Full wwPDB X-ray Structure Validation Report

Feb 19, 2016 – 07:34 PM GMT

PDB ID	:	4U5Z
Title	:	Trichodysplasia spinulosa-associated polyomavirus (TSPyV) VP1
Authors	:	Stroh, L.J.; Stehle, T.
Deposited on	:	2014-07-26
Resolution	:	2.10 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:

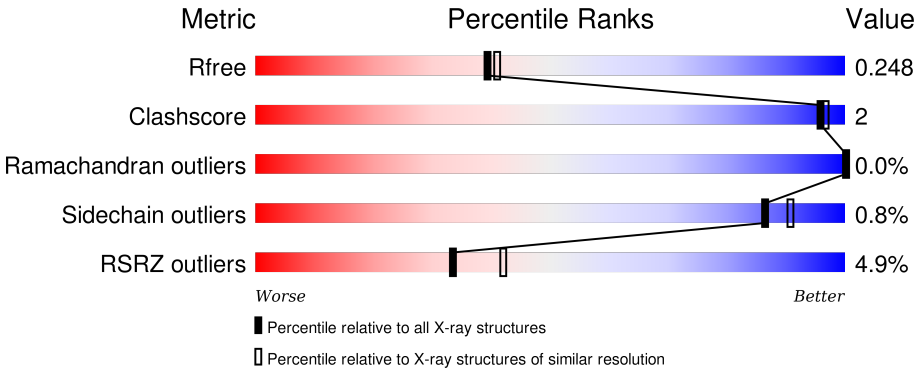
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	280	5% 93% · ·
1	B	280	4% 90% 5% 5%
1	C	280	2% 92% 5% ·
1	D	280	5% 90% · 6%
1	E	280	4% 89% 5% 5%

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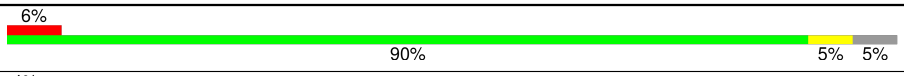
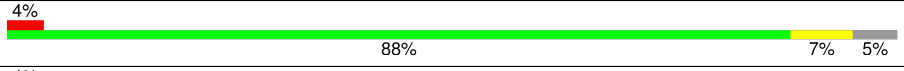
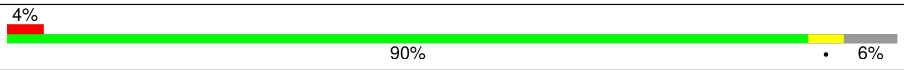
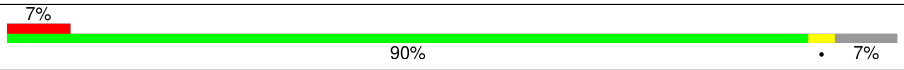
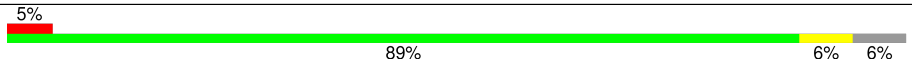
Mol	Chain	Length	Quality of chain
1	F	280	
1	G	280	
1	H	280	
1	I	280	
1	J	280	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20926 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 Structural protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	0
			2096	1318	352	412	14			
1	B	266	Total	C	N	O	S	0	0	0
			2063	1298	346	406	13			
1	C	270	Total	C	N	O	S	0	1	0
			2092	1314	351	413	14			
1	D	263	Total	C	N	O	S	0	0	0
			2017	1274	338	393	12			
1	E	265	Total	C	N	O	S	0	0	0
			2045	1291	341	401	12			
1	F	265	Total	C	N	O	S	0	0	0
			2028	1275	340	400	13			
1	G	265	Total	C	N	O	S	0	0	0
			2030	1280	340	397	13			
1	H	264	Total	C	N	O	S	0	0	0
			2038	1281	341	403	13			
1	I	260	Total	C	N	O	S	0	0	0
			1974	1245	327	390	12			
1	J	264	Total	C	N	O	S	0	0	0
			1992	1257	331	392	12			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	GLY	-	expression tag	UNP E2ESL7
A	25	SER	-	expression tag	UNP E2ESL7
A	26	HIS	-	expression tag	UNP E2ESL7
A	27	MET	-	expression tag	UNP E2ESL7
A	28	ALA	-	expression tag	UNP E2ESL7
A	29	SER	-	expression tag	UNP E2ESL7
B	24	GLY	-	expression tag	UNP E2ESL7
B	25	SER	-	expression tag	UNP E2ESL7
B	26	HIS	-	expression tag	UNP E2ESL7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	27	MET	-	expression tag	UNP E2ESL7
B	28	ALA	-	expression tag	UNP E2ESL7
B	29	SER	-	expression tag	UNP E2ESL7
C	24	GLY	-	expression tag	UNP E2ESL7
C	25	SER	-	expression tag	UNP E2ESL7
C	26	HIS	-	expression tag	UNP E2ESL7
C	27	MET	-	expression tag	UNP E2ESL7
C	28	ALA	-	expression tag	UNP E2ESL7
C	29	SER	-	expression tag	UNP E2ESL7
D	24	GLY	-	expression tag	UNP E2ESL7
D	25	SER	-	expression tag	UNP E2ESL7
D	26	HIS	-	expression tag	UNP E2ESL7
D	27	MET	-	expression tag	UNP E2ESL7
D	28	ALA	-	expression tag	UNP E2ESL7
D	29	SER	-	expression tag	UNP E2ESL7
E	24	GLY	-	expression tag	UNP E2ESL7
E	25	SER	-	expression tag	UNP E2ESL7
E	26	HIS	-	expression tag	UNP E2ESL7
E	27	MET	-	expression tag	UNP E2ESL7
E	28	ALA	-	expression tag	UNP E2ESL7
E	29	SER	-	expression tag	UNP E2ESL7
F	24	GLY	-	expression tag	UNP E2ESL7
F	25	SER	-	expression tag	UNP E2ESL7
F	26	HIS	-	expression tag	UNP E2ESL7
F	27	MET	-	expression tag	UNP E2ESL7
F	28	ALA	-	expression tag	UNP E2ESL7
F	29	SER	-	expression tag	UNP E2ESL7
G	24	GLY	-	expression tag	UNP E2ESL7
G	25	SER	-	expression tag	UNP E2ESL7
G	26	HIS	-	expression tag	UNP E2ESL7
G	27	MET	-	expression tag	UNP E2ESL7
G	28	ALA	-	expression tag	UNP E2ESL7
G	29	SER	-	expression tag	UNP E2ESL7
H	24	GLY	-	expression tag	UNP E2ESL7
H	25	SER	-	expression tag	UNP E2ESL7
H	26	HIS	-	expression tag	UNP E2ESL7
H	27	MET	-	expression tag	UNP E2ESL7
H	28	ALA	-	expression tag	UNP E2ESL7
H	29	SER	-	expression tag	UNP E2ESL7
I	24	GLY	-	expression tag	UNP E2ESL7
I	25	SER	-	expression tag	UNP E2ESL7
I	26	HIS	-	expression tag	UNP E2ESL7

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Chain	Residue	Modelled	Actual	Comment	Reference
I	27	MET	-	expression tag	UNP E2ESL7
I	28	ALA	-	expression tag	UNP E2ESL7
I	29	SER	-	expression tag	UNP E2ESL7
J	24	GLY	-	expression tag	UNP E2ESL7
J	25	SER	-	expression tag	UNP E2ESL7
J	26	HIS	-	expression tag	UNP E2ESL7
J	27	MET	-	expression tag	UNP E2ESL7
J	28	ALA	-	expression tag	UNP E2ESL7
J	29	SER	-	expression tag	UNP E2ESL7

- Molecule 2 is water.

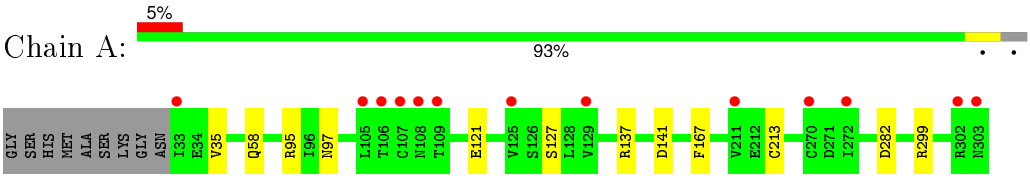
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	86	Total O 86 86	0	0
2	B	89	Total O 89 89	0	0
2	C	88	Total O 88 88	0	0
2	D	48	Total O 48 48	0	0
2	E	89	Total O 89 89	0	0
2	F	26	Total O 26 26	0	0
2	G	41	Total O 41 41	0	0
2	H	34	Total O 34 34	0	0
2	I	17	Total O 17 17	0	0
2	J	33	Total O 33 33	0	0

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.

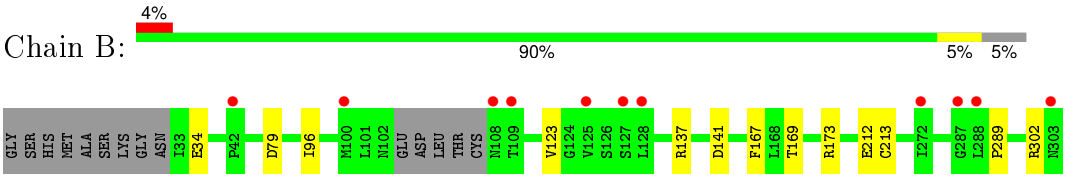
- Molecule 1: Structural protein VP1

Chain A:



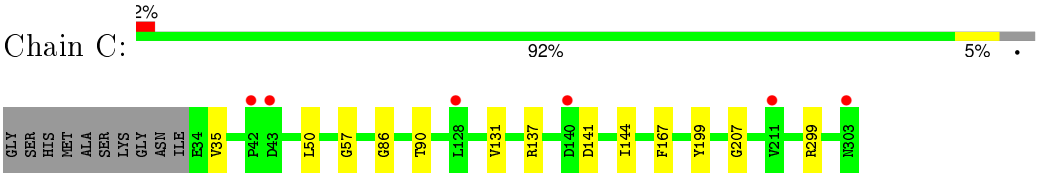
- Molecule 1: Structural protein VP1

Chain B:



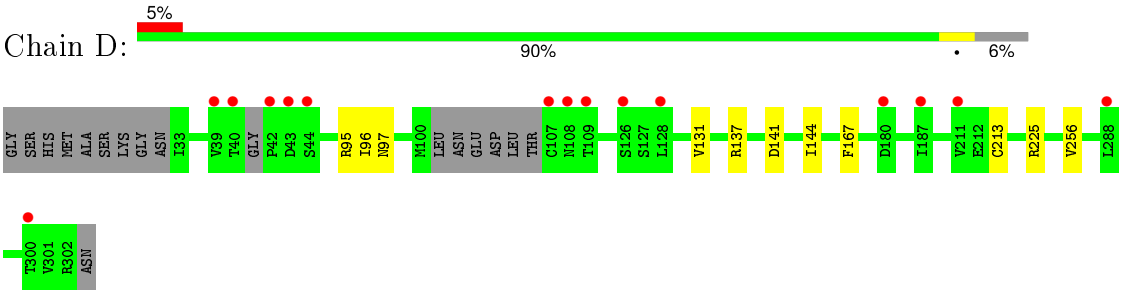
- Molecule 1: Structural protein VP1

Chain C:



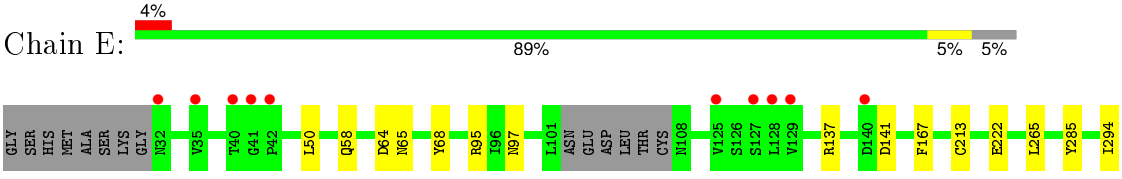
- Molecule 1: Structural protein VP1

Chain D:



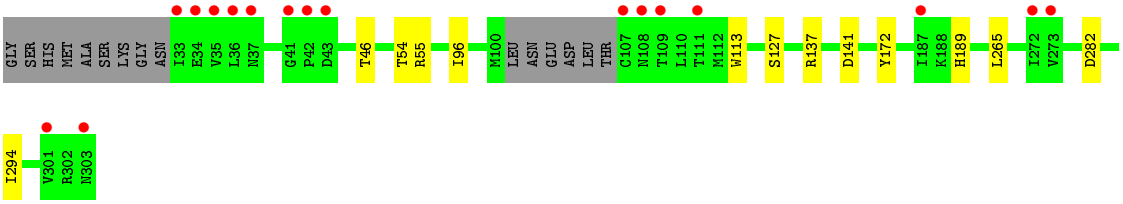
- Molecule 1: Structural protein VP1

Chain E:



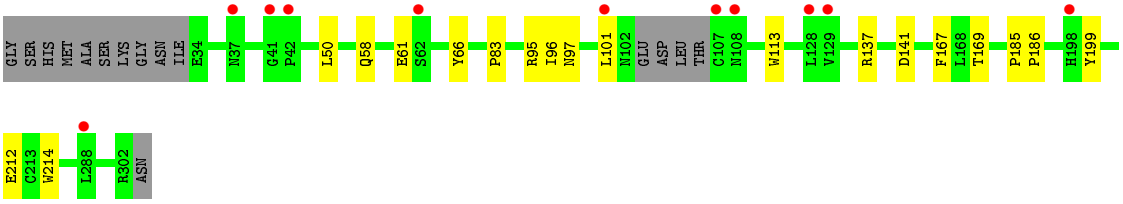
• Molecule 1: Structural protein VP1

Chain F:



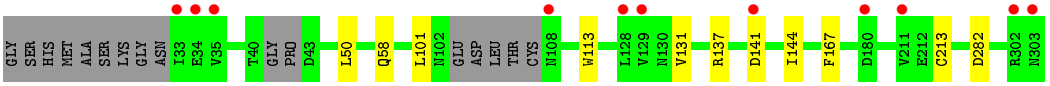
• Molecule 1: Structural protein VP1

Chain G:



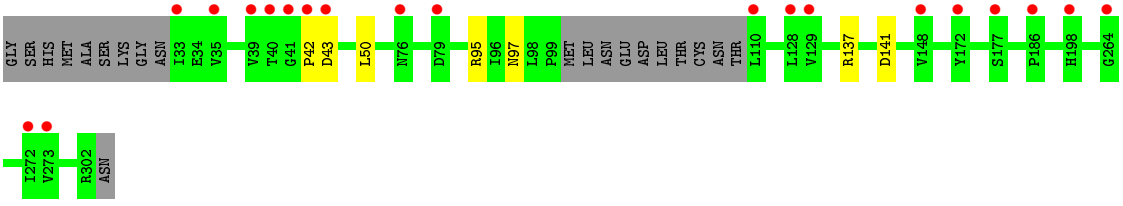
• Molecule 1: Structural protein VP1

Chain H:



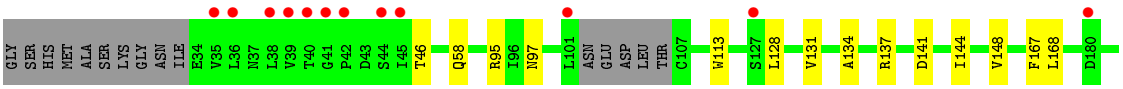
• Molecule 1: Structural protein VP1

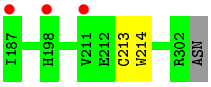
Chain I:



• Molecule 1: Structural protein VP1

Chain J:




I187
H198
V211
E212
C213
W214
R302
ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	64.10Å 153.64Å 143.98Å 90.00° 91.83° 90.00°	Depositor
Resolution (Å)	29.57 – 2.10 29.57 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.57-2.10) 98.3 (29.57-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.205 , 0.249 0.207 , 0.248	Depositor DCC
R_{free} test set	7970 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	37.0	Xtriage
Anisotropy	0.523	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 36.3	EDS
Estimated twinning fraction	0.064 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Outliers	0 of 158871 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	20926	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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	0.47	0/2141	0.67	0/2912
1	B	0.48	0/2107	0.68	0/2864
1	C	0.48	0/2140	0.68	0/2912
1	D	0.42	0/2060	0.63	0/2801
1	E	0.46	0/2089	0.65	0/2842
1	F	0.40	0/2072	0.62	0/2821
1	G	0.42	0/2074	0.65	0/2824
1	H	0.39	0/2080	0.61	0/2829
1	I	0.35	0/2018	0.56	0/2754
1	J	0.39	0/2036	0.61	0/2778
All	All	0.43	0/20817	0.64	0/28337

There are no bond length outliers.

There are no bond angle outliers.

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	2096	0	2040	5	0
1	B	2063	0	1999	7	0
1	C	2092	0	2025	6	0
1	D	2017	0	1945	6	0
1	E	2045	0	1985	7	0
1	F	2028	0	1945	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2030	0	1958	9	0
1	H	2038	0	1956	4	0
1	I	1974	0	1872	3	0
1	J	1992	0	1877	7	0
2	A	86	0	0	0	0
2	B	89	0	0	0	0
2	C	88	0	0	0	0
2	D	48	0	0	0	0
2	E	89	0	0	0	0
2	F	26	0	0	0	0
2	G	41	0	0	0	0
2	H	34	0	0	0	0
2	I	17	0	0	0	0
2	J	33	0	0	0	0
All	All	20926	0	19602	60	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 2.

All (60) 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:B:137:ARG:HG3	1:B:141:ASP:HA	1.72	0.71
1:E:222:GLU:H	1:E:222:GLU:CD	2.06	0.58
1:F:137:ARG:HG3	1:F:141:ASP:HA	1.88	0.55
1:F:265:LEU:HD21	1:F:294:ILE:HD13	1.87	0.54
1:G:95:ARG:NH1	1:G:97:ASN:OD1	2.39	0.54
1:E:64:ASP:O	1:E:65:ASN:HB2	2.08	0.54
1:B:96:ILE:HD12	1:B:96:ILE:N	2.23	0.54
1:A:137:ARG:HG3	1:A:141:ASP:HA	1.91	0.53
1:G:137:ARG:HG3	1:G:141:ASP:HA	1.92	0.52
1:A:95:ARG:NH1	1:A:97:ASN:OD1	2.39	0.51
1:D:167:PHE:CE1	1:D:213:CYS:HB2	2.46	0.50
1:F:46:THR:HG22	1:F:113:TRP:CZ3	2.48	0.49
1:E:95:ARG:NH1	1:E:97:ASN:OD1	2.45	0.49
1:H:101:LEU:HD21	1:H:113:TRP:NE1	2.28	0.49
1:H:137:ARG:HG3	1:H:141:ASP:HA	1.95	0.48
1:J:167:PHE:HB2	1:J:214:TRP:CZ3	2.48	0.48
1:D:225:ARG:NH2	1:D:256:VAL:O	2.47	0.48
1:I:137:ARG:HG3	1:I:141:ASP:HA	1.95	0.48
1:J:137:ARG:HG3	1:J:141:ASP:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:ARG:NH1	1:D:97:ASN:OD1	2.47	0.48
1:G:96:ILE:N	1:G:96:ILE:HD12	2.29	0.47
1:C:57:GLY:HA3	1:C:86:GLY:O	2.15	0.47
1:I:42:PRO:O	1:I:43:ASP:CB	2.63	0.47
1:G:61:GLU:HA	1:G:66:TYR:CD1	2.50	0.47
1:J:95:ARG:NH1	1:J:97:ASN:OD1	2.48	0.47
1:A:35:VAL:HG13	1:A:299:ARG:HD3	1.98	0.46
1:E:137:ARG:HG3	1:E:141:ASP:HA	1.97	0.46
1:D:96:ILE:HD12	1:D:96:ILE:N	2.31	0.46
1:D:137:ARG:HG3	1:D:141:ASP:HA	1.98	0.45
1:H:131:VAL:HB	1:H:144:ILE:HB	1.98	0.45
1:J:46:THR:HG22	1:J:113:TRP:CZ3	2.52	0.45
1:C:137:ARG:HG3	1:C:141:ASP:HA	1.98	0.45
1:I:95:ARG:NH1	1:I:97:ASN:OD1	2.49	0.45
1:F:265:LEU:HD21	1:F:294:ILE:CD1	2.47	0.44
1:B:34:GLU:HB3	1:B:302:ARG:HB3	1.99	0.44
1:G:101:LEU:HD11	1:G:113:TRP:CD1	2.52	0.44
1:E:265:LEU:HD21	1:E:294:ILE:HD13	2.00	0.44
1:B:167:PHE:CE1	1:B:213:CYS:HB2	2.53	0.44
1:F:54:THR:O	1:F:55:ARG:NH1	2.50	0.43
1:G:167:PHE:HB2	1:G:214:TRP:CZ3	2.53	0.43
1:F:127:SER:HA	1:G:212:GLU:O	2.17	0.43
1:E:167:PHE:CE1	1:E:213:CYS:HB2	2.53	0.42
1:H:167:PHE:CE1	1:H:213:CYS:HB2	2.54	0.42
1:J:131:VAL:HB	1:J:144:ILE:HB	1.99	0.42
1:B:123:VAL:HB	1:B:289:PRO:HG2	2.00	0.42
1:J:128:LEU:HD22	1:J:148:VAL:HB	2.02	0.42
1:B:79:ASP:HA	1:B:173:ARG:HD3	2.01	0.42
1:C:167:PHE:HB3	1:C:199:TYR:HB3	2.02	0.41
1:A:127:SER:HA	1:B:212:GLU:O	2.20	0.41
1:F:96:ILE:N	1:F:96:ILE:HD12	2.35	0.41
1:G:167:PHE:HB3	1:G:199:TYR:HB3	2.02	0.41
1:F:172:TYR:HB2	1:F:189:HIS:O	2.20	0.41
1:A:167:PHE:CE1	1:A:213:CYS:HB2	2.56	0.41
1:D:131:VAL:HB	1:D:144:ILE:HB	2.03	0.41
1:J:168:LEU:O	1:J:213:CYS:HA	2.20	0.41
1:C:90:THR:OG1	1:C:207:GLY:HA2	2.21	0.40
1:E:68:TYR:HA	1:E:285:TYR:O	2.21	0.40
1:C:35:VAL:CG1	1:C:299:ARG:HD3	2.50	0.40
1:G:185:PRO:HA	1:G:186:PRO:HD3	2.00	0.40
1:C:131:VAL:HB	1:C:144:ILE:HB	2.02	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	269/280 (96%)	259 (96%)	10 (4%)	0	100	100
1	B	262/280 (94%)	253 (97%)	9 (3%)	0	100	100
1	C	269/280 (96%)	259 (96%)	10 (4%)	0	100	100
1	D	257/280 (92%)	248 (96%)	9 (4%)	0	100	100
1	E	261/280 (93%)	253 (97%)	8 (3%)	0	100	100
1	F	261/280 (93%)	251 (96%)	10 (4%)	0	100	100
1	G	261/280 (93%)	249 (95%)	12 (5%)	0	100	100
1	H	258/280 (92%)	247 (96%)	11 (4%)	0	100	100
1	I	256/280 (91%)	245 (96%)	11 (4%)	0	100	100
1	J	260/280 (93%)	246 (95%)	13 (5%)	1 (0%)	39	37
All	All	2614/2800 (93%)	2510 (96%)	103 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	134	ALA

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	236/246 (96%)	233 (99%)	3 (1%)	76 82
1	B	231/246 (94%)	230 (100%)	1 (0%)	93 96
1	C	235/246 (96%)	234 (100%)	1 (0%)	93 96
1	D	222/246 (90%)	222 (100%)	0	100 100
1	E	228/246 (93%)	226 (99%)	2 (1%)	84 89
1	F	225/246 (92%)	224 (100%)	1 (0%)	93 96
1	G	225/246 (92%)	221 (98%)	4 (2%)	66 72
1	H	227/246 (92%)	224 (99%)	3 (1%)	76 82
1	I	216/246 (88%)	215 (100%)	1 (0%)	92 95
1	J	214/246 (87%)	213 (100%)	1 (0%)	92 95
All	All	2259/2460 (92%)	2242 (99%)	17 (1%)	86 91

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	121	GLU
1	A	282	ASP
1	B	169	THR
1	C	50	LEU
1	E	50	LEU
1	E	58	GLN
1	F	282	ASP
1	G	50	LEU
1	G	58	GLN
1	G	83	PRO
1	G	169	THR
1	H	50	LEU
1	H	58	GLN
1	H	282	ASP
1	I	50	LEU
1	J	58	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	271/280 (96%)	0.05	13 (4%)	34	43	26, 34, 59, 94	0
1	B	266/280 (95%)	-0.01	11 (4%)	41	50	26, 33, 51, 71	0
1	C	270/280 (96%)	-0.08	6 (2%)	65	71	27, 35, 51, 70	0
1	D	263/280 (93%)	0.12	15 (5%)	27	35	29, 39, 64, 93	0
1	E	265/280 (94%)	-0.03	10 (3%)	44	53	25, 35, 56, 86	0
1	F	265/280 (94%)	0.30	17 (6%)	23	30	32, 44, 69, 106	0
1	G	265/280 (94%)	0.14	11 (4%)	40	49	30, 41, 60, 87	0
1	H	264/280 (94%)	0.10	11 (4%)	40	49	31, 45, 63, 77	0
1	I	260/280 (92%)	0.46	20 (7%)	16	22	37, 52, 78, 99	0
1	J	264/280 (94%)	0.23	15 (5%)	27	35	33, 46, 74, 107	0
All	All	2653/2800 (94%)	0.13	129 (4%)	33	42	25, 41, 66, 107	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	110	LEU	7.1
1	A	106	THR	6.4
1	F	107	CYS	6.3
1	J	42	PRO	5.4
1	I	42	PRO	4.8
1	F	36	LEU	4.7
1	I	35	VAL	4.7
1	J	40	THR	4.5
1	I	39	VAL	4.3
1	I	40	THR	4.2
1	E	42	PRO	4.2
1	F	301	VAL	4.2
1	B	100	MET	4.1

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Mol	Chain	Res	Type	RSRZ
1	I	41	GLY	4.0
1	D	39	VAL	3.9
1	D	44	SER	3.9
1	D	107	CYS	3.8
1	D	109	THR	3.8
1	B	42	PRO	3.8
1	G	101	LEU	3.8
1	F	42	PRO	3.8
1	A	272	ILE	3.7
1	J	45	ILE	3.7
1	B	109	THR	3.7
1	E	129	VAL	3.6
1	I	76	ASN	3.5
1	F	111	THR	3.5
1	J	38	LEU	3.5
1	A	107	CYS	3.4
1	F	33	ILE	3.4
1	F	187	ILE	3.4
1	B	128	LEU	3.4
1	F	303	ASN	3.3
1	A	105	LEU	3.3
1	H	303	ASN	3.3
1	I	33	ILE	3.2
1	G	129	VAL	3.2
1	I	129	VAL	3.2
1	D	288	LEU	3.2
1	J	44	SER	3.2
1	B	303	ASN	3.1
1	H	34	GLU	3.1
1	I	177	SER	3.1
1	I	128	LEU	3.1
1	J	35	VAL	3.1
1	F	109	THR	3.0
1	C	42	PRO	3.0
1	D	42	PRO	3.0
1	E	125	VAL	2.9
1	A	33	ILE	2.9
1	H	180	ASP	2.9
1	J	187	ILE	2.9
1	D	211	VAL	2.8
1	E	128	LEU	2.8
1	J	39	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	32	ASN	2.8
1	D	43	ASP	2.8
1	F	108	ASN	2.7
1	H	108	ASN	2.7
1	A	108	ASN	2.6
1	G	42	PRO	2.6
1	I	43	ASP	2.6
1	E	35	VAL	2.6
1	F	35	VAL	2.6
1	H	33	ILE	2.6
1	A	270	CYS	2.6
1	I	186	PRO	2.6
1	E	40	THR	2.6
1	I	79	ASP	2.5
1	A	303	ASN	2.5
1	H	302	ARG	2.5
1	H	129	VAL	2.5
1	I	172	TYR	2.5
1	G	41	GLY	2.5
1	I	273	VAL	2.5
1	J	180	ASP	2.5
1	F	34	GLU	2.5
1	G	288	LEU	2.5
1	D	40	THR	2.5
1	I	264	GLY	2.4
1	G	62	SER	2.4
1	H	35	VAL	2.4
1	B	288	LEU	2.4
1	A	129	VAL	2.4
1	H	128	LEU	2.4
1	C	303	ASN	2.4
1	J	211	VAL	2.4
1	E	140	ASP	2.4
1	C	128	LEU	2.3
1	D	128	LEU	2.3
1	G	128	LEU	2.3
1	A	109	THR	2.3
1	D	108	ASN	2.3
1	E	41	GLY	2.3
1	B	272	ILE	2.3
1	C	140	ASP	2.3
1	B	125	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	41	GLY	2.3
1	B	108	ASN	2.3
1	J	198	HIS	2.3
1	G	107	CYS	2.3
1	C	43	ASP	2.2
1	E	127	SER	2.2
1	J	41	GLY	2.2
1	G	198	HIS	2.2
1	H	141	ASP	2.2
1	J	36	LEU	2.2
1	F	37	ASN	2.2
1	F	272	ILE	2.2
1	B	127	SER	2.2
1	I	198	HIS	2.2
1	A	125	VAL	2.2
1	G	37	ASN	2.1
1	D	187	ILE	2.1
1	G	108	ASN	2.1
1	F	273	VAL	2.1
1	A	211	VAL	2.1
1	C	211	VAL	2.1
1	J	127	SER	2.1
1	H	211	VAL	2.1
1	I	148	VAL	2.1
1	A	302	ARG	2.1
1	D	126	SER	2.0
1	F	43	ASP	2.0
1	J	101	LEU	2.0
1	D	180	ASP	2.0
1	D	300	THR	2.0
1	I	272	ILE	2.0
1	B	287	GLY	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.