Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:53 am BST

PDB ID	:	4GEJ
Title	:	N-terminal domain of VDUP-1
Authors	:	Polekhina, G.; Kok, S.F.; Ascher, D.B.; Waltham, M.
Deposited on	:	2012-08-02
Resolution	:	2.90 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 following versions of software and data (see references ①) were used in the production of this report:

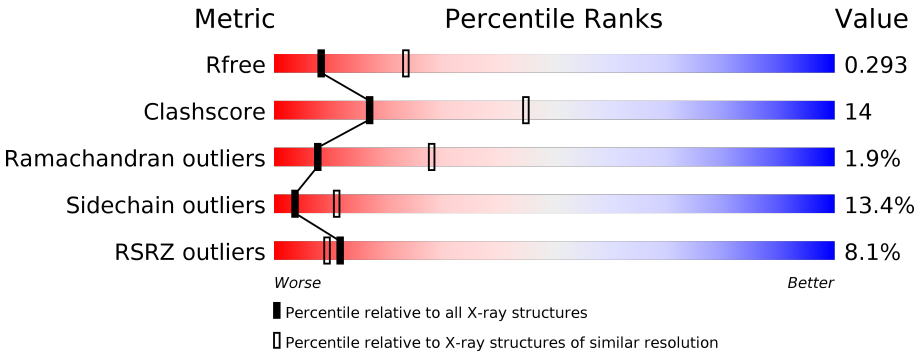
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on 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 <=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	150	18% 60% 21% 8% 11%
1	B	150	% 59% 24% 7% • 9%
1	C	150	3% 61% 23% 7% 9%
1	D	150	9% 60% 27% • 13%
1	E	150	3% 57% 25% 11% • 5%
1	F	150	23% 51% 29% 10% • 9%

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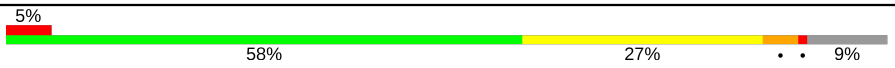
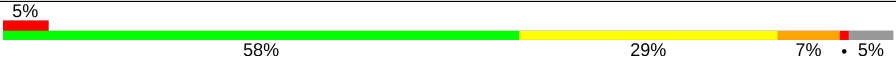
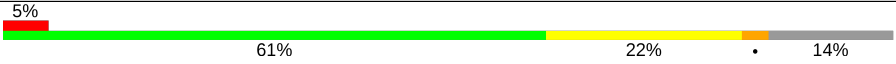
Mol	Chain	Length	Quality of chain
1	G	150	
1	H	150	
1	I	150	
1	J	150	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10938 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 Thioredoxin-interacting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	134	Total	C	N	O	S	0	0	0
			1077	693	179	201	4			
1	B	136	Total	C	N	O	S	0	0	0
			1094	702	181	207	4			
1	C	136	Total	C	N	O	S	0	0	0
			1094	702	181	207	4			
1	D	131	Total	C	N	O	S	0	0	0
			1049	670	174	201	4			
1	E	142	Total	C	N	O	S	0	0	0
			1138	727	189	218	4			
1	F	136	Total	C	N	O	S	0	0	0
			1094	702	181	207	4			
1	G	136	Total	C	N	O	S	0	0	0
			1094	702	181	207	4			
1	H	139	Total	C	N	O	S	0	0	0
			1116	713	184	215	4			
1	I	142	Total	C	N	O	S	0	0	0
			1138	727	189	218	4			
1	J	129	Total	C	N	O	S	0	0	0
			1039	665	172	198	4			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP Q9H3M7
A	1	ASN	-	EXPRESSION TAG	UNP Q9H3M7
A	26	ARG	LYS	SEE REMARK 999	UNP Q9H3M7
A	36	SER	CYS	ENGINEERED MUTATION	UNP Q9H3M7
A	49	SER	CYS	ENGINEERED MUTATION	UNP Q9H3M7
A	120	SER	CYS	ENGINEERED MUTATION	UNP Q9H3M7
B	0	SER	-	EXPRESSION TAG	UNP Q9H3M7
B	1	ASN	-	EXPRESSION TAG	UNP Q9H3M7
B	26	ARG	LYS	SEE REMARK 999	UNP Q9H3M7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	36	SER	CYS	ENGINEERED MUTATION	UNP Q9H3M7
B	49	SER	CYS	ENGINEERED MUTATION	UNP Q9H3M7
B	120	SER	CYS	ENGINEERED MUTATION	UNP Q9H3M7
C	0	SER	-	EXPRESSION TAG	UNP Q9H3M7
C	1	ASN	-	EXPRESSION TAG	UNP Q9H3M7
C	26	ARG	LYS	SEE REMARK 999	UNP Q9H3M7
C	36	SER	CYS	ENGINEERED MUTATION	UNP Q9H3M7
C	49	SER	CYS	ENGINEERED MUTATION	UNP Q9H3M7
C	120	SER	CYS	ENGINEERED MUTATION	UNP Q9H3M7
D	0	SER	-	EXPRESSION TAG	UNP Q9H3M7
D	1	ASN	-	EXPRESSION TAG	UNP Q9H3M7
D	26	ARG	LYS	SEE REMARK 999	UNP Q9H3M7
D	36	SER	CYS	ENGINEERED MUTATION	UNP Q9H3M7
D	49	SER	CYS	ENGINEERED MUTATION	UNP Q9H3M7
D	120	SER	CYS	ENGINEERED MUTATION	UNP Q9H3M7
E	0	SER	-	EXPRESSION TAG	UNP Q9H3M7
E	1	ASN	-	EXPRESSION TAG	UNP Q9H3M7
E	26	ARG	LYS	SEE REMARK 999	UNP Q9H3M7
E	36	SER	CYS	ENGINEERED MUTATION	UNP Q9H3M7
E	49	SER	CYS	ENGINEERED MUTATION	UNP Q9H3M7
E	120	SER	CYS	ENGINEERED MUTATION	UNP Q9H3M7
F	0	SER	-	EXPRESSION TAG	UNP Q9H3M7
F	1	ASN	-	EXPRESSION TAG	UNP Q9H3M7
F	26	ARG	LYS	SEE REMARK 999	UNP Q9H3M7
F	36	SER	CYS	ENGINEERED MUTATION	UNP Q9H3M7
F	49	SER	CYS	ENGINEERED MUTATION	UNP Q9H3M7
F	120	SER	CYS	ENGINEERED MUTATION	UNP Q9H3M7
G	0	SER	-	EXPRESSION TAG	UNP Q9H3M7
G	1	ASN	-	EXPRESSION TAG	UNP Q9H3M7
G	26	ARG	LYS	SEE REMARK 999	UNP Q9H3M7
G	36	SER	CYS	ENGINEERED MUTATION	UNP Q9H3M7
G	49	SER	CYS	ENGINEERED MUTATION	UNP Q9H3M7
G	120	SER	CYS	ENGINEERED MUTATION	UNP Q9H3M7
H	0	SER	-	EXPRESSION TAG	UNP Q9H3M7
H	1	ASN	-	EXPRESSION TAG	UNP Q9H3M7
H	26	ARG	LYS	SEE REMARK 999	UNP Q9H3M7
H	36	SER	CYS	ENGINEERED MUTATION	UNP Q9H3M7
H	49	SER	CYS	ENGINEERED MUTATION	UNP Q9H3M7
H	120	SER	CYS	ENGINEERED MUTATION	UNP Q9H3M7
I	0	SER	-	EXPRESSION TAG	UNP Q9H3M7
I	1	ASN	-	EXPRESSION TAG	UNP Q9H3M7
I	26	ARG	LYS	SEE REMARK 999	UNP Q9H3M7

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Chain	Residue	Modelled	Actual	Comment	Reference
I	36	SER	CYS	ENGINEERED MUTATION	UNP Q9H3M7
I	49	SER	CYS	ENGINEERED MUTATION	UNP Q9H3M7
I	120	SER	CYS	ENGINEERED MUTATION	UNP Q9H3M7
J	0	SER	-	EXPRESSION TAG	UNP Q9H3M7
J	1	ASN	-	EXPRESSION TAG	UNP Q9H3M7
J	26	ARG	LYS	SEE REMARK 999	UNP Q9H3M7
J	36	SER	CYS	ENGINEERED MUTATION	UNP Q9H3M7
J	49	SER	CYS	ENGINEERED MUTATION	UNP Q9H3M7
J	120	SER	CYS	ENGINEERED MUTATION	UNP Q9H3M7

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

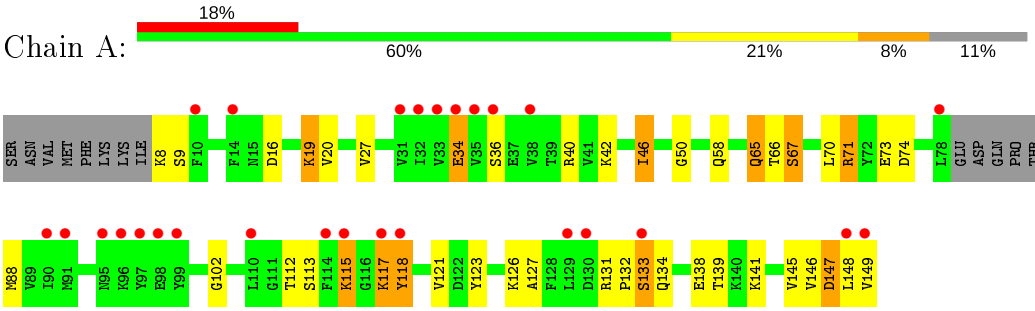
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total Ca 1 1	0	0
2	I	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0

3 Residue-property plots

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

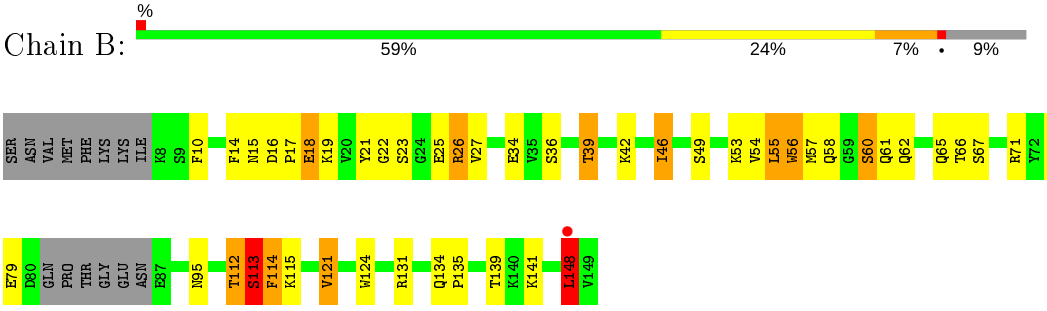
- Molecule 1: Thioredoxin-interacting protein

Chain A:



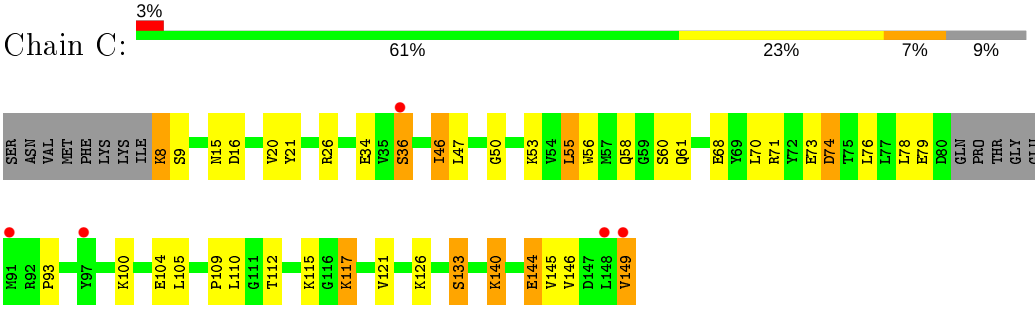
- Molecule 1: Thioredoxin-interacting protein

Chain B:



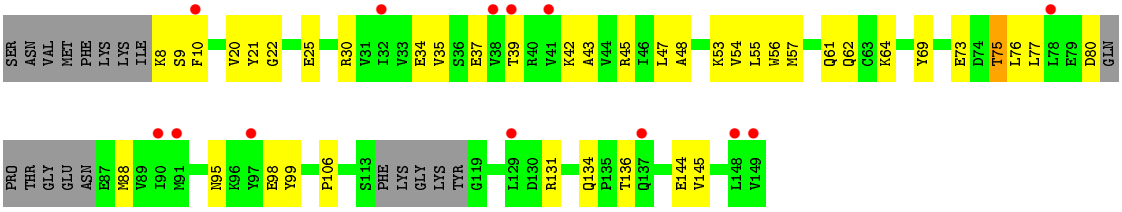
- Molecule 1: Thioredoxin-interacting protein

Chain C:



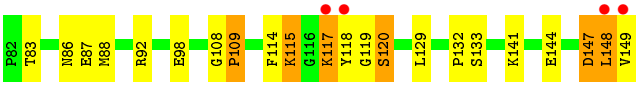
- Molecule 1: Thioredoxin-interacting protein

Chain D:



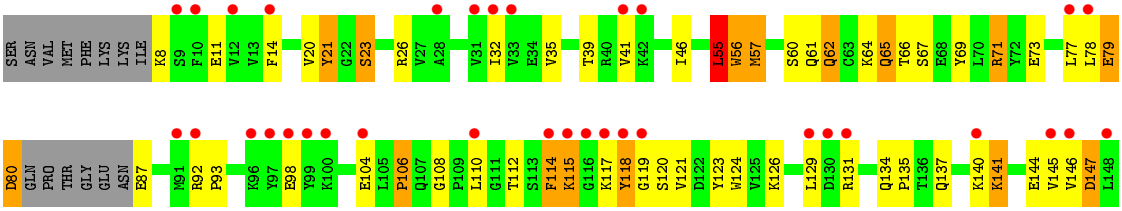
• Molecule 1: Thioredoxin-interacting protein

Chain E:



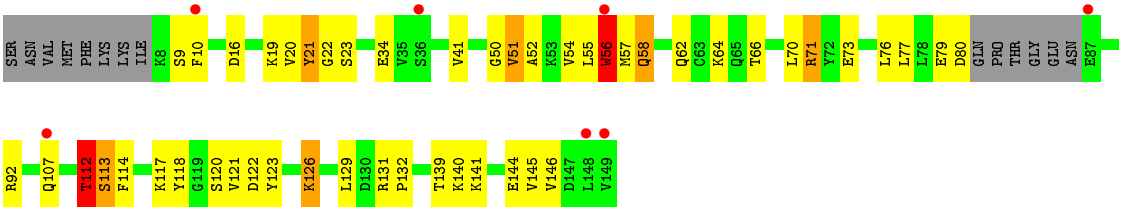
• Molecule 1: Thioredoxin-interacting protein

Chain F:



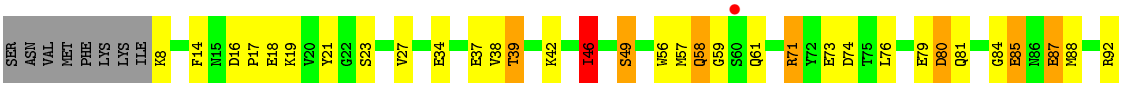
• Molecule 1: Thioredoxin-interacting protein

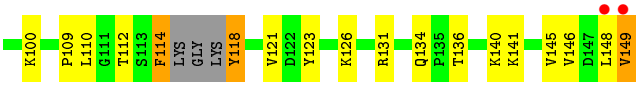
Chain G:



• Molecule 1: Thioredoxin-interacting protein

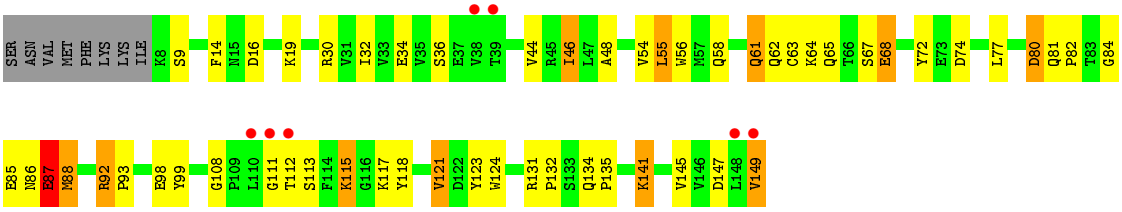
Chain H:





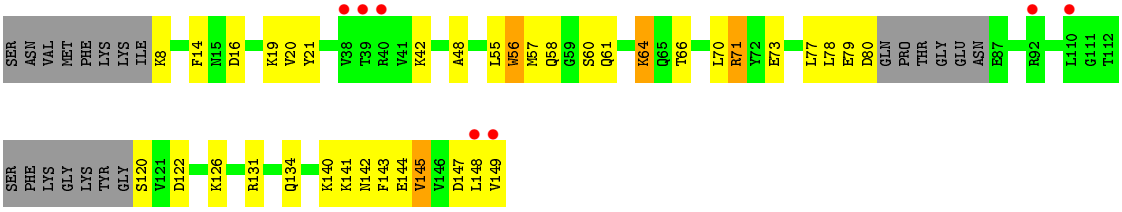
• Molecule 1: Thioredoxin-interacting protein

Chain I:



• Molecule 1: Thioredoxin-interacting protein

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	79.74Å 178.81Å 81.89Å 90.00° 113.32° 90.00°	Depositor
Resolution (Å)	46.00 – 2.90 46.71 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.00-2.90) 99.4 (46.71-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.212 , 0.294 0.220 , 0.293	Depositor DCC
R_{free} test set	2320 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	74.7	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 57.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10938	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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, 0.333 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: CA

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	0.64	0/1099	0.78	0/1479
1	B	0.79	1/1116 (0.1%)	1.02	3/1502 (0.2%)
1	C	0.75	1/1116 (0.1%)	0.93	3/1502 (0.2%)
1	D	0.63	0/1068	0.80	0/1438
1	E	0.81	1/1162 (0.1%)	1.05	7/1567 (0.4%)
1	F	0.66	2/1116 (0.2%)	0.78	2/1502 (0.1%)
1	G	0.70	0/1116	0.89	3/1502 (0.2%)
1	H	0.70	0/1139	0.91	1/1537 (0.1%)
1	I	0.68	2/1162 (0.2%)	0.84	2/1567 (0.1%)
1	J	0.61	1/1058 (0.1%)	0.78	1/1425 (0.1%)
All	All	0.70	8/11152 (0.1%)	0.88	22/15021 (0.1%)

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	C	0	1
1	E	0	2
1	G	0	1
1	I	0	1
All	All	0	5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	56	TRP	CD2-CE2	7.80	1.50	1.41
1	C	56	TRP	CD2-CE2	7.38	1.50	1.41
1	E	56	TRP	CD2-CE2	7.01	1.49	1.41
1	F	56	TRP	CD2-CE2	5.74	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	56	TRP	CD2-CE2	5.63	1.48	1.41
1	F	21	TYR	CG-CD2	5.53	1.46	1.39
1	J	56	TRP	CD2-CE2	5.52	1.48	1.41
1	I	124	TRP	CD2-CE2	5.09	1.47	1.41

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	74	ASP	CB-CG-OD1	9.41	126.77	118.30
1	B	55	LEU	CA-CB-CG	8.93	135.83	115.30
1	H	46	ILE	CG1-CB-CG2	-8.13	93.52	111.40
1	C	55	LEU	CA-CB-CG	8.05	133.81	115.30
1	B	55	LEU	CB-CG-CD2	-7.88	97.60	111.00
1	E	74	ASP	CB-CG-OD2	-7.69	111.38	118.30
1	J	77	LEU	CA-CB-CG	6.06	129.23	115.30
1	E	46	ILE	CG1-CB-CG2	-6.05	98.08	111.40
1	E	45	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	F	55	LEU	CA-CB-CG	5.99	129.07	115.30
1	C	74	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	I	55	LEU	CB-CG-CD2	5.67	120.64	111.00
1	E	55	LEU	CB-CG-CD1	5.60	120.53	111.00
1	E	87	GLU	N-CA-C	-5.48	96.21	111.00
1	F	55	LEU	CB-CG-CD1	5.41	120.19	111.00
1	G	66	THR	N-CA-C	-5.22	96.91	111.00
1	G	56	TRP	N-CA-C	5.22	125.09	111.00
1	C	74	ASP	CB-CG-OD1	5.16	122.95	118.30
1	E	77	LEU	CA-CB-CG	5.15	127.15	115.30
1	I	74	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	B	148	LEU	CA-CB-CG	5.03	126.87	115.30
1	G	51	VAL	CB-CA-C	-5.00	101.89	111.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	15	ASN	Peptide
1	E	79	GLU	Peptide
1	E	80	ASP	Peptide
1	G	56	TRP	Peptide
1	I	85	GLU	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	1077	0	1080	30	0
1	B	1094	0	1090	40	0
1	C	1094	0	1090	19	0
1	D	1049	0	1042	18	0
1	E	1138	0	1128	44	0
1	F	1094	0	1090	45	0
1	G	1094	0	1090	41	0
1	H	1116	0	1098	35	0
1	I	1138	0	1128	42	0
1	J	1039	0	1034	17	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
All	All	10938	0	10870	305	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 14.

All (305) 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:61:GLN:NE2	1:F:56:TRP:HH2	1.34	1.23
1:E:61:GLN:NE2	1:F:56:TRP:CH2	2.19	1.09
1:A:65:GLN:HE22	1:B:60:SER:HB2	0.94	1.08
1:A:65:GLN:NE2	1:B:60:SER:HB2	1.74	1.00
1:B:39:THR:HG21	1:B:131:ARG:HH11	1.31	0.95
1:A:65:GLN:HE22	1:B:60:SER:CB	1.81	0.94
1:I:58:GLN:O	1:I:61:GLN:HB2	1.70	0.91
1:A:147:ASP:HB3	1:A:149:VAL:HG22	1.51	0.91
1:I:55:LEU:HD11	1:I:62:GLN:HB3	1.52	0.88
1:B:39:THR:HG21	1:B:131:ARG:NH1	1.88	0.87
1:B:39:THR:CG2	1:B:131:ARG:HH11	1.88	0.86
1:E:61:GLN:HE22	1:F:56:TRP:HH2	0.86	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:112:THR:H	1:G:121:VAL:HG21	1.37	0.85
1:A:8:LYS:HB3	1:A:34:GLU:O	1.77	0.84
1:G:9:SER:HB3	1:G:34:GLU:HB2	1.58	0.84
1:E:58:GLN:O	1:E:61:GLN:HG3	1.79	0.82
1:I:81:GLN:NE2	1:I:87:GLU:HB3	1.94	0.82
1:I:65:GLN:HG3	1:J:61:GLN:HG2	1.62	0.82
1:B:61:GLN:OE1	1:C:117:LYS:HE2	1.81	0.80
1:D:8:LYS:HB3	1:D:35:VAL:HA	1.61	0.80
1:F:114:PHE:HB3	1:F:119:GLY:HA3	1.64	0.80
1:I:65:GLN:CG	1:J:61:GLN:HG2	2.13	0.79
1:H:56:TRP:HE1	1:H:58:GLN:HE22	1.32	0.78
1:H:118:TYR:CD2	1:H:118:TYR:N	2.52	0.76
1:E:147:ASP:HB3	1:E:149:VAL:HG22	1.69	0.75
1:I:82:PRO:C	1:I:84:GLY:H	1.90	0.75
1:J:14:PHE:HE1	1:J:141:LYS:HG2	1.50	0.75
1:G:50:GLY:HA2	1:G:122:ASP:O	1.87	0.75
1:F:39:THR:CG2	1:F:131:ARG:HH11	2.01	0.73
1:G:112:THR:CG2	1:G:113:SER:HB2	2.19	0.73
1:G:64:LYS:HB2	1:G:64:LYS:NZ	2.04	0.73
1:F:32:ILE:HG12	1:F:98:GLU:HG2	1.71	0.72
1:I:80:ASP:OD1	1:I:80:ASP:N	2.21	0.72
1:B:73:GLU:HB3	1:D:73:GLU:HB3	1.71	0.71
1:E:132:PRO:O	1:E:133:SER:HB2	1.88	0.71
1:H:126:LYS:HE2	1:H:140:LYS:HD2	1.72	0.71
1:H:118:TYR:HD2	1:H:118:TYR:N	1.88	0.70
1:F:65:GLN:HG3	1:F:65:GLN:O	1.89	0.70
1:I:67:SER:O	1:I:68:GLU:HB3	1.92	0.70
1:I:14:PHE:CE1	1:I:141:LYS:HG2	2.27	0.70
1:E:119:GLY:HA2	1:E:120:SER:CB	2.23	0.69
1:A:65:GLN:NE2	1:B:60:SER:CB	2.48	0.69
1:H:46:ILE:HG22	1:H:74:ASP:O	1.93	0.68
1:F:20:VAL:HG22	1:F:144:GLU:HB2	1.76	0.68
1:G:114:PHE:HD1	1:G:144:GLU:OE1	1.76	0.68
1:J:20:VAL:HG13	1:J:144:GLU:HB2	1.74	0.68
1:F:115:LYS:NZ	1:G:118:TYR:OH	2.27	0.68
1:I:115:LYS:O	1:I:118:TYR:HD2	1.77	0.67
1:E:56:TRP:HH2	1:F:61:GLN:HG3	1.59	0.67
1:B:112:THR:O	1:B:113:SER:HB2	1.94	0.66
1:I:14:PHE:HE1	1:I:141:LYS:HG2	1.60	0.66
1:F:65:GLN:C	1:F:65:GLN:HE21	1.98	0.66
1:G:64:LYS:HB2	1:G:64:LYS:HZ2	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:59:GLY:C	1:H:61:GLN:H	2.00	0.65
1:B:61:GLN:OE1	1:C:117:LYS:CE	2.43	0.65
1:I:81:GLN:HG2	1:I:82:PRO:CD	2.27	0.65
1:A:16:ASP:HB3	1:A:19:LYS:HB3	1.79	0.65
1:A:87:GLU:HB2	1:F:26:ARG:HH22	1.62	0.65
1:E:20:VAL:HG22	1:E:144:GLU:HB2	1.79	0.64
1:A:71:ARG:NH2	1:A:73:GLU:OE1	2.31	0.64
1:B:71:ARG:NH2	1:B:73:GLU:OE1	2.30	0.64
1:H:56:TRP:HE1	1:H:58:GLN:NE2	1.95	0.64
1:D:20:VAL:HG22	1:D:144:GLU:HB2	1.80	0.64
1:G:112:THR:HG23	1:G:113:SER:HB2	1.79	0.64
1:B:112:THR:HG23	1:B:121:VAL:CG2	2.27	0.63
1:H:42:LYS:HE2	1:H:88:MET:HE1	1.79	0.63
1:E:38:VAL:HG22	1:E:92:ARG:HG2	1.80	0.63
1:E:119:GLY:CA	1:E:120:SER:HB3	2.30	0.62
1:E:58:GLN:O	1:E:61:GLN:CG	2.47	0.62
1:I:44:VAL:HG21	1:I:99:TYR:CE1	2.36	0.61
1:G:112:THR:N	1:G:121:VAL:HG21	2.11	0.61
1:E:8:LYS:HG2	1:E:9:SER:N	2.12	0.61
1:F:112:THR:HA	1:F:121:VAL:HG21	1.81	0.61
1:E:119:GLY:CA	1:E:120:SER:CB	2.79	0.61
1:J:126:LYS:HG2	1:J:140:LYS:HB2	1.83	0.61
1:A:127:ALA:HB3	1:A:139:THR:HG22	1.82	0.60
1:I:82:PRO:C	1:I:84:GLY:N	2.54	0.60
1:F:69:TYR:O	1:F:106:PRO:HG3	2.02	0.60
1:I:81:GLN:HE22	1:I:87:GLU:HB3	1.62	0.59
1:F:134:GLN:OE1	1:F:135:PRO:HD2	2.03	0.59
1:B:112:THR:HG23	1:B:121:VAL:HG21	1.84	0.58
1:F:8:LYS:HB3	1:F:35:VAL:HA	1.85	0.58
1:H:14:PHE:HE1	1:H:141:LYS:HG2	1.68	0.58
1:B:16:ASP:HB2	1:B:19:LYS:HB2	1.86	0.58
1:A:126:LYS:HD3	1:A:138:GLU:OE1	2.02	0.58
1:F:39:THR:HG23	1:F:131:ARG:HH11	1.69	0.58
1:D:45:ARG:HG3	1:D:75:THR:HG23	1.87	0.57
1:H:134:GLN:OE1	1:H:134:GLN:HA	2.04	0.57
1:F:78:LEU:O	1:F:80:ASP:N	2.34	0.57
1:B:39:THR:CG2	1:B:131:ARG:NH1	2.55	0.57
1:C:36:SER:C	1:C:93:PRO:HG3	2.25	0.57
1:E:30:ARG:NH1	1:E:98:GLU:OE1	2.35	0.57
1:H:92:ARG:HG3	1:H:92:ARG:HH11	1.70	0.56
1:G:126:LYS:HE2	1:G:140:LYS:HD2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:21:TYR:O	1:J:145:VAL:HA	2.05	0.56
1:H:46:ILE:HG21	1:H:76:LEU:HD21	1.87	0.56
1:J:78:LEU:O	1:J:80:ASP:N	2.37	0.56
1:B:54:VAL:HG12	1:B:65:GLN:HB3	1.88	0.55
1:F:26:ARG:HD2	1:F:104:GLU:HG2	1.87	0.55
1:B:10:PHE:CE2	1:B:139:THR:HG22	2.42	0.55
1:B:10:PHE:CD2	1:B:139:THR:HG22	2.42	0.55
1:F:23:SER:OG	1:F:108:GLY:O	2.25	0.55
1:G:21:TYR:CD1	1:G:21:TYR:N	2.74	0.55
1:G:20:VAL:HG22	1:G:144:GLU:HB2	1.89	0.54
1:G:121:VAL:HG11	1:G:123:TYR:CE1	2.42	0.54
1:G:16:ASP:HB3	1:G:19:LYS:HB2	1.89	0.54
1:C:50:GLY:HA3	1:C:70:LEU:HB3	1.89	0.54
1:F:65:GLN:HE21	1:F:66:THR:N	2.05	0.54
1:E:46:ILE:HG22	1:E:74:ASP:O	2.08	0.54
1:F:57:MET:HG2	1:F:62:GLN:HG2	1.88	0.53
1:I:16:ASP:O	1:I:19:LYS:HB2	2.08	0.53
1:D:34:GLU:HG2	1:D:95:ASN:O	2.08	0.53
1:E:13:VAL:HG21	1:E:32:ILE:HD12	1.91	0.53
1:E:119:GLY:HA2	1:E:120:SER:HB2	1.90	0.53
1:H:23:SER:HA	1:H:110:LEU:HD11	1.91	0.53
1:E:19:LYS:HE2	1:E:25:GLU:OE1	2.10	0.53
1:I:84:GLY:C	1:I:86:ASN:H	2.12	0.52
1:B:34:GLU:HG2	1:B:95:ASN:O	2.09	0.52
1:D:22:GLY:O	1:D:25:GLU:HB2	2.09	0.52
1:I:123:TYR:CE1	1:I:145:VAL:HG21	2.44	0.52
1:A:149:VAL:OXT	1:A:149:VAL:HG23	2.10	0.52
1:I:36:SER:O	1:I:93:PRO:HG3	2.10	0.52
1:G:112:THR:HG22	1:G:113:SER:CB	2.39	0.52
1:E:26:ARG:NH2	1:H:84:GLY:O	2.43	0.52
1:B:49:SER:HB2	1:B:124:TRP:CH2	2.46	0.51
1:E:14:PHE:HE1	1:E:141:LYS:HG2	1.75	0.51
1:E:71:ARG:NH2	1:E:73:GLU:OE1	2.44	0.51
1:B:21:TYR:CD2	1:B:27:VAL:HG22	2.46	0.51
1:A:131:ARG:HB2	1:A:134:GLN:HB2	1.92	0.51
1:E:16:ASP:CG	1:E:19:LYS:HB2	2.29	0.51
1:F:129:LEU:HB3	1:F:137:GLN:HB3	1.91	0.51
1:G:112:THR:HG22	1:G:113:SER:HB2	1.89	0.51
1:F:39:THR:HG23	1:F:131:ARG:NH1	2.26	0.50
1:G:10:PHE:CE2	1:G:139:THR:HG22	2.46	0.50
1:G:71:ARG:NH2	1:G:73:GLU:OE1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:16:ASP:CB	1:E:19:LYS:HB2	2.42	0.50
1:E:16:ASP:HB3	1:E:19:LYS:HB2	1.93	0.50
1:I:65:GLN:HG2	1:J:61:GLN:HG2	1.91	0.50
1:H:42:LYS:HG3	1:H:88:MET:HE2	1.93	0.50
1:D:69:TYR:O	1:D:106:PRO:HG3	2.12	0.50
1:I:81:GLN:HG2	1:I:82:PRO:HD3	1.92	0.50
1:E:42:LYS:O	1:E:43:ALA:HB2	2.12	0.50
1:G:54:VAL:HG22	1:G:54:VAL:O	2.12	0.49
1:H:17:PRO:HD2	1:H:18:GLU:H	1.77	0.49
1:A:132:PRO:O	1:A:133:SER:HB2	2.13	0.49
1:A:73:GLU:HB2	1:F:73:GLU:HB3	1.95	0.49
1:G:64:LYS:CB	1:G:64:LYS:NZ	2.74	0.49
1:I:111:GLY:C	1:I:113:SER:H	2.15	0.49
1:I:131:ARG:HB2	1:I:134:GLN:HB2	1.94	0.49
1:J:131:ARG:HB2	1:J:134:GLN:HB2	1.93	0.49
1:C:109:PRO:HD3	1:C:149:VAL:HG11	1.95	0.49
1:E:51:VAL:O	1:E:53:LYS:HE2	2.13	0.49
1:H:21:TYR:O	1:H:145:VAL:HA	2.12	0.49
1:C:8:LYS:HD3	1:C:8:LYS:C	2.33	0.49
1:F:79:GLU:C	1:F:80:ASP:OD2	2.51	0.49
1:I:112:THR:HA	1:I:121:VAL:CG2	2.42	0.49
1:B:10:PHE:O	1:B:139:THR:HG21	2.14	0.48
1:E:117:LYS:NZ	1:E:118:TYR:HE1	2.12	0.48
1:F:118:TYR:HB3	1:G:56:TRP:HE1	1.78	0.48
1:I:112:THR:HA	1:I:121:VAL:HG21	1.96	0.48
1:I:30:ARG:HH11	1:I:98:GLU:CD	2.17	0.48
1:H:8:LYS:HB3	1:H:34:GLU:O	2.13	0.48
1:H:85:GLU:O	1:H:87:GLU:HB2	2.14	0.48
1:J:56:TRP:HD1	1:J:57:MET:O	1.97	0.48
1:F:55:LEU:HG	1:G:57:MET:HB2	1.95	0.48
1:G:55:LEU:HD21	1:G:62:GLN:NE2	2.29	0.48
1:F:147:ASP:HB3	1:F:149:VAL:HG22	1.96	0.48
1:I:61:GLN:NE2	1:I:63:CYS:SG	2.87	0.48
1:B:15:ASN:O	1:B:17:PRO:HD3	2.14	0.48
1:H:38:VAL:O	1:H:39:THR:HG23	2.14	0.48
1:F:64:LYS:HB3	1:F:64:LYS:HE3	1.49	0.47
1:I:81:GLN:HG2	1:I:82:PRO:HD2	1.97	0.47
1:E:117:LYS:CE	1:E:118:TYR:HE1	2.28	0.47
1:F:39:THR:CG2	1:F:131:ARG:NH1	2.75	0.47
1:C:20:VAL:HG13	1:C:144:GLU:HB2	1.97	0.47
1:A:50:GLY:HA3	1:A:70:LEU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:LYS:O	1:D:43:ALA:HB2	2.15	0.47
1:H:21:TYR:CD2	1:H:27:VAL:HG22	2.50	0.47
1:C:9:SER:HB3	1:C:34:GLU:HB2	1.96	0.47
1:G:54:VAL:HG22	1:G:56:TRP:CE3	2.51	0.46
1:E:119:GLY:HA2	1:E:120:SER:HB3	1.92	0.46
1:A:19:LYS:HG3	1:A:20:VAL:N	2.30	0.46
1:J:8:LYS:O	1:J:8:LYS:HG3	2.14	0.46
1:G:121:VAL:CG1	1:G:123:TYR:CE1	2.98	0.46
1:J:64:LYS:HE3	1:J:66:THR:OG1	2.14	0.46
1:D:131:ARG:HB2	1:D:134:GLN:HB2	1.98	0.46
1:E:19:LYS:HE3	1:E:20:VAL:O	2.16	0.46
1:G:54:VAL:HG22	1:G:56:TRP:HE3	1.80	0.46
1:B:112:THR:HG23	1:B:121:VAL:HG23	1.97	0.46
1:I:48:ALA:HB3	1:I:72:TYR:HB3	1.97	0.46
1:G:92:ARG:HG3	1:G:92:ARG:HH11	1.79	0.46
1:D:47:LEU:HD12	1:D:48:ALA:N	2.31	0.46
1:A:66:THR:CG2	1:A:67:SER:N	2.80	0.45
1:D:55:LEU:HD12	1:D:55:LEU:N	2.31	0.45
1:F:124:TRP:CG	1:F:140:LYS:HE3	2.51	0.45
1:A:19:LYS:HE2	1:A:20:VAL:H	1.81	0.45
1:G:131:ARG:HA	1:G:132:PRO:HD2	1.78	0.45
1:F:55:LEU:HD11	1:F:62:GLN:NE2	2.32	0.45
1:I:88:MET:CE	1:I:132:PRO:HG3	2.47	0.45
1:C:46:ILE:HG21	1:C:76:LEU:HD21	1.98	0.45
1:G:41:VAL:HG13	1:G:129:LEU:HD11	1.98	0.45
1:H:131:ARG:NH2	1:H:134:GLN:HG3	2.31	0.45
1:H:42:LYS:HE2	1:H:88:MET:CE	2.44	0.45
1:A:70:LEU:HG	1:A:71:ARG:N	2.31	0.45
1:I:92:ARG:HG3	1:I:92:ARG:NH1	2.32	0.45
1:A:115:LYS:HB2	1:A:118:TYR:OH	2.16	0.45
1:E:117:LYS:CE	1:E:118:TYR:CE1	2.99	0.45
1:F:21:TYR:O	1:F:146:VAL:HG12	2.17	0.45
1:E:147:ASP:HB3	1:E:149:VAL:CG2	2.44	0.45
1:F:71:ARG:HG3	1:F:71:ARG:HH11	1.82	0.45
1:G:52:ALA:HB1	1:G:120:SER:O	2.17	0.45
1:G:112:THR:H	1:G:121:VAL:CG2	2.20	0.44
1:A:123:TYR:CE1	1:A:145:VAL:HG21	2.53	0.44
1:I:46:ILE:HG21	1:I:46:ILE:HD13	1.59	0.44
1:B:18:GLU:HG2	1:B:18:GLU:H	1.53	0.44
1:B:42:LYS:HB2	1:B:42:LYS:NZ	2.32	0.44
1:E:42:LYS:HA	1:E:88:MET:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:58:GLN:HB2	1:G:58:GLN:HE21	1.55	0.44
1:J:48:ALA:HB1	1:J:70:LEU:HD21	1.99	0.44
1:B:131:ARG:HB2	1:B:134:GLN:HB2	2.00	0.44
1:B:22:GLY:O	1:B:25:GLU:HB2	2.17	0.44
1:E:50:GLY:HA3	1:E:70:LEU:HB3	1.99	0.44
1:G:123:TYR:CE1	1:G:145:VAL:HG21	2.53	0.44
1:G:55:LEU:O	1:G:56:TRP:HB3	2.17	0.44
1:I:108:GLY:HA2	1:I:149:VAL:HG13	1.99	0.44
1:J:142:ASN:O	1:J:143:PHE:HB3	2.17	0.44
1:B:113:SER:O	1:B:114:PHE:CB	2.65	0.44
1:D:56:TRP:HD1	1:D:57:MET:O	2.00	0.44
1:I:81:GLN:NE2	1:I:87:GLU:CB	2.74	0.44
1:F:14:PHE:HE1	1:F:141:LYS:HG2	1.82	0.43
1:G:22:GLY:HA2	1:G:146:VAL:O	2.19	0.43
1:G:55:LEU:HD21	1:G:62:GLN:HE21	1.84	0.43
1:H:109:PRO:HD3	1:H:149:VAL:HG11	2.00	0.43
1:H:59:GLY:C	1:H:61:GLN:N	2.67	0.43
1:J:71:ARG:NH2	1:J:73:GLU:OE1	2.51	0.43
1:D:45:ARG:CG	1:D:75:THR:HG23	2.48	0.43
1:C:16:ASP:OD2	1:C:16:ASP:N	2.52	0.43
1:A:117:LYS:HD3	1:D:61:GLN:OE1	2.18	0.43
1:I:9:SER:HB3	1:I:34:GLU:HB2	1.99	0.43
1:E:83:THR:N	1:H:79:GLU:OE2	2.51	0.43
1:A:16:ASP:CG	1:A:19:LYS:HB2	2.39	0.43
1:E:88:MET:HE1	1:E:132:PRO:HD3	2.01	0.43
1:A:112:THR:N	1:A:121:VAL:HG21	2.34	0.43
1:B:19:LYS:HD3	1:B:21:TYR:CE2	2.54	0.43
1:C:126:LYS:HG2	1:C:140:LYS:HB2	2.01	0.43
1:F:71:ARG:CG	1:F:71:ARG:HH11	2.31	0.43
1:D:76:LEU:HD12	1:D:99:TYR:HB3	2.00	0.42
1:F:71:ARG:HD3	1:F:71:ARG:O	2.18	0.42
1:H:71:ARG:NH2	1:H:73:GLU:OE1	2.52	0.42
1:B:54:VAL:CG1	1:B:65:GLN:HB3	2.47	0.42
1:E:83:THR:O	1:H:100:LYS:HD3	2.19	0.42
1:H:17:PRO:CD	1:H:18:GLU:H	2.32	0.42
1:B:14:PHE:HE1	1:B:141:LYS:HG2	1.83	0.42
1:F:41:VAL:O	1:F:41:VAL:HG12	2.18	0.42
1:H:114:PHE:CE1	1:H:118:TYR:CD2	3.07	0.42
1:B:134:GLN:OE1	1:B:135:PRO:HD2	2.20	0.42
1:B:46:ILE:HD12	1:B:46:ILE:HG21	1.81	0.42
1:H:46:ILE:HG21	1:H:46:ILE:HD13	1.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:115:LYS:CE	1:G:118:TYR:OH	2.67	0.42
1:H:16:ASP:CG	1:H:19:LYS:HB2	2.40	0.42
1:B:26:ARG:HH11	1:B:26:ARG:HG2	1.85	0.42
1:C:47:LEU:HD13	1:C:73:GLU:HG3	2.02	0.42
1:D:57:MET:HG3	1:I:55:LEU:HD23	2.01	0.42
1:I:92:ARG:HG3	1:I:92:ARG:HH11	1.85	0.42
1:D:9:SER:HB3	1:D:34:GLU:HB2	2.02	0.42
1:F:78:LEU:C	1:F:80:ASP:H	2.21	0.42
1:H:80:ASP:O	1:H:81:GLN:HG2	2.19	0.42
1:J:16:ASP:OD2	1:J:19:LYS:HB2	2.20	0.42
1:E:54:VAL:HG11	1:E:115:LYS:HD3	2.01	0.41
1:G:55:LEU:HD11	1:G:62:GLN:HE21	1.84	0.41
1:I:108:GLY:HA2	1:I:149:VAL:CG1	2.50	0.41
1:B:26:ARG:HG2	1:B:26:ARG:NH1	2.35	0.41
1:B:113:SER:O	1:B:114:PHE:HB2	2.20	0.41
1:H:49:SER:O	1:H:123:TYR:HA	2.19	0.41
1:E:79:GLU:C	1:E:81:GLN:H	2.24	0.41
1:C:58:GLN:HE21	1:C:61:GLN:NE2	2.18	0.41
1:D:30:ARG:HD2	1:D:98:GLU:OE1	2.20	0.41
1:I:111:GLY:C	1:I:113:SER:N	2.74	0.41
1:I:134:GLN:OE1	1:I:135:PRO:HD2	2.20	0.41
1:A:9:SER:HB3	1:A:34:GLU:HB2	2.03	0.41
1:C:110:LEU:CD1	1:C:145:VAL:HB	2.51	0.41
1:C:46:ILE:HG22	1:C:74:ASP:O	2.20	0.41
1:F:126:LYS:HG2	1:F:140:LYS:HB2	2.02	0.41
1:A:16:ASP:HB3	1:A:19:LYS:CB	2.48	0.41
1:F:23:SER:N	1:F:110:LEU:HD11	2.35	0.41
1:F:123:TYR:CE1	1:F:145:VAL:HG21	2.56	0.41
1:G:56:TRP:O	1:G:62:GLN:HA	2.21	0.41
1:J:141:LYS:HB2	1:J:141:LYS:HE3	1.75	0.41
1:A:46:ILE:HG22	1:A:74:ASP:O	2.21	0.41
1:B:57:MET:HB2	1:E:55:LEU:HG	2.03	0.41
1:E:117:LYS:HZ3	1:E:118:TYR:HE1	1.65	0.41
1:I:84:GLY:O	1:I:86:ASN:N	2.54	0.41
1:C:105:LEU:HD23	1:C:105:LEU:HA	1.71	0.41
1:A:42:LYS:HE2	1:A:88:MET:CE	2.52	0.40
1:B:54:VAL:HG21	1:B:56:TRP:CZ2	2.56	0.40
1:C:21:TYR:O	1:C:145:VAL:HA	2.21	0.40
1:F:92:ARG:HA	1:F:93:PRO:HD3	1.90	0.40
1:G:76:LEU:O	1:G:77:LEU:HD23	2.21	0.40
1:A:27:VAL:O	1:A:102:GLY:HA2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:GLN:HB3	1:C:61:GLN:HB3	2.04	0.40
1:C:71:ARG:NH2	1:C:73:GLU:OE1	2.54	0.40
1:I:32:ILE:HG12	1:I:98:GLU:HG2	2.03	0.40
1:E:108:GLY:HA3	1:E:109:PRO:HD2	1.77	0.40
1:E:44:VAL:HG22	1:E:129:LEU:HD12	2.03	0.40
1:H:92:ARG:HG3	1:H:92:ARG:NH1	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	130/150 (87%)	115 (88%)	11 (8%)	4 (3%)	4 16
1	B	132/150 (88%)	119 (90%)	9 (7%)	4 (3%)	4 17
1	C	132/150 (88%)	123 (93%)	8 (6%)	1 (1%)	19 51
1	D	125/150 (83%)	116 (93%)	8 (6%)	1 (1%)	19 51
1	E	140/150 (93%)	121 (86%)	14 (10%)	5 (4%)	3 14
1	F	132/150 (88%)	119 (90%)	10 (8%)	3 (2%)	6 23
1	G	132/150 (88%)	116 (88%)	13 (10%)	3 (2%)	6 23
1	H	135/150 (90%)	121 (90%)	14 (10%)	0	100 100
1	I	140/150 (93%)	123 (88%)	14 (10%)	3 (2%)	7 26
1	J	123/150 (82%)	114 (93%)	8 (6%)	1 (1%)	19 51
All	All	1321/1500 (88%)	1187 (90%)	109 (8%)	25 (2%)	8 28

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	SER

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Mol	Chain	Res	Type
1	A	117	LYS
1	B	113	SER
1	B	114	PHE
1	E	80	ASP
1	E	120	SER
1	A	118	TYR
1	E	114	PHE
1	F	79	GLU
1	F	114	PHE
1	I	54	VAL
1	B	78	LEU
1	B	148	LEU
1	C	133	SER
1	D	10	PHE
1	E	109	PRO
1	G	113	SER
1	I	68	GLU
1	A	58	GLN
1	E	148	LEU
1	G	112	THR
1	G	117	LYS
1	I	87	GLU
1	J	79	GLU
1	F	106	PRO

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	118/133 (89%)	103 (87%)	15 (13%)	4 13
1	B	120/133 (90%)	101 (84%)	19 (16%)	2 8
1	C	120/133 (90%)	98 (82%)	22 (18%)	1 5
1	D	116/133 (87%)	103 (89%)	13 (11%)	6 18
1	E	125/133 (94%)	108 (86%)	17 (14%)	3 11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	120/133 (90%)	101 (84%)	19 (16%)	2 8
1	G	120/133 (90%)	108 (90%)	12 (10%)	7 23
1	H	123/133 (92%)	105 (85%)	18 (15%)	3 9
1	I	125/133 (94%)	111 (89%)	14 (11%)	6 18
1	J	115/133 (86%)	103 (90%)	12 (10%)	7 21
All	All	1202/1330 (90%)	1041 (87%)	161 (13%)	4 11

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LYS
1	A	34	GLU
1	A	36	SER
1	A	40	ARG
1	A	46	ILE
1	A	65	GLN
1	A	67	SER
1	A	71	ARG
1	A	87	GLU
1	A	115	LYS
1	A	133	SER
1	A	141	LYS
1	A	146	VAL
1	A	147	ASP
1	A	148	LEU
1	B	18	GLU
1	B	23	SER
1	B	26	ARG
1	B	36	SER
1	B	39	THR
1	B	46	ILE
1	B	53	LYS
1	B	55	LEU
1	B	58	GLN
1	B	60	SER
1	B	62	GLN
1	B	66	THR
1	B	67	SER
1	B	79	GLU
1	B	112	THR

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Mol	Chain	Res	Type
1	B	113	SER
1	B	115	LYS
1	B	121	VAL
1	B	148	LEU
1	C	8	LYS
1	C	26	ARG
1	C	36	SER
1	C	46	ILE
1	C	53	LYS
1	C	55	LEU
1	C	60	SER
1	C	68	GLU
1	C	78	LEU
1	C	79	GLU
1	C	90	ILE
1	C	100	LYS
1	C	104	GLU
1	C	112	THR
1	C	115	LYS
1	C	117	LYS
1	C	121	VAL
1	C	133	SER
1	C	140	LYS
1	C	144	GLU
1	C	146	VAL
1	C	149	VAL
1	D	21	TYR
1	D	37	GLU
1	D	39	THR
1	D	53	LYS
1	D	54	VAL
1	D	62	GLN
1	D	64	LYS
1	D	75	THR
1	D	77	LEU
1	D	80	ASP
1	D	88	MET
1	D	136	THR
1	D	145	VAL
1	E	9	SER
1	E	16	ASP
1	E	37	GLU

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Mol	Chain	Res	Type
1	E	46	ILE
1	E	53	LYS
1	E	55	LEU
1	E	58	GLN
1	E	61	GLN
1	E	64	LYS
1	E	71	ARG
1	E	79	GLU
1	E	81	GLN
1	E	86	ASN
1	E	115	LYS
1	E	117	LYS
1	E	147	ASP
1	E	148	LEU
1	F	11	GLU
1	F	23	SER
1	F	46	ILE
1	F	55	LEU
1	F	57	MET
1	F	60	SER
1	F	62	GLN
1	F	65	GLN
1	F	67	SER
1	F	71	ARG
1	F	77	LEU
1	F	80	ASP
1	F	87	GLU
1	F	115	LYS
1	F	117	LYS
1	F	118	TYR
1	F	120	SER
1	F	141	LYS
1	F	147	ASP
1	G	21	TYR
1	G	23	SER
1	G	51	VAL
1	G	58	GLN
1	G	70	LEU
1	G	71	ARG
1	G	79	GLU
1	G	80	ASP
1	G	107	GLN

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Mol	Chain	Res	Type
1	G	112	THR
1	G	126	LYS
1	G	141	LYS
1	H	37	GLU
1	H	39	THR
1	H	46	ILE
1	H	49	SER
1	H	57	MET
1	H	58	GLN
1	H	71	ARG
1	H	80	ASP
1	H	85	GLU
1	H	87	GLU
1	H	112	THR
1	H	114	PHE
1	H	118	TYR
1	H	121	VAL
1	H	136	THR
1	H	146	VAL
1	H	148	LEU
1	H	149	VAL
1	I	46	ILE
1	I	61	GLN
1	I	64	LYS
1	I	77	LEU
1	I	80	ASP
1	I	87	GLU
1	I	88	MET
1	I	92	ARG
1	I	115	LYS
1	I	117	LYS
1	I	121	VAL
1	I	141	LYS
1	I	147	ASP
1	I	149	VAL
1	J	42	LYS
1	J	55	LEU
1	J	58	GLN
1	J	60	SER
1	J	64	LYS
1	J	71	ARG
1	J	120	SER

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Mol	Chain	Res	Type
1	J	122	ASP
1	J	145	VAL
1	J	147	ASP
1	J	148	LEU
1	J	149	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	65	GLN
1	B	58	GLN
1	C	58	GLN
1	C	62	GLN
1	C	95	ASN
1	D	62	GLN
1	E	81	GLN
1	E	107	GLN
1	F	62	GLN
1	F	65	GLN
1	G	58	GLN
1	G	62	GLN
1	G	134	GLN
1	H	58	GLN
1	H	62	GLN
1	H	95	ASN
1	I	58	GLN
1	I	81	GLN
1	I	95	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	134/150 (89%)	1.03	27 (20%) 1 0	47, 101, 172, 203	0
1	B	136/150 (90%)	0.21	2 (1%) 73 73	44, 67, 107, 123	0
1	C	136/150 (90%)	0.35	5 (3%) 41 37	36, 71, 132, 139	0
1	D	131/150 (87%)	0.65	13 (9%) 7 5	46, 94, 146, 173	0
1	E	142/150 (94%)	0.26	4 (2%) 53 49	40, 61, 109, 154	0
1	F	136/150 (90%)	1.22	35 (25%) 0 0	56, 127, 170, 217	0
1	G	136/150 (90%)	0.42	7 (5%) 28 24	56, 82, 121, 150	0
1	H	139/150 (92%)	0.32	3 (2%) 62 59	41, 74, 119, 150	0
1	I	142/150 (94%)	0.54	7 (4%) 29 26	55, 80, 117, 179	0
1	J	129/150 (86%)	0.52	7 (5%) 25 22	54, 92, 133, 170	0
All	All	1361/1500 (90%)	0.55	110 (8%) 12 9	36, 83, 149, 217	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	149	VAL	11.7
1	F	149	VAL	9.1
1	I	149	VAL	8.2
1	E	149	VAL	7.4
1	H	149	VAL	6.5
1	A	148	LEU	6.4
1	D	149	VAL	6.2
1	E	148	LEU	6.2
1	F	100	LYS	6.0
1	J	148	LEU	5.9
1	F	91	MET	5.6
1	H	148	LEU	5.3
1	A	97	TYR	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	91	MET	5.0
1	F	10	PHE	5.0
1	A	38	VAL	4.9
1	A	149	VAL	4.8
1	A	34	GLU	4.7
1	F	115	LYS	4.6
1	A	31	VAL	4.6
1	I	148	LEU	4.3
1	D	90	ILE	4.3
1	D	10	PHE	4.3
1	A	91	MET	4.1
1	F	145	VAL	4.0
1	F	97	TYR	4.0
1	F	148	LEU	3.9
1	C	36	SER	3.8
1	A	98	GLU	3.8
1	A	14	PHE	3.7
1	D	41	VAL	3.7
1	I	39	THR	3.7
1	A	117	LYS	3.6
1	F	31	VAL	3.6
1	C	149	VAL	3.5
1	F	98	GLU	3.5
1	A	118	TYR	3.5
1	I	111	GLY	3.4
1	F	117	LYS	3.4
1	F	28	ALA	3.4
1	F	77	LEU	3.3
1	H	60	SER	3.3
1	F	32	ILE	3.2
1	F	116	GLY	3.2
1	D	38	VAL	3.2
1	A	95	ASN	3.2
1	F	118	TYR	3.2
1	D	129	LEU	3.2
1	F	9	SER	3.1
1	J	110	LEU	3.1
1	G	56	TRP	3.0
1	J	92	ARG	3.0
1	F	33	VAL	2.9
1	A	90	ILE	2.9
1	F	131	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	12	VAL	2.8
1	A	78	LEU	2.8
1	F	129	LEU	2.8
1	J	40	ARG	2.8
1	I	112	THR	2.8
1	B	148	LEU	2.8
1	A	10	PHE	2.8
1	A	96	LYS	2.8
1	C	97	TYR	2.7
1	J	38	VAL	2.7
1	B	77	LEU	2.7
1	F	96	LYS	2.7
1	C	148	LEU	2.7
1	G	148	LEU	2.7
1	D	137	GLN	2.7
1	A	36	SER	2.6
1	J	39	THR	2.6
1	A	129	LEU	2.6
1	A	114	PHE	2.6
1	A	99	TYR	2.6
1	D	97	TYR	2.6
1	A	32	ILE	2.6
1	F	146	VAL	2.5
1	E	118	TYR	2.5
1	F	140	LYS	2.5
1	A	133	SER	2.5
1	F	41	VAL	2.5
1	F	110	LEU	2.4
1	F	104	GLU	2.4
1	A	35	VAL	2.4
1	F	14	PHE	2.4
1	F	119	GLY	2.4
1	G	36	SER	2.4
1	A	33	VAL	2.4
1	I	38	VAL	2.3
1	A	130	ASP	2.3
1	C	91	MET	2.3
1	G	10	PHE	2.3
1	A	115	LYS	2.3
1	F	99	TYR	2.3
1	A	110	LEU	2.2
1	F	42	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	110	LEU	2.2
1	F	92	ARG	2.2
1	F	130	ASP	2.2
1	D	39	THR	2.2
1	F	114	PHE	2.1
1	F	78	LEU	2.1
1	D	148	LEU	2.1
1	G	107	GLN	2.1
1	D	32	ILE	2.1
1	E	117	LYS	2.0
1	D	78	LEU	2.0
1	G	87	GLU	2.0
1	G	149	VAL	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	CA	C	201	1/1	0.83	0.25	74,74,74,74	0
2	CA	I	201	1/1	0.92	0.35	68,68,68,68	0
2	CA	H	201	1/1	0.93	0.34	64,64,64,64	0
2	CA	D	201	1/1	0.96	0.22	77,77,77,77	0
2	CA	A	201	1/1	0.98	0.17	99,99,99,99	0

6.5 Other polymers (i)

There are no such residues in this entry.