



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 02:31 AM UTC

PDB ID : 3FV9 / pdb_00003fv9
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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

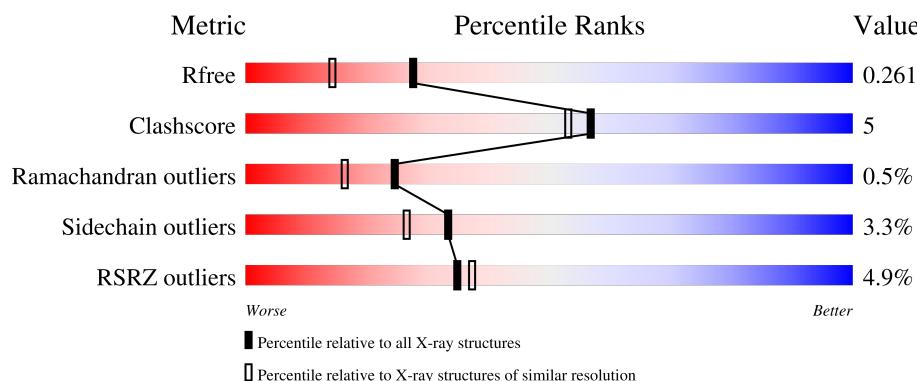
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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	2% 82% 12% 6%
1	B	386	3% 85% 9% 5%
1	C	386	5% 86% 11% ..
1	D	386	% 87% 10% .
1	E	386	6% 85% 11% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	386	11% 84% 12% • •
1	G	386	% 88% 9% •
1	H	386	9% 84% 12% • •

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 (CCD ID: 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

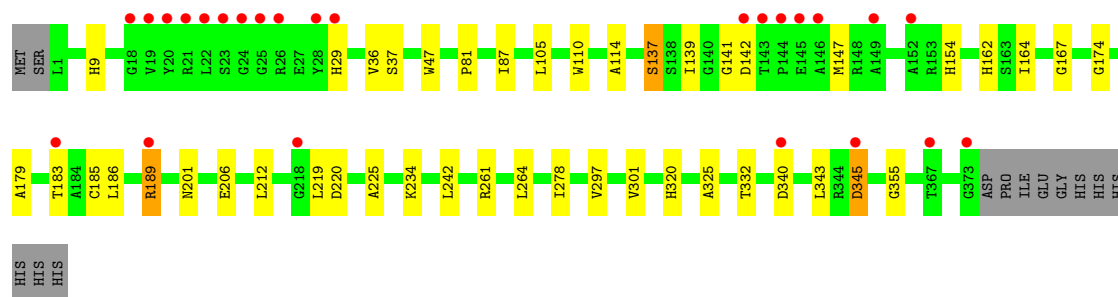
Continued on next page...

Continued from previous page...

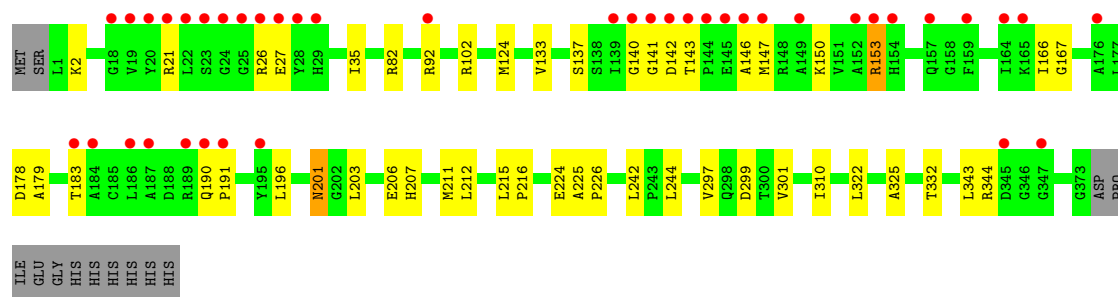
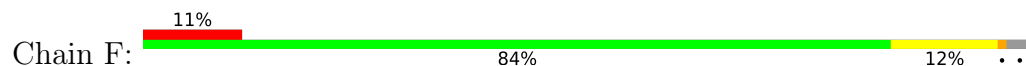
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Mg 1	0	0
2	C	1	Total 1	Mg 1	0	0

- Molecule 3 is water.

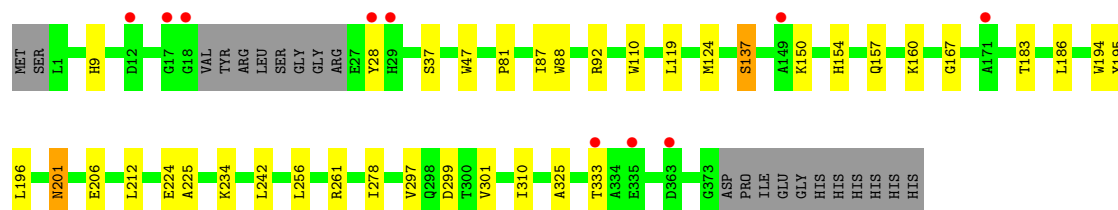
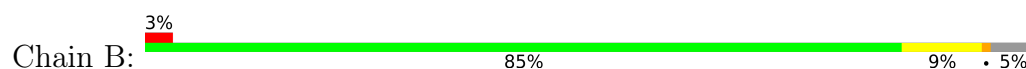
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	2600	Total 2600	O 2600	0	0



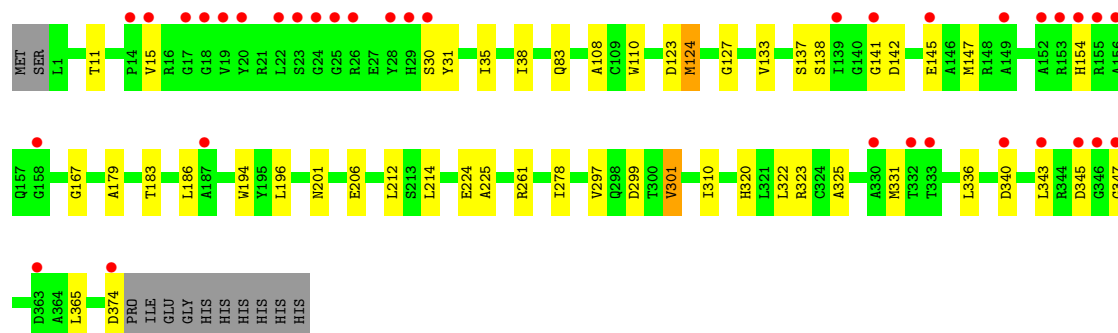
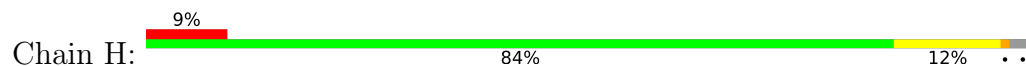
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



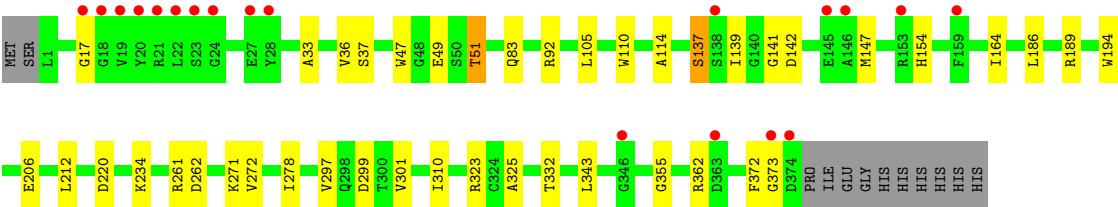
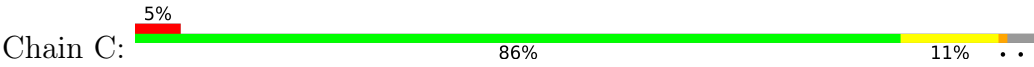
- Molecule 1: Mandelate racemase/muconate lactonizing enzyme



- 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) 95.4 (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)	0.35 , 39.4	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 ⓘ

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	0.59	0/2732	0.80	0/3711
1	B	0.60	0/2750	0.79	0/3735
1	C	0.60	0/2834	0.82	0/3849
1	D	0.58	0/2815	0.79	0/3823
1	E	0.59	0/2815	0.81	2/3823 (0.1%)
1	F	0.69	0/2815	0.83	1/3823 (0.0%)
1	G	0.61	0/2857	0.79	0/3882
1	H	0.58	0/2841	0.81	0/3859
All	All	0.61	0/22459	0.80	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	140	GLY	N-CA-C	7.95	125.74	115.32
1	E	174	GLY	CA-C-N	5.67	125.52	119.28
1	E	174	GLY	C-N-CA	5.67	125.52	119.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2687	0	2710	22	0
1	B	2704	0	2724	22	0
1	C	2782	0	2802	25	0
1	D	2767	0	2791	24	0
1	E	2767	0	2791	24	0
1	F	2767	0	2791	37	0
1	G	2800	0	2824	19	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	204	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 5.

All (204) 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:F:178:ASP:CB	1:F:211:MET:HE2	1.76	1.15
1:C:142:ASP:H	1:C:147:MET:HE3	1.13	1.13
1:F:178:ASP:HB3	1:F:211:MET:HE2	1.16	1.10
3:G:2043:HOH:O	1:E:340:ASP:HB2	1.58	1.03
1:E:142:ASP:H	1:E:147:MET:HE3	1.24	1.01
1:F:141:GLY:HA2	1:F:147:MET:CE	1.90	1.01
1:H:142:ASP:H	1:H:147:MET:HE3	1.29	0.95
1:C:142:ASP:N	1:C:147:MET:HE3	1.81	0.94
1:C:141:GLY:HA2	1:C:147:MET:CE	1.98	0.94
1:D:141:GLY:HA2	1:D:147:MET:HE3	1.51	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:141:GLY:CA	1:F:147:MET:HE3	2.11	0.81
1:F:142:ASP:N	1:F:147:MET:HE3	1.96	0.80
1:F:141:GLY:HA2	1:F:147:MET:HE3	1.62	0.80
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
1:F:141:GLY:HA2	1:F:147:MET:HE1	1.65	0.77
3:G:1833:HOH:O	1:H:340:ASP:HB2	1.85	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:GLY:HA2	1:A:147:MET:HE3	1.65	0.76
1:E:142:ASP:N	1:E:147:MET:HE3	2.00	0.75
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:F:166:ILE:HD12	1:F:211:MET:HE1	1.72	0.71
1:D:142:ASP:H	1:D:147:MET:HE3	1.55	0.71
1:F:142:ASP:H	1:F:147:MET:HE3	1.55	0.71
1:D:142:ASP:N	1:D:147:MET:HE3	2.08	0.69
1:D:141:GLY:CA	1:D:147:MET:HE3	2.24	0.67
1:G:84[B]:HIS:HD2	3:G:1007:HOH:O	1.78	0.67
1:B:194:TRP:CH2	1:B:196:LEU:HG	2.31	0.66
1:C:141:GLY:HA2	1:C:147:MET:HE3	1.75	0.66
1:B:137:SER:OG	1:B:154:HIS:HD2	1.79	0.65
1:H:142:ASP:N	1:H:147:MET:HE3	2.08	0.65
1:H:196:LEU:HD22	1:H:224:GLU:HB2	1.78	0.65
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:92:ARG:HG2	1:F:102:ARG:NH2	2.16	0.61
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: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:H:301:VAL:HG23	1:H:331:MET:HE3	1.87	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:A:141:GLY:CA	1:A:147:MET:HE3	2.36	0.54
1:F:141:GLY:C	1:F:147:MET:HE3	2.33	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1935:HOH:O	1:D:9:HIS:HE1	1.91	0.53
1:F:178:ASP:HB2	1:F:211:MET:HE2	1.82	0.53
1:D:194:TRP:CH2	1:D:196:LEU:HG	2.44	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
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
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:F:178:ASP:CB	1:F:211:MET:CE	2.70	0.50
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: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: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: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
1:C:141:GLY:HA2	1:C:147:MET:HE2	1.90	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1669:HOH:O	1:E:261:ARG:NH2	2.48	0.47
1:C:141:GLY:CA	1:C:147:MET:CE	2.84	0.47
1:F:183:THR:HG22	1:F:216:PRO:CD	2.45	0.47
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
1:C:141:GLY:CA	1:C:147:MET:HE3	2.41	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:D:147:MET:HE1	1:D:165:LYS:O	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:147:MET:HE1	1:A:165:LYS:O	2.17	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:F:141:GLY:H	1:F:147:MET:HE2	1.82	0.44
1:G:136:ILE:HG13	1:G:161:GLY:C	2.43	0.44
1:A:140:GLY:O	1:A:147:MET:HE3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:E:189:ARG:NH1	1:E:220:ASP:HB3	2.34	0.42
1:C:271:LYS:O	1:C:272:VAL:C	2.63	0.42
1:D:271:LYS:O	1:D:272:VAL:C	2.62	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:H:124:MET:HE3	1:H:124:MET:HB3	1.86	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:D:141:GLY:C	1:D:147:MET:HE3	2.45	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:C:234:LYS:HE2	1:C:262:ASP:CG	2.47	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%)	21	13
1	B	361/386 (94%)	351 (97%)	8 (2%)	2 (1%)	21	13
1	C	373/386 (97%)	363 (97%)	8 (2%)	2 (0%)	24	16
1	D	371/386 (96%)	362 (98%)	8 (2%)	1 (0%)	36	29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	371/386 (96%)	361 (97%)	7 (2%)	3 (1%)	16	8
1	F	371/386 (96%)	358 (96%)	11 (3%)	2 (0%)	24	16
1	G	375/386 (97%)	364 (97%)	10 (3%)	1 (0%)	36	29
1	H	374/386 (97%)	364 (97%)	8 (2%)	2 (0%)	24	16
All	All	2955/3088 (96%)	2872 (97%)	68 (2%)	15 (0%)	24	16

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	17	GLY
1	A	301	VAL
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%)	262 (95%)	13 (5%)	23	15
1	B	276/294 (94%)	268 (97%)	8 (3%)	37	31
1	C	284/294 (97%)	275 (97%)	9 (3%)	34	27
1	D	282/294 (96%)	274 (97%)	8 (3%)	38	32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	282/294 (96%)	274 (97%)	8 (3%)	38	32
1	F	282/294 (96%)	269 (95%)	13 (5%)	24	16
1	G	286/294 (97%)	280 (98%)	6 (2%)	47	44
1	H	285/294 (97%)	277 (97%)	8 (3%)	38	32
All	All	2252/2352 (96%)	2179 (97%)	73 (3%)	33	27

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	96	LYS
1	G	206	GLU
1	G	212	LEU
1	G	332	THR
1	G	343	LEU
1	G	362	ARG
1	A	29	HIS
1	A	51	THR
1	A	124	MET
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	332	THR
1	A	345	ASP
1	A	362	ARG
1	A	374	ASP
1	D	19	VAL
1	D	186	LEU
1	D	206	GLU
1	D	212	LEU
1	D	332	THR
1	D	343	LEU
1	D	344	ARG
1	D	362	ARG
1	E	137	SER
1	E	189	ARG
1	E	206	GLU
1	E	212	LEU
1	E	242	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	332	THR
1	E	343	LEU
1	E	345	ASP
1	F	2	LYS
1	F	35	ILE
1	F	124	MET
1	F	137	SER
1	F	150	LYS
1	F	153	ARG
1	F	201	ASN
1	F	206	GLU
1	F	212	LEU
1	F	215	LEU
1	F	242	LEU
1	F	332	THR
1	F	343	LEU
1	B	28	TYR
1	B	137	SER
1	B	150	LYS
1	B	201	ASN
1	B	206	GLU
1	B	212	LEU
1	B	242	LEU
1	B	256	LEU
1	H	124	MET
1	H	138	SER
1	H	145	GLU
1	H	186	LEU
1	H	206	GLU
1	H	212	LEU
1	H	345	ASP
1	H	374	ASP
1	C	51	THR
1	C	137	SER
1	C	186	LEU
1	C	189	ARG
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 (36)

such sidechains are listed below:

Mol	Chain	Res	Type
1	G	9	HIS
1	G	157	GLN
1	G	201	ASN
1	G	320	HIS
1	A	9	HIS
1	A	154	HIS
1	A	157	GLN
1	A	201	ASN
1	A	320	HIS
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	201	ASN
1	E	320	HIS
1	F	9	HIS
1	F	154	HIS
1	F	157	GLN
1	F	190	GLN
1	F	200	ASN
1	F	201	ASN
1	F	320	HIS
1	B	9	HIS
1	B	154	HIS
1	B	157	GLN
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	154	HIS
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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	363/386 (94%)	0.08	8 (2%) 62 66	9, 16, 25, 41	0
1	B	365/386 (94%)	0.13	10 (2%) 56 60	8, 16, 24, 51	0
1	C	374/386 (96%)	0.36	19 (5%) 33 36	8, 17, 30, 48	1 (0%)
1	D	373/386 (96%)	0.28	4 (1%) 78 80	9, 16, 25, 29	0
1	E	373/386 (96%)	0.27	25 (6%) 24 25	10, 17, 29, 46	0
1	F	373/386 (96%)	0.40	41 (10%) 10 11	10, 15, 28, 46	0
1	G	373/386 (96%)	-0.01	3 (0%) 82 85	6, 15, 25, 33	4 (1%)
1	H	374/386 (96%)	0.50	35 (9%) 14 14	7, 16, 31, 49	2 (0%)
All	All	2968/3088 (96%)	0.25	145 (4%) 35 37	6, 16, 27, 51	7 (0%)

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	374	ASP	6.5
1	H	25	GLY	5.8
1	F	18	GLY	5.5
1	B	28	TYR	5.4
1	B	18	GLY	5.3
1	F	19	VAL	5.1
1	F	149	ALA	4.9
1	F	24	GLY	4.8
1	E	24	GLY	4.7
1	C	17	GLY	4.6
1	H	19	VAL	4.5
1	H	345	ASP	4.5
1	B	17	GLY	4.5
1	C	23	SER	4.5
1	H	29	HIS	4.4
1	B	29	HIS	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	158	GLY	4.3
1	E	28	TYR	4.1
1	C	28	TYR	4.0
1	C	24	GLY	4.0
1	C	373	GLY	4.0
1	E	149	ALA	3.8
1	F	147	MET	3.8
1	F	139	ILE	3.8
1	E	22	LEU	3.7
1	E	21	ARG	3.7
1	F	141	GLY	3.6
1	H	28	TYR	3.6
1	H	152	ALA	3.5
1	F	164	ILE	3.4
1	C	22	LEU	3.4
1	A	29	HIS	3.3
1	H	20	TYR	3.3
1	H	149	ALA	3.3
1	H	332[A]	THR	3.3
1	F	143	THR	3.3
1	E	23	SER	3.3
1	H	15	VAL	3.2
1	F	25	GLY	3.2
1	F	159	PHE	3.2
1	E	145	GLU	3.2
1	F	146	ALA	3.2
1	F	184	ALA	3.1
1	F	22	LEU	3.1
1	F	140	GLY	3.1
1	G	363	ASP	3.1
1	E	183	THR	3.1
1	B	333	THR	3.1
1	E	25	GLY	3.1
1	H	30	SER	3.0
1	H	347	GLY	3.0
1	E	152	ALA	3.0
1	H	139	ILE	3.0
1	H	346	GLY	3.0
1	F	187	ALA	3.0
1	D	11	THR	2.9
1	G	333	THR	2.9
1	A	333	THR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	14	PRO	2.9
1	F	154	HIS	2.9
1	H	156	ALA	2.9
1	A	374	ASP	2.9
1	F	20	TYR	2.8
1	E	146	ALA	2.8
1	F	23	SER	2.8
1	F	27	GLU	2.8
1	H	17	GLY	2.8
1	H	145	GLU	2.7
1	B	363	ASP	2.7
1	H	363	ASP	2.7
1	C	146	ALA	2.7
1	F	347	GLY	2.7
1	E	142	ASP	2.7
1	H	343	LEU	2.7
1	H	22	LEU	2.6
1	F	191	PRO	2.6
1	F	21	ARG	2.6
1	C	18	GLY	2.6
1	F	176	ALA	2.6
1	C	19	VAL	2.6
1	F	189	ARG	2.6
1	E	367	THR	2.6
1	F	186	LEU	2.5
1	F	345	ASP	2.5
1	F	190	GLN	2.5
1	F	195	TYR	2.5
1	A	344	ARG	2.5
1	H	187	ALA	2.5
1	F	183	THR	2.5
1	E	345	ASP	2.5
1	H	24	GLY	2.5
1	F	26	ARG	2.5
1	H	153	ARG	2.5
1	F	142	ASP	2.5
1	B	12	ASP	2.5
1	F	28	TYR	2.4
1	F	153	ARG	2.4
1	D	346	GLY	2.4
1	B	171	ALA	2.4
1	H	330	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	26	ARG	2.4
1	E	144	PRO	2.4
1	A	157	GLN	2.4
1	F	92	ARG	2.4
1	D	156	ALA	2.4
1	E	340	ASP	2.3
1	H	374	ASP	2.3
1	H	155	ARG	2.3
1	C	21	ARG	2.3
1	C	159	PHE	2.3
1	H	333	THR	2.3
1	H	141	GLY	2.3
1	H	154	HIS	2.3
1	E	18	GLY	2.3
1	C	346	GLY	2.3
1	E	20	TYR	2.3
1	C	20	TYR	2.3
1	D	363	ASP	2.3
1	E	26	ARG	2.2
1	B	149	ALA	2.2
1	H	18	GLY	2.2
1	F	165	LYS	2.2
1	C	153	ARG	2.2
1	F	145	GLU	2.2
1	H	340	ASP	2.2
1	C	27	GLU	2.2
1	A	373	GLY	2.2
1	F	157	GLN	2.1
1	E	143	THR	2.1
1	H	23	SER	2.1
1	E	189	ARG	2.1
1	F	29	HIS	2.1
1	E	19	VAL	2.1
1	A	145	GLU	2.1
1	B	335	GLU	2.1
1	C	145	GLU	2.1
1	A	345	ASP	2.1
1	C	363	ASP	2.1
1	C	138	SER	2.1
1	E	218	GLY	2.1
1	E	29	HIS	2.1
1	E	373	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	144	PRO	2.0
1	F	152	ALA	2.0
1	G	164	ILE	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 oligosaccharides 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	0.84	0.11	41,41,41,41	0
2	MG	E	501	1/1	0.90	0.09	35,35,35,35	0
2	MG	C	501	1/1	0.91	0.09	37,37,37,37	0
2	MG	B	501	1/1	0.95	0.04	24,24,24,24	0
2	MG	A	501	1/1	0.96	0.06	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.