Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:56 PM GMT

PDB ID	:	3S7V
Title	:	Unassembled KI Polyomavirus VP1 Pentamer
Authors	:	Neu, U.; Stehle, T.
Deposited on	:	2011-05-27
Resolution	:	2.55 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:

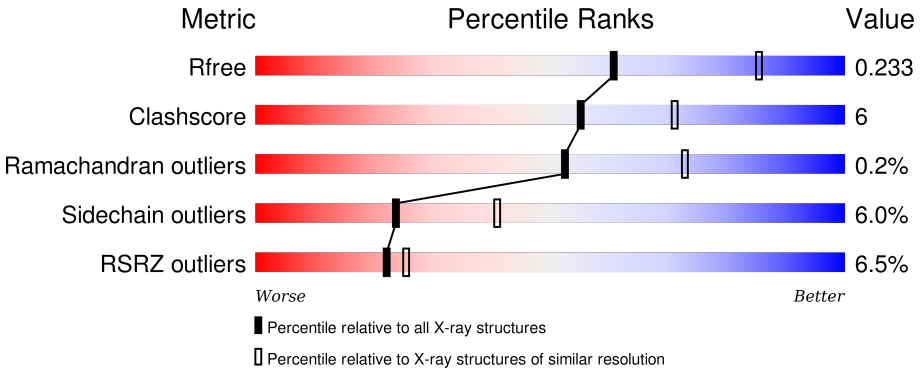
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.55 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	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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	277	4% 79% 12% • 7%
1	B	277	3% 81% 12% • 5%
1	C	277	3% 83% 12% • •
1	D	277	6% 80% 12% • 6%
1	E	277	12% 79% 13% • 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	277	7% 78% 16%
1	G	277	8% 79% 12% 7%
1	H	277	5% 81% 13%
1	I	277	8% 79% 12% 8%
1	J	277	5% 80% 12% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20343 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 Major capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			1987	1261	340	378	8			
1	B	262	Total	C	N	O	S	0	0	0
			2024	1283	350	384	7			
1	C	268	Total	C	N	O	S	0	0	0
			2072	1310	356	397	9			
1	D	261	Total	C	N	O	S	0	0	0
			2019	1280	347	384	8			
1	E	261	Total	C	N	O	S	0	0	0
			2017	1277	348	385	7			
1	F	266	Total	C	N	O	S	0	0	0
			2061	1303	355	394	9			
1	G	258	Total	C	N	O	S	0	0	0
			1995	1265	341	381	8			
1	H	265	Total	C	N	O	S	0	0	0
			2049	1298	349	393	9			
1	I	256	Total	C	N	O	S	0	0	0
			1979	1256	339	377	7			
1	J	261	Total	C	N	O	S	0	0	0
			2023	1281	346	388	8			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	GLY	-	EXPRESSION TAG	UNP A3R4N3
A	29	SER	-	EXPRESSION TAG	UNP A3R4N3
A	30	HIS	-	EXPRESSION TAG	UNP A3R4N3
A	31	MET	-	EXPRESSION TAG	UNP A3R4N3
B	28	GLY	-	EXPRESSION TAG	UNP A3R4N3
B	29	SER	-	EXPRESSION TAG	UNP A3R4N3
B	30	HIS	-	EXPRESSION TAG	UNP A3R4N3
B	31	MET	-	EXPRESSION TAG	UNP A3R4N3
C	28	GLY	-	EXPRESSION TAG	UNP A3R4N3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	29	SER	-	EXPRESSION TAG	UNP A3R4N3
C	30	HIS	-	EXPRESSION TAG	UNP A3R4N3
C	31	MET	-	EXPRESSION TAG	UNP A3R4N3
D	28	GLY	-	EXPRESSION TAG	UNP A3R4N3
D	29	SER	-	EXPRESSION TAG	UNP A3R4N3
D	30	HIS	-	EXPRESSION TAG	UNP A3R4N3
D	31	MET	-	EXPRESSION TAG	UNP A3R4N3
E	28	GLY	-	EXPRESSION TAG	UNP A3R4N3
E	29	SER	-	EXPRESSION TAG	UNP A3R4N3
E	30	HIS	-	EXPRESSION TAG	UNP A3R4N3
E	31	MET	-	EXPRESSION TAG	UNP A3R4N3
F	28	GLY	-	EXPRESSION TAG	UNP A3R4N3
F	29	SER	-	EXPRESSION TAG	UNP A3R4N3
F	30	HIS	-	EXPRESSION TAG	UNP A3R4N3
F	31	MET	-	EXPRESSION TAG	UNP A3R4N3
G	28	GLY	-	EXPRESSION TAG	UNP A3R4N3
G	29	SER	-	EXPRESSION TAG	UNP A3R4N3
G	30	HIS	-	EXPRESSION TAG	UNP A3R4N3
G	31	MET	-	EXPRESSION TAG	UNP A3R4N3
H	28	GLY	-	EXPRESSION TAG	UNP A3R4N3
H	29	SER	-	EXPRESSION TAG	UNP A3R4N3
H	30	HIS	-	EXPRESSION TAG	UNP A3R4N3
H	31	MET	-	EXPRESSION TAG	UNP A3R4N3
I	28	GLY	-	EXPRESSION TAG	UNP A3R4N3
I	29	SER	-	EXPRESSION TAG	UNP A3R4N3
I	30	HIS	-	EXPRESSION TAG	UNP A3R4N3
I	31	MET	-	EXPRESSION TAG	UNP A3R4N3
J	28	GLY	-	EXPRESSION TAG	UNP A3R4N3
J	29	SER	-	EXPRESSION TAG	UNP A3R4N3
J	30	HIS	-	EXPRESSION TAG	UNP A3R4N3
J	31	MET	-	EXPRESSION TAG	UNP A3R4N3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	6	Total O 6 6	0	0
2	B	8	Total O 8 8	0	0
2	C	14	Total O 14 14	0	0
2	D	9	Total O 9 9	0	0

Continued on next page...

Continued from previous page...

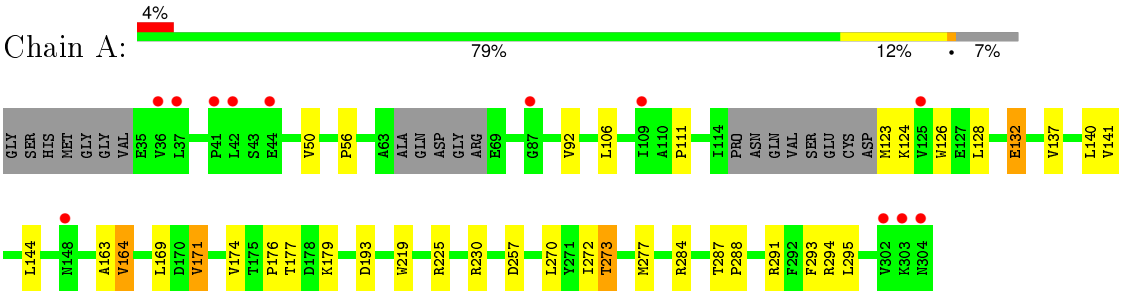
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	4	Total O 4 4	0	0
2	F	18	Total O 18 18	0	0
2	G	13	Total O 13 13	0	0
2	H	6	Total O 6 6	0	0
2	I	23	Total O 23 23	0	0
2	J	16	Total O 16 16	0	0

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.

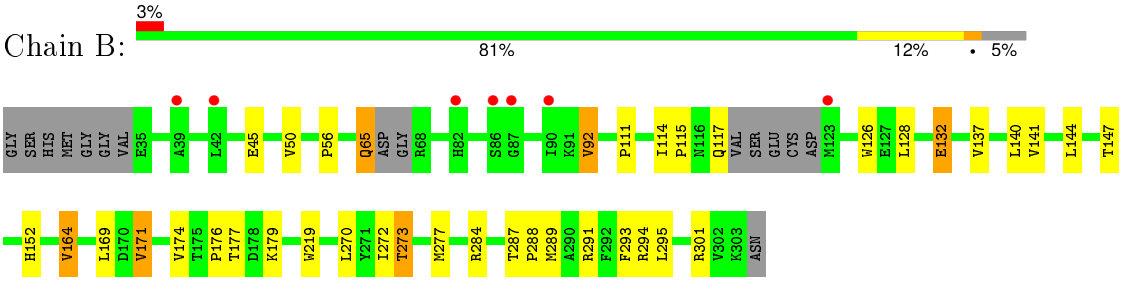
- Molecule 1: Major capsid protein VP1

Chain A:



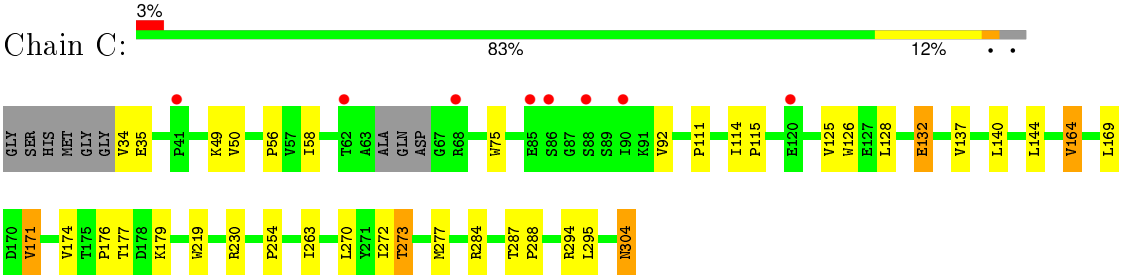
- Molecule 1: Major capsid protein VP1

Chain B:



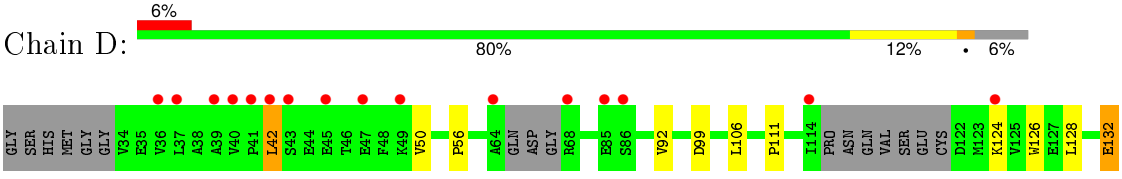
- Molecule 1: Major capsid protein VP1

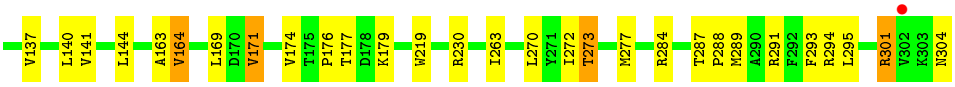
Chain C:



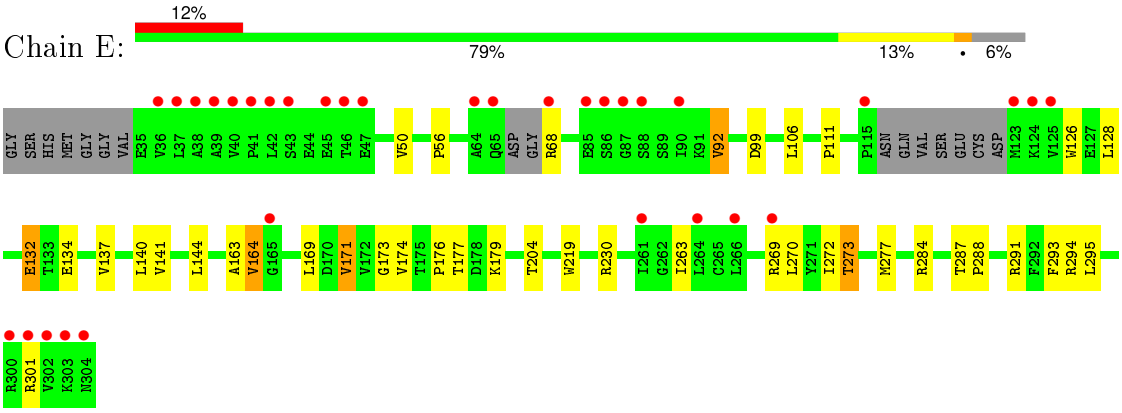
- Molecule 1: Major capsid protein VP1

Chain D:

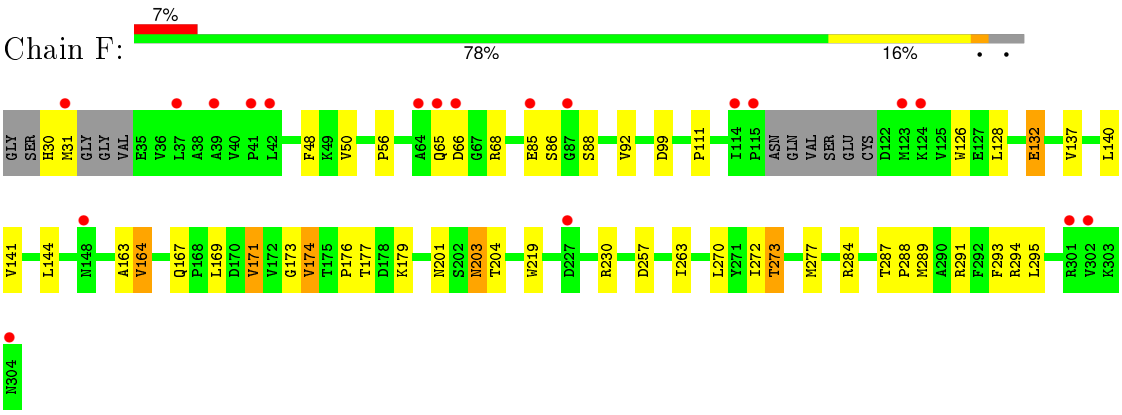




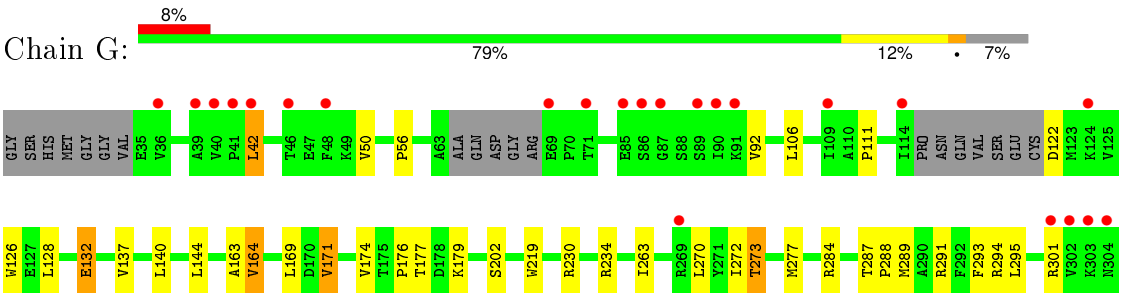
• Molecule 1: Major capsid protein VP1



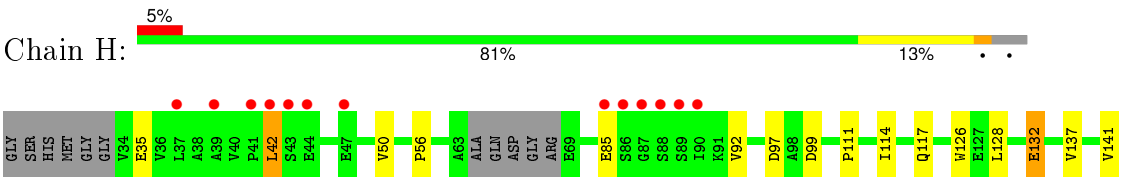
• Molecule 1: Major capsid protein VP1



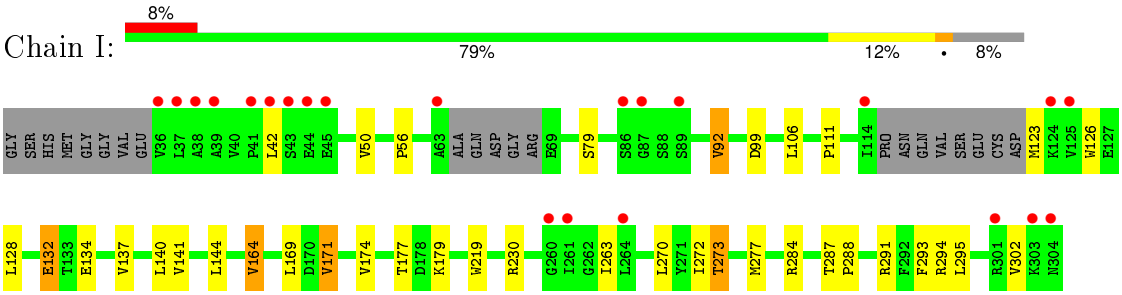
• Molecule 1: Major capsid protein VP1



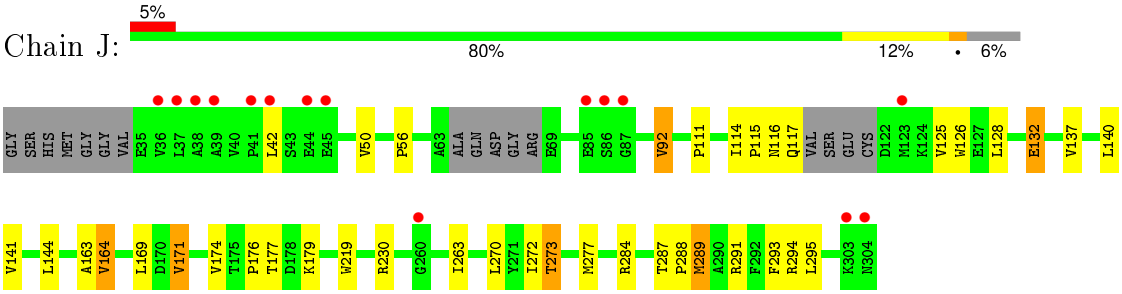
• Molecule 1: Major capsid protein VP1



• Molecule 1: Major capsid protein VP1



• Molecule 1: Major capsid protein VP1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	70.33Å 82.78Å 142.06Å 87.01° 98.23° 108.65°	Depositor
Resolution (Å)	49.27 – 2.55 49.26 – 2.55	Depositor EDS
% Data completeness (in resolution range)	95.9 (49.27-2.55) 95.8 (49.26-2.55)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.202 , 0.219 0.213 , 0.233	Depositor DCC
R_{free} test set	4647 reflections (5.20%)	DCC
Wilson B-factor (Å^2)	56.4	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 93979 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	20343	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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	0.43	0/2037	0.60	0/2783
1	B	0.46	0/2075	0.60	0/2837
1	C	0.46	0/2124	0.63	0/2903
1	D	0.44	0/2069	0.60	1/2826 (0.0%)
1	E	0.44	0/2068	0.60	0/2826
1	F	0.46	0/2113	0.62	0/2885
1	G	0.46	0/2045	0.61	0/2794
1	H	0.48	0/2101	0.63	0/2874
1	I	0.48	0/2029	0.62	0/2773
1	J	0.49	0/2074	0.62	0/2834
All	All	0.46	0/20735	0.61	1/28335 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	42	LEU	CA-CB-CG	5.10	127.04	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1987	0	1955	29	0
1	B	2024	0	1989	24	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2072	0	2032	30	0
1	D	2019	0	1988	24	0
1	E	2017	0	1976	28	0
1	F	2061	0	2019	37	0
1	G	1995	0	1959	27	0
1	H	2049	0	2013	26	0
1	I	1979	0	1946	28	0
1	J	2023	0	1984	26	0
2	A	6	0	0	3	0
2	B	8	0	0	1	0
2	C	14	0	0	4	0
2	D	9	0	0	3	0
2	E	4	0	0	0	0
2	F	18	0	0	2	0
2	G	13	0	0	3	0
2	H	6	0	0	1	0
2	I	23	0	0	5	0
2	J	16	0	0	1	0
All	All	20343	0	19861	254	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 6.

All (254) 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:C:177:THR:HG22	1:C:179:LYS:H	1.13	1.13
1:B:177:THR:HG22	1:B:179:LYS:H	1.18	1.07
1:J:177:THR:HG22	1:J:179:LYS:H	1.12	1.06
1:G:177:THR:HG22	1:G:179:LYS:H	1.19	1.05
1:I:177:THR:HG22	1:I:179:LYS:H	1.20	1.04
1:H:177:THR:HG22	1:H:179:LYS:H	1.19	1.04
1:A:177:THR:HG22	1:A:179:LYS:H	1.20	1.02
1:F:177:THR:HG22	1:F:179:LYS:H	1.21	1.01
1:D:177:THR:HG22	1:D:179:LYS:H	1.19	1.00
1:E:177:THR:HG22	1:E:179:LYS:H	1.20	1.00
1:B:56:PRO:HB3	1:B:287:THR:HG21	1.44	0.99
1:H:56:PRO:HB3	1:H:287:THR:HG21	1.42	0.98
1:E:56:PRO:HB3	1:E:287:THR:HG21	1.46	0.98
1:F:56:PRO:HB3	1:F:287:THR:HG21	1.45	0.97
1:A:56:PRO:HB3	1:A:287:THR:HG21	1.45	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:56:PRO:HB3	1:I:287:THR:HG21	1.46	0.97
1:G:56:PRO:HB3	1:G:287:THR:HG21	1.46	0.95
1:J:56:PRO:HB3	1:J:287:THR:HG21	1.47	0.95
1:D:56:PRO:HB3	1:D:287:THR:HG21	1.46	0.95
1:C:56:PRO:HB3	1:C:287:THR:HG21	1.47	0.95
1:A:123:MET:HG2	1:A:124:LYS:H	1.32	0.91
1:G:56:PRO:CB	1:G:287:THR:HG21	2.01	0.90
1:A:56:PRO:CB	1:A:287:THR:HG21	2.01	0.90
1:H:56:PRO:CB	1:H:287:THR:HG21	2.02	0.89
1:C:56:PRO:CB	1:C:287:THR:HG21	2.02	0.89
1:C:49:LYS:HE3	2:C:306:HOH:O	1.71	0.89
1:C:34:VAL:HG12	1:C:35:GLU:H	1.37	0.88
1:J:56:PRO:CB	1:J:287:THR:HG21	2.02	0.88
1:E:56:PRO:CB	1:E:287:THR:HG21	2.03	0.88
1:F:56:PRO:CB	1:F:287:THR:HG21	2.04	0.87
1:I:56:PRO:CB	1:I:287:THR:HG21	2.04	0.86
1:B:56:PRO:CB	1:B:287:THR:HG21	2.05	0.85
1:F:287:THR:HG22	1:F:288:PRO:O	1.77	0.85
1:H:287:THR:HG22	1:H:288:PRO:O	1.76	0.85
1:D:56:PRO:CB	1:D:287:THR:HG21	2.06	0.85
1:J:287:THR:HG22	1:J:288:PRO:O	1.78	0.84
1:C:287:THR:HG22	1:C:288:PRO:O	1.78	0.83
1:D:287:THR:HG22	1:D:288:PRO:O	1.77	0.83
1:E:287:THR:HG22	1:E:288:PRO:O	1.79	0.82
1:I:287:THR:HG22	1:I:288:PRO:O	1.81	0.81
1:G:287:THR:HG22	1:G:288:PRO:O	1.80	0.81
1:B:287:THR:HG22	1:B:288:PRO:O	1.81	0.80
1:A:287:THR:HG22	1:A:288:PRO:O	1.82	0.79
1:E:269:ARG:HH21	1:F:68:ARG:HG2	1.46	0.79
1:I:273:THR:HG22	2:I:315:HOH:O	1.82	0.79
1:C:254:PRO:HD2	2:C:310:HOH:O	1.83	0.77
1:B:114:ILE:HB	1:B:117:GLN:HG2	1.66	0.76
1:C:177:THR:HG22	1:C:179:LYS:N	1.97	0.75
1:J:177:THR:HG22	1:J:179:LYS:N	1.96	0.74
1:C:277:MET:HE1	2:C:312:HOH:O	1.87	0.74
1:D:272:ILE:HD11	1:D:295:LEU:HD11	1.70	0.73
1:F:272:ILE:HD11	1:F:295:LEU:HD11	1.71	0.73
1:C:230:ARG:HG2	1:C:263:ILE:HD11	1.70	0.72
1:E:177:THR:HG22	1:E:179:LYS:N	2.03	0.72
1:G:177:THR:HG22	1:G:179:LYS:N	2.01	0.72
1:H:177:THR:HG22	1:H:179:LYS:N	2.01	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:272:ILE:HD11	1:H:295:LEU:HD11	1.73	0.71
1:B:177:THR:HG22	1:B:179:LYS:N	2.01	0.71
1:G:42:LEU:HD13	1:G:42:LEU:H	1.56	0.70
1:D:177:THR:HG22	1:D:179:LYS:N	2.02	0.69
1:F:201:ASN:OD1	1:F:203:ASN:HB2	1.92	0.69
1:E:272:ILE:HD11	1:E:295:LEU:HD11	1.74	0.69
1:C:272:ILE:HD11	1:C:295:LEU:HD11	1.73	0.69
1:G:272:ILE:HD11	1:G:295:LEU:HD11	1.74	0.69
1:J:272:ILE:HD11	1:J:295:LEU:HD11	1.74	0.69
1:I:272:ILE:HD11	1:I:295:LEU:HD11	1.75	0.68
1:A:272:ILE:HD11	1:A:295:LEU:HD11	1.76	0.68
1:B:65:GLN:HA	1:B:65:GLN:HE21	1.58	0.68
1:F:273:THR:HG22	2:F:306:HOH:O	1.95	0.67
2:I:309:HOH:O	1:J:92:VAL:HG13	1.95	0.67
2:H:310:HOH:O	1:I:92:VAL:HG13	1.95	0.66
1:B:272:ILE:HD11	1:B:295:LEU:HD11	1.76	0.66
1:A:123:MET:CG	1:A:124:LYS:H	2.08	0.65
1:J:56:PRO:HB3	1:J:287:THR:CG2	2.25	0.65
1:A:177:THR:HG22	1:A:179:LYS:N	2.03	0.65
1:F:273:THR:CG2	2:F:306:HOH:O	2.44	0.64
1:G:56:PRO:HB3	1:G:287:THR:CG2	2.24	0.64
1:I:177:THR:HG22	1:I:179:LYS:N	2.03	0.64
1:E:230:ARG:HG2	1:E:263:ILE:HD11	1.80	0.63
1:J:117:GLN:HA	1:J:117:GLN:OE1	1.97	0.63
1:J:230:ARG:HG2	1:J:263:ILE:HD11	1.82	0.62
1:C:56:PRO:HB3	1:C:287:THR:CG2	2.27	0.61
1:G:277:MET:CE	2:G:305:HOH:O	2.48	0.61
1:I:273:THR:CG2	2:I:315:HOH:O	2.42	0.61
1:E:56:PRO:HB3	1:E:287:THR:CG2	2.26	0.61
2:A:306:HOH:O	1:B:92:VAL:HG13	1.99	0.61
1:A:225:ARG:NH2	1:G:202:SER:O	2.33	0.61
1:C:34:VAL:HG12	1:C:35:GLU:N	2.14	0.60
1:A:56:PRO:HB3	1:A:287:THR:CG2	2.25	0.60
1:C:304:ASN:ND2	1:C:304:ASN:H	1.99	0.60
1:C:277:MET:CE	2:C:312:HOH:O	2.45	0.60
1:H:56:PRO:HB3	1:H:287:THR:CG2	2.24	0.59
1:A:123:MET:HG2	1:A:124:LYS:N	2.09	0.59
1:I:56:PRO:HB3	1:I:287:THR:CG2	2.27	0.58
1:D:56:PRO:HB3	1:D:287:THR:CG2	2.28	0.58
1:G:277:MET:HE1	2:G:305:HOH:O	2.02	0.58
2:A:307:HOH:O	1:E:134:GLU:HG2	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:LEU:HB2	1:A:273:THR:HG21	1.86	0.58
1:F:177:THR:HG22	1:F:179:LYS:N	2.04	0.57
1:B:56:PRO:HB3	1:B:287:THR:CG2	2.28	0.57
1:H:42:LEU:H	1:H:42:LEU:HD22	1.69	0.57
1:D:287:THR:HG23	1:D:288:PRO:HD2	1.87	0.57
1:F:287:THR:HG23	1:F:288:PRO:HD2	1.88	0.56
1:B:287:THR:HG23	1:B:288:PRO:HD2	1.88	0.56
1:H:35:GLU:HB3	1:H:303:LYS:HB3	1.89	0.55
1:F:164:VAL:HG22	1:F:270:LEU:HD21	1.89	0.55
1:F:56:PRO:HB3	1:F:287:THR:CG2	2.27	0.55
1:J:169:LEU:HB2	1:J:273:THR:HG21	1.88	0.55
1:H:169:LEU:HB2	1:H:273:THR:HG21	1.87	0.55
1:I:169:LEU:HB2	1:I:273:THR:HG21	1.90	0.54
1:B:171:VAL:HG13	1:B:219:TRP:CE3	2.43	0.54
1:F:230:ARG:NH2	1:F:257:ASP:HB3	2.23	0.54
1:G:169:LEU:HB2	1:G:273:THR:HG21	1.91	0.53
1:A:164:VAL:HG22	1:A:270:LEU:HD21	1.90	0.53
1:I:164:VAL:HG22	1:I:270:LEU:HD21	1.89	0.53
1:F:169:LEU:HB2	1:F:273:THR:HG21	1.90	0.53
1:D:164:VAL:HG22	1:D:270:LEU:HD21	1.91	0.53
1:C:164:VAL:HG22	1:C:270:LEU:HD21	1.90	0.53
1:C:171:VAL:HG13	1:C:219:TRP:CE3	2.44	0.53
1:D:169:LEU:HB2	1:D:273:THR:HG21	1.89	0.52
1:E:164:VAL:HG22	1:E:270:LEU:HD21	1.91	0.52
1:E:171:VAL:HG13	1:E:219:TRP:CE3	2.45	0.52
1:E:169:LEU:HB2	1:E:273:THR:HG21	1.91	0.52
1:F:30:HIS:CE1	1:F:167:GLN:HG3	2.44	0.52
1:H:287:THR:HG23	1:H:288:PRO:HD2	1.90	0.52
1:A:171:VAL:HG13	1:A:219:TRP:CE3	2.45	0.52
1:F:171:VAL:HG13	1:F:219:TRP:CE3	2.45	0.52
1:B:164:VAL:HG22	1:B:270:LEU:HD21	1.91	0.51
1:B:169:LEU:HB2	1:B:273:THR:HG21	1.90	0.51
1:F:111:PRO:HB2	1:F:126:TRP:CD1	2.45	0.51
1:C:140:LEU:HD22	1:D:176:PRO:HB3	1.93	0.51
1:A:230:ARG:NH2	1:A:257:ASP:HB3	2.25	0.51
1:A:140:LEU:HD22	1:B:176:PRO:HB3	1.93	0.51
1:I:171:VAL:HG13	1:I:219:TRP:CE3	2.45	0.51
1:G:171:VAL:HG13	1:G:219:TRP:CE3	2.46	0.51
2:I:22:HOH:O	1:J:230:ARG:HD2	2.11	0.50
1:F:30:HIS:O	1:F:31:MET:HB2	2.11	0.50
1:H:171:VAL:HG13	1:H:219:TRP:CE3	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:THR:HG23	1:A:288:PRO:HD2	1.94	0.50
1:B:171:VAL:HG13	1:B:219:TRP:HE3	1.77	0.50
1:D:171:VAL:HG13	1:D:219:TRP:CE3	2.46	0.50
1:E:287:THR:HG23	1:E:288:PRO:HD2	1.93	0.50
1:F:140:LEU:HD22	1:G:176:PRO:HB3	1.94	0.50
1:I:230:ARG:HG2	1:I:263:ILE:HD11	1.93	0.49
1:H:141:VAL:HG21	1:I:277:MET:CE	2.42	0.49
1:I:134:GLU:HG2	2:J:309:HOH:O	2.11	0.49
1:H:230:ARG:HG2	1:H:263:ILE:HD11	1.94	0.49
1:J:171:VAL:HG13	1:J:219:TRP:CE3	2.47	0.49
1:A:171:VAL:HG13	1:A:219:TRP:HE3	1.78	0.49
1:I:171:VAL:HG13	1:I:219:TRP:HE3	1.78	0.48
1:F:132:GLU:HG2	1:F:294:ARG:HB3	1.96	0.48
1:A:111:PRO:HB2	1:A:126:TRP:CD1	2.49	0.48
1:G:287:THR:HG23	1:G:288:PRO:HD2	1.96	0.48
1:A:176:PRO:HB3	1:E:140:LEU:HD22	1.95	0.48
1:I:141:VAL:HG21	1:J:277:MET:CE	2.43	0.48
1:H:164:VAL:HG22	1:H:270:LEU:HD21	1.96	0.47
1:C:169:LEU:HB2	1:C:273:THR:HG21	1.95	0.47
1:C:287:THR:HG23	1:C:288:PRO:HD2	1.95	0.47
1:E:111:PRO:HB2	1:E:126:TRP:CD1	2.50	0.47
1:F:173:GLY:O	1:F:204:THR:HG23	2.15	0.47
1:F:171:VAL:HG13	1:F:219:TRP:HE3	1.80	0.47
1:F:291:ARG:HG2	1:F:293:PHE:CE1	2.50	0.47
1:I:287:THR:HG23	1:I:288:PRO:HD2	1.96	0.47
1:I:277:MET:HE1	2:I:310:HOH:O	2.14	0.47
2:D:305:HOH:O	1:E:92:VAL:HG13	2.15	0.47
1:J:164:VAL:HG22	1:J:270:LEU:HD21	1.97	0.47
1:D:230:ARG:HG2	1:D:263:ILE:HD11	1.96	0.47
1:D:163:ALA:HB3	1:D:273:THR:HG23	1.97	0.46
1:J:287:THR:HG23	1:J:288:PRO:HD2	1.96	0.46
1:C:132:GLU:HG2	1:C:294:ARG:HB3	1.97	0.46
1:G:234:ARG:HD2	2:G:25:HOH:O	2.14	0.46
1:G:164:VAL:HG22	1:G:270:LEU:HD21	1.98	0.46
1:G:291:ARG:HG2	1:G:293:PHE:CE1	2.51	0.46
1:C:171:VAL:HG13	1:C:219:TRP:HE3	1.79	0.46
1:B:291:ARG:HG2	1:B:293:PHE:CE1	2.51	0.46
1:G:230:ARG:HG2	1:G:263:ILE:HD11	1.98	0.46
1:H:201:ASN:H	1:H:204:THR:HG1	1.63	0.46
1:G:171:VAL:HG13	1:G:219:TRP:HE3	1.80	0.45
1:A:193:ASP:OD2	1:F:48:PHE:HD1	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:171:VAL:HG13	1:H:219:TRP:HE3	1.82	0.45
1:C:114:ILE:HA	1:C:115:PRO:HD3	1.74	0.45
1:E:171:VAL:HG13	1:E:219:TRP:HE3	1.79	0.45
1:D:111:PRO:HB2	1:D:126:TRP:CD1	2.52	0.45
1:B:132:GLU:HG2	1:B:294:ARG:HB3	1.97	0.45
1:B:111:PRO:HB2	1:B:126:TRP:CD1	2.52	0.45
1:J:111:PRO:HB2	1:J:126:TRP:CD1	2.52	0.45
1:F:176:PRO:HB3	1:J:140:LEU:HD22	1.98	0.45
1:H:132:GLU:HG2	1:H:294:ARG:HB3	1.98	0.45
1:D:171:VAL:HG13	1:D:219:TRP:HE3	1.80	0.45
1:J:132:GLU:HG2	1:J:294:ARG:HB3	1.99	0.45
1:H:163:ALA:HB3	1:H:273:THR:HG23	1.97	0.45
1:F:230:ARG:HG2	1:F:263:ILE:HD11	1.99	0.45
1:A:291:ARG:HG2	1:A:293:PHE:CE1	2.52	0.45
1:G:132:GLU:HG2	1:G:294:ARG:HB3	1.99	0.44
1:I:140:LEU:HD22	1:J:176:PRO:HB3	1.99	0.44
1:B:114:ILE:O	1:B:115:PRO:C	2.56	0.44
1:D:132:GLU:HG2	1:D:294:ARG:HB3	1.98	0.44
1:E:269:ARG:NH2	1:F:68:ARG:HG2	2.24	0.44
1:G:111:PRO:HB2	1:G:126:TRP:CD1	2.53	0.44
1:H:111:PRO:HB2	1:H:126:TRP:CD1	2.52	0.44
1:A:277:MET:HE1	2:A:309:HOH:O	2.17	0.44
1:D:141:VAL:HG21	1:E:277:MET:CE	2.47	0.44
1:I:132:GLU:HG2	1:I:294:ARG:HB3	2.00	0.44
2:B:306:HOH:O	1:C:230:ARG:HD2	2.18	0.44
1:A:132:GLU:HG2	1:A:294:ARG:HB3	2.00	0.44
1:E:173:GLY:O	1:E:204:THR:HG23	2.18	0.43
1:F:65:GLN:HG3	1:F:68:ARG:HB2	2.00	0.43
1:D:277:MET:HE1	2:D:308:HOH:O	2.18	0.43
1:B:141:VAL:HG21	1:C:277:MET:CE	2.48	0.43
1:C:111:PRO:HB2	1:C:126:TRP:CD1	2.53	0.43
1:B:140:LEU:HD22	1:C:176:PRO:HB3	1.99	0.43
1:B:147:THR:OG1	1:B:152:HIS:NE2	2.48	0.43
1:J:171:VAL:HG13	1:J:219:TRP:HE3	1.83	0.43
1:G:163:ALA:HB3	1:G:273:THR:HG23	2.00	0.43
1:G:140:LEU:HD22	1:H:176:PRO:HB3	2.01	0.43
1:H:141:VAL:HG21	1:I:277:MET:HE1	2.00	0.43
1:F:277:MET:CE	1:J:141:VAL:HG21	2.48	0.43
1:E:132:GLU:HG2	1:E:294:ARG:HB3	2.00	0.43
1:G:106:LEU:HD23	1:G:273:THR:HB	2.01	0.42
1:F:85:GLU:HG2	1:F:88:SER:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:LEU:HD22	1:C:295:LEU:HD13	2.02	0.42
1:E:291:ARG:HG2	1:E:293:PHE:CE1	2.54	0.42
1:F:65:GLN:CG	1:F:68:ARG:HB2	2.49	0.42
1:I:111:PRO:HB2	1:I:126:TRP:CD1	2.54	0.42
1:A:277:MET:HE1	1:E:141:VAL:HG21	2.01	0.42
1:I:123:MET:O	1:I:302:VAL:HG22	2.19	0.42
1:H:270:LEU:HD22	1:H:295:LEU:HD13	2.02	0.42
1:J:163:ALA:HB3	1:J:273:THR:HG23	2.01	0.41
1:A:277:MET:CE	1:E:141:VAL:HG21	2.50	0.41
1:A:141:VAL:HG21	1:B:277:MET:CE	2.49	0.41
1:H:114:ILE:O	1:H:117:GLN:HB2	2.19	0.41
1:H:230:ARG:NH2	1:H:257:ASP:HB3	2.36	0.41
1:F:141:VAL:HG21	1:G:277:MET:HE1	2.02	0.41
1:F:163:ALA:HB3	1:F:273:THR:HG23	2.02	0.41
1:I:79:SER:HB2	1:I:99:ASP:HB3	2.03	0.41
1:H:97:ASP:HB3	1:H:99:ASP:HB2	2.03	0.41
1:F:66:ASP:O	1:F:68:ARG:HD2	2.20	0.41
1:F:174:VAL:CG2	1:J:289:MET:HG2	2.51	0.41
1:E:106:LEU:HD23	1:E:273:THR:HB	2.02	0.41
1:I:106:LEU:HD23	1:I:273:THR:HB	2.03	0.41
1:F:141:VAL:HG21	1:G:277:MET:CE	2.51	0.41
1:A:106:LEU:HD23	1:A:273:THR:HB	2.03	0.41
1:D:106:LEU:HD23	1:D:273:THR:HB	2.03	0.41
1:D:124:LYS:HE2	1:D:301:ARG:HH22	1.86	0.41
1:I:291:ARG:HG2	1:I:293:PHE:CE1	2.56	0.41
1:D:140:LEU:HD22	1:E:176:PRO:HB3	2.01	0.41
1:J:114:ILE:HA	1:J:115:PRO:HD2	1.92	0.41
1:C:304:ASN:H	1:C:304:ASN:HD22	1.69	0.40
1:A:163:ALA:HB3	1:A:273:THR:HG23	2.03	0.40
1:D:277:MET:CE	2:D:308:HOH:O	2.69	0.40
1:C:58:ILE:HD12	1:C:75:TRP:HB2	2.03	0.40
1:J:291:ARG:HG2	1:J:293:PHE:CE1	2.57	0.40
1:E:163:ALA:HB3	1:E:273:THR:HG23	2.04	0.40
1:D:291:ARG:HG2	1:D:293:PHE:CE1	2.56	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	251/277 (91%)	242 (96%)	9 (4%)	0	100	100
1	B	256/277 (92%)	246 (96%)	10 (4%)	0	100	100
1	C	264/277 (95%)	254 (96%)	10 (4%)	0	100	100
1	D	255/277 (92%)	244 (96%)	10 (4%)	1 (0%)	39	60
1	E	255/277 (92%)	245 (96%)	9 (4%)	1 (0%)	39	60
1	F	260/277 (94%)	250 (96%)	8 (3%)	2 (1%)	24	40
1	G	252/277 (91%)	240 (95%)	12 (5%)	0	100	100
1	H	261/277 (94%)	248 (95%)	13 (5%)	0	100	100
1	I	250/277 (90%)	241 (96%)	8 (3%)	1 (0%)	39	60
1	J	255/277 (92%)	245 (96%)	9 (4%)	1 (0%)	39	60
All	All	2559/2770 (92%)	2455 (96%)	98 (4%)	6 (0%)	52	73

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	86	SER
1	F	99	ASP
1	J	42	LEU
1	D	99	ASP
1	E	99	ASP
1	I	42	LEU

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	220/236 (93%)	209 (95%)	11 (5%)	30	51
1	B	223/236 (94%)	208 (93%)	15 (7%)	20	35
1	C	230/236 (98%)	217 (94%)	13 (6%)	25	44
1	D	223/236 (94%)	208 (93%)	15 (7%)	20	35
1	E	222/236 (94%)	209 (94%)	13 (6%)	24	42
1	F	228/236 (97%)	215 (94%)	13 (6%)	25	44
1	G	221/236 (94%)	206 (93%)	15 (7%)	20	34
1	H	229/236 (97%)	214 (93%)	15 (7%)	21	36
1	I	219/236 (93%)	208 (95%)	11 (5%)	30	51
1	J	225/236 (95%)	211 (94%)	14 (6%)	23	39
All	All	2240/2360 (95%)	2105 (94%)	135 (6%)	24	41

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	VAL
1	A	92	VAL
1	A	128	LEU
1	A	132	GLU
1	A	137	VAL
1	A	144	LEU
1	A	164	VAL
1	A	171	VAL
1	A	174	VAL
1	A	273	THR
1	A	284	ARG
1	B	45	GLU
1	B	50	VAL
1	B	65	GLN
1	B	92	VAL
1	B	128	LEU
1	B	132	GLU
1	B	137	VAL
1	B	144	LEU
1	B	164	VAL
1	B	171	VAL
1	B	174	VAL
1	B	273	THR
1	B	284	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	289	MET
1	B	301	ARG
1	C	50	VAL
1	C	92	VAL
1	C	125	VAL
1	C	128	LEU
1	C	132	GLU
1	C	137	VAL
1	C	144	LEU
1	C	164	VAL
1	C	171	VAL
1	C	174	VAL
1	C	273	THR
1	C	284	ARG
1	C	304	ASN
1	D	42	LEU
1	D	50	VAL
1	D	92	VAL
1	D	128	LEU
1	D	132	GLU
1	D	137	VAL
1	D	144	LEU
1	D	164	VAL
1	D	171	VAL
1	D	174	VAL
1	D	273	THR
1	D	284	ARG
1	D	289	MET
1	D	301	ARG
1	D	304	ASN
1	E	50	VAL
1	E	68	ARG
1	E	92	VAL
1	E	128	LEU
1	E	132	GLU
1	E	137	VAL
1	E	144	LEU
1	E	164	VAL
1	E	171	VAL
1	E	174	VAL
1	E	273	THR
1	E	284	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	301	ARG
1	F	50	VAL
1	F	92	VAL
1	F	128	LEU
1	F	132	GLU
1	F	137	VAL
1	F	144	LEU
1	F	164	VAL
1	F	171	VAL
1	F	174	VAL
1	F	203	ASN
1	F	273	THR
1	F	284	ARG
1	F	289	MET
1	G	42	LEU
1	G	50	VAL
1	G	92	VAL
1	G	122	ASP
1	G	128	LEU
1	G	132	GLU
1	G	137	VAL
1	G	144	LEU
1	G	164	VAL
1	G	171	VAL
1	G	174	VAL
1	G	273	THR
1	G	284	ARG
1	G	289	MET
1	G	301	ARG
1	H	42	LEU
1	H	50	VAL
1	H	85	GLU
1	H	92	VAL
1	H	128	LEU
1	H	132	GLU
1	H	137	VAL
1	H	144	LEU
1	H	164	VAL
1	H	171	VAL
1	H	174	VAL
1	H	273	THR
1	H	284	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	289	MET
1	H	303	LYS
1	I	50	VAL
1	I	92	VAL
1	I	128	LEU
1	I	132	GLU
1	I	137	VAL
1	I	144	LEU
1	I	164	VAL
1	I	171	VAL
1	I	174	VAL
1	I	273	THR
1	I	284	ARG
1	J	50	VAL
1	J	92	VAL
1	J	116	ASN
1	J	125	VAL
1	J	128	LEU
1	J	132	GLU
1	J	137	VAL
1	J	144	LEU
1	J	164	VAL
1	J	171	VAL
1	J	174	VAL
1	J	273	THR
1	J	284	ARG
1	J	289	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	286	HIS
1	B	65	GLN
1	B	142	ASN
1	B	286	HIS
1	C	142	ASN
1	C	304	ASN
1	D	142	ASN
1	D	286	HIS
1	D	304	ASN
1	E	142	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	286	HIS
1	F	142	ASN
1	F	286	HIS
1	G	142	ASN
1	G	286	HIS
1	H	142	ASN
1	H	286	HIS
1	I	142	ASN
1	J	142	ASN
1	J	286	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 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	257/277 (92%)	0.57	12 (4%) 35 41	40, 61, 94, 127	0
1	B	262/277 (94%)	0.34	7 (2%) 58 63	38, 60, 87, 114	0
1	C	268/277 (96%)	0.35	8 (2%) 54 60	38, 56, 82, 99	0
1	D	261/277 (94%)	0.52	17 (6%) 22 25	39, 64, 100, 115	0
1	E	261/277 (94%)	0.69	33 (12%) 5 5	39, 62, 97, 130	0
1	F	266/277 (96%)	0.49	19 (7%) 19 22	37, 58, 95, 124	0
1	G	258/277 (93%)	0.60	23 (8%) 12 13	36, 60, 93, 127	0
1	H	265/277 (95%)	0.44	14 (5%) 30 35	36, 60, 97, 121	0
1	I	256/277 (92%)	0.51	22 (8%) 13 14	35, 55, 88, 114	0
1	J	261/277 (94%)	0.53	15 (5%) 27 32	35, 56, 87, 116	0
All	All	2615/2770 (94%)	0.50	170 (6%) 22 25	35, 59, 95, 130	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	42	LEU	6.6
1	E	64	ALA	6.4
1	E	41	PRO	5.8
1	A	304	ASN	5.7
1	A	37	LEU	5.6
1	G	89	SER	5.6
1	J	304	ASN	5.3
1	I	304	ASN	5.3
1	A	42	LEU	5.2
1	D	41	PRO	5.1
1	G	41	PRO	5.1
1	E	42	LEU	4.9
1	F	302	VAL	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	39	ALA	4.7
1	E	304	ASN	4.6
1	E	37	LEU	4.5
1	J	41	PRO	4.5
1	E	266	LEU	4.4
1	F	42	LEU	4.4
1	F	64	ALA	4.4
1	G	87	GLY	4.3
1	G	86	SER	4.3
1	E	40	VAL	4.2
1	J	39	ALA	4.1
1	I	41	PRO	4.1
1	F	37	LEU	4.1
1	E	38	ALA	4.1
1	A	302	VAL	4.0
1	E	125	VAL	4.0
1	D	85	GLU	4.0
1	H	39	ALA	4.0
1	B	39	ALA	3.9
1	C	41	PRO	3.9
1	G	90	ILE	3.9
1	E	88	SER	3.9
1	E	303	LYS	3.8
1	D	114	ILE	3.8
1	J	37	LEU	3.7
1	G	124	LYS	3.7
1	I	42	LEU	3.7
1	J	44	GLU	3.7
1	H	87	GLY	3.6
1	F	115	PRO	3.6
1	I	37	LEU	3.6
1	D	86	SER	3.6
1	C	90	ILE	3.6
1	E	43	SER	3.6
1	E	87	GLY	3.5
1	I	87	GLY	3.5
1	I	36	VAL	3.5
1	G	40	VAL	3.5
1	E	46	THR	3.4
1	J	86	SER	3.4
1	C	68	ARG	3.4
1	A	109	ILE	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	49	LYS	3.4
1	B	90	ILE	3.4
1	H	89	SER	3.3
1	I	86	SER	3.3
1	A	36	VAL	3.3
1	H	85	GLU	3.3
1	A	41	PRO	3.2
1	H	41	PRO	3.2
1	I	43	SER	3.2
1	F	301	ARG	3.2
1	J	87	GLY	3.2
1	F	87	GLY	3.2
1	I	303	LYS	3.2
1	G	304	ASN	3.1
1	H	42	LEU	3.1
1	E	264	LEU	3.1
1	E	261	ILE	3.1
1	D	45	GLU	3.0
1	E	85	GLU	3.0
1	J	42	LEU	3.0
1	J	45	GLU	3.0
1	I	63	ALA	3.0
1	G	42	LEU	3.0
1	B	87	GLY	2.9
1	I	44	GLU	2.9
1	J	38	ALA	2.9
1	D	36	VAL	2.9
1	H	86	SER	2.9
1	D	124	LYS	2.9
1	I	264	LEU	2.9
1	B	86	SER	2.8
1	J	303	LYS	2.8
1	I	39	ALA	2.8
1	D	64	ALA	2.8
1	D	43	SER	2.8
1	E	165	GLY	2.8
1	J	123	MET	2.8
1	I	45	GLU	2.8
1	G	85	GLU	2.8
1	D	40	VAL	2.7
1	G	36	VAL	2.7
1	E	124	LYS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	300	ARG	2.7
1	J	85	GLU	2.7
1	E	68	ARG	2.7
1	E	86	SER	2.7
1	I	125	VAL	2.7
1	A	87	GLY	2.6
1	A	44	GLU	2.6
1	E	39	ALA	2.6
1	F	66	ASP	2.6
1	I	38	ALA	2.6
1	G	91	LYS	2.6
1	G	39	ALA	2.6
1	C	86	SER	2.6
1	E	123	MET	2.6
1	J	36	VAL	2.6
1	E	269	ARG	2.5
1	A	303	LYS	2.5
1	B	123	MET	2.5
1	G	69	GLU	2.5
1	G	46	THR	2.5
1	F	31	MET	2.5
1	A	148	ASN	2.5
1	H	44	GLU	2.5
1	G	109	ILE	2.4
1	F	123	MET	2.4
1	F	85	GLU	2.4
1	I	124	LYS	2.4
1	H	90	ILE	2.4
1	I	261	ILE	2.4
1	H	88	SER	2.4
1	E	301	ARG	2.4
1	E	302	VAL	2.4
1	G	71	THR	2.4
1	J	260	GLY	2.3
1	D	47	GLU	2.3
1	D	302	VAL	2.3
1	F	304	ASN	2.3
1	D	37	LEU	2.3
1	F	114	ILE	2.3
1	I	89	SER	2.3
1	B	42	LEU	2.3
1	C	62	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	301	ARG	2.2
1	F	65	GLN	2.2
1	E	65	GLN	2.2
1	E	45	GLU	2.2
1	I	260	GLY	2.2
1	E	47	GLU	2.2
1	H	37	LEU	2.2
1	F	39	ALA	2.1
1	I	114	ILE	2.1
1	F	41	PRO	2.1
1	C	85	GLU	2.1
1	F	124	LYS	2.1
1	H	47	GLU	2.1
1	F	148	ASN	2.1
1	F	227	ASP	2.1
1	D	68	ARG	2.1
1	E	115	PRO	2.1
1	C	88	SER	2.1
1	G	303	LYS	2.1
1	E	36	VAL	2.1
1	G	48	PHE	2.1
1	H	302	VAL	2.0
1	G	114	ILE	2.0
1	G	301	ARG	2.0
1	A	125	VAL	2.0
1	G	302	VAL	2.0
1	E	90	ILE	2.0
1	C	120	GLU	2.0
1	G	269	ARG	2.0
1	B	82	HIS	2.0
1	H	43	SER	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.