Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 04:16 PM EDT

PDB ID	:	4WYV
Title	:	Crystal Structure of Human Translin in Open Conformation
Authors	:	Dvir, H.; Eliahoo, E.; Alian, A.
Deposited on	:	2014-11-18
Resolution	:	3.00 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

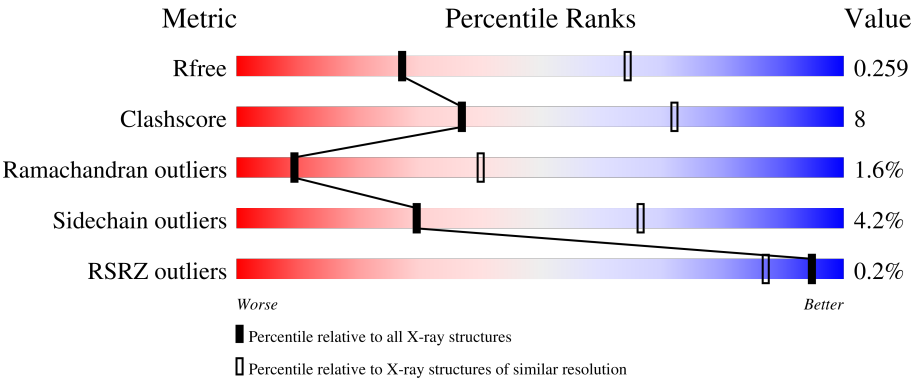
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	240	71% 16% • 11%
1	B	240	72% 14% • 12%
1	C	240	68% 17% • 12%
1	D	240	71% 15% • 11%
1	E	240	68% 19% • 11%

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Mol	Chain	Length	Quality of chain
1	F	240	
1	G	240	
1	H	240	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13935 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 Translin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1741	1116	300	323	2			
1	B	212	Total	C	N	O	S	0	0	0
			1737	1114	299	322	2			
1	C	210	Total	C	N	O	S	0	0	0
			1717	1100	296	319	2			
1	D	214	Total	C	N	O	S	0	0	0
			1741	1113	301	325	2			
1	E	213	Total	C	N	O	S	0	0	0
			1743	1117	300	324	2			
1	F	212	Total	C	N	O	S	0	0	0
			1737	1114	299	322	2			
1	G	216	Total	C	N	O	S	0	0	0
			1767	1133	304	328	2			
1	H	212	Total	C	N	O	S	0	0	0
			1734	1112	298	322	2			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP Q15631
A	-10	ARG	-	expression tag	UNP Q15631
A	-9	GLY	-	expression tag	UNP Q15631
A	-8	SER	-	expression tag	UNP Q15631
A	-7	HIS	-	expression tag	UNP Q15631
A	-6	HIS	-	expression tag	UNP Q15631
A	-5	HIS	-	expression tag	UNP Q15631
A	-4	HIS	-	expression tag	UNP Q15631
A	-3	HIS	-	expression tag	UNP Q15631
A	-2	HIS	-	expression tag	UNP Q15631
A	-1	GLY	-	expression tag	UNP Q15631
A	0	SER	-	expression tag	UNP Q15631
B	-11	MET	-	initiating methionine	UNP Q15631

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	ARG	-	expression tag	UNP Q15631
B	-9	GLY	-	expression tag	UNP Q15631
B	-8	SER	-	expression tag	UNP Q15631
B	-7	HIS	-	expression tag	UNP Q15631
B	-6	HIS	-	expression tag	UNP Q15631
B	-5	HIS	-	expression tag	UNP Q15631
B	-4	HIS	-	expression tag	UNP Q15631
B	-3	HIS	-	expression tag	UNP Q15631
B	-2	HIS	-	expression tag	UNP Q15631
B	-1	GLY	-	expression tag	UNP Q15631
B	0	SER	-	expression tag	UNP Q15631
C	-11	MET	-	initiating methionine	UNP Q15631
C	-10	ARG	-	expression tag	UNP Q15631
C	-9	GLY	-	expression tag	UNP Q15631
C	-8	SER	-	expression tag	UNP Q15631
C	-7	HIS	-	expression tag	UNP Q15631
C	-6	HIS	-	expression tag	UNP Q15631
C	-5	HIS	-	expression tag	UNP Q15631
C	-4	HIS	-	expression tag	UNP Q15631
C	-3	HIS	-	expression tag	UNP Q15631
C	-2	HIS	-	expression tag	UNP Q15631
C	-1	GLY	-	expression tag	UNP Q15631
C	0	SER	-	expression tag	UNP Q15631
D	-11	MET	-	initiating methionine	UNP Q15631
D	-10	ARG	-	expression tag	UNP Q15631
D	-9	GLY	-	expression tag	UNP Q15631
D	-8	SER	-	expression tag	UNP Q15631
D	-7	HIS	-	expression tag	UNP Q15631
D	-6	HIS	-	expression tag	UNP Q15631
D	-5	HIS	-	expression tag	UNP Q15631
D	-4	HIS	-	expression tag	UNP Q15631
D	-3	HIS	-	expression tag	UNP Q15631
D	-2	HIS	-	expression tag	UNP Q15631
D	-1	GLY	-	expression tag	UNP Q15631
D	0	SER	-	expression tag	UNP Q15631
E	-11	MET	-	initiating methionine	UNP Q15631
E	-10	ARG	-	expression tag	UNP Q15631
E	-9	GLY	-	expression tag	UNP Q15631
E	-8	SER	-	expression tag	UNP Q15631
E	-7	HIS	-	expression tag	UNP Q15631
E	-6	HIS	-	expression tag	UNP Q15631
E	-5	HIS	-	expression tag	UNP Q15631

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	HIS	-	expression tag	UNP Q15631
E	-3	HIS	-	expression tag	UNP Q15631
E	-2	HIS	-	expression tag	UNP Q15631
E	-1	GLY	-	expression tag	UNP Q15631
E	0	SER	-	expression tag	UNP Q15631
F	-11	MET	-	initiating methionine	UNP Q15631
F	-10	ARG	-	expression tag	UNP Q15631
F	-9	GLY	-	expression tag	UNP Q15631
F	-8	SER	-	expression tag	UNP Q15631
F	-7	HIS	-	expression tag	UNP Q15631
F	-6	HIS	-	expression tag	UNP Q15631
F	-5	HIS	-	expression tag	UNP Q15631
F	-4	HIS	-	expression tag	UNP Q15631
F	-3	HIS	-	expression tag	UNP Q15631
F	-2	HIS	-	expression tag	UNP Q15631
F	-1	GLY	-	expression tag	UNP Q15631
F	0	SER	-	expression tag	UNP Q15631
G	-11	MET	-	initiating methionine	UNP Q15631
G	-10	ARG	-	expression tag	UNP Q15631
G	-9	GLY	-	expression tag	UNP Q15631
G	-8	SER	-	expression tag	UNP Q15631
G	-7	HIS	-	expression tag	UNP Q15631
G	-6	HIS	-	expression tag	UNP Q15631
G	-5	HIS	-	expression tag	UNP Q15631
G	-4	HIS	-	expression tag	UNP Q15631
G	-3	HIS	-	expression tag	UNP Q15631
G	-2	HIS	-	expression tag	UNP Q15631
G	-1	GLY	-	expression tag	UNP Q15631
G	0	SER	-	expression tag	UNP Q15631
H	-11	MET	-	initiating methionine	UNP Q15631
H	-10	ARG	-	expression tag	UNP Q15631
H	-9	GLY	-	expression tag	UNP Q15631
H	-8	SER	-	expression tag	UNP Q15631
H	-7	HIS	-	expression tag	UNP Q15631
H	-6	HIS	-	expression tag	UNP Q15631
H	-5	HIS	-	expression tag	UNP Q15631
H	-4	HIS	-	expression tag	UNP Q15631
H	-3	HIS	-	expression tag	UNP Q15631
H	-2	HIS	-	expression tag	UNP Q15631
H	-1	GLY	-	expression tag	UNP Q15631
H	0	SER	-	expression tag	UNP Q15631

- Molecule 2 is water.

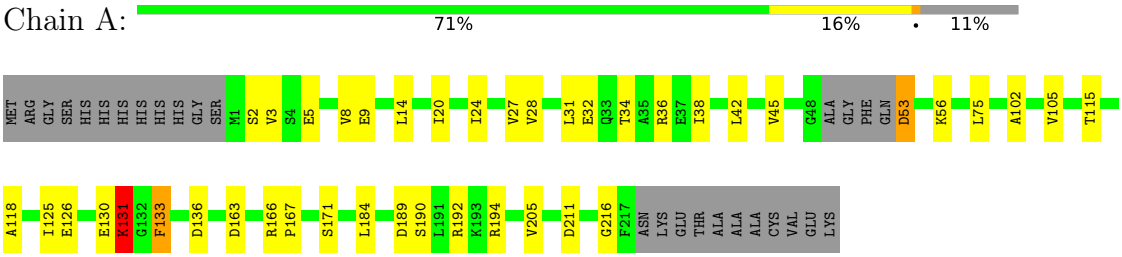
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	7	Total O 7 7	0	0
2	B	2	Total O 2 2	0	0
2	C	2	Total O 2 2	0	0
2	D	2	Total O 2 2	0	0
2	E	2	Total O 2 2	0	0
2	F	2	Total O 2 2	0	0
2	G	1	Total O 1 1	0	0

3 Residue-property plots (i)

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

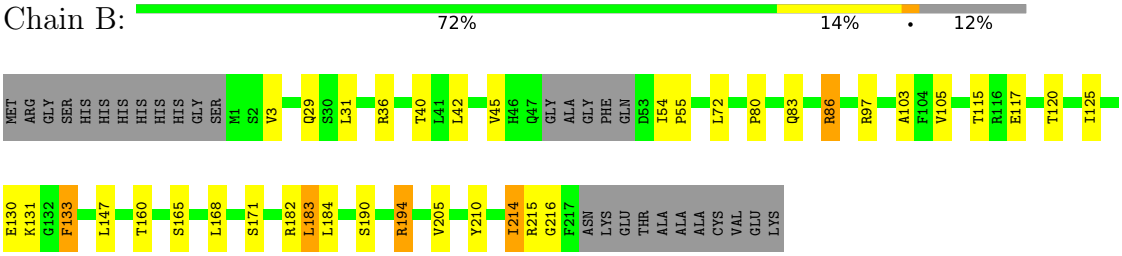
- Molecule 1: Translin

Chain A:



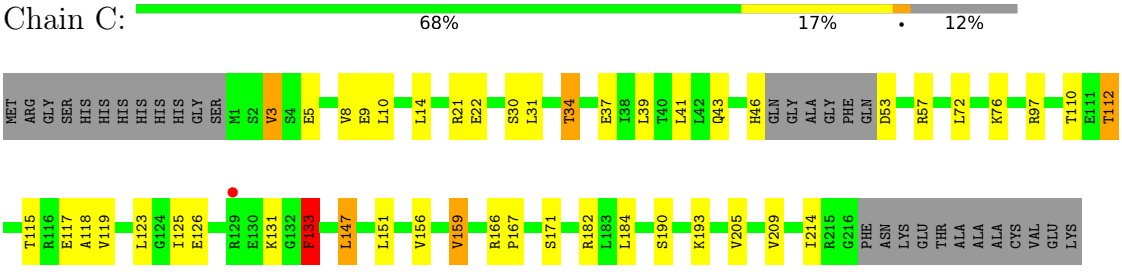
- Molecule 1: Translin

Chain B:



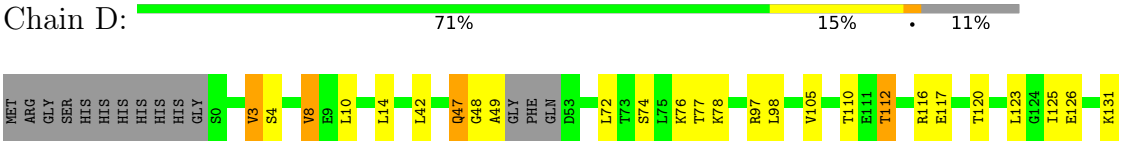
- Molecule 1: Translin

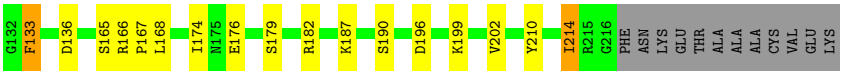
Chain C:



- Molecule 1: Translin

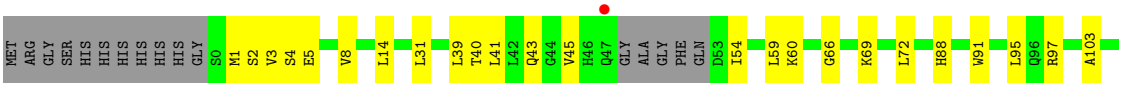
Chain D:





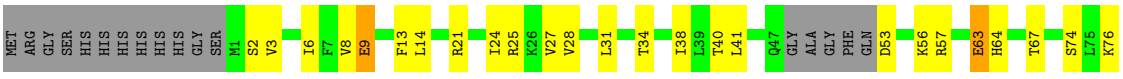
• Molecule 1: Translin

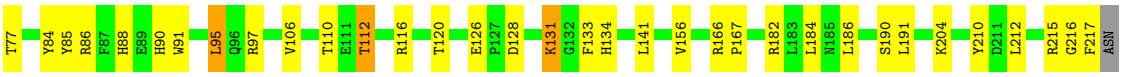
Chain E:



• Molecule 1: Translin

Chain F:



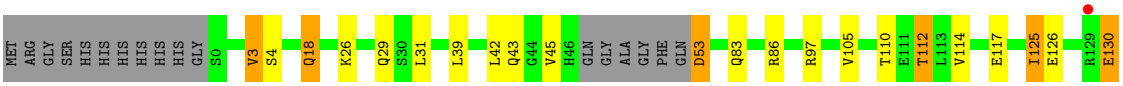


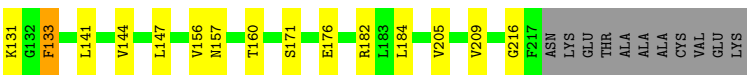
• Molecule 1: Translin

Chain G:

• Molecule 1: Translin

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	82.31Å 82.31Å 635.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.00 – 3.00 57.96 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (58.00-3.00) 98.6 (57.96-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.93 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.226 , 0.272 0.215 , 0.259	Depositor DCC
R_{free} test set	2272 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	76.8	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 47.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13935	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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

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	0.91	3/1772 (0.2%)	0.76	1/2390 (0.0%)
1	B	0.88	2/1768 (0.1%)	0.79	2/2385 (0.1%)
1	C	0.94	5/1747 (0.3%)	0.75	2/2357 (0.1%)
1	D	0.83	0/1771	0.73	0/2389
1	E	0.76	0/1774	0.68	0/2393
1	F	0.84	3/1768 (0.2%)	0.72	1/2385 (0.0%)
1	G	0.93	4/1799 (0.2%)	0.77	3/2426 (0.1%)
1	H	0.83	2/1765 (0.1%)	0.71	0/2381
All	All	0.87	19/14164 (0.1%)	0.74	9/19106 (0.0%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	46	HIS	C-O	12.28	1.46	1.23
1	A	9	GLU	CD-OE1	12.14	1.39	1.25
1	G	69	LYS	CG-CD	10.11	1.86	1.52
1	H	4	SER	CB-OG	9.42	1.54	1.42
1	B	194	ARG	CZ-NH1	7.98	1.43	1.33
1	F	63	GLU	CD-OE1	-7.65	1.17	1.25
1	F	9	GLU	CD-OE1	7.62	1.34	1.25
1	C	37	GLU	CB-CG	6.51	1.64	1.52
1	G	56	LYS	CD-CE	6.39	1.67	1.51
1	G	129	ARG	CZ-NH1	6.00	1.40	1.33
1	G	-1	GLY	N-CA	5.80	1.54	1.46
1	B	130	GLU	CB-CG	5.70	1.62	1.52
1	F	9	GLU	CG-CD	5.61	1.60	1.51
1	C	9	GLU	CD-OE1	5.54	1.31	1.25
1	C	117	GLU	CG-CD	5.43	1.60	1.51
1	C	193	LYS	CG-CD	5.38	1.70	1.52
1	A	131	LYS	CE-NZ	5.20	1.62	1.49
1	H	4	SER	CA-CB	5.13	1.60	1.52
1	A	9	GLU	CD-OE2	5.01	1.31	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	194	ARG	NE-CZ-NH2	-9.94	115.33	120.30
1	G	129	ARG	NE-CZ-NH1	9.67	125.13	120.30
1	G	129	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	B	183	LEU	CA-CB-CG	6.52	130.29	115.30
1	G	21	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	C	21	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	A	194	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	C	21	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	F	86	ARG	NE-CZ-NH2	-5.05	117.77	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1741	0	1761	25	0
1	B	1737	0	1758	26	0
1	C	1717	0	1741	37	0
1	D	1741	0	1762	24	0
1	E	1743	0	1763	30	0
1	F	1737	0	1758	40	0
1	G	1767	0	1783	38	0
1	H	1734	0	1755	28	0
2	A	7	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	1	0	0	0	0
All	All	13935	0	14081	218	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 8.

All (218) 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:69:LYS:CD	1:G:69:LYS:CG	1.86	1.50
1:F:110:THR:CG2	1:F:112:THR:HG22	1.81	1.09
1:F:110:THR:HG23	1:F:112:THR:HG22	1.37	1.03
1:E:72:LEU:HD23	1:E:125:ILE:HD11	1.52	0.91
1:C:39:LEU:HD11	1:C:43:GLN:HE21	1.43	0.83
1:B:80:PRO:HG2	1:B:83:GLN:HE21	1.44	0.82
1:B:183:LEU:HD11	1:F:8:VAL:HG22	1.62	0.82
1:E:1:MET:O	1:E:5:GLU:HB2	1.79	0.82
1:C:41:LEU:HB3	1:C:57:ARG:CZ	2.11	0.81
1:H:110:THR:OG1	1:H:112:THR:HG22	1.81	0.80
1:C:41:LEU:HB2	1:C:57:ARG:NH2	1.96	0.80
1:D:72:LEU:O	1:D:76:LYS:HG3	1.81	0.80
1:G:54:ILE:HG13	1:G:55:PRO:HD3	1.65	0.79
1:E:110:THR:OG1	1:E:112:THR:HG22	1.82	0.78
1:A:53:ASP:O	1:A:56:LYS:HB2	1.84	0.78
1:F:34:THR:O	1:F:38:ILE:HD12	1.86	0.76
1:D:74:SER:O	1:D:77:THR:HB	1.88	0.73
1:B:80:PRO:CG	1:B:83:GLN:HE21	2.00	0.73
1:C:110:THR:OG1	1:C:112:THR:HG22	1.89	0.72
1:B:210:TYR:O	1:B:214:ILE:HG22	1.90	0.72
1:G:69:LYS:CD	1:G:69:LYS:CB	2.67	0.72
1:F:110:THR:HG23	1:F:112:THR:CG2	2.15	0.72
1:F:110:THR:HG21	1:F:112:THR:HG22	1.73	0.71
1:C:41:LEU:CB	1:C:57:ARG:CZ	2.69	0.71
1:H:42:LEU:O	1:H:45:VAL:HG22	1.92	0.70
1:B:40:THR:HG23	1:C:182:ARG:HD2	1.74	0.70
1:A:36:ARG:HD2	1:B:182:ARG:O	1.93	0.68
1:D:110:THR:OG1	1:D:112:THR:HG22	1.92	0.68
1:F:215:ARG:HB2	1:F:217:PHE:HE1	1.58	0.68
1:F:34:THR:O	1:F:38:ILE:CD1	2.42	0.67
1:C:3:VAL:HG21	1:G:176:GLU:HB3	1.75	0.67
1:F:182:ARG:HD2	1:G:40:THR:HG23	1.78	0.66
1:B:42:LEU:O	1:B:45:VAL:HG13	1.96	0.65
1:A:42:LEU:O	1:A:45:VAL:HG13	1.98	0.63
1:F:21:ARG:HH11	1:F:90:HIS:HE1	1.47	0.62
1:E:115:THR:HG23	1:E:118:ALA:H	1.65	0.62
1:B:117:GLU:O	1:B:120:THR:HG22	2.00	0.61
1:D:14:LEU:HD12	1:H:184:LEU:HD22	1.82	0.61
1:A:34:THR:O	1:A:38:ILE:HD12	2.01	0.61
1:E:72:LEU:CD2	1:E:125:ILE:HD11	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:53:ASP:O	1:F:56:LYS:HB2	2.00	0.60
1:D:165:SER:HA	1:D:168:LEU:HD12	1.81	0.60
1:A:53:ASP:HB2	1:A:56:LYS:HD3	1.84	0.60
1:H:39:LEU:HD21	1:H:43:GLN:CD	2.22	0.60
1:A:115:THR:HG23	1:A:118:ALA:H	1.66	0.60
1:E:40:THR:HG23	1:H:182:ARG:HD2	1.84	0.59
1:C:3:VAL:CG2	1:G:176:GLU:HB3	2.32	0.59
1:C:41:LEU:HB3	1:C:57:ARG:NE	2.16	0.59
1:F:76:LYS:NZ	1:F:126:GLU:OE2	2.35	0.59
1:C:14:LEU:CD1	1:G:137:VAL:HG11	2.32	0.59
1:A:125:ILE:HG23	1:A:133:PHE:O	2.02	0.59
1:B:72:LEU:HD13	1:B:125:ILE:HD11	1.84	0.59
1:C:125:ILE:HG23	1:C:133:PHE:O	2.02	0.59
1:E:160:THR:HG21	1:H:209:VAL:HG12	1.84	0.59
1:C:41:LEU:CB	1:C:57:ARG:NH2	2.66	0.58
1:C:166:ARG:HB3	1:C:167:PRO:HD3	1.85	0.58
1:C:156:VAL:O	1:C:159:VAL:HG12	2.04	0.58
1:F:156:VAL:HG21	1:F:204:LYS:HE2	1.85	0.58
1:G:125:ILE:HG22	1:G:126:GLU:N	2.18	0.58
1:B:171:SER:HA	1:B:205:VAL:HG11	1.88	0.56
1:F:21:ARG:HH11	1:F:90:HIS:CE1	2.23	0.56
1:F:128:ASP:HA	1:F:134:HIS:CD2	2.39	0.56
1:G:125:ILE:HG23	1:G:133:PHE:O	2.05	0.56
1:B:215:ARG:CZ	1:C:214:ILE:HD12	2.36	0.56
1:C:125:ILE:HG22	1:C:126:GLU:N	2.20	0.56
1:B:165:SER:HA	1:B:168:LEU:HD12	1.88	0.56
1:B:184:LEU:HD22	1:F:14:LEU:HD12	1.87	0.55
1:B:210:TYR:O	1:B:214:ILE:CG2	2.53	0.55
1:G:52:GLN:O	1:G:53:ASP:HB3	2.06	0.54
1:C:147:LEU:HD22	1:C:151:LEU:HG	1.89	0.54
1:D:116:ARG:O	1:D:120:THR:HG23	2.08	0.54
1:E:45:VAL:HG23	1:E:54:ILE:HD11	1.90	0.54
1:G:166:ARG:HB3	1:G:167:PRO:HD3	1.90	0.53
1:E:174:ILE:HG22	1:E:202:VAL:HG22	1.90	0.53
1:F:24:ILE:O	1:F:28:VAL:HG23	2.08	0.53
1:F:184:LEU:HD23	1:F:186:LEU:HD21	1.90	0.53
1:A:125:ILE:HG22	1:A:126:GLU:N	2.24	0.53
1:H:125:ILE:HD13	1:H:125:ILE:N	2.24	0.53
1:E:125:ILE:HG22	1:E:126:GLU:N	2.24	0.52
1:G:42:LEU:O	1:G:45:VAL:HG13	2.08	0.52
1:G:69:LYS:CG	1:G:69:LYS:CE	2.80	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:171:SER:HA	1:H:205:VAL:HG11	1.92	0.52
1:D:125:ILE:HG22	1:D:126:GLU:N	2.23	0.52
1:A:28:VAL:O	1:A:32:GLU:HG3	2.10	0.52
1:A:125:ILE:CG2	1:A:133:PHE:O	2.59	0.51
1:H:125:ILE:HG22	1:H:126:GLU:N	2.25	0.51
1:E:180:GLY:O	1:E:183:LEU:HB2	2.10	0.51
1:G:52:GLN:O	1:G:52:GLN:HG2	2.10	0.51
1:G:190:SER:O	1:G:193:LYS:HE2	2.11	0.51
1:H:39:LEU:C	1:H:39:LEU:HD23	2.32	0.51
1:D:3:VAL:HG21	1:H:176:GLU:HB3	1.93	0.50
1:A:171:SER:HA	1:A:205:VAL:HG11	1.93	0.50
1:D:77:THR:HG22	1:D:78:LYS:HD3	1.94	0.50
1:F:9:GLU:HG2	1:F:13:PHE:HE2	1.77	0.50
1:D:174:ILE:HG22	1:D:202:VAL:HG22	1.94	0.50
1:E:160:THR:CG2	1:H:209:VAL:HG12	2.42	0.50
1:F:141:LEU:HD12	1:F:191:LEU:HD21	1.94	0.50
1:D:196:ASP:O	1:D:199:LYS:HG2	2.12	0.50
1:F:131:LYS:HD2	1:F:134:HIS:HE1	1.76	0.50
1:C:41:LEU:C	1:C:57:ARG:HE	2.15	0.49
1:A:189:ASP:OD1	1:A:192:ARG:NH2	2.46	0.49
1:E:129:ARG:HH11	1:E:129:ARG:HB3	1.77	0.49
1:E:115:THR:CG2	1:E:118:ALA:HB2	2.42	0.48
1:B:182:ARG:HH11	1:B:182:ARG:HG2	1.78	0.48
1:A:27:VAL:HG13	1:A:75:LEU:HD13	1.95	0.48
1:H:125:ILE:HG23	1:H:133:PHE:O	2.13	0.48
1:C:184:LEU:HA	1:G:11:GLN:OE1	2.14	0.48
1:F:215:ARG:HB2	1:F:217:PHE:CE1	2.43	0.48
1:A:184:LEU:HD22	1:E:14:LEU:HD12	1.95	0.48
1:D:4:SER:O	1:D:8:VAL:HG13	2.14	0.48
1:H:157:ASN:O	1:H:160:THR:HB	2.13	0.48
1:G:71:HIS:O	1:G:74:SER:HB3	2.14	0.48
1:E:66:GLY:HA2	1:E:69:LYS:NZ	2.29	0.47
1:H:53:ASP:OD1	1:H:53:ASP:C	2.52	0.47
1:C:14:LEU:HD11	1:G:137:VAL:HG11	1.96	0.47
1:D:187:LYS:HG3	1:H:18:GLN:HG2	1.95	0.47
1:F:116:ARG:O	1:F:120:THR:HG23	2.14	0.47
1:D:10:LEU:HD13	1:H:141:LEU:HD21	1.96	0.47
1:G:125:ILE:CG2	1:G:126:GLU:N	2.77	0.47
1:F:38:ILE:HD11	1:F:64:HIS:HB3	1.95	0.47
1:D:125:ILE:CG2	1:D:126:GLU:N	2.77	0.47
1:E:39:LEU:HD11	1:E:43:GLN:HE21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:LEU:HD23	1:B:31:LEU:HA	1.74	0.47
1:C:5:GLU:O	1:C:8:VAL:HG12	2.13	0.47
1:C:115:THR:HG23	1:C:118:ALA:H	1.80	0.46
1:C:72:LEU:HD13	1:C:125:ILE:HD11	1.96	0.46
1:A:53:ASP:OD1	1:A:53:ASP:C	2.54	0.46
1:C:30:SER:O	1:C:34:THR:HG22	2.14	0.46
1:C:125:ILE:CG2	1:C:126:GLU:N	2.78	0.46
1:G:69:LYS:HG3	1:G:124:GLY:HA3	1.98	0.46
1:B:36:ARG:HD2	1:C:182:ARG:O	2.16	0.46
1:G:115:THR:HG23	1:G:118:ALA:H	1.81	0.45
1:G:88:HIS:HE1	1:G:92:ARG:NH1	2.14	0.45
1:H:125:ILE:HD13	1:H:125:ILE:H	1.82	0.45
1:H:114:VAL:HG13	1:H:114:VAL:O	2.17	0.45
1:G:98:LEU:HB3	1:G:123:LEU:HD21	1.98	0.45
1:H:42:LEU:HD11	1:H:105:VAL:HG23	1.98	0.45
1:F:38:ILE:HD12	1:F:38:ILE:H	1.80	0.45
1:C:10:LEU:HD13	1:G:141:LEU:HD21	1.99	0.45
1:H:83:GLN:OE1	1:H:86:ARG:HD2	2.17	0.45
1:A:130:GLU:O	1:A:131:LYS:O	2.35	0.44
1:F:91:TRP:O	1:F:95:LEU:HB2	2.17	0.44
1:G:69:LYS:CD	1:G:69:LYS:HB3	2.43	0.44
1:C:14:LEU:HD11	1:G:137:VAL:CG1	2.48	0.44
1:H:126:GLU:HB3	1:H:130:GLU:HB3	2.00	0.44
1:F:88:HIS:HA	1:F:91:TRP:CZ2	2.52	0.44
1:F:106:VAL:O	1:F:110:THR:HG22	2.17	0.44
1:B:80:PRO:HG3	1:B:83:GLN:HE21	1.82	0.44
1:E:115:THR:HG23	1:E:118:ALA:CB	2.47	0.44
1:E:126:GLU:HB3	1:E:130:GLU:HB3	1.98	0.44
1:E:196:ASP:O	1:E:199:LYS:HG2	2.17	0.44
1:F:2:SER:O	1:F:6:ILE:HG13	2.17	0.44
1:F:212:LEU:O	1:F:217:PHE:HD1	2.01	0.44
1:A:166:ARG:HB3	1:A:167:PRO:HD3	2.00	0.43
1:D:176:GLU:HB3	1:H:3:VAL:HG21	1.99	0.43
1:B:40:THR:CG2	1:C:182:ARG:HD2	2.45	0.43
1:B:103:ALA:HB1	1:B:147:LEU:HD22	2.00	0.43
1:E:41:LEU:HD21	1:E:60:LYS:HB3	2.00	0.43
1:D:42:LEU:HD11	1:D:105:VAL:HG23	2.01	0.43
1:G:116:ARG:O	1:G:120:THR:HG23	2.18	0.43
1:H:144:VAL:O	1:H:147:LEU:HB3	2.18	0.43
1:G:126:GLU:HB3	1:G:130:GLU:HB3	2.01	0.43
1:H:26:LYS:O	1:H:29:GLN:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ASP:HB3	1:B:214:ILE:HD12	2.01	0.43
1:F:131:LYS:HD2	1:F:131:LYS:HA	1.85	0.43
1:G:196:ASP:O	1:G:199:LYS:HG2	2.19	0.43
1:E:66:GLY:HA2	1:E:69:LYS:HZ2	1.84	0.43
1:F:84:TYR:HD1	1:F:85:TYR:CD1	2.37	0.43
1:C:171:SER:HA	1:C:205:VAL:HG11	2.01	0.42
1:E:72:LEU:HD23	1:E:125:ILE:CD1	2.36	0.42
1:C:41:LEU:HB2	1:C:57:ARG:CZ	2.41	0.42
1:G:20:ILE:O	1:G:24:ILE:HG13	2.19	0.42
1:B:54:ILE:N	1:B:55:PRO:CD	2.83	0.42
1:E:117:GLU:O	1:E:120:THR:HB	2.19	0.42
1:A:20:ILE:O	1:A:24:ILE:HG13	2.20	0.42
1:D:166:ARG:HB3	1:D:167:PRO:HD3	2.00	0.42
1:C:119:VAL:O	1:C:123:LEU:HG	2.20	0.42
1:D:210:TYR:CZ	1:D:214:ILE:HD12	2.54	0.42
1:G:144:VAL:O	1:G:147:LEU:HB3	2.19	0.42
1:A:5:GLU:O	1:A:8:VAL:HG22	2.19	0.42
1:F:74:SER:O	1:F:77:THR:HB	2.19	0.42
1:G:125:ILE:CG2	1:G:133:PHE:O	2.68	0.42
1:F:110:THR:CG2	1:F:112:THR:CG2	2.73	0.42
1:A:14:LEU:HD11	1:E:137:VAL:HG21	2.02	0.42
1:A:14:LEU:HD22	1:E:184:LEU:HD22	2.02	0.42
1:D:117:GLU:O	1:D:120:THR:OG1	2.27	0.42
1:G:170:ILE:HG22	1:G:205:VAL:HG21	2.02	0.42
1:H:171:SER:HA	1:H:205:VAL:CG1	2.50	0.42
1:C:14:LEU:HD13	1:G:137:VAL:HG11	2.00	0.41
1:G:88:HIS:CE1	1:G:92:ARG:NH1	2.88	0.41
1:A:163:ASP:C	1:A:163:ASP:OD1	2.59	0.41
1:B:83:GLN:O	1:B:86:ARG:HB2	2.21	0.41
1:F:25:ARG:HE	1:F:90:HIS:CD2	2.37	0.41
1:B:42:LEU:HD11	1:B:105:VAL:HG23	2.01	0.41
1:E:59:LEU:HD23	1:E:59:LEU:HA	1.95	0.41
1:F:128:ASP:HA	1:F:134:HIS:HD2	1.81	0.41
1:C:39:LEU:CD1	1:C:43:GLN:HE21	2.24	0.41
1:D:179:SER:O	1:D:182:ARG:HB2	2.21	0.41
1:F:210:TYR:CD2	1:G:156:VAL:HG13	2.56	0.41
1:B:125:ILE:HG23	1:B:133:PHE:O	2.21	0.41
1:C:76:LYS:NZ	1:C:126:GLU:OE2	2.53	0.41
1:E:88:HIS:HA	1:E:91:TRP:CZ2	2.55	0.41
1:F:166:ARG:HB3	1:F:167:PRO:HD3	2.03	0.41
1:G:27:VAL:HG11	1:G:75:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:117:GLU:H	1:H:117:GLU:CD	2.23	0.41
1:A:102:ALA:O	1:A:105:VAL:HG22	2.20	0.41
1:A:125:ILE:CG2	1:A:126:GLU:N	2.84	0.41
1:D:125:ILE:HG23	1:D:133:PHE:O	2.20	0.41
1:F:41:LEU:O	1:F:57:ARG:NH1	2.54	0.41
1:F:34:THR:O	1:F:38:ILE:HD13	2.21	0.40
1:B:160:THR:CG2	1:C:209:VAL:HG12	2.52	0.40
1:D:98:LEU:HB3	1:D:123:LEU:HD21	2.03	0.40
1:E:103:ALA:HB1	1:E:147:LEU:HD22	2.03	0.40
1:G:189:ASP:OD1	1:G:192:ARG:NH2	2.54	0.40
1:H:39:LEU:HD21	1:H:43:GLN:OE1	2.22	0.40
1:C:22:GLU:OE1	1:C:22:GLU:HA	2.21	0.40
1:D:47:GLN:O	1:D:49:ALA:N	2.55	0.40
1:E:4:SER:O	1:E:8:VAL:HG23	2.21	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	209/240 (87%)	201 (96%)	4 (2%)	4 (2%)	8 36
1	B	208/240 (87%)	202 (97%)	4 (2%)	2 (1%)	15 53
1	C	206/240 (86%)	198 (96%)	6 (3%)	2 (1%)	15 53
1	D	210/240 (88%)	202 (96%)	4 (2%)	4 (2%)	8 36
1	E	209/240 (87%)	199 (95%)	5 (2%)	5 (2%)	6 29
1	F	208/240 (87%)	201 (97%)	4 (2%)	3 (1%)	11 43
1	G	212/240 (88%)	204 (96%)	5 (2%)	3 (1%)	11 43
1	H	208/240 (87%)	199 (96%)	5 (2%)	4 (2%)	8 36
All	All	1670/1920 (87%)	1606 (96%)	37 (2%)	27 (2%)	9 40

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	LYS
1	A	133	PHE
1	B	133	PHE
1	C	133	PHE
1	D	133	PHE
1	F	131	LYS
1	F	133	PHE
1	G	53	ASP
1	G	133	PHE
1	H	125	ILE
1	H	131	LYS
1	H	133	PHE
1	C	131	LYS
1	D	48	GLY
1	D	136	ASP
1	E	2	SER
1	E	133	PHE
1	G	131	LYS
1	A	136	ASP
1	A	216	GLY
1	D	131	LYS
1	E	131	LYS
1	E	136	ASP
1	F	216	GLY
1	B	216	GLY
1	E	216	GLY
1	H	216	GLY

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	192/212 (91%)	187 (97%)	5 (3%)	46	78
1	B	192/212 (91%)	183 (95%)	9 (5%)	26	63
1	C	190/212 (90%)	180 (95%)	10 (5%)	22	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	192/212 (91%)	185 (96%)	7 (4%)	35 70
1	E	193/212 (91%)	184 (95%)	9 (5%)	26 63
1	F	192/212 (91%)	182 (95%)	10 (5%)	23 59
1	G	195/212 (92%)	189 (97%)	6 (3%)	40 75
1	H	192/212 (91%)	184 (96%)	8 (4%)	30 66
All	All	1538/1696 (91%)	1474 (96%)	64 (4%)	30 66

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	3	VAL
1	A	31	LEU
1	A	53	ASP
1	A	190	SER
1	B	3	VAL
1	B	29	GLN
1	B	86	ARG
1	B	97	ARG
1	B	115	THR
1	B	131	LYS
1	B	190	SER
1	B	194	ARG
1	B	214	ILE
1	C	3	VAL
1	C	31	LEU
1	C	34	THR
1	C	53	ASP
1	C	97	ARG
1	C	112	THR
1	C	133	PHE
1	C	147	LEU
1	C	159	VAL
1	C	190	SER
1	D	3	VAL
1	D	8	VAL
1	D	47	GLN
1	D	97	ARG
1	D	112	THR
1	D	190	SER

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Mol	Chain	Res	Type
1	D	214	ILE
1	E	3	VAL
1	E	31	LEU
1	E	95	LEU
1	E	97	ARG
1	E	112	THR
1	E	129	ARG
1	E	137	VAL
1	E	174	ILE
1	E	190	SER
1	F	3	VAL
1	F	27	VAL
1	F	31	LEU
1	F	40	THR
1	F	63	GLU
1	F	67	THR
1	F	95	LEU
1	F	97	ARG
1	F	112	THR
1	F	190	SER
1	G	51	PHE
1	G	97	ARG
1	G	119	VAL
1	G	131	LYS
1	G	189	ASP
1	G	190	SER
1	H	3	VAL
1	H	18	GLN
1	H	31	LEU
1	H	53	ASP
1	H	97	ARG
1	H	112	THR
1	H	130	GLU
1	H	156	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	11	GLN
1	B	83	GLN
1	C	43	GLN
1	D	11	GLN

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Mol	Chain	Res	Type
1	D	47	GLN
1	E	43	GLN
1	E	83	GLN
1	F	90	HIS
1	F	134	HIS
1	H	157	ASN
1	H	169	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	213/240 (88%)	-0.36	0 100 100	40, 72, 106, 127	0
1	B	212/240 (88%)	-0.39	0 100 100	44, 74, 104, 128	0
1	C	210/240 (87%)	-0.22	1 (0%) 91 75	46, 80, 112, 125	0
1	D	214/240 (89%)	-0.33	0 100 100	47, 73, 109, 131	0
1	E	213/240 (88%)	-0.34	1 (0%) 91 75	59, 85, 114, 134	0
1	F	212/240 (88%)	-0.21	0 100 100	60, 91, 122, 136	0
1	G	216/240 (90%)	-0.34	0 100 100	50, 79, 110, 132	0
1	H	212/240 (88%)	-0.18	1 (0%) 91 75	59, 85, 105, 121	0
All	All	1702/1920 (88%)	-0.30	3 (0%) 95 87	40, 81, 112, 136	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	129	ARG	3.2
1	C	129	ARG	2.6
1	E	47	GLN	2.4

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.