Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:40 PM GMT

PDB ID	:	4FQB
Title	:	crystal structure of toxic effector Tse1 in complex with immune protein Tsi1
Authors	:	Wang, T.; Li, L.; Zhang, W.
Deposited on	:	2012-06-25
Resolution	:	2.69 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

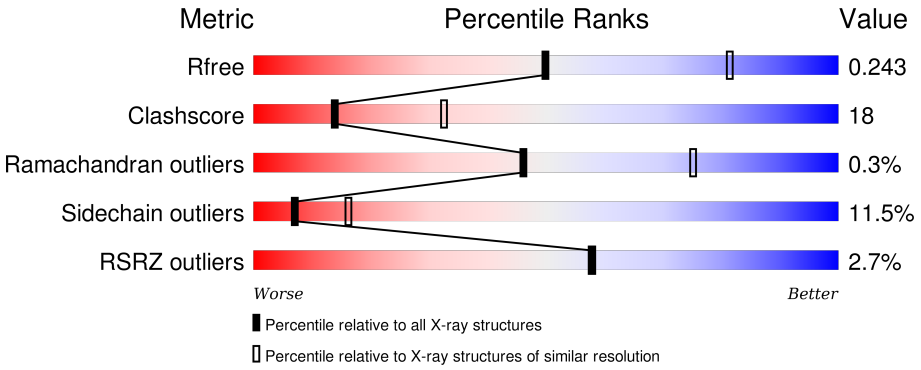
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 <=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	162	69% 19% 10%
1	C	162	3% 59% 26% 6% 10%
1	E	162	2% 57% 25% 6% 10%
1	G	162	7% 64% 20% 6% 10%
2	B	162	62% 25% 9%

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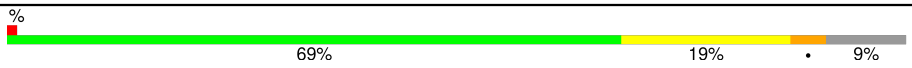
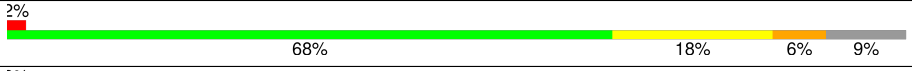
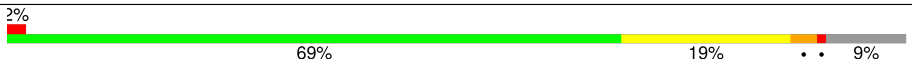
Mol	Chain	Length	Quality of chain
2	D	162	
2	F	162	
2	H	162	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9004 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 toxic effector Tse1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	1	0	0
			1091	682	195	205	9			
1	C	146	Total	C	N	O	S	0	0	0
			1091	682	195	205	9			
1	E	146	Total	C	N	O	S	0	0	0
			1091	682	195	205	9			
1	G	146	Total	C	N	O	S	0	0	0
			1091	682	195	205	9			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	155	LEU	-	EXPRESSION TAG	UNP Q9I2Q1
A	156	GLU	-	EXPRESSION TAG	UNP Q9I2Q1
A	157	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
A	158	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
A	159	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
A	160	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
A	161	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
A	162	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
C	155	LEU	-	EXPRESSION TAG	UNP Q9I2Q1
C	156	GLU	-	EXPRESSION TAG	UNP Q9I2Q1
C	157	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
C	158	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
C	159	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
C	160	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
C	161	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
C	162	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
E	155	LEU	-	EXPRESSION TAG	UNP Q9I2Q1
E	156	GLU	-	EXPRESSION TAG	UNP Q9I2Q1
E	157	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
E	158	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
E	159	HIS	-	EXPRESSION TAG	UNP Q9I2Q1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	160	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
E	161	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
E	162	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
G	155	LEU	-	EXPRESSION TAG	UNP Q9I2Q1
G	156	GLU	-	EXPRESSION TAG	UNP Q9I2Q1
G	157	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
G	158	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
G	159	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
G	160	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
G	161	HIS	-	EXPRESSION TAG	UNP Q9I2Q1
G	162	HIS	-	EXPRESSION TAG	UNP Q9I2Q1

- Molecule 2 is a protein called immune protein Tsi1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	148	Total	C	N	O	S	0	0	0
			1142	701	202	230	9			
2	D	148	Total	C	N	O	S	0	0	0
			1142	701	202	230	9			
2	F	148	Total	C	N	O	S	0	0	0
			1142	701	202	230	9			
2	H	148	Total	C	N	O	S	0	0	0
			1142	701	202	230	9			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	19	MET	-	EXPRESSION TAG	UNP Q9I2Q0
B	173	LEU	-	EXPRESSION TAG	UNP Q9I2Q0
B	174	GLU	-	EXPRESSION TAG	UNP Q9I2Q0
B	175	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
B	176	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
B	177	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
B	178	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
B	179	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
B	180	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
D	19	MET	-	EXPRESSION TAG	UNP Q9I2Q0
D	173	LEU	-	EXPRESSION TAG	UNP Q9I2Q0
D	174	GLU	-	EXPRESSION TAG	UNP Q9I2Q0
D	175	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
D	176	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
D	177	HIS	-	EXPRESSION TAG	UNP Q9I2Q0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	178	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
D	179	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
D	180	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
F	19	MET	-	EXPRESSION TAG	UNP Q9I2Q0
F	173	LEU	-	EXPRESSION TAG	UNP Q9I2Q0
F	174	GLU	-	EXPRESSION TAG	UNP Q9I2Q0
F	175	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
F	176	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
F	177	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
F	178	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
F	179	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
F	180	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
H	19	MET	-	EXPRESSION TAG	UNP Q9I2Q0
H	173	LEU	-	EXPRESSION TAG	UNP Q9I2Q0
H	174	GLU	-	EXPRESSION TAG	UNP Q9I2Q0
H	175	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
H	176	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
H	177	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
H	178	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
H	179	HIS	-	EXPRESSION TAG	UNP Q9I2Q0
H	180	HIS	-	EXPRESSION TAG	UNP Q9I2Q0

- Molecule 3 is water.

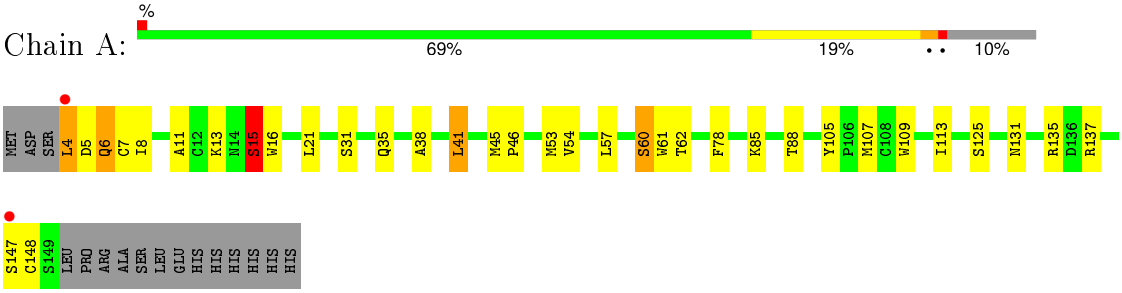
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	9	Total O 9 9	0	0
3	B	17	Total O 17 17	0	0
3	C	5	Total O 5 5	0	0
3	D	15	Total O 15 15	0	0
3	E	2	Total O 2 2	0	0
3	F	14	Total O 14 14	0	0
3	G	1	Total O 1 1	0	0
3	H	9	Total O 9 9	0	0

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.

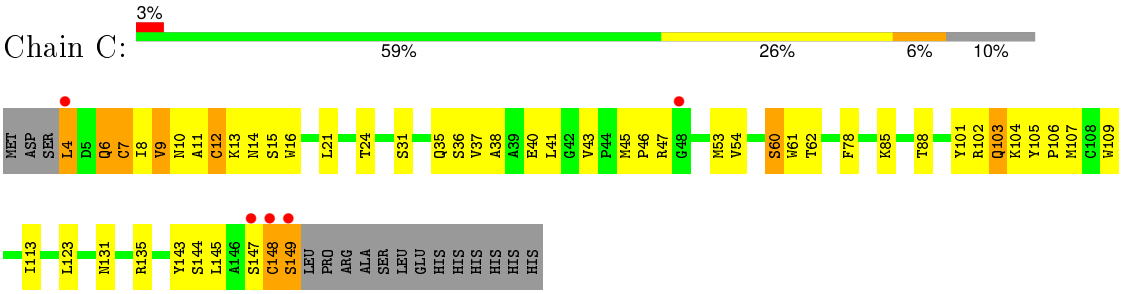
- Molecule 1: toxic effector Tse1

Chain A:



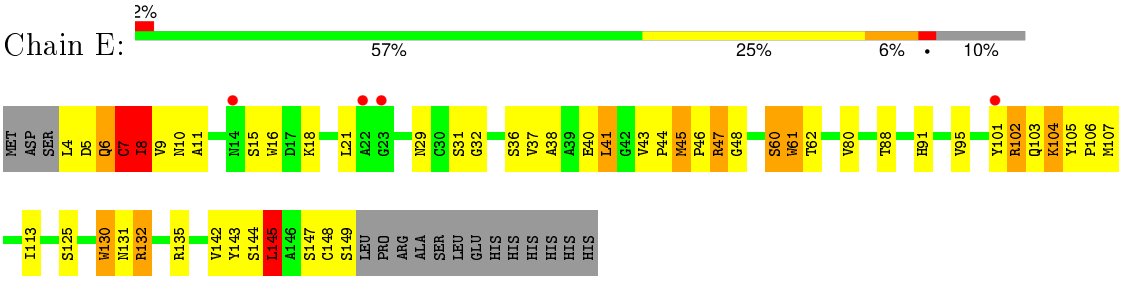
- Molecule 1: toxic effector Tse1

Chain C:



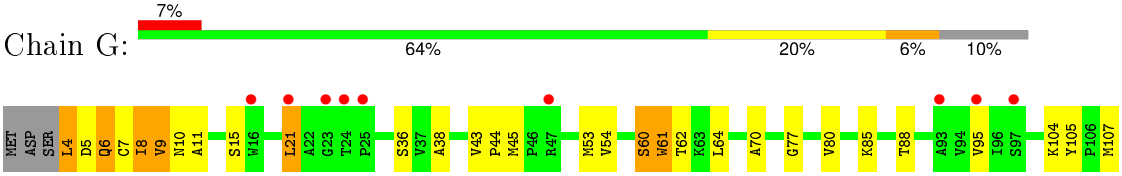
- Molecule 1: toxic effector Tse1

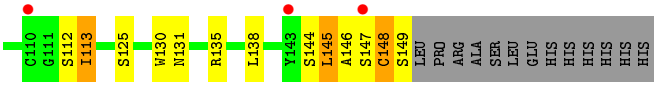
Chain E:



- Molecule 1: toxic effector Tse1

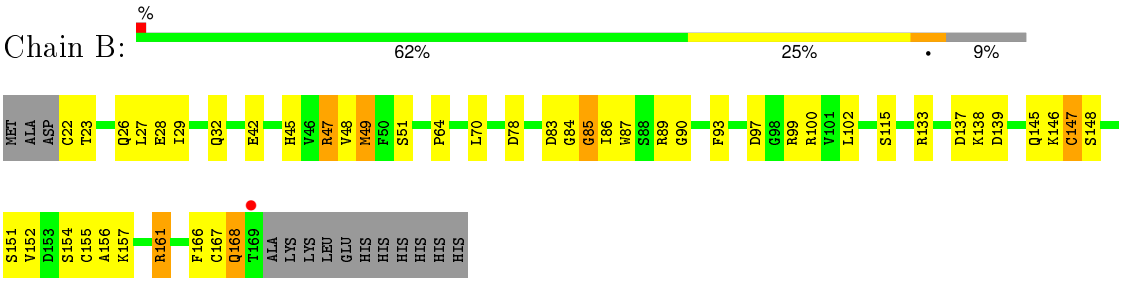
Chain G:





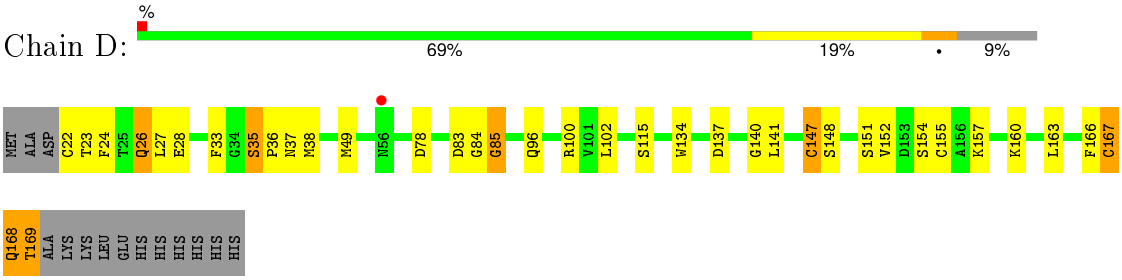
• Molecule 2: immune protein Tsi1

Chain B:



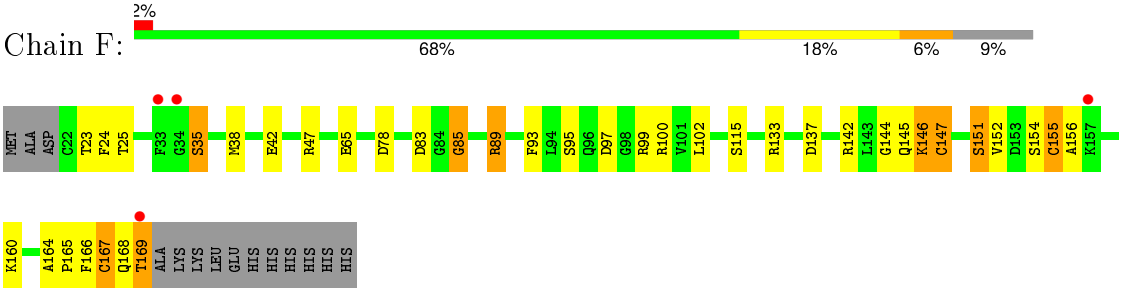
• Molecule 2: immune protein Tsi1

Chain D:



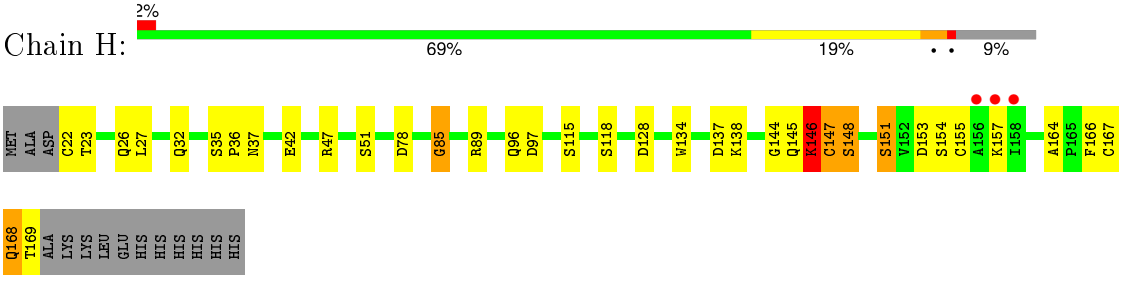
• Molecule 2: immune protein Tsi1

Chain F:



• Molecule 2: immune protein Tsi1

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	97.71Å 97.71Å 293.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.69 29.77 – 2.69	Depositor EDS
% Data completeness (in resolution range)	93.6 (30.00-2.69) 93.7 (29.77-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.201 , 0.245 0.207 , 0.243	Depositor DCC
R_{free} test set	2336 reflections (5.70%)	DCC
Wilson B-factor (Å^2)	69.8	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 37.4	EDS
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 43193 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9004	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.83	3/1113 (0.3%)	0.87	2/1508 (0.1%)
1	C	0.79	2/1113 (0.2%)	0.86	3/1508 (0.2%)
1	E	0.79	3/1113 (0.3%)	0.80	1/1508 (0.1%)
1	G	0.70	1/1113 (0.1%)	0.75	0/1508
2	B	1.03	3/1166 (0.3%)	1.06	4/1575 (0.3%)
2	D	1.02	1/1166 (0.1%)	0.94	1/1575 (0.1%)
2	F	0.90	0/1166	0.96	4/1575 (0.3%)
2	H	0.92	2/1166 (0.2%)	1.12	6/1575 (0.4%)
All	All	0.88	15/9116 (0.2%)	0.93	21/12332 (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
2	B	0	1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	134	TRP	CD2-CE2	6.98	1.49	1.41
2	B	28	GLU	CD-OE1	6.85	1.33	1.25
1	C	16	TRP	CD2-CE2	5.68	1.48	1.41
2	H	118	SER	CB-OG	-5.37	1.35	1.42
1	A	16	TRP	CD2-CE2	5.37	1.47	1.41
1	C	109	TRP	CD2-CE2	5.36	1.47	1.41
2	B	85	GLY	C-O	5.29	1.32	1.23
1	A	15	SER	CB-OG	-5.25	1.35	1.42
1	E	16	TRP	CD2-CE2	5.14	1.47	1.41
2	B	85	GLY	N-CA	5.10	1.53	1.46
1	E	61	TRP	CD2-CE2	5.09	1.47	1.41
2	H	134	TRP	CD2-CE2	5.08	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	61	TRP	CD2-CE2	5.06	1.47	1.41
1	E	130	TRP	CD2-CE2	5.03	1.47	1.41
1	A	109	TRP	CD2-CE2	5.01	1.47	1.41

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	145	GLN	CB-CA-C	-19.52	71.35	110.40
2	H	146	LYS	N-CA-C	-11.42	80.15	111.00
1	C	148	CYS	N-CA-CB	-10.22	92.20	110.60
2	H	145	GLN	N-CA-C	9.14	135.69	111.00
2	B	85	GLY	N-CA-C	-8.87	90.92	113.10
2	D	85	GLY	N-CA-C	-7.81	93.58	113.10
1	E	145	LEU	CA-CB-CG	-7.40	98.27	115.30
2	F	85	GLY	N-CA-C	-7.16	95.20	113.10
2	B	47	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	C	7	CYS	CB-CA-C	-7.06	96.28	110.40
1	A	137	ARG	NE-CZ-NH1	6.62	123.61	120.30
2	F	89	ARG	C-N-CA	-6.45	108.75	122.30
2	B	133	ARG	NE-CZ-NH1	6.24	123.42	120.30
2	H	128	ASP	CB-CG-OD2	5.92	123.62	118.30
1	A	15	SER	CA-CB-OG	-5.71	95.80	111.20
2	H	85	GLY	N-CA-C	-5.68	98.89	113.10
1	C	9	VAL	CB-CA-C	-5.45	101.04	111.40
2	B	97	ASP	CB-CG-OD1	5.41	123.17	118.30
2	F	97	ASP	CB-CG-OD1	5.39	123.15	118.30
2	F	167	CYS	CA-CB-SG	-5.17	104.69	114.00
2	H	89	ARG	C-N-CA	-5.13	111.53	122.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	90	GLY	Peptide

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	1091	0	1069	34	0
1	C	1091	0	1069	57	0
1	E	1091	0	1069	62	0
1	G	1091	0	1069	50	0
2	B	1142	0	1061	35	0
2	D	1142	0	1061	23	1
2	F	1142	0	1061	41	0
2	H	1142	0	1061	27	0
3	A	9	0	0	0	0
3	B	17	0	0	2	0
3	C	5	0	0	0	0
3	D	15	0	0	0	0
3	E	2	0	0	0	0
3	F	14	0	0	3	0
3	G	1	0	0	0	0
3	H	9	0	0	1	0
All	All	9004	0	8520	321	1

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 18.

All (321) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:144:SER:C	1:G:145:LEU:HD12	1.38	1.44
1:E:45:MET:CE	1:E:46:PRO:HD2	1.58	1.32
1:E:45:MET:HA	1:E:45:MET:CE	1.67	1.24
2:F:152:VAL:HG12	3:F:213:HOH:O	1.45	1.15
1:E:45:MET:HE1	1:E:46:PRO:HD2	1.21	1.13
1:E:45:MET:CA	1:E:45:MET:HE3	1.79	1.13
1:E:45:MET:CE	1:E:46:PRO:CD	2.30	1.09
1:A:6:GLN:HA	1:A:6:GLN:NE2	1.59	1.09
1:E:145:LEU:N	1:E:145:LEU:HD12	1.66	1.08
2:B:161:ARG:CG	2:B:161:ARG:HH11	1.68	1.06
1:C:9:VAL:HG13	1:C:10:ASN:N	1.70	1.05
1:C:6:GLN:O	1:C:9:VAL:HG12	1.57	1.04
1:E:45:MET:CE	1:E:45:MET:CA	2.30	1.03
2:H:96:GLN:HG2	2:H:97:ASP:N	1.74	1.02
1:C:6:GLN:NE2	1:C:9:VAL:HG11	1.74	1.02
2:H:36:PRO:O	2:H:37:ASN:HB2	1.57	1.02
2:B:161:ARG:HG3	2:B:161:ARG:HH11	1.18	1.01
1:G:144:SER:C	1:G:145:LEU:CD1	2.30	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:144:SER:O	1:G:145:LEU:HD12	1.63	0.97
1:G:6:GLN:HG3	1:G:10:ASN:HD21	1.26	0.97
1:A:6:GLN:CA	1:A:6:GLN:HE21	1.75	0.96
1:G:145:LEU:N	1:G:145:LEU:HD12	1.77	0.95
1:G:145:LEU:CD1	1:G:145:LEU:N	2.30	0.95
1:E:145:LEU:H	1:E:145:LEU:HD12	1.26	0.93
2:F:145:GLN:N	2:F:155:CYS:SG	2.42	0.92
1:A:4:LEU:O	1:A:148:CYS:SG	2.29	0.91
1:E:144:SER:HB2	1:E:145:LEU:HD11	1.50	0.91
1:A:6:GLN:CA	1:A:6:GLN:NE2	2.30	0.90
2:D:22:CYS:SG	2:D:167:CYS:O	2.29	0.90
1:E:45:MET:HA	1:E:45:MET:HE3	0.91	0.90
2:F:99:ARG:NH1	2:F:168:GLN:O	2.04	0.90
2:B:167:CYS:SG	2:B:167:CYS:O	2.30	0.89
1:C:37:VAL:O	1:C:41:LEU:HD12	1.72	0.89
2:F:167:CYS:O	2:F:167:CYS:SG	2.30	0.89
2:F:89:ARG:HD3	3:F:210:HOH:O	1.71	0.89
2:F:168:GLN:HG2	2:F:169:THR:O	1.70	0.89
1:A:131:ASN:HD22	2:B:85:GLY:HA2	1.36	0.89
1:C:14:ASN:HD22	1:C:40:GLU:CD	1.77	0.87
1:C:9:VAL:CG1	1:C:10:ASN:N	2.38	0.86
1:A:6:GLN:HA	1:A:6:GLN:HE21	1.33	0.85
2:F:146:LYS:HB2	2:F:156:ALA:HB3	1.57	0.85
1:E:145:LEU:N	1:E:145:LEU:CD1	2.30	0.85
1:E:45:MET:HE2	1:E:46:PRO:N	1.93	0.84
1:G:77:GLY:O	1:G:148:CYS:HB2	1.77	0.83
1:G:6:GLN:HG3	1:G:10:ASN:ND2	1.94	0.82
1:E:45:MET:HE3	1:E:46:PRO:HD2	1.60	0.82
2:F:146:LYS:CB	2:F:156:ALA:HB3	2.10	0.82
1:C:14:ASN:ND2	1:C:40:GLU:OE2	2.13	0.82
2:H:96:GLN:HG2	2:H:97:ASP:H	1.43	0.81
1:A:4:LEU:N	1:A:4:LEU:HD23	1.95	0.81
2:H:148:SER:H	2:H:154:SER:HB2	1.45	0.81
1:A:11:ALA:HB2	1:A:41:LEU:HD21	1.60	0.81
1:G:6:GLN:CG	1:G:10:ASN:HD21	1.91	0.81
1:E:105:TYR:CE1	1:E:135:ARG:HG2	2.15	0.81
1:C:105:TYR:CE1	1:C:135:ARG:HG2	2.17	0.80
1:E:7:CYS:O	1:E:10:ASN:N	2.14	0.80
2:F:152:VAL:O	2:F:155:CYS:HB2	1.82	0.80
2:F:42:GLU:OE1	2:F:47:ARG:NH2	2.15	0.79
2:D:26:GLN:HG3	2:D:27:LEU:N	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:169:THR:CG2	2:D:169:THR:O	2.30	0.79
1:C:4:LEU:HD12	1:C:4:LEU:O	1.83	0.78
2:H:147:CYS:SG	2:H:155:CYS:N	2.56	0.77
1:C:8:ILE:CD1	1:C:78:PHE:O	2.32	0.77
1:C:6:GLN:HE22	1:C:9:VAL:HG11	1.49	0.76
1:A:38:ALA:CB	1:A:45:MET:HG3	2.15	0.76
1:E:144:SER:HB2	1:E:145:LEU:CD1	2.17	0.74
1:C:6:GLN:O	1:C:9:VAL:CG1	2.32	0.74
2:F:151:SER:O	2:F:154:SER:OG	2.05	0.74
2:D:169:THR:HG22	2:D:169:THR:O	1.88	0.73
1:A:60:SER:HB2	1:A:61:TRP:HD1	1.53	0.73
1:E:45:MET:CA	1:E:45:MET:HE2	2.16	0.72
1:C:4:LEU:CG	1:C:4:LEU:O	2.37	0.72
2:F:25:THR:HB	3:F:212:HOH:O	1.89	0.71
1:C:6:GLN:HA	1:C:6:GLN:NE2	2.05	0.71
2:D:22:CYS:SG	2:D:167:CYS:C	2.67	0.71
1:E:41:LEU:HD23	1:E:41:LEU:N	2.04	0.71
1:E:45:MET:CE	1:E:46:PRO:N	2.51	0.71
1:G:105:TYR:CE1	1:G:135:ARG:HG2	2.26	0.71
1:E:7:CYS:O	1:E:8:ILE:C	2.30	0.70
2:B:157:LYS:HE3	2:D:157:LYS:HE3	1.73	0.70
1:C:11:ALA:CB	1:C:41:LEU:HD11	2.23	0.69
1:C:4:LEU:HG	1:C:4:LEU:O	1.90	0.69
1:G:45:MET:HE1	1:G:53:MET:HE2	1.74	0.69
1:C:4:LEU:O	1:C:4:LEU:CD1	2.40	0.69
1:A:131:ASN:O	1:A:135:ARG:HB2	1.91	0.69
2:D:115:SER:HB2	2:D:166:PHE:HD1	1.58	0.69
1:C:9:VAL:HG13	1:C:10:ASN:H	1.56	0.68
1:A:11:ALA:CB	1:A:41:LEU:HD21	2.23	0.68
2:F:164:ALA:N	2:F:165:PRO:HD2	2.09	0.68
1:C:6:GLN:CA	1:C:6:GLN:HE21	2.06	0.68
1:G:146:ALA:O	1:G:148:CYS:O	2.11	0.68
1:A:38:ALA:HB2	1:A:45:MET:HG3	1.76	0.67
1:C:9:VAL:CG1	1:C:10:ASN:H	2.06	0.67
1:E:144:SER:C	1:E:145:LEU:HG	2.15	0.67
1:G:45:MET:HE1	1:G:53:MET:CE	2.25	0.67
1:G:38:ALA:CB	1:G:45:MET:HG3	2.25	0.67
2:B:137:ASP:OD2	2:B:139:ASP:N	2.29	0.66
1:G:6:GLN:O	1:G:7:CYS:C	2.30	0.66
1:C:6:GLN:C	1:C:9:VAL:HG12	2.15	0.66
1:C:102:ARG:O	1:C:103:GLN:HB2	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:MET:HE3	1:E:46:PRO:CD	2.13	0.65
1:G:146:ALA:C	1:G:148:CYS:O	2.34	0.65
2:H:42:GLU:OE1	2:H:47:ARG:NH2	2.29	0.65
1:E:142:VAL:CG2	1:E:143:TYR:N	2.59	0.65
1:C:6:GLN:NE2	1:C:9:VAL:CG1	2.54	0.65
1:G:8:ILE:O	1:G:11:ALA:N	2.30	0.65
2:H:153:ASP:O	2:H:155:CYS:N	2.29	0.65
2:H:168:GLN:NE2	2:H:168:GLN:O	2.30	0.65
1:E:5:ASP:OD1	1:E:5:ASP:N	2.30	0.65
1:E:5:ASP:O	1:E:7:CYS:N	2.30	0.65
1:E:11:ALA:CB	1:E:41:LEU:HD21	2.27	0.65
2:B:161:ARG:CG	2:B:161:ARG:NH1	2.37	0.65
1:A:4:LEU:N	1:A:4:LEU:CD2	2.59	0.65
1:E:45:MET:HE2	1:E:45:MET:C	2.17	0.64
2:B:161:ARG:NH1	2:B:161:ARG:HG3	2.01	0.64
1:E:142:VAL:HG22	1:E:143:TYR:N	2.11	0.64
1:A:6:GLN:O	1:A:7:CYS:C	2.35	0.64
1:G:146:ALA:CB	1:G:148:CYS:O	2.46	0.64
1:A:11:ALA:HB2	1:A:41:LEU:CD2	2.28	0.64
2:B:22:CYS:O	2:B:22:CYS:SG	2.57	0.63
1:A:11:ALA:O	1:A:15:SER:HB2	2.00	0.62
1:C:6:GLN:HA	1:C:6:GLN:HE21	1.64	0.62
2:D:147:CYS:HA	2:D:155:CYS:HA	1.83	0.61
2:F:99:ARG:NH2	2:F:168:GLN:O	2.33	0.61
1:C:11:ALA:HB3	1:C:41:LEU:HD11	1.82	0.61
2:B:99:ARG:NH1	2:B:168:GLN:O	2.21	0.61
1:E:37:VAL:O	1:E:41:LEU:HG	2.01	0.60
2:F:133:ARG:HG3	2:F:147:CYS:SG	2.42	0.60
1:A:6:GLN:O	1:A:8:ILE:N	2.35	0.60
1:G:131:ASN:HB2	2:H:85:GLY:HA2	1.83	0.60
1:G:9:VAL:HG12	1:G:10:ASN:N	2.15	0.60
1:E:43:VAL:HG13	1:E:44:PRO:HD2	1.84	0.59
2:F:146:LYS:HB3	2:F:156:ALA:CB	2.33	0.59
1:G:112:SER:HA	3:H:206:HOH:O	2.02	0.59
1:E:5:ASP:O	1:E:6:GLN:C	2.41	0.59
2:H:167:CYS:O	2:H:168:GLN:CB	2.50	0.59
2:F:144:GLY:C	2:F:155:CYS:SG	2.81	0.59
1:A:105:TYR:CZ	1:A:135:ARG:HG2	2.37	0.59
1:A:105:TYR:CE1	1:A:135:ARG:HG2	2.38	0.58
2:H:36:PRO:O	2:H:37:ASN:CB	2.36	0.58
2:F:168:GLN:HG2	2:F:169:THR:N	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:153:ASP:O	2:H:154:SER:C	2.42	0.58
1:E:47:ARG:HG2	1:E:48:GLY:N	2.19	0.58
2:B:161:ARG:NH1	2:B:161:ARG:HG2	2.18	0.58
2:F:146:LYS:HB3	2:F:156:ALA:HB3	1.85	0.57
1:G:146:ALA:HB1	1:G:148:CYS:O	2.04	0.57
1:E:8:ILE:O	1:E:9:VAL:C	2.41	0.57
1:E:103:GLN:OE1	1:E:103:GLN:HA	2.04	0.57
1:C:43:VAL:HG13	1:C:143:TYR:CD2	2.40	0.57
1:A:6:GLN:C	1:A:6:GLN:HE21	2.07	0.57
2:F:144:GLY:O	2:F:145:GLN:HG2	2.04	0.56
1:A:5:ASP:N	1:A:5:ASP:OD1	2.38	0.56
2:B:161:ARG:HG2	2:B:161:ARG:HH11	1.67	0.56
1:C:14:ASN:HB2	1:C:40:GLU:OE1	2.05	0.56
2:H:167:CYS:O	2:H:168:GLN:HB3	2.05	0.56
2:B:45:HIS:HD2	3:B:210:HOH:O	1.88	0.56
1:C:45:MET:HE1	1:C:53:MET:HE2	1.87	0.56
1:A:131:ASN:ND2	2:B:85:GLY:HA2	2.16	0.56
1:C:8:ILE:HD12	1:C:78:PHE:O	2.04	0.56
2:D:24:PHE:CE1	2:D:102:LEU:HB2	2.41	0.56
1:E:40:GLU:C	1:E:41:LEU:HD23	2.25	0.55
1:E:101:TYR:OH	2:F:65:GLU:OE2	2.20	0.55
2:F:99:ARG:CZ	2:F:168:GLN:O	2.54	0.55
1:C:60:SER:HB2	1:C:61:TRP:HD1	1.71	0.55
1:E:11:ALA:HB2	1:E:41:LEU:HD21	1.88	0.55
2:F:145:GLN:O	2:F:146:LYS:HB2	2.07	0.55
2:H:151:SER:OG	2:H:153:ASP:OD1	2.23	0.55
2:H:148:SER:N	2:H:154:SER:HB2	2.19	0.55
1:C:131:ASN:O	1:C:135:ARG:HB2	2.06	0.55
1:G:105:TYR:CZ	1:G:135:ARG:HG2	2.41	0.55
1:G:8:ILE:O	1:G:9:VAL:C	2.46	0.54
1:G:131:ASN:O	1:G:135:ARG:HB2	2.07	0.54
1:A:8:ILE:CD1	1:A:78:PHE:O	2.56	0.54
2:H:32:GLN:OE1	2:H:47:ARG:NH1	2.41	0.54
1:C:105:TYR:CZ	1:C:135:ARG:HG2	2.43	0.53
1:C:35:GLN:NE2	1:C:46:PRO:O	2.39	0.53
2:F:146:LYS:CB	2:F:156:ALA:CB	2.85	0.53
1:C:144:SER:C	1:C:145:LEU:HG	2.28	0.53
1:E:131:ASN:O	1:E:135:ARG:HB2	2.10	0.52
2:B:148:SER:OG	2:B:154:SER:HB2	2.10	0.52
1:C:43:VAL:HG13	1:C:143:TYR:CE2	2.44	0.52
1:G:107:MET:HA	1:G:125:SER:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LEU:HD12	1:A:147:SER:CB	2.39	0.52
1:E:132:ARG:HG2	1:E:135:ARG:NH2	2.25	0.52
2:F:35:SER:HB2	2:F:38:MET:HB2	1.91	0.51
2:H:147:CYS:HA	2:H:155:CYS:HA	1.93	0.51
1:G:131:ASN:CB	2:H:85:GLY:HA2	2.41	0.51
1:G:54:VAL:HG11	1:G:85:LYS:HG3	1.93	0.51
1:E:60:SER:HB2	1:E:61:TRP:HD1	1.76	0.50
2:H:115:SER:HB2	2:H:166:PHE:HD1	1.76	0.50
2:D:168:GLN:NE2	2:D:169:THR:C	2.65	0.50
1:E:102:ARG:O	1:E:103:GLN:HB2	2.10	0.50
2:F:24:PHE:CE1	2:F:95:SER:HB3	2.46	0.50
1:E:95:VAL:HG13	1:E:106:PRO:HB2	1.94	0.50
2:D:36:PRO:O	2:D:37:ASN:HB2	2.12	0.50
2:B:147:CYS:HA	2:B:155:CYS:HA	1.93	0.50
1:E:45:MET:CE	1:E:45:MET:C	2.75	0.50
1:G:77:GLY:HA3	1:G:148:CYS:CB	2.41	0.50
1:C:148:CYS:O	1:C:149:SER:O	2.30	0.50
1:E:132:ARG:NH2	2:F:83:ASP:OD2	2.41	0.50
1:G:145:LEU:N	1:G:145:LEU:HD13	2.24	0.50
1:E:144:SER:C	1:E:145:LEU:HD12	2.29	0.50
1:C:43:VAL:CG1	1:C:143:TYR:CD2	2.95	0.50
2:F:146:LYS:O	2:F:156:ALA:N	2.42	0.49
1:C:38:ALA:CB	1:C:45:MET:HG3	2.42	0.49
2:B:84:GLY:C	2:B:85:GLY:O	2.48	0.49
1:A:35:GLN:NE2	1:A:46:PRO:O	2.39	0.49
1:C:45:MET:HE1	1:C:53:MET:CE	2.42	0.49
2:B:48:VAL:C	2:B:49:MET:HG2	2.31	0.49
2:H:164:ALA:O	2:H:167:CYS:O	2.30	0.49
1:G:43:VAL:HG12	1:G:44:PRO:N	2.26	0.49
1:A:54:VAL:HG11	1:A:85:LYS:HG3	1.95	0.49
2:F:147:CYS:HA	2:F:155:CYS:HA	1.94	0.48
1:G:8:ILE:O	1:G:11:ALA:HB3	2.13	0.48
2:F:164:ALA:N	2:F:165:PRO:CD	2.76	0.48
2:D:148:SER:OG	2:D:154:SER:HB2	2.13	0.48
2:B:137:ASP:OD2	2:B:139:ASP:HB2	2.13	0.48
2:H:146:LYS:O	2:H:155:CYS:HA	2.13	0.48
1:A:41:LEU:HD12	1:A:147:SER:HB3	1.95	0.48
2:D:147:CYS:SG	2:D:155:CYS:N	2.86	0.47
2:F:144:GLY:HA3	2:F:155:CYS:SG	2.54	0.47
1:G:6:GLN:O	1:G:8:ILE:N	2.47	0.47
2:H:168:GLN:NE2	2:H:168:GLN:C	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:ARG:HG3	2:B:167:CYS:HA	1.96	0.47
1:E:105:TYR:CZ	1:E:135:ARG:HG2	2.49	0.47
2:F:115:SER:HB2	2:F:166:PHE:HD1	1.79	0.47
1:C:105:TYR:HA	1:C:106:PRO:HD2	1.78	0.47
1:E:6:GLN:O	1:E:7:CYS:O	2.33	0.47
2:D:152:VAL:O	2:D:155:CYS:HB2	2.15	0.47
2:F:146:LYS:HD2	2:F:146:LYS:HA	1.40	0.47
1:A:11:ALA:CB	1:A:41:LEU:CD2	2.89	0.47
1:E:15:SER:HA	1:E:18:LYS:HD2	1.97	0.47
1:E:15:SER:HB3	1:E:36:SER:HB2	1.95	0.47
1:G:80:VAL:HB	1:G:95:VAL:HB	1.97	0.47
2:D:38:MET:HB3	2:D:49:MET:CE	2.45	0.46
1:G:60:SER:HB2	1:G:61:TRP:HD1	1.80	0.46
1:C:14:ASN:CB	1:C:40:GLU:OE1	2.63	0.46
1:C:101:TYR:N	1:C:105:TYR:O	2.44	0.46
1:E:107:MET:HA	1:E:125:SER:HA	1.97	0.46
1:C:45:MET:CE	1:C:53:MET:CE	2.94	0.46
2:B:49:MET:HE2	2:B:49:MET:HB3	1.83	0.46
1:G:77:GLY:HA3	1:G:148:CYS:HB3	1.98	0.46
2:B:152:VAL:O	2:B:155:CYS:HB2	2.15	0.46
2:B:84:GLY:HA3	2:B:87:TRP:CZ2	2.51	0.46
1:G:5:ASP:HA	1:G:148:CYS:SG	2.56	0.46
2:F:164:ALA:HB3	2:F:165:PRO:HD3	1.97	0.46
2:B:147:CYS:SG	2:B:155:CYS:N	2.88	0.45
1:C:148:CYS:O	1:C:149:SER:C	2.55	0.45
1:A:8:ILE:HD11	1:A:78:PHE:O	2.17	0.45
2:H:96:GLN:CG	2:H:97:ASP:N	2.60	0.45
1:E:7:CYS:O	1:E:10:ASN:HB2	2.17	0.45
1:E:80:VAL:HB	1:E:95:VAL:HB	1.98	0.45
2:B:42:GLU:OE1	2:B:47:ARG:NH2	2.49	0.45
1:G:8:ILE:HG22	1:G:9:VAL:N	2.32	0.45
1:C:144:SER:O	1:C:145:LEU:HG	2.15	0.45
2:B:84:GLY:HA3	2:B:87:TRP:CH2	2.52	0.45
1:C:6:GLN:HA	1:C:9:VAL:CG1	2.47	0.44
1:C:6:GLN:HE21	1:C:9:VAL:CG1	2.31	0.44
2:B:115:SER:HB2	2:B:166:PHE:HD1	1.82	0.44
2:F:100:ARG:HG3	2:F:167:CYS:CB	2.47	0.44
2:F:93:PHE:HB2	2:F:102:LEU:HB3	1.98	0.44
1:E:131:ASN:HD22	2:F:85:GLY:HA2	1.83	0.44
2:B:45:HIS:CD2	3:B:210:HOH:O	2.68	0.44
2:B:48:VAL:O	2:B:49:MET:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:141:LEU:HB2	2:D:163:LEU:HD21	2.00	0.44
2:D:100:ARG:HG3	2:D:167:CYS:HB2	1.99	0.44
1:G:4:LEU:HD12	1:G:4:LEU:O	2.18	0.44
1:C:148:CYS:C	1:C:149:SER:O	2.56	0.44
2:F:164:ALA:HB3	2:F:165:PRO:CD	2.48	0.43
1:C:15:SER:HB3	1:C:36:SER:HB2	2.00	0.43
1:C:6:GLN:CA	1:C:9:VAL:HG12	2.48	0.43
2:B:64:PRO:HB3	2:B:86:ILE:HG12	2.00	0.43
1:C:8:ILE:HD11	1:C:78:PHE:O	2.16	0.43
1:G:21:LEU:HA	1:G:21:LEU:HD22	1.86	0.43
1:E:38:ALA:CB	1:E:45:MET:HG2	2.49	0.43
2:D:49:MET:HB3	2:D:49:MET:HE2	1.73	0.43
1:G:45:MET:HE1	1:G:53:MET:HE3	1.99	0.43
1:C:9:VAL:O	1:C:12:CYS:HB2	2.19	0.42
2:F:142:ARG:HG2	2:F:160:LYS:HG2	2.00	0.42
1:A:53:MET:O	1:A:57:LEU:HG	2.18	0.42
2:B:146:LYS:HB2	2:B:156:ALA:HB3	2.01	0.42
2:B:29:ILE:HB	2:B:89:ARG:HG3	2.01	0.42
1:E:91:HIS:HD2	1:E:130:TRP:CH2	2.37	0.42
1:C:6:GLN:HA	1:C:9:VAL:HG12	2.01	0.42
2:D:168:GLN:HE21	2:D:169:THR:C	2.23	0.42
1:A:107:MET:HA	1:A:125:SER:HA	2.01	0.42
2:H:153:ASP:C	2:H:155:CYS:N	2.71	0.42
2:B:32:GLN:HG3	2:B:49:MET:HE1	2.01	0.42
1:G:6:GLN:C	1:G:8:ILE:N	2.68	0.42
1:C:45:MET:CE	1:C:53:MET:HE2	2.47	0.42
1:E:91:HIS:HD2	1:E:130:TRP:CZ2	2.37	0.42
2:D:169:THR:O	2:D:169:THR:HG23	2.14	0.42
1:G:104:LYS:HE3	1:G:104:LYS:HB2	1.78	0.41
1:A:6:GLN:C	1:A:8:ILE:N	2.70	0.41
1:A:5:ASP:O	1:A:6:GLN:C	2.59	0.41
2:H:144:GLY:C	2:H:155:CYS:SG	2.99	0.41
2:B:48:VAL:HG22	2:B:70:LEU:HD22	2.02	0.41
2:D:168:GLN:HE21	2:D:169:THR:H	1.68	0.41
1:E:144:SER:C	1:E:145:LEU:CD1	2.85	0.41
2:H:22:CYS:HB2	2:H:167:CYS:HB3	1.99	0.41
2:F:168:GLN:CG	2:F:169:THR:O	2.57	0.41
1:G:5:ASP:N	1:G:5:ASP:OD1	2.54	0.41
1:G:64:LEU:CD1	1:G:70:ALA:HA	2.51	0.41
1:E:6:GLN:O	1:E:7:CYS:C	2.59	0.41
2:B:93:PHE:HB2	2:B:102:LEU:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:ILE:HG12	1:E:148:CYS:SG	2.61	0.41
1:G:45:MET:CE	1:G:53:MET:HE3	2.51	0.41
1:G:113:ILE:HG12	1:G:113:ILE:H	1.61	0.41
2:D:84:GLY:C	2:D:85:GLY:O	2.57	0.41
2:F:146:LYS:O	2:F:156:ALA:HB2	2.21	0.41
2:D:140:GLY:HA2	2:D:163:LEU:HD12	2.03	0.41
1:E:104:LYS:HB2	1:E:104:LYS:HE2	1.28	0.40
1:E:47:ARG:HG2	1:E:48:GLY:H	1.86	0.40
1:G:130:TRP:CD2	1:G:138:LEU:HD21	2.56	0.40
1:C:54:VAL:HG11	1:C:85:LYS:HG3	2.02	0.40
2:H:26:GLN:HG2	2:H:27:LEU:N	2.35	0.40
1:E:29:ASN:OD1	1:E:32:GLY:N	2.52	0.40
1:C:102:ARG:C	1:C:104:LYS:H	2.24	0.40
1:C:104:LYS:HB2	1:C:104:LYS:HE3	1.77	0.40
1:G:43:VAL:CG1	1:G:44:PRO:N	2.85	0.40
1:G:15:SER:HB3	1:G:36:SER:HB2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:33:PHE:O	2:D:35:SER:OG[4_555]	2.12	0.08

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	144/162 (89%)	133 (92%)	11 (8%)	0	100 100
1	C	144/162 (89%)	134 (93%)	10 (7%)	0	100 100
1	E	144/162 (89%)	134 (93%)	8 (6%)	2 (1%)	14 35
1	G	144/162 (89%)	128 (89%)	16 (11%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	146/162 (90%)	142 (97%)	4 (3%)	0	100 100
2	D	146/162 (90%)	142 (97%)	4 (3%)	0	100 100
2	F	146/162 (90%)	138 (94%)	8 (6%)	0	100 100
2	H	146/162 (90%)	138 (94%)	7 (5%)	1 (1%)	26 55
All	All	1160/1296 (90%)	1089 (94%)	68 (6%)	3 (0%)	46 75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	7	CYS
1	E	8	ILE
2	H	146	LYS

5.3.2 Protein sidechains (i)

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	113/128 (88%)	102 (90%)	11 (10%)	10 23
1	C	113/128 (88%)	95 (84%)	18 (16%)	3 8
1	E	113/128 (88%)	94 (83%)	19 (17%)	2 6
1	G	113/128 (88%)	100 (88%)	13 (12%)	7 16
2	B	127/139 (91%)	114 (90%)	13 (10%)	9 21
2	D	127/139 (91%)	113 (89%)	14 (11%)	8 18
2	F	127/139 (91%)	118 (93%)	9 (7%)	18 41
2	H	127/139 (91%)	114 (90%)	13 (10%)	9 21
All	All	960/1068 (90%)	850 (88%)	110 (12%)	7 16

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU

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Mol	Chain	Res	Type
1	A	6	GLN
1	A	13	LYS
1	A	15	SER
1	A	21	LEU
1	A	31	SER
1	A	41	LEU
1	A	60	SER
1	A	62	THR
1	A	88	THR
1	A	113	ILE
2	B	23	THR
2	B	26	GLN
2	B	27	LEU
2	B	49	MET
2	B	51	SER
2	B	78	ASP
2	B	83	ASP
2	B	138	LYS
2	B	145	GLN
2	B	147	CYS
2	B	151	SER
2	B	161	ARG
2	B	168	GLN
1	C	4	LEU
1	C	6	GLN
1	C	7	CYS
1	C	12	CYS
1	C	13	LYS
1	C	21	LEU
1	C	24	THR
1	C	31	SER
1	C	47	ARG
1	C	60	SER
1	C	62	THR
1	C	88	THR
1	C	103	GLN
1	C	107	MET
1	C	113	ILE
1	C	123	LEU
1	C	147	SER
1	C	149	SER
2	D	23	THR

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Mol	Chain	Res	Type
2	D	26	GLN
2	D	28	GLU
2	D	35	SER
2	D	78	ASP
2	D	83	ASP
2	D	96	GLN
2	D	137	ASP
2	D	147	CYS
2	D	151	SER
2	D	160	LYS
2	D	167	CYS
2	D	168	GLN
2	D	169	THR
1	E	4	LEU
1	E	6	GLN
1	E	7	CYS
1	E	8	ILE
1	E	21	LEU
1	E	31	SER
1	E	41	LEU
1	E	45	MET
1	E	47	ARG
1	E	60	SER
1	E	62	THR
1	E	88	THR
1	E	102	ARG
1	E	104	LYS
1	E	113	ILE
1	E	132	ARG
1	E	145	LEU
1	E	147	SER
1	E	149	SER
2	F	23	THR
2	F	35	SER
2	F	78	ASP
2	F	137	ASP
2	F	146	LYS
2	F	147	CYS
2	F	151	SER
2	F	155	CYS
2	F	169	THR
1	G	4	LEU

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Mol	Chain	Res	Type
1	G	6	GLN
1	G	8	ILE
1	G	9	VAL
1	G	21	LEU
1	G	60	SER
1	G	62	THR
1	G	88	THR
1	G	113	ILE
1	G	145	LEU
1	G	147	SER
1	G	148	CYS
1	G	149	SER
2	H	23	THR
2	H	35	SER
2	H	51	SER
2	H	78	ASP
2	H	137	ASP
2	H	138	LYS
2	H	146	LYS
2	H	147	CYS
2	H	148	SER
2	H	151	SER
2	H	157	LYS
2	H	168	GLN
2	H	169	THR

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

Mol	Chain	Res	Type
1	A	6	GLN
2	B	45	HIS
1	C	6	GLN
1	C	14	ASN
2	D	132	GLN
2	D	168	GLN
1	E	6	GLN
1	G	10	ASN
2	H	37	ASN
2	H	168	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 95^{th} 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	146/162 (90%)	-0.09	2 (1%)	78	77	46, 80, 124, 149	1 (0%)
1	C	146/162 (90%)	0.05	5 (3%)	49	49	55, 91, 139, 168	0
1	E	146/162 (90%)	-0.02	4 (2%)	58	58	57, 97, 140, 175	0
1	G	146/162 (90%)	0.25	12 (8%)	14	11	63, 102, 149, 175	0
2	B	148/162 (91%)	-0.27	1 (0%)	89	90	42, 63, 98, 160	0
2	D	148/162 (91%)	-0.33	1 (0%)	89	90	43, 63, 92, 153	0
2	F	148/162 (91%)	-0.09	4 (2%)	58	58	45, 69, 121, 146	0
2	H	148/162 (91%)	-0.09	3 (2%)	68	69	44, 68, 134, 168	0
All	All	1176/1296 (90%)	-0.08	32 (2%)	58	58	42, 78, 137, 175	1 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	149	SER	5.4
1	E	23	GLY	4.9
1	C	4	LEU	4.1
1	C	147	SER	4.0
2	H	156	ALA	3.8
1	G	147	SER	3.6
1	A	4	LEU	3.6
1	A	147	SER	3.4
2	B	169	THR	3.4
1	G	23	GLY	3.0
1	C	48	GLY	2.6
1	G	47	ARG	2.6
2	F	33	PHE	2.6
1	G	143	TYR	2.5
1	G	97	SER	2.5
2	F	157	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	21	LEU	2.4
2	H	158	ILE	2.4
1	E	22	ALA	2.4
1	G	93	ALA	2.4
1	G	110	CYS	2.4
1	G	25	PRO	2.3
1	E	14	ASN	2.3
2	H	157	LYS	2.3
1	G	16	TRP	2.3
1	C	148	CYS	2.2
1	G	95	VAL	2.2
2	F	169	THR	2.2
1	E	101	TYR	2.1
2	F	34	GLY	2.1
1	G	24	THR	2.0
2	D	56	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.