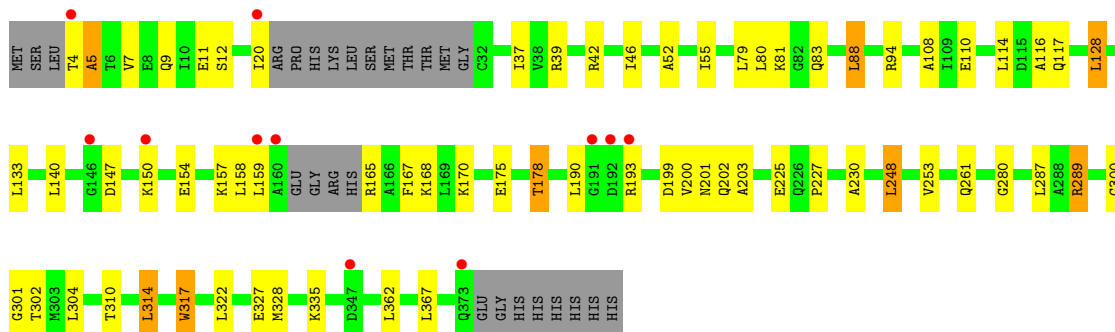
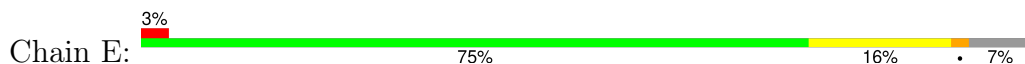




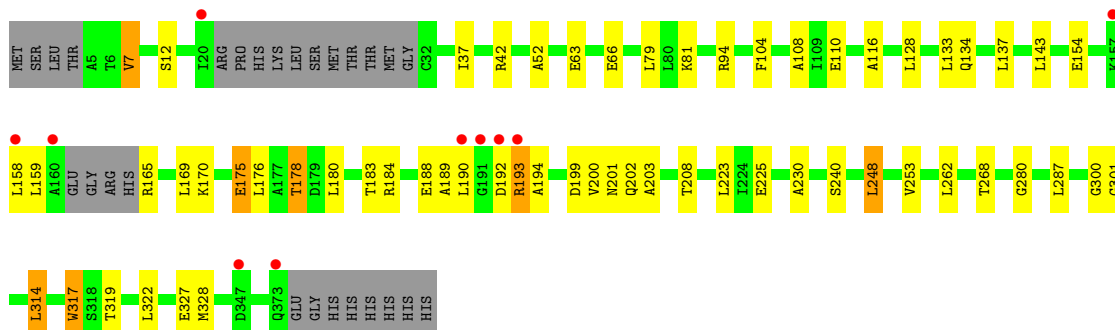
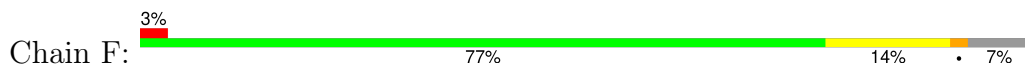
- Molecule 1: L-Ala-D/L-Glu epimerase, a muconate lactonizing enzyme



- Molecule 1: L-Ala-D/L-Glu epimerase, a muconate lactonizing enzyme

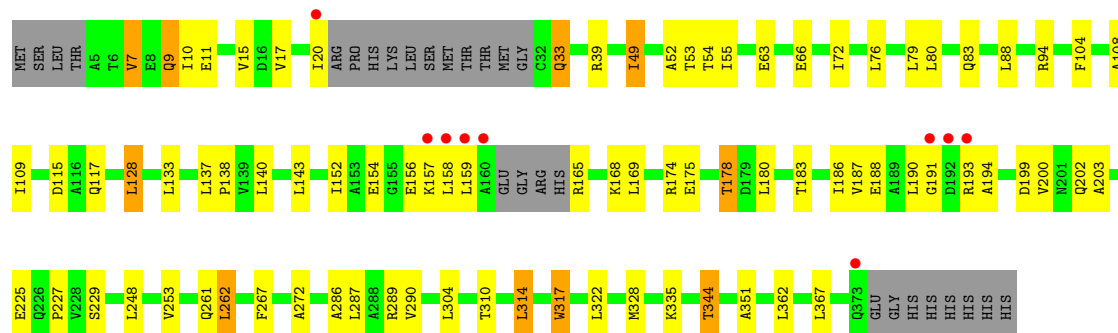


- Molecule 1: L-Ala-D/L-Glu epimerase, a muconate lactonizing enzyme




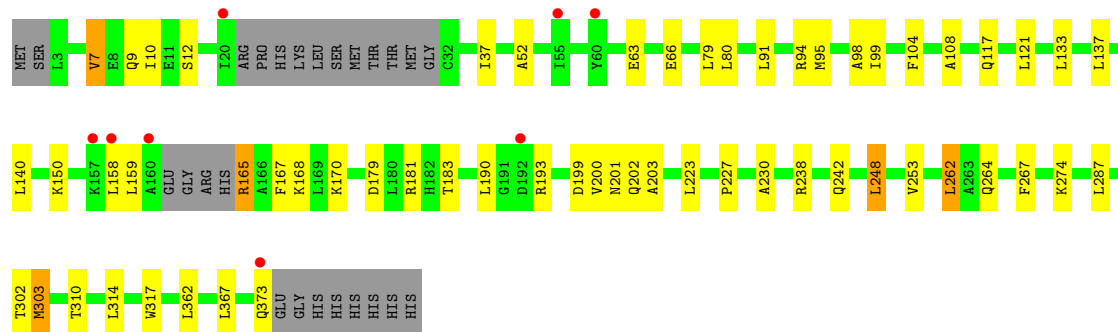
- Molecule 1: L-Ala-D/L-Glu epimerase, a muconate lactonizing enzyme

Chain G:  2% 71% 19% 7%



- Molecule 1: L-Ala-D/L-Glu epimerase, a muconate lactonizing enzyme

Chain H:  2% 78% 14% 7%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.32Å 122.73Å 193.54Å 90.00° 93.04° 90.00°	Depositor
Resolution (Å)	24.94 – 1.80 39.60 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (24.94-1.80) 99.1 (39.60-1.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.15 (at 1.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.229 , 0.250 0.228 , 0.249	Depositor DCC
$R_{free}$ test set	17054 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.4	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	21638	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.34	1/2649 (0.0%)	0.61	0/3606
1	B	0.33	0/2634	0.60	0/3585
1	C	0.32	0/2634	0.59	0/3585
1	D	0.30	0/2634	0.59	0/3585
1	E	0.32	0/2641	0.60	0/3595
1	F	0.34	0/2634	0.61	0/3585
1	G	0.31	0/2634	0.60	0/3585
1	H	0.31	0/2649	0.60	0/3606
All	All	0.32	1/21109 (0.0%)	0.60	0/28732

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	328	MET	SD-CE	-5.38	1.47	1.77

There are no bond angle outliers.

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	2611	0	2655	49	0
1	B	2596	0	2637	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2596	0	2637	47	0
1	D	2596	0	2637	41	0
1	E	2603	0	2644	55	0
1	F	2596	0	2637	47	0
1	G	2596	0	2637	62	0
1	H	2611	0	2655	47	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	114	0	0	2	0
3	B	116	0	0	0	0
3	C	94	0	0	0	0
3	D	91	0	0	1	0
3	E	97	0	0	0	0
3	F	121	0	0	1	0
3	G	89	0	0	2	0
3	H	103	0	0	1	0
All	All	21638	0	21139	410	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 10.

All (410) 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:A:302:THR:HB	1:A:328:MET:CE	1.75	1.16
1:A:302:THR:HB	1:A:328:MET:HE1	1.30	1.10
1:G:225:GLU:HG3	1:G:248:LEU:HD12	1.38	1.03
1:B:202:GLN:HE21	1:B:230:ALA:H	1.08	0.95
1:E:202:GLN:HE21	1:E:230:ALA:H	1.09	0.93
1:G:33:GLN:HA	1:G:33:GLN:HE21	1.33	0.93
1:D:202:GLN:HE21	1:D:230:ALA:H	1.18	0.92
1:F:202:GLN:HE21	1:F:230:ALA:H	1.13	0.91
1:H:202:GLN:HE21	1:H:230:ALA:H	1.17	0.88
1:H:9:GLN:HE21	1:H:10:ILE:H	1.22	0.86
1:C:202:GLN:HE21	1:C:230:ALA:H	1.20	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:MET:HA	1:B:303:MET:HE2	1.60	0.83
1:G:55:ILE:HG21	1:G:304:LEU:HD12	1.60	0.83
1:A:202:GLN:HE21	1:A:230:ALA:H	1.22	0.83
1:G:248:LEU:HD11	1:G:272:ALA:HB2	1.59	0.82
1:A:328:MET:HE2	1:A:328:MET:HA	1.62	0.80
1:A:302:THR:CB	1:A:328:MET:HE1	2.09	0.80
1:H:310:THR:O	1:H:314:LEU:HD23	1.82	0.79
1:H:79:LEU:HD11	1:H:94:ARG:HG2	1.66	0.77
1:F:159:LEU:HD12	1:F:190:LEU:HD12	1.66	0.77
1:E:202:GLN:NE2	1:E:230:ALA:H	1.83	0.76
1:B:202:GLN:NE2	1:B:230:ALA:H	1.85	0.75
1:A:79:LEU:HD11	1:A:94:ARG:HG2	1.71	0.73
1:A:9:GLN:HE21	1:A:10:ILE:H	1.36	0.72
1:A:184:ARG:O	1:A:188:GLU:HG3	1.91	0.71
1:E:11:GLU:OE1	1:E:39:ARG:HD2	1.90	0.71
1:E:79:LEU:HD11	1:E:94:ARG:HG2	1.71	0.71
1:E:20:ILE:HG22	1:E:335:LYS:HZ2	1.53	0.71
1:B:274:LYS:NZ	1:B:303:MET:HE1	2.07	0.70
1:H:303:MET:HA	1:H:303:MET:CE	2.21	0.70
1:G:33:GLN:HE21	1:G:33:GLN:CA	2.05	0.69
1:B:303:MET:HA	1:B:303:MET:CE	2.22	0.69
1:D:154:GLU:O	1:D:158:LEU:HD13	1.93	0.69
1:A:302:THR:HB	1:A:328:MET:HE2	1.75	0.68
1:F:202:GLN:HE21	1:F:230:ALA:N	1.91	0.68
1:F:202:GLN:NE2	1:F:230:ALA:H	1.90	0.68
1:G:154:GLU:O	1:G:158:LEU:HD13	1.93	0.68
1:D:9:GLN:HE21	1:D:10:ILE:H	1.42	0.68
1:E:202:GLN:HE21	1:E:230:ALA:N	1.88	0.67
1:B:302:THR:HB	1:B:328:MET:HE2	1.75	0.67
1:G:159:LEU:HD13	1:G:193:ARG:HG3	1.77	0.67
1:D:202:GLN:NE2	1:D:230:ALA:H	1.92	0.67
1:B:170:LYS:HE2	1:B:199:ASP:OD2	1.95	0.66
1:F:79:LEU:HD11	1:F:94:ARG:HG2	1.77	0.66
1:H:303:MET:HA	1:H:303:MET:HE2	1.77	0.66
1:B:320:LEU:O	1:B:322:LEU:HD12	1.95	0.66
1:A:193:ARG:HD3	1:A:193:ARG:H	1.61	0.65
1:B:274:LYS:NZ	1:B:303:MET:CE	2.59	0.65
1:G:262:LEU:HD22	1:G:267:PHE:HB2	1.78	0.64
1:E:154:GLU:O	1:E:157:LYS:HG2	1.98	0.64
1:B:274:LYS:HZ2	1:B:303:MET:HE1	1.62	0.64
1:G:159:LEU:HD12	1:G:190:LEU:HD12	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:327:GLU:H	1:E:328:MET:HE3	1.64	0.63
1:E:42:ARG:HG3	1:E:46:ILE:O	1.99	0.63
1:A:91:LEU:O	1:A:95:MET:HG3	1.98	0.63
1:H:202:GLN:NE2	1:H:230:ALA:H	1.94	0.62
1:H:302:THR:O	1:H:303:MET:HE3	1.98	0.62
1:E:168:LYS:HE3	1:E:199:ASP:HB2	1.80	0.62
1:D:200:VAL:HB	1:D:227:PRO:HA	1.81	0.62
1:B:202:GLN:HE21	1:B:230:ALA:N	1.90	0.62
1:B:274:LYS:HZ3	1:B:303:MET:CE	2.13	0.61
1:G:79:LEU:HD11	1:G:94:ARG:HG2	1.82	0.61
1:B:301:GLY:C	1:B:328:MET:HE1	2.20	0.61
1:G:20:ILE:HA	1:G:335:LYS:HE2	1.82	0.61
1:B:335:LYS:HB3	1:B:335:LYS:NZ	2.15	0.61
1:F:193:ARG:HD3	1:F:193:ARG:N	2.16	0.61
1:D:202:GLN:HE21	1:D:230:ALA:N	1.94	0.60
1:A:147:ASP:OD2	1:A:150:LYS:HG3	2.01	0.60
1:E:147:ASP:OD2	1:E:150:LYS:HG3	2.01	0.60
1:F:184:ARG:O	1:F:188:GLU:HG3	2.01	0.60
1:C:77:THR:HG22	1:C:81:LYS:HE2	1.83	0.60
1:H:179:ASP:O	1:H:183:THR:HG23	2.01	0.60
1:D:168:LYS:HE3	1:D:199:ASP:HB2	1.83	0.60
1:D:223:LEU:HD21	1:D:248:LEU:HG	1.83	0.60
1:G:186:ILE:HG23	1:G:190:LEU:HD23	1.83	0.60
1:E:20:ILE:HG22	1:E:335:LYS:NZ	2.17	0.59
1:H:9:GLN:NE2	1:H:10:ILE:H	1.96	0.59
1:G:143:LEU:HD12	1:G:169:LEU:CD2	2.32	0.59
1:E:158:LEU:HD12	1:E:167:PHE:HE1	1.68	0.59
1:B:135:THR:HG22	1:B:135:THR:O	2.03	0.58
1:E:159:LEU:HD13	1:E:193:ARG:HG3	1.85	0.58
1:G:344:THR:HG23	1:G:351:ALA:HB3	1.84	0.58
1:C:154:GLU:O	1:C:158:LEU:HD13	2.03	0.58
1:E:175:GLU:O	1:E:178:THR:HG23	2.03	0.58
1:A:137:LEU:HD22	1:A:314:LEU:HD12	1.85	0.58
1:F:327:GLU:H	1:F:328:MET:HE3	1.68	0.58
1:B:314:LEU:CD1	1:B:328:MET:HG3	2.34	0.58
1:D:362:LEU:HD21	1:D:367:LEU:HD22	1.86	0.57
1:G:253:VAL:CG1	1:G:262:LEU:HD12	2.34	0.57
1:B:184:ARG:O	1:B:188:GLU:HG3	2.05	0.57
1:B:200:VAL:HG12	1:B:203:ALA:HB3	1.86	0.57
1:E:317:TRP:HB3	1:E:322:LEU:HD11	1.85	0.57
1:G:157:LYS:O	1:G:158:LEU:HD12	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:ARG:HD3	1:E:116:ALA:HB1	1.85	0.56
1:A:7:VAL:HG22	1:A:81:LYS:HA	1.86	0.56
1:B:89:ASN:HB3	1:D:133:LEU:HD11	1.87	0.56
1:E:88:LEU:HD21	1:E:114:LEU:HD21	1.86	0.56
1:F:159:LEU:HD21	1:F:194:ALA:HB2	1.87	0.56
1:G:190:LEU:HD22	1:G:190:LEU:N	2.20	0.56
1:F:133:LEU:HD13	1:F:319:THR:HA	1.88	0.56
1:C:11:GLU:OE1	1:C:39:ARG:HD2	2.05	0.56
1:C:223:LEU:HD21	1:C:248:LEU:HG	1.88	0.56
1:D:79:LEU:HD11	1:D:94:ARG:HG2	1.87	0.56
1:A:262:LEU:HD22	1:A:267:PHE:HB2	1.87	0.56
1:G:49:ILE:HD13	1:G:49:ILE:H	1.71	0.56
1:D:179:ASP:O	1:D:183:THR:HG23	2.05	0.56
1:B:190:LEU:N	1:B:190:LEU:HD12	2.21	0.55
1:F:200:VAL:HG12	1:F:203:ALA:HB3	1.88	0.55
1:C:362:LEU:HD21	1:C:367:LEU:HD22	1.87	0.55
1:D:39:ARG:NH2	1:D:362:LEU:HD23	2.22	0.55
1:F:192:ASP:HB3	1:F:193:ARG:HD3	1.88	0.55
1:H:52:ALA:HB2	1:H:108:ALA:HB2	1.89	0.55
1:G:248:LEU:C	1:G:248:LEU:HD13	2.27	0.55
1:H:262:LEU:HD22	1:H:267:PHE:HB2	1.87	0.55
1:C:327:GLU:H	1:C:328:MET:HE3	1.71	0.55
1:G:9:GLN:HG2	1:G:10:ILE:N	2.21	0.55
1:G:33:GLN:HA	1:G:33:GLN:NE2	2.14	0.55
1:A:190:LEU:HD12	1:A:190:LEU:N	2.22	0.55
1:E:9:GLN:HA	1:E:81:LYS:HE2	1.88	0.55
1:E:4:THR:O	1:E:5:ALA:CB	2.55	0.54
1:H:150:LYS:NZ	1:H:150:LYS:HB2	2.22	0.54
1:C:193:ARG:HD3	1:C:193:ARG:N	2.21	0.54
1:E:4:THR:O	1:E:5:ALA:HB2	2.07	0.54
1:F:137:LEU:HD12	1:F:314:LEU:HD12	1.90	0.54
1:H:137:LEU:HD12	1:H:314:LEU:HD12	1.88	0.54
1:C:154:GLU:O	1:C:157:LYS:HB3	2.08	0.54
1:D:20:ILE:HD12	1:D:20:ILE:O	2.08	0.54
1:E:289:ARG:HD2	1:E:289:ARG:N	2.23	0.54
1:C:89:ASN:HB3	1:F:133:LEU:HD11	1.89	0.53
1:B:154:GLU:O	1:B:158:LEU:HD13	2.08	0.53
1:F:301:GLY:C	1:F:328:MET:HE1	2.29	0.53
1:B:180:LEU:HA	1:B:183:THR:HG22	1.91	0.53
1:B:302:THR:O	1:B:303:MET:HE3	2.08	0.53
1:H:274:LYS:NZ	1:H:303:MET:HE1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LEU:HD22	1:A:193:ARG:HG2	1.91	0.53
1:C:9:GLN:HE21	1:C:10:ILE:H	1.57	0.53
1:C:202:GLN:NE2	1:C:230:ALA:H	1.99	0.53
1:F:314:LEU:HD13	1:F:328:MET:HG3	1.91	0.53
1:D:157:LYS:HZ3	1:D:157:LYS:HB3	1.74	0.53
1:F:180:LEU:HA	1:F:183:THR:HG22	1.90	0.53
1:H:170:LYS:HD3	1:H:199:ASP:HB3	1.91	0.52
1:D:9:GLN:NE2	1:D:10:ILE:H	2.05	0.52
1:E:20:ILE:HA	1:E:335:LYS:NZ	2.24	0.52
1:F:300:GLY:O	1:F:328:MET:CE	2.56	0.52
1:E:300:GLY:O	1:E:328:MET:HE1	2.10	0.52
1:F:52:ALA:HB2	1:F:108:ALA:HB2	1.92	0.52
1:F:327:GLU:C	1:F:328:MET:HE2	2.29	0.52
1:A:223:LEU:HD21	1:A:248:LEU:HG	1.90	0.52
1:F:165:ARG:HG2	1:F:165:ARG:HH11	1.74	0.52
1:H:274:LYS:NZ	1:H:303:MET:CE	2.73	0.52
1:A:362:LEU:HD21	1:A:367:LEU:HD22	1.91	0.52
1:C:202:GLN:HE21	1:C:230:ALA:N	2.00	0.52
1:C:300:GLY:O	1:C:328:MET:CE	2.58	0.52
1:D:20:ILE:HG13	1:D:333:LEU:O	2.10	0.52
1:G:310:THR:O	1:G:314:LEU:HD22	2.10	0.52
1:A:337:ASP:O	1:A:366:LYS:HD3	2.09	0.52
1:D:121:LEU:HD12	1:D:128:LEU:HD11	1.92	0.52
1:E:301:GLY:C	1:E:328:MET:HE1	2.30	0.52
1:G:362:LEU:HD21	1:G:367:LEU:HD22	1.92	0.52
1:D:314:LEU:HD13	1:D:328:MET:HG3	1.90	0.52
1:C:147:ASP:OD2	1:C:150:LYS:HG3	2.10	0.51
1:C:192:ASP:HB3	1:C:193:ARG:HD3	1.91	0.51
1:E:300:GLY:O	1:E:328:MET:CE	2.59	0.51
1:G:7:VAL:CG1	1:G:80:LEU:O	2.58	0.51
1:C:300:GLY:O	1:C:328:MET:HE1	2.11	0.51
1:H:168:LYS:HE3	1:H:199:ASP:HB2	1.91	0.51
1:B:170:LYS:HD3	1:B:199:ASP:HB3	1.92	0.51
1:D:140:LEU:C	1:D:140:LEU:HD12	2.31	0.51
1:D:157:LYS:HB3	1:D:157:LYS:NZ	2.25	0.51
1:G:152:ILE:O	1:G:156:GLU:HG2	2.11	0.51
1:E:327:GLU:C	1:E:328:MET:HE2	2.31	0.51
1:B:9:GLN:HE21	1:B:10:ILE:H	1.57	0.51
1:F:300:GLY:O	1:F:328:MET:HE1	2.10	0.51
1:H:238:ARG:O	1:H:242:GLN:HG3	2.11	0.51
1:B:66:GLU:CD	1:B:66:GLU:H	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:117:GLN:HE21	1:H:121:LEU:HG	1.76	0.51
1:A:154:GLU:O	1:A:158:LEU:HD23	2.11	0.50
1:C:139:VAL:HG23	1:C:139:VAL:O	2.10	0.50
1:G:117:GLN:HE21	1:G:128:LEU:HG	1.76	0.50
1:H:223:LEU:HD21	1:H:248:LEU:HG	1.92	0.50
1:B:327:GLU:H	1:B:328:MET:HE3	1.76	0.50
1:E:225:GLU:HG3	1:E:248:LEU:HD13	1.92	0.50
1:G:168:LYS:HE3	1:G:199:ASP:HB2	1.93	0.50
1:H:190:LEU:HD12	1:H:190:LEU:N	2.26	0.50
1:B:86:ASP:OD1	1:B:117:GLN:OE1	2.30	0.50
1:H:66:GLU:H	1:H:66:GLU:CD	2.15	0.50
1:E:175:GLU:HB2	1:E:178:THR:HG22	1.94	0.50
1:D:66:GLU:CD	1:D:66:GLU:H	2.15	0.50
1:A:180:LEU:HA	1:A:183:THR:HG22	1.94	0.50
1:C:91:LEU:O	1:C:95:MET:HG3	2.12	0.50
1:D:39:ARG:HH21	1:D:362:LEU:HD23	1.77	0.50
1:H:200:VAL:HB	1:H:227:PRO:HA	1.93	0.50
1:B:7:VAL:HG13	1:B:80:LEU:O	2.12	0.49
1:H:170:LYS:HE2	1:H:199:ASP:OD2	2.12	0.49
1:C:66:GLU:H	1:C:66:GLU:CD	2.14	0.49
1:G:253:VAL:O	1:G:253:VAL:HG23	2.12	0.49
1:B:168:LYS:HE3	1:B:199:ASP:HB2	1.92	0.49
1:C:168:LYS:HE3	1:C:199:ASP:HB2	1.94	0.49
1:A:200:VAL:HG12	1:A:203:ALA:HB3	1.94	0.49
1:A:193:ARG:H	1:A:193:ARG:CD	2.24	0.49
1:D:317:TRP:HB3	1:D:322:LEU:HD11	1.93	0.49
1:G:7:VAL:HG12	1:G:83:GLN:O	2.13	0.49
1:A:52:ALA:HB2	1:A:108:ALA:HB2	1.94	0.49
1:E:190:LEU:O	1:E:193:ARG:HG2	2.13	0.49
1:H:158:LEU:HD23	1:H:167:PHE:HE1	1.77	0.49
1:C:317:TRP:HB3	1:C:322:LEU:HD11	1.94	0.49
1:G:180:LEU:HA	1:G:183:THR:HG22	1.94	0.49
1:B:7:VAL:CG1	1:B:80:LEU:O	2.60	0.48
1:C:193:ARG:HH11	1:C:193:ARG:HG3	1.77	0.48
1:G:7:VAL:HG11	1:G:80:LEU:O	2.13	0.48
1:B:335:LYS:HB3	1:B:335:LYS:HZ3	1.76	0.48
1:A:328:MET:CE	1:A:328:MET:HA	2.40	0.48
1:B:193:ARG:HG2	1:B:193:ARG:HH11	1.78	0.48
1:C:52:ALA:HB2	1:C:108:ALA:HB2	1.94	0.48
1:G:11:GLU:OE1	1:G:39:ARG:HD2	2.13	0.48
1:G:225:GLU:CG	1:G:248:LEU:HD12	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:362:LEU:HD21	1:E:367:LEU:HD22	1.95	0.48
1:C:7:VAL:CG1	1:C:80:LEU:O	2.62	0.48
1:C:200:VAL:HB	1:C:227:PRO:HA	1.95	0.48
1:C:327:GLU:C	1:C:328:MET:HE2	2.34	0.48
1:F:317:TRP:HB3	1:F:322:LEU:HD11	1.96	0.48
1:B:11:GLU:OE1	1:B:39:ARG:HD2	2.14	0.48
1:G:63:GLU:OE1	1:G:104:PHE:HB2	2.13	0.48
1:G:140:LEU:C	1:G:140:LEU:HD12	2.34	0.48
1:F:134:GLN:HG3	1:F:137:LEU:CD2	2.44	0.48
1:F:190:LEU:N	1:F:190:LEU:HD22	2.28	0.48
1:G:79:LEU:C	1:G:79:LEU:HD13	2.34	0.48
1:F:199:ASP:HA	1:F:225:GLU:HB3	1.96	0.47
1:H:91:LEU:O	1:H:95:MET:HG3	2.15	0.47
1:A:179:ASP:O	1:A:183:THR:HG22	2.14	0.47
1:B:165:ARG:HG2	1:B:165:ARG:HH11	1.79	0.47
1:C:302:THR:HB	1:C:328:MET:HE2	1.96	0.47
1:A:79:LEU:HD13	1:A:79:LEU:C	2.34	0.47
1:D:52:ALA:HB2	1:D:108:ALA:HB2	1.97	0.47
1:E:12:SER:HA	1:E:37:ILE:O	2.15	0.47
1:F:170:LYS:HD2	1:F:199:ASP:HB3	1.96	0.47
1:F:193:ARG:HG3	1:F:193:ARG:HH11	1.79	0.47
1:G:15:VAL:HG12	1:G:17:VAL:HG13	1.97	0.47
1:A:168:LYS:HE3	1:A:199:ASP:HB2	1.97	0.47
1:B:147:ASP:OD2	1:B:150:LYS:HG3	2.15	0.47
1:C:140:LEU:HD12	1:C:140:LEU:C	2.36	0.47
1:H:274:LYS:HZ2	1:H:303:MET:HE1	1.80	0.47
1:G:200:VAL:HB	1:G:227:PRO:HA	1.97	0.46
1:F:154:GLU:O	1:F:158:LEU:HD13	2.15	0.46
1:B:322:LEU:HD12	1:B:322:LEU:N	2.30	0.46
1:E:20:ILE:HA	1:E:335:LYS:HZ3	1.80	0.46
1:H:373:GLN:HA	1:H:373:GLN:NE2	2.30	0.46
1:E:253:VAL:O	1:E:253:VAL:HG13	2.16	0.46
1:G:183:THR:O	1:G:187:VAL:HG23	2.16	0.46
1:E:110:GLU:OE1	1:E:280:GLY:HA3	2.16	0.46
1:F:176:LEU:HD22	1:F:208:THR:HG23	1.97	0.46
1:H:274:LYS:HZ3	1:H:303:MET:CE	2.28	0.46
1:E:200:VAL:HG12	1:E:203:ALA:HB3	1.98	0.46
1:E:314:LEU:HD13	1:E:328:MET:HG3	1.98	0.46
1:F:223:LEU:HD21	1:F:248:LEU:HG	1.97	0.46
1:B:133:LEU:HD11	1:D:89:ASN:HB3	1.97	0.46
1:E:52:ALA:HB2	1:E:108:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:12:SER:HA	1:H:37:ILE:O	2.16	0.46
1:A:201:ASN:O	1:A:202:GLN:HB2	2.16	0.45
1:G:317:TRP:HB3	1:G:322:LEU:HD11	1.97	0.45
1:A:202:GLN:NE2	1:A:230:ALA:H	2.01	0.45
1:D:240:SER:HB2	1:D:268:THR:O	2.17	0.45
1:A:63:GLU:OE1	1:A:104:PHE:HB2	2.16	0.45
1:A:66:GLU:H	1:A:66:GLU:CD	2.20	0.45
1:A:80:LEU:HD22	1:A:91:LEU:HD22	1.99	0.45
1:A:9:GLN:NE2	1:A:10:ILE:H	2.11	0.45
1:B:159:LEU:HD13	1:B:193:ARG:HG3	1.98	0.45
1:D:168:LYS:HE3	1:D:199:ASP:CB	2.46	0.45
1:H:117:GLN:NE2	1:H:121:LEU:HG	2.32	0.45
1:A:137:LEU:N	1:A:137:LEU:HD12	2.32	0.45
1:B:190:LEU:N	1:B:190:LEU:CD1	2.80	0.45
1:D:63:GLU:OE1	1:D:104:PHE:HB2	2.17	0.45
1:D:110:GLU:OE1	1:D:280:GLY:HA3	2.17	0.45
1:G:200:VAL:HG12	1:G:203:ALA:HB3	1.99	0.45
1:H:165:ARG:HG2	1:H:165:ARG:HH11	1.82	0.45
1:C:104:PHE:HZ	1:C:303:MET:CE	2.30	0.45
1:C:225:GLU:HG3	1:C:248:LEU:HD13	1.99	0.45
1:E:200:VAL:HB	1:E:227:PRO:HA	1.99	0.45
1:A:302:THR:CA	1:A:328:MET:HE1	2.47	0.45
1:C:314:LEU:HD13	1:C:328:MET:HG3	1.98	0.45
1:D:199:ASP:HA	1:D:225:GLU:HB3	1.98	0.45
1:A:240:SER:HB2	1:A:268:THR:O	2.17	0.44
1:B:314:LEU:HB3	1:B:352:LEU:HD13	1.99	0.44
1:F:189:ALA:HB3	1:F:190:LEU:HD22	1.99	0.44
1:F:240:SER:HB2	1:F:268:THR:O	2.17	0.44
1:A:4:THR:HG22	3:A:956:HOH:O	2.16	0.44
1:B:143:LEU:HD12	1:B:169:LEU:HD21	2.00	0.44
1:C:104:PHE:HZ	1:C:303:MET:HE3	1.81	0.44
1:E:302:THR:HB	1:E:328:MET:HE2	1.98	0.44
1:F:175:GLU:O	1:F:178:THR:HG23	2.17	0.44
1:H:362:LEU:HD21	1:H:367:LEU:HD22	2.00	0.44
1:C:137:LEU:N	1:C:137:LEU:HD12	2.32	0.44
1:E:79:LEU:HD13	1:E:79:LEU:C	2.37	0.44
1:G:52:ALA:HB2	1:G:108:ALA:HB2	1.98	0.44
1:G:66:GLU:CD	1:G:66:GLU:H	2.21	0.44
1:G:310:THR:HG23	1:G:328:MET:HB3	2.00	0.44
1:H:158:LEU:HD23	1:H:167:PHE:CE1	2.52	0.44
1:C:301:GLY:C	1:C:328:MET:HE1	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:143:LEU:HD12	1:F:169:LEU:HD21	1.98	0.44
1:C:169:LEU:HD13	1:C:186:ILE:HD12	1.98	0.44
1:G:33:GLN:CA	1:G:33:GLN:NE2	2.78	0.44
1:B:274:LYS:NZ	1:B:303:MET:HE3	2.31	0.44
1:D:183:THR:O	1:D:187:VAL:HG23	2.18	0.44
1:E:55:ILE:HD11	1:E:304:LEU:HG	1.99	0.44
1:E:140:LEU:HD12	1:E:140:LEU:C	2.38	0.44
1:F:110:GLU:OE1	1:F:280:GLY:HA3	2.18	0.44
1:A:225:GLU:HG3	1:A:248:LEU:HD13	1.99	0.44
1:G:202:GLN:HB3	1:G:229:SER:HA	1.99	0.44
1:G:344:THR:HG22	3:G:824:HOH:O	2.17	0.44
1:H:63:GLU:OE1	1:H:104:PHE:HB2	2.17	0.44
1:D:12:SER:HA	1:D:37:ILE:O	2.18	0.44
1:G:261:GLN:HG3	3:H:565:HOH:O	2.17	0.44
1:B:140:LEU:C	1:B:140:LEU:HD12	2.38	0.43
1:C:165:ARG:HG2	1:C:165:ARG:HH11	1.82	0.43
1:F:253:VAL:O	1:F:253:VAL:HG13	2.17	0.43
1:H:140:LEU:HD12	1:H:140:LEU:C	2.37	0.43
1:H:201:ASN:O	1:H:202:GLN:HB2	2.18	0.43
1:G:79:LEU:HD13	1:G:79:LEU:O	2.18	0.43
1:B:91:LEU:O	1:B:95:MET:HG3	2.19	0.43
1:E:327:GLU:N	1:E:328:MET:HE3	2.32	0.43
1:G:165:ARG:O	1:G:194:ALA:HA	2.18	0.43
1:F:7:VAL:HG22	1:F:81:LYS:HA	1.99	0.43
1:B:179:ASP:O	1:B:183:THR:HG22	2.18	0.43
1:C:199:ASP:HA	1:C:225:GLU:HB3	1.99	0.43
1:C:201:ASN:O	1:C:202:GLN:HB2	2.19	0.43
1:H:253:VAL:HG13	1:H:253:VAL:O	2.19	0.43
1:A:328:MET:HE2	1:A:328:MET:CA	2.40	0.43
1:F:63:GLU:OE1	1:F:104:PHE:HB2	2.19	0.43
1:B:274:LYS:HZ3	1:B:303:MET:HE3	1.82	0.43
1:C:168:LYS:HE3	1:C:199:ASP:CB	2.49	0.43
1:E:7:VAL:CG1	1:E:80:LEU:O	2.67	0.43
1:F:225:GLU:HG3	1:F:248:LEU:HD13	2.00	0.43
1:D:147:ASP:HB3	1:D:150:LYS:HD2	2.00	0.43
1:E:7:VAL:HG12	1:E:83:GLN:O	2.18	0.43
1:A:310:THR:O	1:A:314:LEU:HD22	2.19	0.43
1:A:253:VAL:HG13	1:A:253:VAL:O	2.19	0.42
1:F:159:LEU:CD1	1:F:190:LEU:HD12	2.44	0.42
1:E:201:ASN:O	1:E:202:GLN:HB2	2.19	0.42
1:E:327:GLU:C	1:E:328:MET:CE	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:49:ILE:HD12	3:G:721:HOH:O	2.17	0.42
1:H:274:LYS:HZ3	1:H:303:MET:HE3	1.83	0.42
1:B:302:THR:HB	1:B:328:MET:CE	2.44	0.42
1:D:201:ASN:O	1:D:202:GLN:HB2	2.19	0.42
1:E:117:GLN:HE21	1:E:128:LEU:HG	1.85	0.42
1:E:310:THR:HG23	1:E:328:MET:HB3	2.02	0.42
1:E:199:ASP:HA	1:E:225:GLU:HB3	2.00	0.42
1:A:310:THR:O	1:A:314:LEU:CD2	2.68	0.42
1:B:38:VAL:CG2	1:B:72:ILE:HD13	2.50	0.42
1:B:193:ARG:HG2	1:B:193:ARG:NH1	2.34	0.42
1:B:201:ASN:O	1:B:202:GLN:HB2	2.20	0.42
1:C:253:VAL:HG13	1:C:253:VAL:O	2.19	0.42
1:D:7:VAL:CG1	1:D:80:LEU:O	2.68	0.42
1:C:65:PRO:HD2	1:C:66:GLU:OE1	2.20	0.42
1:C:147:ASP:OD2	1:C:149:ALA:HB3	2.20	0.42
1:D:310:THR:HG23	1:D:328:MET:HB3	2.02	0.42
1:G:53:THR:HG22	1:G:54:THR:N	2.35	0.41
1:B:261:GLN:HG3	3:D:406:HOH:O	2.20	0.41
1:D:19:THR:O	1:D:335:LYS:HG3	2.20	0.41
1:A:317:TRP:HB3	1:A:322:LEU:HD11	2.02	0.41
1:F:66:GLU:CD	1:F:66:GLU:H	2.23	0.41
1:F:193:ARG:HD3	1:F:193:ARG:H	1.84	0.41
1:G:72:ILE:HA	1:G:76:LEU:HB2	2.02	0.41
1:A:190:LEU:N	1:A:190:LEU:CD1	2.83	0.41
1:B:20:ILE:HA	1:B:335:LYS:HD3	2.02	0.41
1:E:170:LYS:HB3	1:E:170:LYS:NZ	2.35	0.41
1:G:159:LEU:CD1	1:G:190:LEU:HD12	2.46	0.41
1:H:200:VAL:HG12	1:H:203:ALA:HB3	2.02	0.41
1:A:327:GLU:C	1:A:328:MET:HE3	2.41	0.41
1:B:273:LEU:CD2	1:B:287:LEU:HD13	2.50	0.41
1:H:202:GLN:HE21	1:H:230:ALA:N	1.99	0.41
1:A:198:VAL:HG21	1:A:216:LEU:HD13	2.02	0.41
3:A:433:HOH:O	1:E:261:GLN:HG3	2.20	0.41
1:F:12:SER:HA	1:F:37:ILE:O	2.20	0.41
1:G:49:ILE:HD13	1:G:115:ASP:OD2	2.21	0.41
1:H:7:VAL:HG13	1:H:80:LEU:O	2.20	0.41
1:B:135:THR:O	1:B:135:THR:CG2	2.68	0.41
1:B:189:ALA:C	1:B:190:LEU:HD12	2.41	0.41
1:B:300:GLY:O	1:B:328:MET:CE	2.69	0.41
1:C:7:VAL:HG11	1:C:80:LEU:O	2.20	0.41
1:C:53:THR:HG22	1:C:54:THR:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:ILE:HD12	1:D:20:ILE:C	2.41	0.41
1:F:42:ARG:CD	1:F:116:ALA:HB1	2.51	0.41
1:G:157:LYS:C	1:G:158:LEU:HD12	2.40	0.41
1:G:174:ARG:HG3	1:G:174:ARG:HH11	1.83	0.41
1:G:175:GLU:O	1:G:178:THR:HG23	2.21	0.41
1:H:98:ALA:O	1:H:99:ILE:HD13	2.20	0.41
1:A:328:MET:CE	1:A:328:MET:CA	2.98	0.41
1:B:223:LEU:HD21	1:B:248:LEU:HG	2.03	0.41
1:B:274:LYS:HD3	1:B:303:MET:HE3	2.01	0.41
1:E:165:ARG:HH11	1:E:165:ARG:HG2	1.86	0.41
1:E:170:LYS:HD2	1:E:199:ASP:HB3	2.02	0.41
1:F:201:ASN:O	1:F:202:GLN:HB2	2.21	0.41
1:H:79:LEU:HD13	1:H:79:LEU:C	2.41	0.41
1:B:177:ALA:O	1:B:181:ARG:HG3	2.21	0.41
1:C:240:SER:HB2	1:C:268:THR:O	2.21	0.41
1:G:76:LEU:HD13	1:G:109:ILE:HG13	2.03	0.41
1:G:253:VAL:HG13	1:G:262:LEU:HD12	2.03	0.41
1:B:88:LEU:HD11	1:B:110:GLU:HG3	2.03	0.40
1:C:154:GLU:HA	1:C:157:LYS:HB3	2.02	0.40
1:F:134:GLN:HG2	3:F:503:HOH:O	2.22	0.40
1:H:190:LEU:N	1:H:190:LEU:CD1	2.84	0.40
1:B:199:ASP:HA	1:B:225:GLU:HB3	2.02	0.40
1:G:286:ALA:O	1:G:290:VAL:HG23	2.21	0.40
1:D:253:VAL:O	1:D:253:VAL:HG13	2.21	0.40
1:G:137:LEU:HA	1:G:138:PRO:HD3	1.91	0.40
1:B:9:GLN:NE2	1:B:10:ILE:H	2.19	0.40
1:B:253:VAL:O	1:B:253:VAL:HG13	2.21	0.40
1:B:58:LEU:HD21	1:B:64:SER:HB3	2.03	0.40
1:D:169:LEU:HD13	1:D:186:ILE:HD12	2.04	0.40
1:H:159:LEU:HD13	1:H:193:ARG:NE	2.37	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	350/381 (92%)	336 (96%)	13 (4%)	1 (0%)	41	27
1	B	348/381 (91%)	339 (97%)	9 (3%)	0	100	100
1	C	348/381 (91%)	337 (97%)	11 (3%)	0	100	100
1	D	348/381 (91%)	337 (97%)	11 (3%)	0	100	100
1	E	349/381 (92%)	341 (98%)	7 (2%)	1 (0%)	41	27
1	F	348/381 (91%)	340 (98%)	8 (2%)	0	100	100
1	G	348/381 (91%)	336 (97%)	11 (3%)	1 (0%)	41	27
1	H	350/381 (92%)	340 (97%)	10 (3%)	0	100	100
All	All	2789/3048 (92%)	2706 (97%)	80 (3%)	3 (0%)	51	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	GLY
1	E	5	ALA
1	G	191	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	266/288 (92%)	258 (97%)	8 (3%)	41	27
1	B	264/288 (92%)	257 (97%)	7 (3%)	44	31
1	C	264/288 (92%)	255 (97%)	9 (3%)	37	22
1	D	264/288 (92%)	260 (98%)	4 (2%)	65	56
1	E	265/288 (92%)	256 (97%)	9 (3%)	37	22
1	F	264/288 (92%)	254 (96%)	10 (4%)	33	18
1	G	264/288 (92%)	249 (94%)	15 (6%)	20	8
1	H	266/288 (92%)	256 (96%)	10 (4%)	33	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2117/2304 (92%)	2045 (97%)	72 (3%)	37 22

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	133	LEU
1	A	193	ARG
1	A	248	LEU
1	A	262	LEU
1	A	287	LEU
1	A	317	TRP
1	A	328	MET
1	B	7	VAL
1	B	165	ARG
1	B	248	LEU
1	B	287	LEU
1	B	314	LEU
1	B	317	TRP
1	B	347	ASP
1	C	133	LEU
1	C	190	LEU
1	C	193	ARG
1	C	248	LEU
1	C	287	LEU
1	C	289	ARG
1	C	314	LEU
1	C	317	TRP
1	C	361	GLU
1	D	248	LEU
1	D	287	LEU
1	D	314	LEU
1	D	317	TRP
1	E	88	LEU
1	E	128	LEU
1	E	133	LEU
1	E	178	THR
1	E	248	LEU
1	E	287	LEU
1	E	289	ARG
1	E	314	LEU
1	E	317	TRP

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Mol	Chain	Res	Type
1	F	7	VAL
1	F	128	LEU
1	F	175	GLU
1	F	178	THR
1	F	193	ARG
1	F	248	LEU
1	F	262	LEU
1	F	287	LEU
1	F	314	LEU
1	F	317	TRP
1	G	7	VAL
1	G	9	GLN
1	G	33	GLN
1	G	49	ILE
1	G	88	LEU
1	G	128	LEU
1	G	133	LEU
1	G	178	THR
1	G	188	GLU
1	G	262	LEU
1	G	287	LEU
1	G	289	ARG
1	G	314	LEU
1	G	317	TRP
1	G	344	THR
1	H	7	VAL
1	H	133	LEU
1	H	165	ARG
1	H	181	ARG
1	H	248	LEU
1	H	262	LEU
1	H	264	GLN
1	H	287	LEU
1	H	303	MET
1	H	317	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	134	GLN
1	A	202	GLN

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Mol	Chain	Res	Type
1	A	233	ASN
1	A	241	GLN
1	A	354	GLN
1	B	117	GLN
1	B	134	GLN
1	B	202	GLN
1	B	233	ASN
1	C	9	GLN
1	C	202	GLN
1	C	233	ASN
1	C	242	GLN
1	C	265	GLN
1	C	373	GLN
1	D	9	GLN
1	D	117	GLN
1	D	202	GLN
1	D	233	ASN
1	D	242	GLN
1	D	373	GLN
1	E	117	GLN
1	E	202	GLN
1	E	233	ASN
1	F	74	HIS
1	F	202	GLN
1	F	233	ASN
1	F	241	GLN
1	F	368	HIS
1	G	33	GLN
1	G	117	GLN
1	G	233	ASN
1	H	9	GLN
1	H	202	GLN
1	H	233	ASN
1	H	261	GLN
1	H	264	GLN
1	H	373	GLN

### 5.3.3 RNA ⓘ

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 monosaccharides 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	356/381 (93%)	-0.17	7 (1%) 65 61	19, 27, 45, 70	0
1	B	354/381 (92%)	-0.22	6 (1%) 70 66	20, 27, 45, 71	0
1	C	354/381 (92%)	-0.09	14 (3%) 38 32	20, 29, 48, 69	0
1	D	354/381 (92%)	-0.14	10 (2%) 53 47	20, 30, 47, 74	0
1	E	355/381 (93%)	-0.17	11 (3%) 49 43	20, 28, 49, 71	0
1	F	354/381 (92%)	-0.22	10 (2%) 53 47	19, 28, 47, 72	0
1	G	354/381 (92%)	-0.11	9 (2%) 57 52	21, 30, 48, 76	0
1	H	356/381 (93%)	-0.21	8 (2%) 62 57	20, 28, 47, 72	0
All	All	2837/3048 (93%)	-0.17	75 (2%) 56 51	19, 28, 47, 76	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	160	ALA	7.8
1	G	373	GLN	5.8
1	E	160	ALA	5.7
1	C	160	ALA	5.6
1	A	373	GLN	5.5
1	H	373	GLN	5.1
1	F	157	LYS	4.7
1	G	192	ASP	4.6
1	D	373	GLN	4.4
1	C	373	GLN	4.2
1	C	146	GLY	4.2
1	E	192	ASP	4.1
1	F	373	GLN	4.0
1	A	160	ALA	4.0
1	C	20	ILE	3.8
1	B	373	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	H	160	ALA	3.6
1	G	191	GLY	3.6
1	D	160	ALA	3.5
1	B	160	ALA	3.5
1	E	373	GLN	3.5
1	F	193	ARG	3.3
1	F	191	GLY	3.3
1	A	192	ASP	3.3
1	G	20	ILE	3.2
1	F	190	LEU	3.2
1	C	192	ASP	3.1
1	D	159	LEU	2.9
1	D	192	ASP	2.9
1	E	20	ILE	2.9
1	G	159	LEU	2.8
1	A	20	ILE	2.8
1	E	193	ARG	2.8
1	F	160	ALA	2.8
1	A	193	ARG	2.7
1	C	159	LEU	2.7
1	E	4	THR	2.7
1	D	60	TYR	2.6
1	E	159	LEU	2.6
1	D	20	ILE	2.6
1	C	154	GLU	2.6
1	B	20	ILE	2.6
1	F	20	ILE	2.6
1	C	191	GLY	2.5
1	G	157	LYS	2.5
1	F	158	LEU	2.5
1	H	55	ILE	2.5
1	F	192	ASP	2.4
1	H	158	LEU	2.4
1	A	191	GLY	2.4
1	C	193	ARG	2.4
1	E	150	LYS	2.4
1	B	347	ASP	2.3
1	D	181	ARG	2.3
1	C	150	LYS	2.3
1	H	192	ASP	2.3
1	G	158	LEU	2.3
1	F	347	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	60	TYR	2.2
1	H	157	LYS	2.2
1	D	158	LEU	2.2
1	C	153	ALA	2.2
1	D	193	ARG	2.2
1	E	146	GLY	2.2
1	H	20	ILE	2.2
1	C	147	ASP	2.2
1	D	368	HIS	2.1
1	E	347	ASP	2.1
1	B	158	LEU	2.1
1	C	158	LEU	2.1
1	H	60	TYR	2.1
1	G	193	ARG	2.1
1	E	191	GLY	2.1
1	B	157	LYS	2.0
1	C	60	TYR	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	A	382	1/1	0.99	0.10	17,17,17,17	0
2	MG	D	382	1/1	0.99	0.13	19,19,19,19	0
2	MG	E	382	1/1	0.99	0.16	18,18,18,18	0
2	MG	F	382	1/1	0.99	0.09	20,20,20,20	0
2	MG	G	382	1/1	0.99	0.14	21,21,21,21	0
2	MG	H	382	1/1	0.99	0.12	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	C	382	1/1	1.00	0.14	17,17,17,17	0
2	MG	B	382	1/1	1.00	0.13	16,16,16,16	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.