



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:51 AM GMT

PDB ID : 2EK1
Title : Crystal structure of RNA-binding motif of human rna-binding protein 12
Authors : Ihsanawati; Bessho, Y.; Shirouzu, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2007-03-22
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

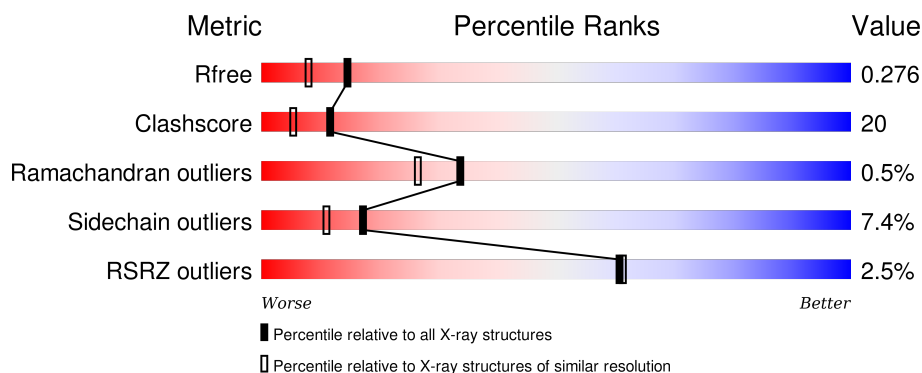
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	95	<div> <div> <div></div> <div>59%</div> <div>21%</div> <div>•</div> <div>17%</div> </div> </div>
1	B	95	<div> <div>2%</div> <div> <div></div> <div>61%</div> <div>18%</div> <div>•</div> <div>18%</div> </div> </div>
1	C	95	<div> <div> <div></div> <div>57%</div> <div>20%</div> <div>6%</div> <div>17%</div> </div> </div>
1	D	95	<div> <div> <div></div> <div>61%</div> <div>19%</div> <div>•</div> <div>17%</div> </div> </div>
1	E	95	<div> <div>3%</div> <div> <div></div> <div>46%</div> <div>29%</div> <div>6%</div> <div>•</div> <div>17%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	95	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>59%</div><div>21%</div><div>•</div><div>17%</div></div></div>
1	G	95	<div><div><div></div><div></div><div></div><div></div></div><div><div>4%</div><div>48%</div><div>31%</div><div>•</div><div>19%</div></div></div>
1	H	95	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>49%</div><div>28%</div><div>5%</div><div>17%</div></div></div>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 5266 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 RNA-binding protein 12.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	79	Total	C	N	O	S	Se	0	0	0
			606	387	98	117	1	3			
1	B	78	Total	C	N	O	S	Se	0	0	0
			600	384	97	115	1	3			
1	C	79	Total	C	N	O	S	Se	0	0	0
			606	387	98	117	1	3			
1	D	79	Total	C	N	O	S	Se	0	0	0
			604	386	98	116	1	3			
1	E	79	Total	C	N	O	S	Se	0	0	0
			606	387	98	117	1	3			
1	F	79	Total	C	N	O	S	Se	0	0	0
			606	387	98	117	1	3			
1	G	77	Total	C	N	O	S	Se	0	0	0
			593	379	96	114	1	3			
1	H	79	Total	C	N	O	S	Se	0	0	0
			606	387	98	117	1	3			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	861	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
A	862	SER	-	EXPRESSION TAG	UNP Q9NTZ6
A	863	SER	-	EXPRESSION TAG	UNP Q9NTZ6
A	864	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
A	865	SER	-	EXPRESSION TAG	UNP Q9NTZ6
A	866	SER	-	EXPRESSION TAG	UNP Q9NTZ6
A	867	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
A	950	SER	-	EXPRESSION TAG	UNP Q9NTZ6
A	951	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
A	952	PRO	-	EXPRESSION TAG	UNP Q9NTZ6
A	953	SER	-	EXPRESSION TAG	UNP Q9NTZ6
A	954	SER	-	EXPRESSION TAG	UNP Q9NTZ6
A	955	GLY	-	EXPRESSION TAG	UNP Q9NTZ6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	861	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
B	862	SER	-	EXPRESSION TAG	UNP Q9NTZ6
B	863	SER	-	EXPRESSION TAG	UNP Q9NTZ6
B	864	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
B	865	SER	-	EXPRESSION TAG	UNP Q9NTZ6
B	866	SER	-	EXPRESSION TAG	UNP Q9NTZ6
B	867	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
B	950	SER	-	EXPRESSION TAG	UNP Q9NTZ6
B	951	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
B	952	PRO	-	EXPRESSION TAG	UNP Q9NTZ6
B	953	SER	-	EXPRESSION TAG	UNP Q9NTZ6
B	954	SER	-	EXPRESSION TAG	UNP Q9NTZ6
B	955	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
C	861	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
C	862	SER	-	EXPRESSION TAG	UNP Q9NTZ6
C	863	SER	-	EXPRESSION TAG	UNP Q9NTZ6
C	864	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
C	865	SER	-	EXPRESSION TAG	UNP Q9NTZ6
C	866	SER	-	EXPRESSION TAG	UNP Q9NTZ6
C	867	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
C	950	SER	-	EXPRESSION TAG	UNP Q9NTZ6
C	951	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
C	952	PRO	-	EXPRESSION TAG	UNP Q9NTZ6
C	953	SER	-	EXPRESSION TAG	UNP Q9NTZ6
C	954	SER	-	EXPRESSION TAG	UNP Q9NTZ6
C	955	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
D	861	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
D	862	SER	-	EXPRESSION TAG	UNP Q9NTZ6
D	863	SER	-	EXPRESSION TAG	UNP Q9NTZ6
D	864	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
D	865	SER	-	EXPRESSION TAG	UNP Q9NTZ6
D	866	SER	-	EXPRESSION TAG	UNP Q9NTZ6
D	867	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
D	950	SER	-	EXPRESSION TAG	UNP Q9NTZ6
D	951	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
D	952	PRO	-	EXPRESSION TAG	UNP Q9NTZ6
D	953	SER	-	EXPRESSION TAG	UNP Q9NTZ6
D	954	SER	-	EXPRESSION TAG	UNP Q9NTZ6
D	955	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
E	861	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
E	862	SER	-	EXPRESSION TAG	UNP Q9NTZ6
E	863	SER	-	EXPRESSION TAG	UNP Q9NTZ6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	864	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
E	865	SER	-	EXPRESSION TAG	UNP Q9NTZ6
E	866	SER	-	EXPRESSION TAG	UNP Q9NTZ6
E	867	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
E	950	SER	-	EXPRESSION TAG	UNP Q9NTZ6
E	951	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
E	952	PRO	-	EXPRESSION TAG	UNP Q9NTZ6
E	953	SER	-	EXPRESSION TAG	UNP Q9NTZ6
E	954	SER	-	EXPRESSION TAG	UNP Q9NTZ6
E	955	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
F	861	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
F	862	SER	-	EXPRESSION TAG	UNP Q9NTZ6
F	863	SER	-	EXPRESSION TAG	UNP Q9NTZ6
F	864	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
F	865	SER	-	EXPRESSION TAG	UNP Q9NTZ6
F	866	SER	-	EXPRESSION TAG	UNP Q9NTZ6
F	867	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
F	950	SER	-	EXPRESSION TAG	UNP Q9NTZ6
F	951	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
F	952	PRO	-	EXPRESSION TAG	UNP Q9NTZ6
F	953	SER	-	EXPRESSION TAG	UNP Q9NTZ6
F	954	SER	-	EXPRESSION TAG	UNP Q9NTZ6
F	955	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
G	861	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
G	862	SER	-	EXPRESSION TAG	UNP Q9NTZ6
G	863	SER	-	EXPRESSION TAG	UNP Q9NTZ6
G	864	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
G	865	SER	-	EXPRESSION TAG	UNP Q9NTZ6
G	866	SER	-	EXPRESSION TAG	UNP Q9NTZ6
G	867	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
G	950	SER	-	EXPRESSION TAG	UNP Q9NTZ6
G	951	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
G	952	PRO	-	EXPRESSION TAG	UNP Q9NTZ6
G	953	SER	-	EXPRESSION TAG	UNP Q9NTZ6
G	954	SER	-	EXPRESSION TAG	UNP Q9NTZ6
G	955	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
H	861	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
H	862	SER	-	EXPRESSION TAG	UNP Q9NTZ6
H	863	SER	-	EXPRESSION TAG	UNP Q9NTZ6
H	864	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
H	865	SER	-	EXPRESSION TAG	UNP Q9NTZ6
H	866	SER	-	EXPRESSION TAG	UNP Q9NTZ6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	867	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
H	950	SER	-	EXPRESSION TAG	UNP Q9NTZ6
H	951	GLY	-	EXPRESSION TAG	UNP Q9NTZ6
H	952	PRO	-	EXPRESSION TAG	UNP Q9NTZ6
H	953	SER	-	EXPRESSION TAG	UNP Q9NTZ6
H	954	SER	-	EXPRESSION TAG	UNP Q9NTZ6
H	955	GLY	-	EXPRESSION TAG	UNP Q9NTZ6

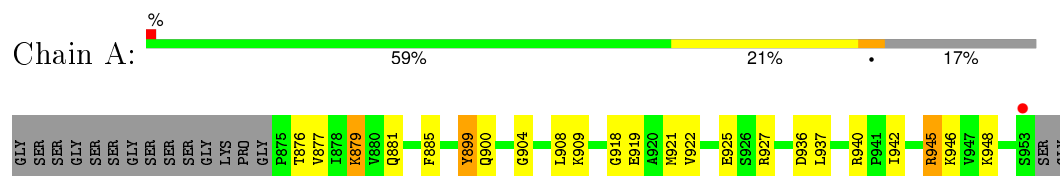
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	67	Total O 67 67	0	0
2	B	54	Total O 54 54	0	0
2	C	64	Total O 64 64	0	0
2	D	52	Total O 52 52	0	0
2	E	48	Total O 48 48	0	0
2	F	51	Total O 51 51	0	0
2	G	48	Total O 48 48	0	0
2	H	55	Total O 55 55	0	0

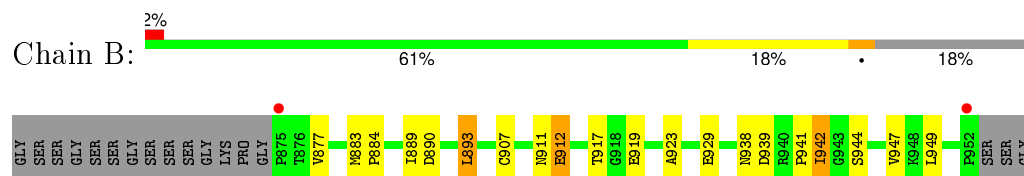
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

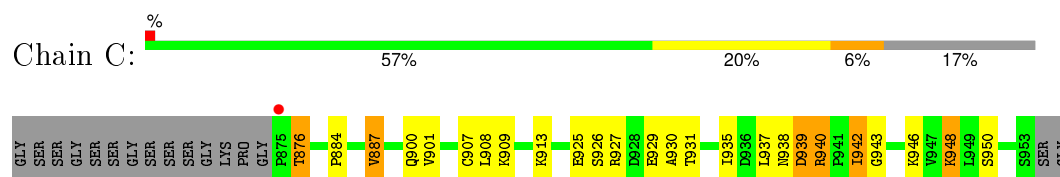
• Molecule 1: RNA-binding protein 12



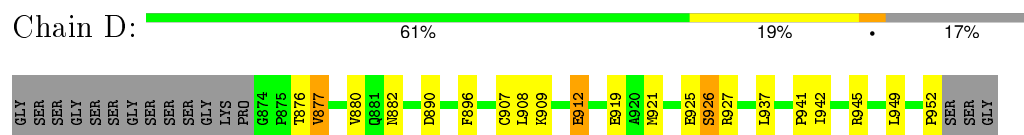
• Molecule 1: RNA-binding protein 12



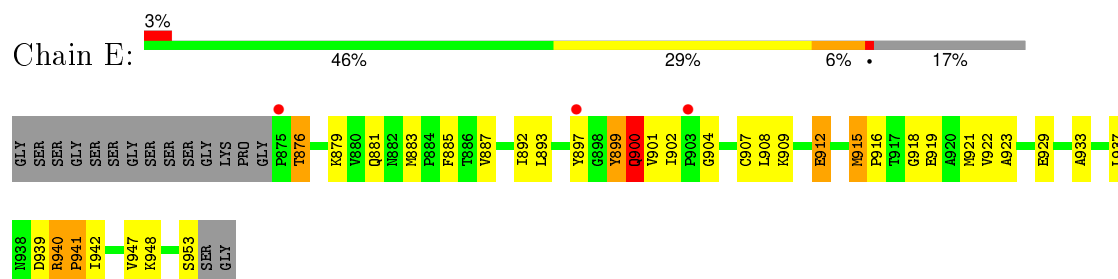
• Molecule 1: RNA-binding protein 12



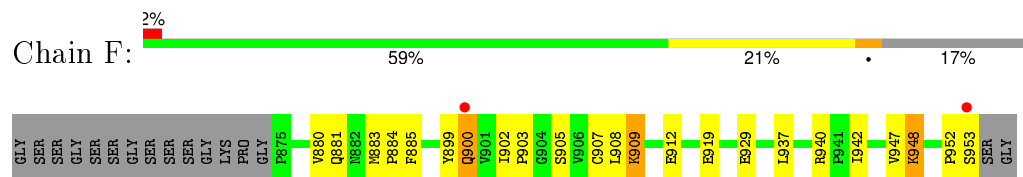
• Molecule 1: RNA-binding protein 12



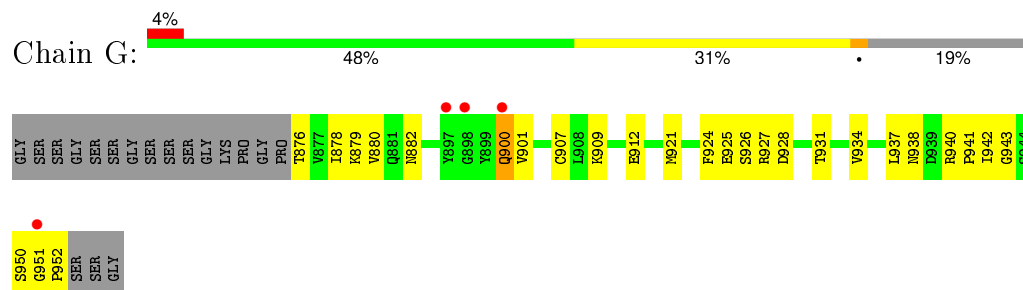
• Molecule 1: RNA-binding protein 12



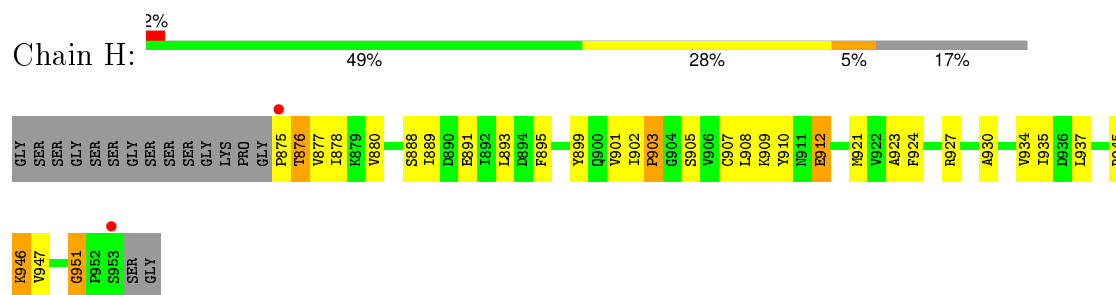
- Molecule 1: RNA-binding protein 12



- Molecule 1: RNA-binding protein 12



- Molecule 1: RNA-binding protein 12



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.88Å 103.23Å 62.19Å 90.00° 91.50° 90.00°	Depositor
Resolution (Å)	29.76 – 2.00 31.08 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.3 (29.76-2.00) 90.5 (31.08-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.208 , 0.274 0.210 , 0.276	Depositor DCC
R_{free} test set	1988 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.3	EDS
Estimated twinning fraction	0.146 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 39738 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5266	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	1.29	0/615	1.15	1/827 (0.1%)
1	B	1.31	1/609 (0.2%)	1.20	3/819 (0.4%)
1	C	1.19	2/615 (0.3%)	1.16	0/827
1	D	1.35	2/613 (0.3%)	1.18	2/825 (0.2%)
1	E	1.19	1/615 (0.2%)	1.19	2/827 (0.2%)
1	F	1.21	2/615 (0.3%)	1.10	1/827 (0.1%)
1	G	1.03	0/601	1.03	1/808 (0.1%)
1	H	1.26	2/615 (0.3%)	1.18	1/827 (0.1%)
All	All	1.23	10/4898 (0.2%)	1.15	11/6587 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	1
1	H	0	1
All	All	0	3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	896	PHE	CE2-CZ	7.06	1.50	1.37
1	E	887	VAL	CB-CG1	6.14	1.65	1.52
1	H	899	TYR	CD1-CE1	5.79	1.48	1.39
1	H	899	TYR	CD2-CE2	5.71	1.48	1.39
1	F	919	GLU	CB-CG	5.54	1.62	1.52
1	D	925	GLU	CG-CD	5.51	1.60	1.51
1	C	950	SER	CB-OG	-5.18	1.35	1.42
1	B	941	PRO	CG-CD	5.04	1.67	1.50
1	F	912	GLU	CG-CD	5.03	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	887	VAL	CB-CG1	-5.01	1.42	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	890	ASP	CB-CG-OD1	7.55	125.09	118.30
1	B	942	ILE	N-CA-C	-5.81	95.32	111.00
1	E	915	MSE	CG-SE-CE	-5.51	86.77	98.90
1	E	941	PRO	N-CA-C	5.51	126.43	112.10
1	A	942	ILE	N-CA-C	-5.38	96.47	111.00
1	F	942	ILE	N-CA-C	-5.29	96.72	111.00
1	B	890	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	D	942	ILE	N-CA-C	-5.22	96.91	111.00
1	H	945	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	D	909	LYS	CD-CE-NZ	-5.06	100.07	111.70
1	G	921	MSE	CG-SE-CE	-5.02	87.85	98.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	899	TYR	Sidechain
1	E	899	TYR	Sidechain
1	H	910	TYR	Sidechain

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	606	0	607	28	0
1	B	600	0	602	18	0
1	C	606	0	607	28	0
1	D	604	0	604	10	0
1	E	606	0	607	37	0
1	F	606	0	607	25	0
1	G	593	0	594	39	0
1	H	606	0	607	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	67	0	0	10	0
2	B	54	0	0	2	0
2	C	64	0	0	3	0
2	D	52	0	0	1	0
2	E	48	0	0	6	0
2	F	51	0	0	2	0
2	G	48	0	0	9	0
2	H	55	0	0	4	0
All	All	5266	0	4835	196	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 20.

All (196) 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:E:883:MSE:HE1	1:E:892:ILE:HG12	1.27	1.15
1:C:876:THR:HG21	1:C:927:ARG:HA	1.41	1.03
1:G:882:ASN:HD21	1:G:945:ARG:HH11	0.97	0.96
1:F:900:GLN:NE2	1:F:929:GLU:HG3	1.83	0.93
1:C:927:ARG:HG2	2:C:984:HOH:O	1.66	0.93
1:H:946:LYS:HD2	1:H:946:LYS:H	1.35	0.92
1:E:909:LYS:HG2	1:F:907:CYS:HB3	1.56	0.88
1:E:909:LYS:NZ	1:E:921:MSE:HE3	1.89	0.86
1:G:879:LYS:HB3	1:G:950:SER:HB3	1.58	0.86
1:G:942:ILE:HG12	1:G:947:VAL:HG21	1.54	0.85
1:C:876:THR:HG21	1:C:927:ARG:CA	2.06	0.85
1:C:909:LYS:HG2	1:D:907:CYS:HB3	1.59	0.85
1:D:882:ASN:HD21	1:D:945:ARG:HH21	1.22	0.83
1:A:904:GLY:N	2:A:1001:HOH:O	1.96	0.82
1:G:927:ARG:O	1:G:931:THR:HG22	1.78	0.82
1:G:882:ASN:ND2	1:G:945:ARG:HH11	1.78	0.81
1:D:882:ASN:ND2	1:D:945:ARG:HH21	1.77	0.81
1:B:912:GLU:OE2	1:B:912:GLU:N	2.14	0.81
1:B:912:GLU:H	1:B:912:GLU:CD	1.85	0.79
1:G:882:ASN:HD21	1:G:945:ARG:NH1	1.78	0.79
1:D:912:GLU:HG2	2:D:976:HOH:O	1.83	0.78
1:G:907:CYS:HB3	1:H:909:LYS:CG	2.13	0.77
1:A:876:THR:HA	2:A:977:HOH:O	1.83	0.77
1:D:882:ASN:HD21	1:D:945:ARG:NH2	1.83	0.76
1:G:934:VAL:HG13	1:G:949:LEU:O	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:900:GLN:CD	1:F:929:GLU:HG3	2.06	0.75
1:H:912:GLU:HG2	2:H:960:HOH:O	1.87	0.75
1:G:952:PRO:HG2	2:G:990:HOH:O	1.86	0.74
1:E:907:CYS:HB3	1:F:909:LYS:HD2	1.70	0.73
1:G:945:ARG:NH2	2:G:983:HOH:O	2.21	0.72
1:G:907:CYS:HB3	1:H:909:LYS:HG2	1.70	0.72
1:A:945:ARG:HD2	2:A:1013:HOH:O	1.89	0.72
1:E:904:GLY:N	2:E:971:HOH:O	2.21	0.72
1:H:946:LYS:N	1:H:946:LYS:HD2	2.06	0.70
1:H:878:ILE:HD11	1:H:930:ALA:HB1	1.74	0.70
1:E:909:LYS:CE	1:E:921:MSE:HE3	2.22	0.69
1:C:925:GLU:OE1	2:C:1016:HOH:O	2.11	0.69
1:E:876:THR:HG22	2:E:984:HOH:O	1.92	0.69
1:A:945:ARG:HG2	1:A:945:ARG:HH21	1.57	0.69
1:G:934:VAL:HG21	1:G:951:GLY:HA2	1.74	0.68
1:F:900:GLN:NE2	1:F:929:GLU:CG	2.56	0.68
1:F:903:PRO:HA	2:F:1005:HOH:O	1.94	0.68
1:D:876:THR:CG2	1:D:952:PRO:HB3	2.24	0.68
1:H:878:ILE:CD1	1:H:930:ALA:HB1	2.24	0.67
1:A:940:ARG:HD3	2:A:980:HOH:O	1.93	0.67
1:F:881:GLN:O	1:F:947:VAL:HG23	1.97	0.65
1:H:878:ILE:HD13	1:H:934:VAL:HG23	1.79	0.65
1:E:883:MSE:HE1	1:E:892:ILE:CG1	2.17	0.65
1:G:907:CYS:HB3	1:H:909:LYS:HG3	1.78	0.65
1:A:945:ARG:HG2	1:A:945:ARG:NH2	2.11	0.65
1:A:948:LYS:HD2	2:A:1021:HOH:O	1.98	0.64
1:G:925:GLU:OE1	1:G:925:GLU:HA	1.98	0.64
1:F:948:LYS:HD2	1:F:948:LYS:N	2.13	0.63
1:G:926:SER:HB3	2:G:996:HOH:O	1.99	0.63
1:F:940:ARG:NE	2:F:997:HOH:O	2.28	0.62
1:E:909:LYS:HZ2	1:E:921:MSE:HE3	1.64	0.62
1:E:900:GLN:HB2	1:E:929:GLU:HG3	1.82	0.61
1:C:876:THR:HG21	1:C:927:ARG:N	2.15	0.61
1:E:909:LYS:CG	1:F:907:CYS:HB3	2.29	0.61
1:E:940:ARG:HH11	1:E:940:ARG:CG	2.14	0.61
1:H:878:ILE:HD13	1:H:934:VAL:CG2	2.30	0.61
1:C:900:GLN:O	1:C:925:GLU:HG2	2.00	0.61
1:E:879:LYS:HG3	1:E:921:MSE:HE1	1.83	0.60
1:A:909:LYS:CG	1:B:907:CYS:HB3	2.32	0.60
1:E:940:ARG:NH1	1:E:940:ARG:HG3	2.16	0.60
1:G:942:ILE:CG1	1:G:947:VAL:HG21	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:944:SER:OG	1:C:913:LYS:HD2	2.02	0.60
1:G:934:VAL:O	1:G:938:ASN:HB2	2.01	0.59
1:H:888:SER:OG	1:H:891:GLU:HG3	2.03	0.59
1:H:934:VAL:HG21	1:H:951:GLY:HA2	1.84	0.59
1:H:907:CYS:SG	1:H:921:MSE:HB2	2.43	0.59
1:B:911:ASN:HB2	1:B:912:GLU:OE2	2.04	0.58
1:A:879:LYS:HE3	2:A:1014:HOH:O	2.04	0.57
1:F:883:MSE:HB3	1:F:884:PRO:HD2	1.87	0.57
1:E:940:ARG:HD2	2:E:998:HOH:O	2.05	0.56
1:F:900:GLN:NE2	1:F:929:GLU:CB	2.68	0.56
1:F:937:LEU:HA	1:F:940:ARG:HD2	1.87	0.56
1:G:880:VAL:HG22	1:G:949:LEU:CD2	2.35	0.56
1:A:940:ARG:CD	2:A:980:HOH:O	2.51	0.56
1:A:909:LYS:HG2	1:B:907:CYS:HB3	1.86	0.56
1:B:877:VAL:HG12	1:B:923:ALA:HB2	1.86	0.56
1:C:937:LEU:O	1:C:940:ARG:HB2	2.06	0.56
1:B:938:ASN:CG	2:B:977:HOH:O	2.43	0.56
1:F:881:GLN:O	1:F:947:VAL:CG2	2.53	0.55
1:A:936:ASP:O	1:A:940:ARG:NH1	2.40	0.55
1:C:948:LYS:HD3	1:C:948:LYS:N	2.21	0.55
1:A:881:GLN:HG2	1:A:919:GLU:HG2	1.87	0.55
1:A:945:ARG:CG	1:A:945:ARG:HH21	2.20	0.54
1:G:931:THR:HB	1:G:952:PRO:HG3	1.90	0.54
1:E:881:GLN:HG2	1:E:919:GLU:HG2	1.90	0.54
1:G:912:GLU:HB2	2:G:967:HOH:O	2.07	0.54
1:G:880:VAL:HG13	1:G:947:VAL:CG1	2.38	0.53
1:A:946:LYS:HB3	1:A:946:LYS:NZ	2.23	0.53
1:G:909:LYS:HB3	2:G:956:HOH:O	2.08	0.53
1:B:929:GLU:HG3	2:B:1000:HOH:O	2.09	0.53
1:C:901:VAL:O	1:C:901:VAL:HG13	2.08	0.53
1:C:938:ASN:O	1:C:939:ASP:HB2	2.08	0.52
1:G:937:LEU:HD22	1:G:940:ARG:HD2	1.90	0.52
1:F:952:PRO:O	1:F:953:SER:CB	2.57	0.52
1:G:900:GLN:HB3	1:G:925:GLU:HG2	1.92	0.52
1:C:946:LYS:HE2	1:C:948:LYS:NZ	2.25	0.52
1:C:946:LYS:HE2	1:C:948:LYS:HZ3	1.75	0.52
1:B:917:THR:HG23	1:B:919:GLU:H	1.75	0.52
1:H:946:LYS:CD	1:H:946:LYS:H	2.15	0.52
1:B:917:THR:HG23	1:B:919:GLU:N	2.25	0.51
1:D:877:VAL:HG23	1:D:921:MSE:HE3	1.93	0.51
1:C:876:THR:HG21	1:C:926:SER:C	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:907:CYS:HB3	1:F:909:LYS:CD	2.39	0.51
1:E:942:ILE:HG13	1:E:947:VAL:HG21	1.93	0.51
1:A:946:LYS:HB3	1:A:946:LYS:HZ3	1.77	0.50
1:H:875:PRO:HA	1:H:924:PHE:O	2.11	0.50
1:E:907:CYS:CB	1:F:909:LYS:HD2	2.39	0.50
1:E:912:GLU:HG2	2:E:959:HOH:O	2.11	0.49
1:H:877:VAL:HG11	1:H:921:MSE:HE2	1.94	0.49
1:E:899:TYR:O	1:E:901:VAL:N	2.36	0.49
1:B:942:ILE:HD12	1:B:947:VAL:HG21	1.93	0.49
1:E:940:ARG:NH1	1:E:940:ARG:CG	2.71	0.49
1:H:889:ILE:HD11	1:H:908:LEU:HD11	1.95	0.49
1:G:882:ASN:C	2:G:985:HOH:O	2.51	0.48
1:E:902:ILE:HG22	1:E:904:GLY:H	1.77	0.48
1:C:900:GLN:NE2	1:C:929:GLU:CD	2.67	0.48
1:D:937:LEU:HB2	1:D:949:LEU:HD11	1.95	0.48
1:A:899:TYR:HB3	2:A:961:HOH:O	2.13	0.48
1:A:946:LYS:NZ	1:A:946:LYS:CB	2.77	0.47
1:G:909:LYS:HE2	2:H:983:HOH:O	2.14	0.47
1:G:882:ASN:ND2	2:G:997:HOH:O	2.36	0.47
1:A:877:VAL:HG11	1:A:921:MSE:HE2	1.96	0.47
1:C:884:PRO:HG3	1:C:942:ILE:HG22	1.97	0.47
1:C:931:THR:O	1:C:935:ILE:HG13	2.15	0.47
1:E:902:ILE:HG22	1:E:902:ILE:O	2.15	0.46
1:H:876:THR:OG1	1:H:927:ARG:HA	2.15	0.46
1:C:940:ARG:HG3	1:C:940:ARG:NH2	2.30	0.46
1:B:889:ILE:HG22	1:B:893:LEU:HD22	1.98	0.46
1:C:942:ILE:HG22	1:C:943:GLY:N	2.30	0.46
1:F:899:TYR:CD2	1:F:899:TYR:N	2.83	0.46
1:G:948:LYS:HD2	2:G:995:HOH:O	2.15	0.46
1:E:940:ARG:HH11	1:E:940:ARG:HG3	1.78	0.46
1:E:881:GLN:OE1	1:E:948:LYS:HE2	2.16	0.45
1:H:880:VAL:HG13	1:H:947:VAL:CG1	2.46	0.45
1:E:933:ALA:O	1:E:937:LEU:HB2	2.16	0.45
1:G:926:SER:OG	1:G:928:ASP:HB2	2.17	0.45
1:G:937:LEU:CD2	1:G:940:ARG:HD2	2.46	0.45
1:E:918:GLY:HA3	2:E:969:HOH:O	2.16	0.45
1:F:952:PRO:O	1:F:953:SER:HB2	2.16	0.45
1:G:876:THR:HA	2:G:984:HOH:O	2.17	0.44
1:C:876:THR:CG2	1:C:926:SER:C	2.86	0.44
1:A:940:ARG:NE	2:A:980:HOH:O	2.50	0.44
1:F:880:VAL:CG1	1:F:947:VAL:HG21	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:884:PRO:HD2	1:C:942:ILE:HG21	1.98	0.44
1:H:895:PHE:HA	2:H:962:HOH:O	2.18	0.44
1:A:918:GLY:HA2	2:A:966:HOH:O	2.17	0.44
1:E:883:MSE:CE	1:E:942:ILE:CD1	2.96	0.44
1:C:907:CYS:HB3	2:C:990:HOH:O	2.17	0.44
1:D:926:SER:O	1:D:927:ARG:C	2.56	0.44
1:H:905:SER:HB2	1:H:923:ALA:HB3	2.00	0.43
1:E:885:PHE:HA	2:E:966:HOH:O	2.17	0.43
1:E:907:CYS:SG	1:E:921:MSE:HB2	2.58	0.43
1:G:876:THR:OG1	1:G:924:PHE:O	2.33	0.43
1:G:901:VAL:HB	1:G:924:PHE:CE1	2.54	0.43
1:C:900:GLN:HB3	1:C:925:GLU:HG3	2.00	0.43
1:E:915:MSE:HG3	1:E:916:PRO:HD2	2.01	0.43
1:E:922:VAL:HG12	1:E:923:ALA:N	2.34	0.43
1:H:902:ILE:HA	1:H:903:PRO:HD2	1.71	0.43
1:G:900:GLN:O	1:G:924:PHE:HD1	2.02	0.42
1:B:883:MSE:HB3	1:B:884:PRO:HD2	2.00	0.42
1:H:880:VAL:HG13	1:H:947:VAL:HG11	2.02	0.42
1:C:876:THR:HG23	1:C:930:ALA:HB2	2.01	0.42
1:C:884:PRO:CD	1:C:942:ILE:CG2	2.98	0.42
1:G:941:PRO:HA	1:G:945:ARG:O	2.19	0.42
1:G:942:ILE:HG12	1:G:947:VAL:CG2	2.38	0.42
1:A:937:LEU:HA	1:A:940:ARG:HG3	2.01	0.42
1:H:935:ILE:HA	1:H:935:ILE:HD13	1.77	0.42
1:G:879:LYS:HB3	1:G:950:SER:CB	2.38	0.42
1:A:885:PHE:CD2	1:A:885:PHE:C	2.90	0.42
1:A:925:GLU:HA	1:A:925:GLU:OE2	2.20	0.42
1:E:907:CYS:HB3	1:F:909:LYS:CE	2.49	0.42
1:G:942:ILE:HG23	1:G:942:ILE:HD12	1.76	0.42
1:B:917:THR:CG2	1:B:919:GLU:HB2	2.49	0.42
1:D:880:VAL:O	1:D:919:GLU:HA	2.19	0.42
1:H:937:LEU:HA	1:H:937:LEU:HD23	1.87	0.42
1:C:940:ARG:HH21	1:C:940:ARG:HG3	1.84	0.41
1:E:883:MSE:CE	1:E:942:ILE:HD12	2.50	0.41
1:E:909:LYS:NZ	1:E:921:MSE:CE	2.72	0.41
1:A:908:LEU:C	1:B:907:CYS:HB2	2.40	0.41
1:F:902:ILE:CG2	1:F:903:PRO:HD2	2.51	0.41
1:F:902:ILE:HG23	1:F:903:PRO:HD2	2.02	0.41
1:B:947:VAL:HG12	1:B:949:LEU:CD1	2.51	0.41
1:H:901:VAL:HG11	2:H:965:HOH:O	2.20	0.41
1:A:900:GLN:CD	1:A:900:GLN:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:900:GLN:NE2	1:F:929:GLU:HB3	2.35	0.41
1:F:902:ILE:HB	1:F:905:SER:HB3	2.03	0.41
1:A:909:LYS:HG3	1:B:907:CYS:HB3	2.01	0.41
1:C:887:VAL:HG13	1:C:887:VAL:O	2.21	0.41
1:A:876:THR:HG21	1:A:927:ARG:HA	2.02	0.40
1:G:943:GLY:C	1:G:945:ARG:H	2.23	0.40
1:E:940:ARG:CB	1:E:940:ARG:HH11	2.35	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	77/95 (81%)	76 (99%)	1 (1%)	0	100	100
1	B	76/95 (80%)	74 (97%)	2 (3%)	0	100	100
1	C	77/95 (81%)	74 (96%)	3 (4%)	0	100	100
1	D	77/95 (81%)	76 (99%)	1 (1%)	0	100	100
1	E	77/95 (81%)	74 (96%)	2 (3%)	1 (1%)	15	7
1	F	77/95 (81%)	75 (97%)	2 (3%)	0	100	100
1	G	75/95 (79%)	69 (92%)	6 (8%)	0	100	100
1	H	77/95 (81%)	74 (96%)	1 (1%)	2 (3%)	7	2
All	All	613/760 (81%)	592 (97%)	18 (3%)	3 (0%)	34	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	900	GLN
1	H	951	GLY
1	H	903	PRO

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	68/75 (91%)	65 (96%)	3 (4%)	35	30
1	B	67/75 (89%)	64 (96%)	3 (4%)	34	29
1	C	68/75 (91%)	62 (91%)	6 (9%)	12	7
1	D	67/75 (89%)	61 (91%)	6 (9%)	12	7
1	E	68/75 (91%)	58 (85%)	10 (15%)	4	2
1	F	68/75 (91%)	63 (93%)	5 (7%)	17	11
1	G	66/75 (88%)	63 (96%)	3 (4%)	34	29
1	H	68/75 (91%)	64 (94%)	4 (6%)	24	18
All	All	540/600 (90%)	500 (93%)	40 (7%)	17	11

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	879	LYS
1	A	922	VAL
1	A	945	ARG
1	B	893	LEU
1	B	912	GLU
1	B	939	ASP
1	C	876	THR
1	C	908	LEU
1	C	939	ASP
1	C	940	ARG
1	C	942	ILE
1	C	948	LYS
1	D	877	VAL
1	D	890	ASP
1	D	908	LEU
1	D	912	GLU
1	D	926	SER
1	D	941	PRO
1	E	876	THR

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Mol	Chain	Res	Type
1	E	893	LEU
1	E	897	TYR
1	E	900	GLN
1	E	908	LEU
1	E	912	GLU
1	E	939	ASP
1	E	940	ARG
1	E	941	PRO
1	E	953	SER
1	F	885	PHE
1	F	900	GLN
1	F	908	LEU
1	F	909	LYS
1	F	948	LYS
1	G	878	ILE
1	G	900	GLN
1	G	948	LYS
1	H	876	THR
1	H	893	LEU
1	H	912	GLU
1	H	946	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	900	GLN
1	B	882	ASN
1	B	900	GLN
1	C	900	GLN
1	D	882	ASN
1	F	900	GLN
1	G	882	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	76/95 (80%)	-0.07	1 (1%) 79 80	14, 23, 38, 55	0
1	B	75/95 (78%)	-0.18	2 (2%) 58 58	14, 24, 41, 45	0
1	C	76/95 (80%)	0.04	1 (1%) 79 80	15, 28, 41, 49	0
1	D	76/95 (80%)	-0.11	0 100 100	16, 28, 39, 45	0
1	E	76/95 (80%)	-0.02	3 (3%) 43 45	19, 26, 45, 51	0
1	F	76/95 (80%)	-0.05	2 (2%) 59 60	18, 27, 45, 56	0
1	G	74/95 (77%)	0.48	4 (5%) 29 31	21, 42, 63, 66	0
1	H	76/95 (80%)	0.08	2 (2%) 59 60	19, 28, 45, 52	0
All	All	605/760 (79%)	0.02	15 (2%) 61 61	14, 27, 49, 66	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	953	SER	4.8
1	H	953	SER	3.6
1	G	900	GLN	3.2
1	C	875	PRO	2.9
1	G	951	GLY	2.9
1	E	875	PRO	2.9
1	E	903	PRO	2.7
1	B	875	PRO	2.7
1	G	897	TYR	2.7
1	F	953	SER	2.4
1	H	875	PRO	2.3
1	B	952	PRO	2.2
1	G	898	GLY	2.1
1	E	897	TYR	2.1
1	F	900	GLN	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.