



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 07:29 PM EDT

PDB ID : 3FV9
Title : Crystal structure of putative mandelate racemase/muconatelactonizing enzyme from ROSEOVARIUS NUBINHIBENS ISM complexed with magnesium
Authors : Malashkevich, V.N.; Rutter, M.; Bain, K.T.; Lau, C.; Ozyurt, S.; Smith, D.; Wasserman, S.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2009-01-15
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-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

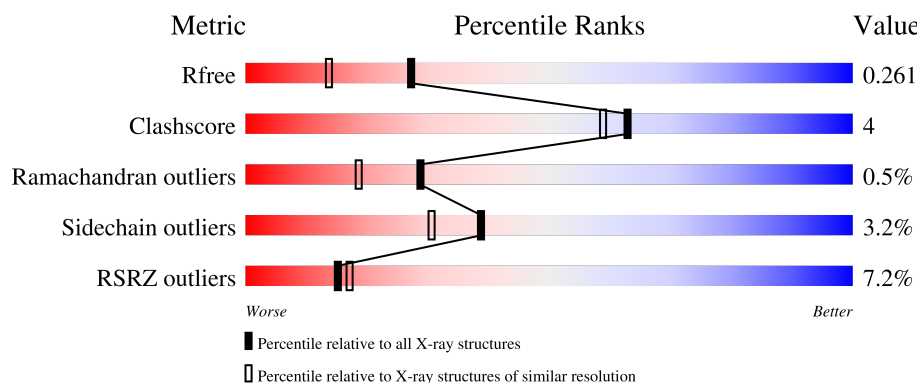
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	386	<div> <div>4%</div> <div>83%</div> <div>10%</div> <div>6%</div> </div>
1	B	386	<div> <div>3%</div> <div>85%</div> <div>9%</div> <div>5%</div> </div>
1	C	386	<div> <div>9%</div> <div>87%</div> <div>10%</div> <div>•</div> </div>
1	D	386	<div> <div>4%</div> <div>88%</div> <div>9%</div> <div>•</div> </div>
1	E	386	<div> <div>9%</div> <div>85%</div> <div>11%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	386	<div><div></div><div>10%</div><div>85%</div><div>11%</div><div></div><div></div></div>
1	G	386	<div><div></div><div>%</div><div>88%</div><div>8%</div><div></div><div></div></div>
1	H	386	<div><div></div><div>16%</div><div>84%</div><div>12%</div><div></div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24665 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Mandelate racemase/muconate lactonizing enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	373	Total	C	N	O	S	0	4	0
			2800	1743	515	526	16			
1	A	363	Total	C	N	O	S	0	0	0
			2687	1667	494	510	16			
1	D	373	Total	C	N	O	S	0	0	0
			2767	1718	510	523	16			
1	E	373	Total	C	N	O	S	0	0	0
			2767	1718	510	523	16			
1	F	373	Total	C	N	O	S	0	0	0
			2767	1718	510	523	16			
1	B	365	Total	C	N	O	S	0	0	0
			2704	1679	496	513	16			
1	H	374	Total	C	N	O	S	0	2	0
			2786	1730	513	527	16			
1	C	374	Total	C	N	O	S	0	1	0
			2782	1727	513	526	16			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	MET	-	expression tag	UNP A3SNG0
G	0	SER	-	expression tag	UNP A3SNG0
G	1	LEU	-	expression tag	UNP A3SNG0
G	377	GLU	-	expression tag	UNP A3SNG0
G	378	GLY	-	expression tag	UNP A3SNG0
G	379	HIS	-	expression tag	UNP A3SNG0
G	380	HIS	-	expression tag	UNP A3SNG0
G	381	HIS	-	expression tag	UNP A3SNG0
G	382	HIS	-	expression tag	UNP A3SNG0
G	383	HIS	-	expression tag	UNP A3SNG0
G	384	HIS	-	expression tag	UNP A3SNG0
A	-1	MET	-	expression tag	UNP A3SNG0
A	0	SER	-	expression tag	UNP A3SNG0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1	LEU	-	expression tag	UNP A3SNG0
A	377	GLU	-	expression tag	UNP A3SNG0
A	378	GLY	-	expression tag	UNP A3SNG0
A	379	HIS	-	expression tag	UNP A3SNG0
A	380	HIS	-	expression tag	UNP A3SNG0
A	381	HIS	-	expression tag	UNP A3SNG0
A	382	HIS	-	expression tag	UNP A3SNG0
A	383	HIS	-	expression tag	UNP A3SNG0
A	384	HIS	-	expression tag	UNP A3SNG0
D	-1	MET	-	expression tag	UNP A3SNG0
D	0	SER	-	expression tag	UNP A3SNG0
D	1	LEU	-	expression tag	UNP A3SNG0
D	377	GLU	-	expression tag	UNP A3SNG0
D	378	GLY	-	expression tag	UNP A3SNG0
D	379	HIS	-	expression tag	UNP A3SNG0
D	380	HIS	-	expression tag	UNP A3SNG0
D	381	HIS	-	expression tag	UNP A3SNG0
D	382	HIS	-	expression tag	UNP A3SNG0
D	383	HIS	-	expression tag	UNP A3SNG0
D	384	HIS	-	expression tag	UNP A3SNG0
E	-1	MET	-	expression tag	UNP A3SNG0
E	0	SER	-	expression tag	UNP A3SNG0
E	1	LEU	-	expression tag	UNP A3SNG0
E	377	GLU	-	expression tag	UNP A3SNG0
E	378	GLY	-	expression tag	UNP A3SNG0
E	379	HIS	-	expression tag	UNP A3SNG0
E	380	HIS	-	expression tag	UNP A3SNG0
E	381	HIS	-	expression tag	UNP A3SNG0
E	382	HIS	-	expression tag	UNP A3SNG0
E	383	HIS	-	expression tag	UNP A3SNG0
E	384	HIS	-	expression tag	UNP A3SNG0
F	-1	MET	-	expression tag	UNP A3SNG0
F	0	SER	-	expression tag	UNP A3SNG0
F	1	LEU	-	expression tag	UNP A3SNG0
F	377	GLU	-	expression tag	UNP A3SNG0
F	378	GLY	-	expression tag	UNP A3SNG0
F	379	HIS	-	expression tag	UNP A3SNG0
F	380	HIS	-	expression tag	UNP A3SNG0
F	381	HIS	-	expression tag	UNP A3SNG0
F	382	HIS	-	expression tag	UNP A3SNG0
F	383	HIS	-	expression tag	UNP A3SNG0
F	384	HIS	-	expression tag	UNP A3SNG0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	MET	-	expression tag	UNP A3SNG0
B	0	SER	-	expression tag	UNP A3SNG0
B	1	LEU	-	expression tag	UNP A3SNG0
B	377	GLU	-	expression tag	UNP A3SNG0
B	378	GLY	-	expression tag	UNP A3SNG0
B	379	HIS	-	expression tag	UNP A3SNG0
B	380	HIS	-	expression tag	UNP A3SNG0
B	381	HIS	-	expression tag	UNP A3SNG0
B	382	HIS	-	expression tag	UNP A3SNG0
B	383	HIS	-	expression tag	UNP A3SNG0
B	384	HIS	-	expression tag	UNP A3SNG0
H	-1	MET	-	expression tag	UNP A3SNG0
H	0	SER	-	expression tag	UNP A3SNG0
H	1	LEU	-	expression tag	UNP A3SNG0
H	377	GLU	-	expression tag	UNP A3SNG0
H	378	GLY	-	expression tag	UNP A3SNG0
H	379	HIS	-	expression tag	UNP A3SNG0
H	380	HIS	-	expression tag	UNP A3SNG0
H	381	HIS	-	expression tag	UNP A3SNG0
H	382	HIS	-	expression tag	UNP A3SNG0
H	383	HIS	-	expression tag	UNP A3SNG0
H	384	HIS	-	expression tag	UNP A3SNG0
C	-1	MET	-	expression tag	UNP A3SNG0
C	0	SER	-	expression tag	UNP A3SNG0
C	1	LEU	-	expression tag	UNP A3SNG0
C	377	GLU	-	expression tag	UNP A3SNG0
C	378	GLY	-	expression tag	UNP A3SNG0
C	379	HIS	-	expression tag	UNP A3SNG0
C	380	HIS	-	expression tag	UNP A3SNG0
C	381	HIS	-	expression tag	UNP A3SNG0
C	382	HIS	-	expression tag	UNP A3SNG0
C	383	HIS	-	expression tag	UNP A3SNG0
C	384	HIS	-	expression tag	UNP A3SNG0

- 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	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

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

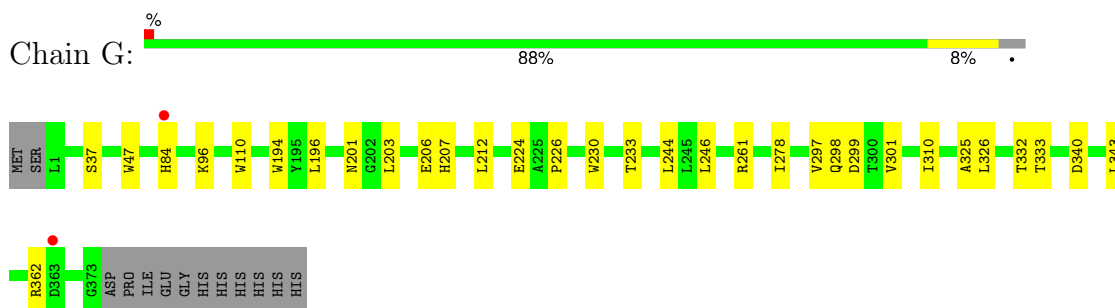
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	2600	Total 2600	O 2600	0	0

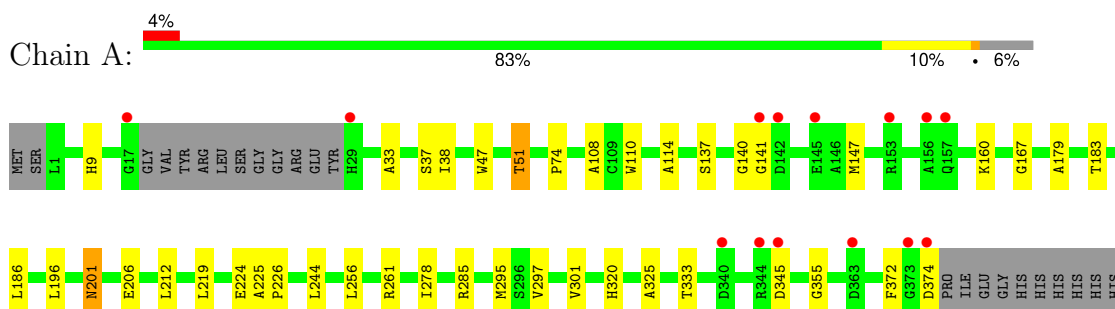
3 Residue-property plots [i](#)

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.

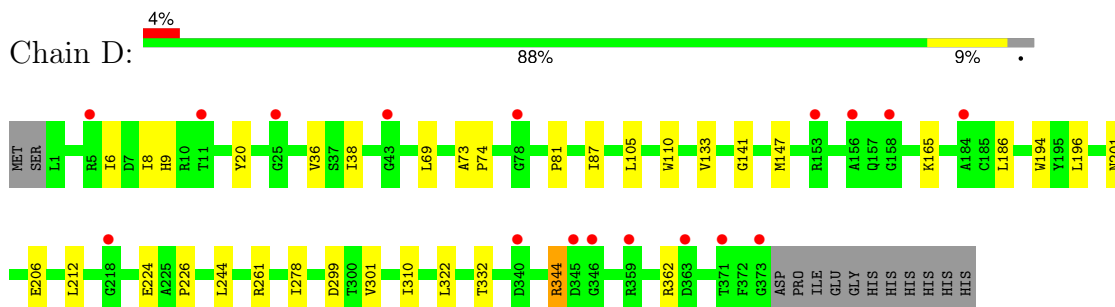
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



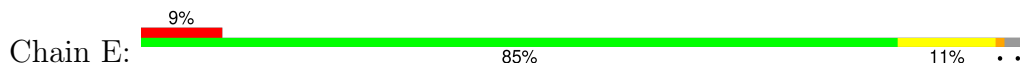
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

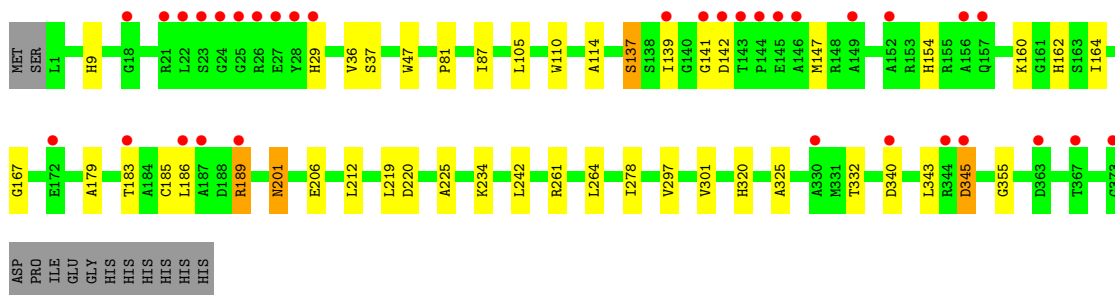


- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

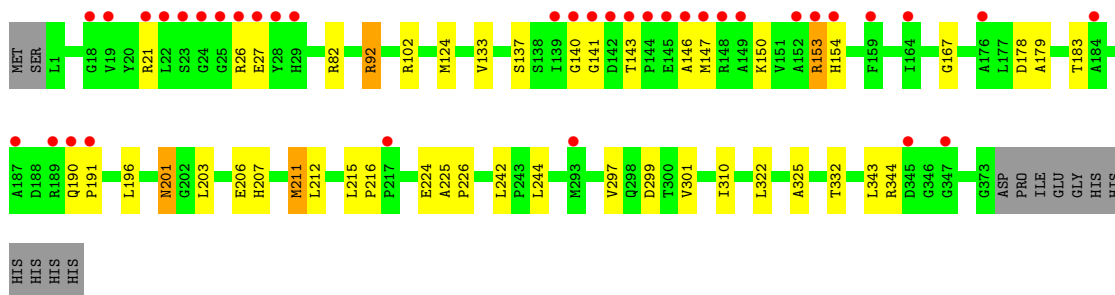
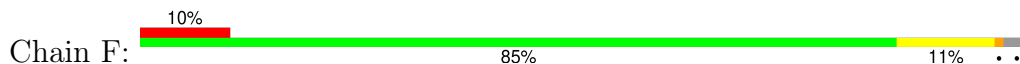


- Molecule 1: Mandelate racemase/muconate lactonizing enzyme

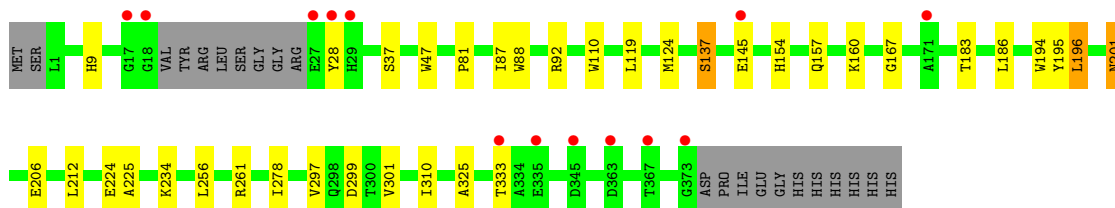
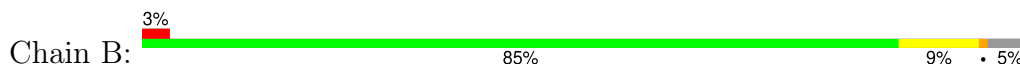




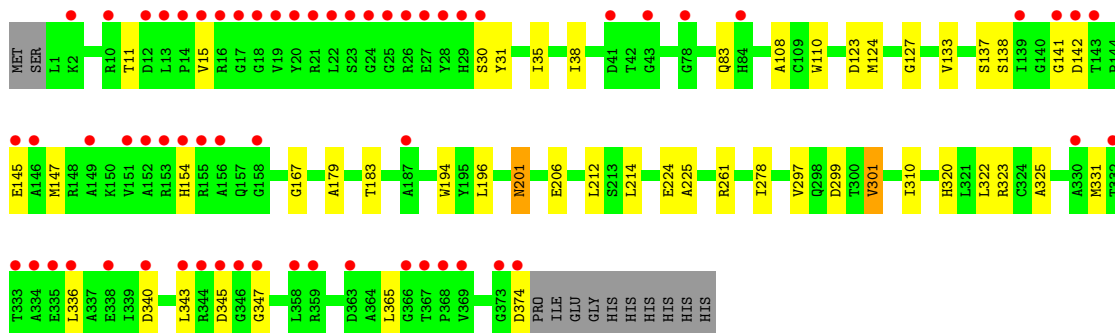
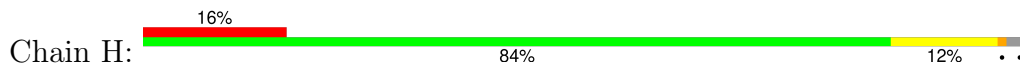
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



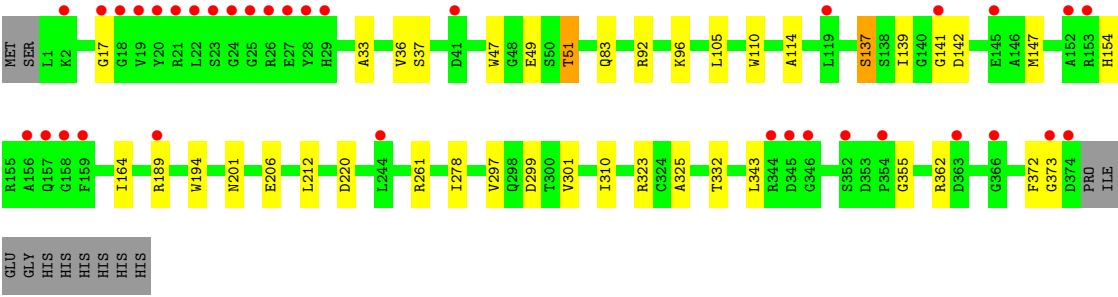
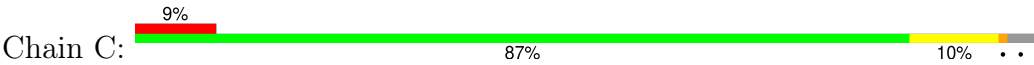
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	169.08Å 174.57Å 108.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.7 (20.00-1.90) 95.7 (20.00-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.49 (at 1.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.203 , 0.241 0.228 , 0.261	Depositor DCC
R_{free} test set	12030 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24665	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 13.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.43	0/2732	0.59	0/3711
1	B	0.46	0/2750	0.59	1/3735 (0.0%)
1	C	0.45	0/2834	0.61	0/3849
1	D	0.43	0/2815	0.59	0/3823
1	E	0.43	0/2815	0.60	0/3823
1	F	0.51	0/2815	0.63	2/3823 (0.1%)
1	G	0.45	0/2857	0.60	0/3882
1	H	0.42	0/2841	0.59	0/3859
All	All	0.45	0/22459	0.60	3/30505 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	211	MET	CG-SD-CE	6.82	111.11	100.20
1	B	196	LEU	CA-CB-CG	5.37	127.66	115.30
1	F	140	GLY	N-CA-C	5.06	125.74	113.10

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	2687	0	2710	21	0
1	B	2704	0	2724	22	0
1	C	2782	0	2802	23	0
1	D	2767	0	2791	20	0
1	E	2767	0	2791	24	0
1	F	2767	0	2791	33	0
1	G	2800	0	2824	18	0
1	H	2786	0	2809	33	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	G	2600	0	0	32	0
All	All	24665	0	22242	192	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (192) 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)
3:G:2043:HOH:O	1:E:340:ASP:HB2	1.58	1.03
1:F:141:GLY:HA2	1:F:147:MET:CE	1.90	1.01
1:F:141:GLY:HA2	1:F:147:MET:HE3	1.40	0.99
1:C:141:GLY:HA2	1:C:147:MET:CE	1.98	0.94
1:F:178:ASP:HB3	1:F:211:MET:HE1	1.48	0.93
1:D:141:GLY:HA2	1:D:147:MET:CE	1.99	0.91
1:D:344:ARG:HH11	1:D:344:ARG:HG2	1.35	0.89
1:C:33:ALA:HA	1:C:51:THR:HB	1.55	0.88
1:F:178:ASP:HB3	1:F:211:MET:CE	2.11	0.79
1:F:141:GLY:CA	1:F:147:MET:CE	2.60	0.79
1:A:33:ALA:HA	1:A:51:THR:HB	1.63	0.78
3:G:1833:HOH:O	1:H:340:ASP:HB2	1.85	0.77
3:G:1231:HOH:O	1:H:261:ARG:NH1	2.20	0.75
1:F:143:THR:HG23	1:F:146:ALA:H	1.52	0.73
1:F:92:ARG:HG2	1:F:102:ARG:CZ	2.20	0.72
1:D:141:GLY:HA2	1:D:147:MET:HE3	1.71	0.71
1:D:141:GLY:HA2	1:D:147:MET:HE1	1.72	0.70
1:F:178:ASP:CB	1:F:211:MET:CE	2.70	0.70
1:C:141:GLY:HA2	1:C:147:MET:HE2	1.73	0.69
1:G:84[B]:HIS:HD2	3:G:1007:HOH:O	1.78	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:TRP:CH2	1:B:196:LEU:HG	2.31	0.66
1:C:142:ASP:H	1:C:147:MET:CE	2.08	0.66
1:B:137:SER:OG	1:B:154:HIS:HD2	1.79	0.65
1:E:142:ASP:H	1:E:147:MET:HE3	1.61	0.65
1:H:196:LEU:HD22	1:H:224:GLU:HB2	1.78	0.65
1:C:142:ASP:N	1:C:147:MET:HE2	2.13	0.64
1:A:140:GLY:O	1:A:147:MET:HE3	1.98	0.63
1:H:110:TRP:CD1	1:H:278:ILE:HB	2.34	0.63
1:D:344:ARG:HG2	1:D:344:ARG:NH1	2.03	0.63
1:F:92:ARG:HG2	1:F:102:ARG:NH1	2.14	0.63
1:D:196:LEU:HD22	1:D:224:GLU:HB2	1.81	0.62
1:H:299:ASP:HB2	1:H:310:ILE:HD11	1.82	0.62
1:F:178:ASP:CB	1:F:211:MET:HE2	2.30	0.62
1:F:141:GLY:CA	1:F:147:MET:HE2	2.29	0.61
1:F:92:ARG:HG2	1:F:102:ARG:NH2	2.16	0.61
1:E:142:ASP:H	1:E:147:MET:CE	2.14	0.60
1:D:299:ASP:HB2	1:D:310:ILE:HD11	1.84	0.59
1:E:234:LYS:HG2	1:E:264:LEU:HD13	1.85	0.59
1:A:141:GLY:HA2	1:A:147:MET:CE	2.34	0.58
1:F:179:ALA:O	1:F:183:THR:HG23	2.04	0.57
1:H:137:SER:HB2	1:H:154:HIS:CD2	2.40	0.57
3:G:1912:HOH:O	1:E:29:HIS:O	2.18	0.57
1:C:141:GLY:CA	1:C:147:MET:HE2	2.34	0.56
1:C:142:ASP:H	1:C:147:MET:HE2	1.67	0.56
1:G:299:ASP:HB2	1:G:310:ILE:HD11	1.87	0.56
1:H:179:ALA:O	1:H:183:THR:HG23	2.06	0.56
1:B:196:LEU:HD22	1:B:224:GLU:HB2	1.86	0.56
3:G:2148:HOH:O	1:F:26:ARG:HD2	2.06	0.55
3:G:2715:HOH:O	1:A:261:ARG:NH1	2.39	0.54
1:H:142:ASP:H	1:H:147:MET:HE2	1.73	0.54
1:B:297:VAL:O	1:B:325:ALA:HA	2.08	0.54
1:G:194:TRP:CH2	1:G:196[A]:LEU:HG	2.43	0.54
1:D:133:VAL:HG13	1:D:322:LEU:HD21	1.89	0.54
1:H:11:THR:HG22	1:H:35:ILE:HD13	1.89	0.54
3:G:2607:HOH:O	1:A:9:HIS:HE1	1.92	0.53
1:H:301:VAL:HG23	1:H:331:MET:HE3	1.88	0.53
3:G:1935:HOH:O	1:D:9:HIS:HE1	1.91	0.53
1:D:194:TRP:CH2	1:D:196:LEU:HG	2.44	0.53
1:A:141:GLY:HA2	1:A:147:MET:HE3	1.91	0.53
1:A:179:ALA:O	1:A:183:THR:HG23	2.08	0.52
1:E:186:LEU:HD12	1:E:219:LEU:HD22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:GLY:CA	1:D:147:MET:HE3	2.39	0.52
1:E:179:ALA:O	1:E:183:THR:HG23	2.10	0.52
1:A:201:ASN:HD22	1:A:225:ALA:HB1	1.75	0.52
1:F:92:ARG:NE	1:F:102:ARG:HH12	2.08	0.51
1:B:299:ASP:HB2	1:B:310:ILE:HD11	1.92	0.51
3:G:1392:HOH:O	1:C:261:ARG:NH2	2.44	0.51
1:G:261:ARG:NH1	3:G:1569:HOH:O	2.30	0.51
1:D:110:TRP:CD1	1:D:278:ILE:HB	2.46	0.51
1:B:154:HIS:HA	1:B:157:GLN:HE21	1.75	0.51
1:F:178:ASP:CB	1:F:211:MET:HE1	2.27	0.51
3:G:788:HOH:O	1:D:261:ARG:NH1	2.41	0.51
1:H:11:THR:HG22	1:H:35:ILE:CD1	2.41	0.51
1:H:201:ASN:HD22	1:H:225:ALA:HB1	1.75	0.51
1:C:139:ILE:HB	1:C:164:ILE:HG22	1.93	0.50
1:E:37:SER:HB3	1:E:47:TRP:CZ3	2.47	0.50
1:F:178:ASP:HB2	1:F:211:MET:HE2	1.93	0.50
1:A:186:LEU:HD12	1:A:219:LEU:HD22	1.93	0.50
1:B:201:ASN:HD22	1:B:225:ALA:HB1	1.77	0.50
1:H:142:ASP:H	1:H:147:MET:CE	2.24	0.50
1:H:133:VAL:HG13	1:H:322:LEU:HD21	1.94	0.50
1:E:81:PRO:HA	1:E:87:ILE:HD11	1.94	0.49
1:C:137:SER:HB2	1:C:154:HIS:CD2	2.47	0.49
1:F:226:PRO:HG3	1:F:244:LEU:HD11	1.94	0.49
3:G:1508:HOH:O	1:C:92:ARG:HD3	2.12	0.49
3:G:975:HOH:O	1:B:234:LYS:HE3	2.11	0.49
1:A:114:ALA:HB3	1:A:355:GLY:HA2	1.95	0.49
1:C:114:ALA:HB3	1:C:355:GLY:HA2	1.93	0.49
1:H:15:VAL:HG22	1:H:31:TYR:CE1	2.47	0.48
1:H:141:GLY:HA2	1:H:147:MET:CE	2.43	0.48
1:E:141:GLY:HA2	1:E:147:MET:CE	2.43	0.48
1:B:110:TRP:CD1	1:B:278:ILE:HB	2.48	0.48
3:G:1788:HOH:O	1:E:261:ARG:NH1	2.42	0.48
1:F:190:GLN:HG3	1:F:191:PRO:HD2	1.95	0.48
1:C:141:GLY:HA2	1:C:147:MET:HE3	1.93	0.48
1:G:196[A]:LEU:HD22	1:G:224:GLU:HB2	1.95	0.48
1:C:110:TRP:CD1	1:C:278:ILE:HB	2.49	0.48
3:G:2254:HOH:O	1:E:9:HIS:HE1	1.97	0.47
3:G:695:HOH:O	1:E:320:HIS:HD2	1.97	0.47
1:H:194:TRP:CH2	1:H:196:LEU:HG	2.50	0.47
3:G:1669:HOH:O	1:E:261:ARG:NH2	2.48	0.47
1:F:183:THR:HG22	1:F:216:PRO:CD	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:2117:HOH:O	1:B:261:ARG:NH2	2.47	0.47
1:B:37:SER:HB3	1:B:47:TRP:CZ3	2.50	0.47
1:D:6:ILE:HG12	1:D:38:ILE:HG12	1.96	0.46
3:G:2406:HOH:O	1:H:183:THR:HG21	2.15	0.46
1:F:21:ARG:HG2	1:F:27:GLU:HG2	1.98	0.46
1:E:201:ASN:HD22	1:E:225:ALA:HB1	1.81	0.46
3:G:1864:HOH:O	1:C:83:GLN:HG2	2.14	0.46
1:H:15:VAL:HG23	1:H:30:SER:HA	1.98	0.46
1:C:49:GLU:OE2	1:C:51:THR:CG2	2.64	0.46
3:G:1260:HOH:O	1:B:9:HIS:HE1	1.98	0.46
1:C:372:PHE:HA	1:C:373:GLY:HA3	1.58	0.46
1:G:333:THR:HG22	1:G:333:THR:O	2.15	0.46
1:A:110:TRP:CD1	1:A:278:ILE:HB	2.51	0.46
1:E:110:TRP:CD1	1:E:278:ILE:HB	2.51	0.46
1:G:37:SER:HB3	1:G:47:TRP:CZ3	2.51	0.45
1:D:20:TYR:OH	1:D:165:LYS:HE3	2.16	0.45
1:E:36:VAL:HG11	1:E:105:LEU:HD23	1.98	0.45
1:E:297:VAL:O	1:E:325:ALA:HA	2.17	0.45
3:G:879:HOH:O	1:B:183:THR:HG21	2.16	0.45
1:A:74:PRO:HG3	1:A:372:PHE:CE1	2.52	0.45
1:F:196:LEU:HD11	1:F:224:GLU:HB2	1.99	0.45
1:F:299:ASP:HB2	1:F:310:ILE:HD11	1.99	0.45
1:F:201:ASN:HD22	1:F:225:ALA:HB1	1.82	0.45
1:E:139:ILE:HD13	1:E:164:ILE:HG22	1.99	0.45
1:C:299:ASP:HB2	1:C:310:ILE:HD11	1.99	0.45
1:A:297:VAL:O	1:A:325:ALA:HA	2.17	0.45
1:G:110:TRP:CD1	1:G:278:ILE:HB	2.52	0.44
1:A:333:THR:O	1:A:333:THR:HG22	2.18	0.44
1:B:88:TRP:CD1	1:B:92:ARG:HD2	2.52	0.44
1:C:36:VAL:HG11	1:C:105:LEU:HD23	2.00	0.44
1:C:194:TRP:CE2	1:C:323:ARG:HD2	2.52	0.44
1:B:333:THR:O	1:B:333:THR:CG2	2.66	0.44
1:H:38:ILE:HD12	1:H:108:ALA:HB3	1.99	0.43
1:G:340:ASP:HB2	3:G:1521:HOH:O	2.18	0.43
1:A:141:GLY:HA2	1:A:147:MET:HE1	1.99	0.43
1:A:37:SER:HB3	1:A:47:TRP:CZ3	2.53	0.43
1:B:196:LEU:HD13	1:B:224:GLU:OE1	2.18	0.43
1:H:133:VAL:O	1:H:347:GLY:HA3	2.19	0.43
1:H:196:LEU:HD13	1:H:224:GLU:OE1	2.18	0.43
1:D:8:ILE:HD12	1:D:69:LEU:HD13	2.01	0.43
3:G:739:HOH:O	1:B:160:LYS:HE3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:2733:HOH:O	1:F:153:ARG:HD3	2.17	0.43
1:F:183:THR:HG22	1:F:216:PRO:HD2	2.00	0.43
1:B:119:LEU:HB2	1:B:124:MET:HG2	2.00	0.43
1:F:297:VAL:O	1:F:325:ALA:HA	2.18	0.43
1:H:194:TRP:CE2	1:H:323:ARG:HD2	2.54	0.42
1:C:37:SER:HB3	1:C:47:TRP:CZ3	2.54	0.42
1:D:226:PRO:HG3	1:D:244:LEU:HD11	2.01	0.42
1:F:183:THR:CG2	1:F:216:PRO:CD	2.97	0.42
1:H:142:ASP:N	1:H:147:MET:HE2	2.35	0.42
1:E:189:ARG:NH1	1:E:220:ASP:HB3	2.34	0.42
1:B:333:THR:O	1:B:333:THR:HG22	2.19	0.42
1:A:196:LEU:HD11	1:A:224:GLU:HB2	2.02	0.42
3:G:655:HOH:O	1:H:320:HIS:HD2	2.02	0.42
1:A:38:ILE:HD12	1:A:108:ALA:HB3	2.02	0.42
1:D:36:VAL:HG11	1:D:105:LEU:HD23	2.01	0.42
1:H:123:ASP:HA	1:H:127:GLY:HA2	2.02	0.42
1:G:233:THR:HG21	1:G:246:LEU:HD21	2.02	0.42
1:D:73:ALA:HB3	1:D:74:PRO:HD3	2.02	0.42
1:H:214:LEU:HD21	1:C:220:ASP:HB2	2.01	0.42
1:H:301:VAL:HG23	1:H:331:MET:CE	2.50	0.42
1:A:285:ARG:HG3	1:A:295:MET:SD	2.60	0.41
3:G:1784:HOH:O	1:H:83:GLN:NE2	2.53	0.41
1:E:114:ALA:HB3	1:E:355:GLY:HA2	2.02	0.41
1:E:147:MET:HB3	1:E:185:CYS:SG	2.61	0.41
1:F:203:LEU:HD22	1:F:207:HIS:CD2	2.56	0.41
1:F:141:GLY:N	1:F:147:MET:CE	2.83	0.41
1:H:343:LEU:HA	1:H:347:GLY:O	2.20	0.41
1:G:194:TRP:CZ3	1:G:196[A]:LEU:HG	2.56	0.41
1:G:226:PRO:HG3	1:G:244:LEU:HD11	2.01	0.41
3:G:656:HOH:O	1:F:344:ARG:NH1	2.53	0.41
1:F:82:ARG:CZ	1:B:119:LEU:HD21	2.51	0.41
1:G:297:VAL:O	1:G:325:ALA:HA	2.21	0.41
1:G:299:ASP:CB	1:G:310:ILE:HD11	2.51	0.41
1:A:226:PRO:HG3	1:A:244:LEU:HD11	2.02	0.41
3:G:816:HOH:O	1:A:320:HIS:HD2	2.04	0.41
1:E:137:SER:OG	1:E:154:HIS:HD2	2.04	0.41
1:H:297:VAL:O	1:H:325:ALA:HA	2.21	0.41
1:D:81:PRO:HA	1:D:87:ILE:HD11	2.04	0.41
1:F:133:VAL:HG13	1:F:322:LEU:HD21	2.02	0.40
1:H:336:LEU:HD22	1:H:365:LEU:HD23	2.01	0.40
1:G:203:LEU:HD22	1:G:207:HIS:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:139:ILE:CD1	1:E:162:HIS:HB3	2.51	0.40
1:B:186:LEU:HD22	1:B:195:TYR:CG	2.57	0.40
1:C:297:VAL:O	1:C:325:ALA:HA	2.21	0.40
1:G:84[B]:HIS:CD2	3:G:1007:HOH:O	2.64	0.40
1:H:194:TRP:CH2	1:H:323:ARG:HB3	2.56	0.40
1:G:230[B]:TRP:HD1	3:G:1048:HOH:O	2.03	0.40
1:G:298:GLN:HG2	1:G:326:LEU:HB2	2.03	0.40
1:B:81:PRO:HA	1:B:87:ILE:HD11	2.03	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	359/386 (93%)	349 (97%)	8 (2%)	2 (1%)	25	15
1	B	361/386 (94%)	351 (97%)	8 (2%)	2 (1%)	25	15
1	C	373/386 (97%)	363 (97%)	8 (2%)	2 (0%)	29	18
1	D	371/386 (96%)	362 (98%)	8 (2%)	1 (0%)	41	31
1	E	371/386 (96%)	361 (97%)	7 (2%)	3 (1%)	19	9
1	F	371/386 (96%)	358 (96%)	11 (3%)	2 (0%)	29	18
1	G	375/386 (97%)	364 (97%)	10 (3%)	1 (0%)	41	31
1	H	374/386 (97%)	364 (97%)	8 (2%)	2 (0%)	29	18
All	All	2955/3088 (96%)	2872 (97%)	68 (2%)	15 (0%)	29	18

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	17	GLY
1	A	301	VAL

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Mol	Chain	Res	Type
1	F	301	VAL
1	B	301	VAL
1	C	301	VAL
1	A	167	GLY
1	E	345	ASP
1	H	301	VAL
1	D	301	VAL
1	B	167	GLY
1	G	301	VAL
1	E	167	GLY
1	H	167	GLY
1	E	301	VAL
1	F	167	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	275/294 (94%)	266 (97%)	9 (3%)	38	29
1	B	276/294 (94%)	269 (98%)	7 (2%)	47	41
1	C	284/294 (97%)	274 (96%)	10 (4%)	36	27
1	D	282/294 (96%)	275 (98%)	7 (2%)	47	41
1	E	282/294 (96%)	272 (96%)	10 (4%)	36	27
1	F	282/294 (96%)	269 (95%)	13 (5%)	27	17
1	G	286/294 (97%)	279 (98%)	7 (2%)	49	43
1	H	285/294 (97%)	277 (97%)	8 (3%)	43	36
All	All	2252/2352 (96%)	2181 (97%)	71 (3%)	39	30

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	96	LYS
1	G	201	ASN

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Mol	Chain	Res	Type
1	G	206	GLU
1	G	212	LEU
1	G	332	THR
1	G	343	LEU
1	G	362	ARG
1	A	51	THR
1	A	137	SER
1	A	160	LYS
1	A	201	ASN
1	A	206	GLU
1	A	212	LEU
1	A	256	LEU
1	A	345	ASP
1	A	374	ASP
1	D	186	LEU
1	D	201	ASN
1	D	206	GLU
1	D	212	LEU
1	D	332	THR
1	D	344	ARG
1	D	362	ARG
1	E	137	SER
1	E	160	LYS
1	E	189	ARG
1	E	201	ASN
1	E	206	GLU
1	E	212	LEU
1	E	242	LEU
1	E	332	THR
1	E	343	LEU
1	E	345	ASP
1	F	92	ARG
1	F	124	MET
1	F	137	SER
1	F	150	LYS
1	F	153	ARG
1	F	154	HIS
1	F	201	ASN
1	F	206	GLU
1	F	212	LEU
1	F	215	LEU
1	F	242	LEU

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Mol	Chain	Res	Type
1	F	332	THR
1	F	343	LEU
1	B	28	TYR
1	B	137	SER
1	B	145	GLU
1	B	201	ASN
1	B	206	GLU
1	B	212	LEU
1	B	256	LEU
1	H	124	MET
1	H	138	SER
1	H	145	GLU
1	H	201	ASN
1	H	206	GLU
1	H	212	LEU
1	H	345	ASP
1	H	374	ASP
1	C	51	THR
1	C	96	LYS
1	C	137	SER
1	C	189	ARG
1	C	201	ASN
1	C	206	GLU
1	C	212	LEU
1	C	332	THR
1	C	343	LEU
1	C	362	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	9	HIS
1	G	83	GLN
1	G	157	GLN
1	G	201	ASN
1	G	320	HIS
1	A	9	HIS
1	A	83	GLN
1	A	154	HIS
1	A	157	GLN
1	A	201	ASN
1	A	320	HIS

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Mol	Chain	Res	Type
1	D	9	HIS
1	D	201	ASN
1	D	320	HIS
1	E	9	HIS
1	E	83	GLN
1	E	154	HIS
1	E	157	GLN
1	E	201	ASN
1	E	320	HIS
1	F	9	HIS
1	F	154	HIS
1	F	201	ASN
1	F	320	HIS
1	B	9	HIS
1	B	83	GLN
1	B	154	HIS
1	B	157	GLN
1	B	190	GLN
1	B	200	ASN
1	B	201	ASN
1	H	9	HIS
1	H	83	GLN
1	H	201	ASN
1	H	320	HIS
1	C	9	HIS
1	C	83	GLN
1	C	201	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 5 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	363/386 (94%)	0.31	14 (3%) 39 42	9, 16, 25, 41	0
1	B	365/386 (94%)	0.36	13 (3%) 42 45	8, 16, 24, 51	0
1	C	374/386 (96%)	0.64	35 (9%) 8 9	8, 17, 30, 48	0
1	D	373/386 (96%)	0.47	17 (4%) 32 35	9, 16, 25, 29	0
1	E	373/386 (96%)	0.50	33 (8%) 10 11	10, 17, 29, 46	0
1	F	373/386 (96%)	0.63	37 (9%) 7 8	10, 15, 28, 46	0
1	G	373/386 (96%)	0.23	2 (0%) 91 92	9, 15, 25, 33	0
1	H	374/386 (96%)	0.87	62 (16%) 1 1	8, 16, 31, 49	0
All	All	2968/3088 (96%)	0.50	213 (7%) 15 17	8, 16, 27, 51	0

All (213) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	374	ASP	10.2
1	H	19	VAL	8.7
1	B	18	GLY	8.1
1	C	24	GLY	7.9
1	H	29	HIS	7.6
1	H	25	GLY	7.6
1	B	28	TYR	7.2
1	B	17	GLY	7.2
1	F	18	GLY	7.0
1	H	345	ASP	7.0
1	F	24	GLY	6.3
1	E	22	LEU	6.1
1	E	21	ARG	6.1
1	E	25	GLY	6.0
1	C	22	LEU	5.7
1	C	17	GLY	5.7

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Mol	Chain	Res	Type	RSRZ
1	H	18	GLY	5.7
1	C	373	GLY	5.6
1	H	28	TYR	5.6
1	H	374	ASP	5.5
1	B	29	HIS	5.3
1	E	145	GLU	5.3
1	E	24	GLY	5.3
1	C	27	GLU	5.1
1	H	149	ALA	5.1
1	A	374	ASP	5.1
1	H	363	ASP	5.0
1	H	24	GLY	4.7
1	F	19	VAL	4.5
1	H	158	GLY	4.5
1	F	149	ALA	4.4
1	H	156	ALA	4.4
1	C	23	SER	4.4
1	H	145	GLU	4.4
1	H	17	GLY	4.4
1	H	153	ARG	4.3
1	E	345	ASP	4.3
1	D	373	GLY	4.2
1	H	20	TYR	4.0
1	G	363	ASP	4.0
1	E	367	THR	4.0
1	E	149	ALA	4.0
1	H	14	PRO	4.0
1	A	29	HIS	4.0
1	F	22	LEU	3.9
1	C	21	ARG	3.9
1	C	28	TYR	3.8
1	H	152	ALA	3.8
1	D	156	ALA	3.8
1	E	28	TYR	3.8
1	F	191	PRO	3.7
1	C	344	ARG	3.7
1	F	25	GLY	3.6
1	D	346	GLY	3.6
1	H	373	GLY	3.6
1	A	344	ARG	3.6
1	E	29	HIS	3.6
1	H	15	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	H	141	GLY	3.6
1	H	346	GLY	3.6
1	D	184	ALA	3.5
1	H	367	THR	3.5
1	C	363	ASP	3.5
1	E	156	ALA	3.5
1	H	30	SER	3.5
1	D	345	ASP	3.5
1	H	27	GLU	3.5
1	E	152	ALA	3.4
1	B	171	ALA	3.4
1	B	27	GLU	3.4
1	F	147	MET	3.4
1	F	21	ARG	3.4
1	F	187	ALA	3.4
1	H	146	ALA	3.3
1	H	139	ILE	3.3
1	H	343	LEU	3.3
1	H	333	THR	3.3
1	H	344	ARG	3.3
1	D	363	ASP	3.2
1	B	363	ASP	3.2
1	C	18	GLY	3.2
1	H	369	VAL	3.2
1	E	27	GLU	3.2
1	H	26	ARG	3.2
1	F	139	ILE	3.2
1	A	17	GLY	3.2
1	D	158	GLY	3.2
1	H	347	GLY	3.1
1	E	187	ALA	3.1
1	F	190	GLN	3.1
1	C	26	ARG	3.1
1	H	187	ALA	3.1
1	F	140	GLY	3.1
1	H	368	PRO	3.0
1	F	23	SER	3.0
1	E	189	ARG	3.0
1	E	146	ALA	3.0
1	E	23	SER	3.0
1	H	340	ASP	3.0
1	F	145	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	154	HIS	3.0
1	D	11	THR	3.0
1	F	141	GLY	3.0
1	E	26	ARG	3.0
1	F	159	PHE	3.0
1	C	156	ALA	3.0
1	F	142	ASP	3.0
1	F	189	ARG	2.9
1	C	159	PHE	2.9
1	H	2	LYS	2.8
1	C	145	GLU	2.8
1	D	359	ARG	2.8
1	F	143	THR	2.8
1	H	332[A]	THR	2.8
1	F	345	ASP	2.8
1	H	335	GLU	2.8
1	F	26	ARG	2.8
1	A	345	ASP	2.7
1	H	12	ASP	2.7
1	H	43	GLY	2.7
1	H	366	GLY	2.7
1	E	340	ASP	2.7
1	C	354	PRO	2.7
1	H	151	VAL	2.7
1	A	156	ALA	2.6
1	A	340	ASP	2.6
1	E	183	THR	2.6
1	A	145	GLU	2.6
1	E	142	ASP	2.6
1	G	84[A]	HIS	2.6
1	H	41	ASP	2.6
1	H	16	ARG	2.6
1	H	78	GLY	2.6
1	F	29	HIS	2.6
1	H	338	GLU	2.6
1	H	22	LEU	2.6
1	F	146	ALA	2.6
1	E	344	ARG	2.6
1	F	153	ARG	2.5
1	H	13	LEU	2.5
1	B	373	GLY	2.5
1	C	152	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	347	GLY	2.5
1	H	21	ARG	2.5
1	C	158	GLY	2.5
1	C	352	SER	2.5
1	F	144	PRO	2.5
1	D	78	GLY	2.5
1	C	346	GLY	2.5
1	E	172	GLU	2.5
1	C	189	ARG	2.5
1	A	157	GLN	2.4
1	C	29	HIS	2.4
1	C	41	ASP	2.4
1	H	23	SER	2.4
1	H	84[A]	HIS	2.4
1	C	20	TYR	2.4
1	A	142	ASP	2.4
1	H	10	ARG	2.4
1	H	154	HIS	2.4
1	C	141	GLY	2.4
1	E	18	GLY	2.4
1	C	25	GLY	2.3
1	F	148	ARG	2.3
1	E	373	GLY	2.3
1	A	363	ASP	2.3
1	A	373	GLY	2.3
1	B	145	GLU	2.3
1	C	345	ASP	2.3
1	D	43	GLY	2.2
1	F	293	MET	2.2
1	E	363	ASP	2.2
1	D	340	ASP	2.2
1	C	19	VAL	2.2
1	H	336	LEU	2.2
1	H	155	ARG	2.2
1	H	359	ARG	2.2
1	C	119	LEU	2.2
1	E	330	ALA	2.2
1	H	330	ALA	2.2
1	F	27	GLU	2.2
1	H	143	THR	2.2
1	E	141	GLY	2.2
1	A	153	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	5	ARG	2.2
1	F	152	ALA	2.2
1	E	157	GLN	2.2
1	E	144	PRO	2.1
1	D	153	ARG	2.1
1	C	153	ARG	2.1
1	A	141	GLY	2.1
1	H	142	ASP	2.1
1	F	28	TYR	2.1
1	D	218	GLY	2.1
1	D	371	THR	2.1
1	B	345	ASP	2.1
1	B	367	THR	2.1
1	E	186	LEU	2.1
1	F	176	ALA	2.1
1	F	164	ILE	2.1
1	C	157	GLN	2.1
1	C	366	GLY	2.1
1	E	139	ILE	2.1
1	H	334	ALA	2.1
1	F	217	PRO	2.1
1	B	335	GLU	2.1
1	D	25	GLY	2.1
1	C	2	LYS	2.1
1	E	143	THR	2.0
1	F	184	ALA	2.0
1	C	244	LEU	2.0
1	B	333	THR	2.0
1	H	358	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	F	501	1/1	0.82	0.20	41,41,41,41	0
2	MG	E	501	1/1	0.91	0.11	35,35,35,35	0
2	MG	C	501	1/1	0.94	0.09	37,37,37,37	0
2	MG	B	501	1/1	0.95	0.05	24,24,24,24	0
2	MG	A	501	1/1	0.95	0.09	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.