Full wwPDB X-ray Structure Validation Report (i)

Sep 9, 2023 – 11:42 PM EDT

PDB ID	:	4H5L
Title	:	Crystal Structure of Toscana Virus Nucleocapsid Protein Hexamer
Authors	:	Raymond, D.D.; Smith, J.L.
Deposited on	:	2012-09-18
Resolution	:	2.75 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 (i) 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 (1)) were used in the production of this report:

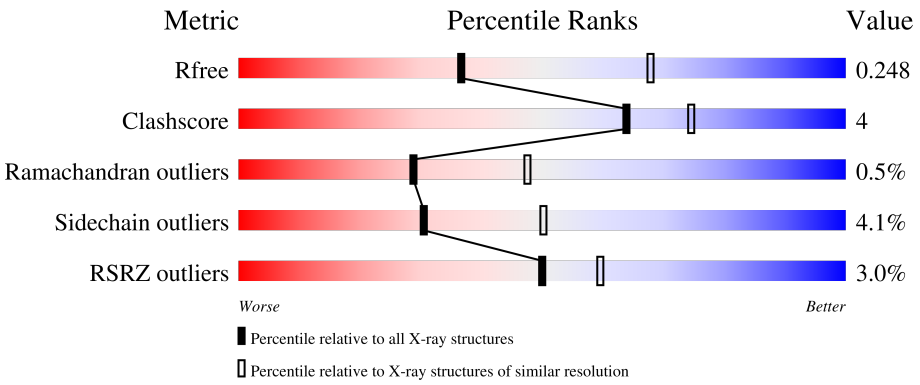
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	253	2%, 81%, 14%
1	B	253	%, 83%, 13%
1	C	253	9%, 85%, 11%
1	D	253	80%, 16%
1	E	253	2%, 82%, 14%

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Mol	Chain	Length	Quality of chain
1	F	253	4% 85% 11%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11238 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 Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	243	1869	1186	325	347	11	0	0	0
1	B	244	1870	1187	325	347	11	0	0	0
1	C	244	1873	1188	326	348	11	0	0	0
1	D	244	1873	1188	326	348	11	0	0	0
1	E	244	1873	1188	326	348	11	0	0	0
1	F	244	1863	1182	322	348	11	0	0	0

- Molecule 2 is water.

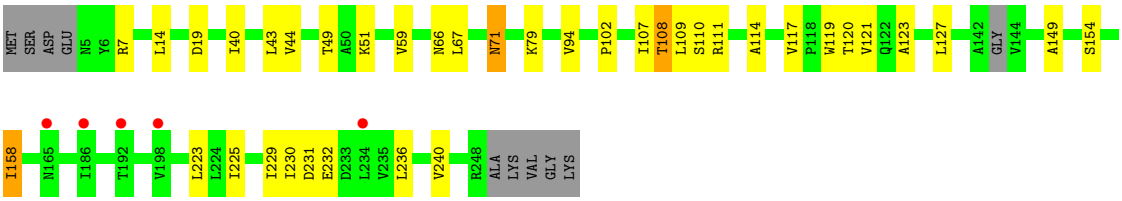
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	1	1	1	0	0
2	B	2	2	2	0	0
2	C	2	2	2	0	0
2	D	5	5	5	0	0
2	E	3	3	3	0	0
2	F	4	4	4	0	0

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.

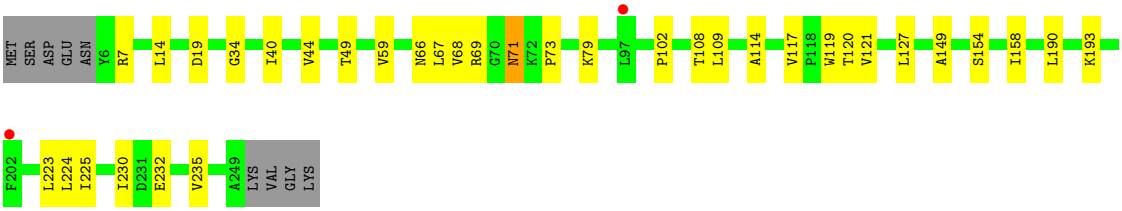
• Molecule 1: Nucleoprotein

Chain A:



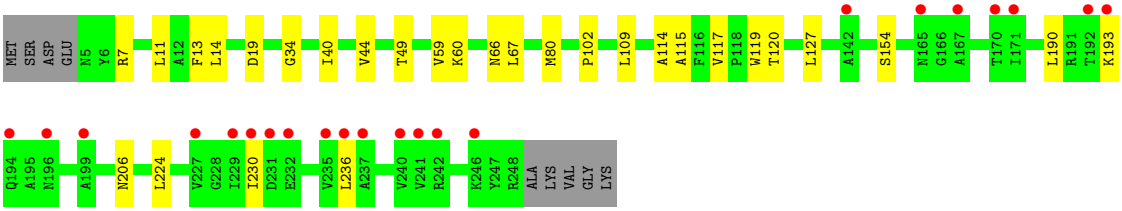
• Molecule 1: Nucleoprotein

Chain B:



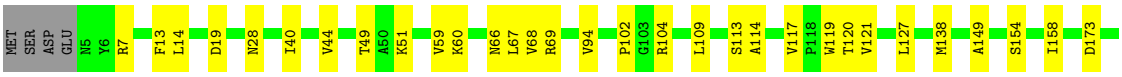
• Molecule 1: Nucleoprotein

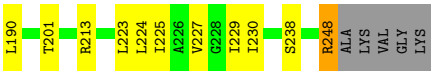
Chain C:



• Molecule 1: Nucleoprotein

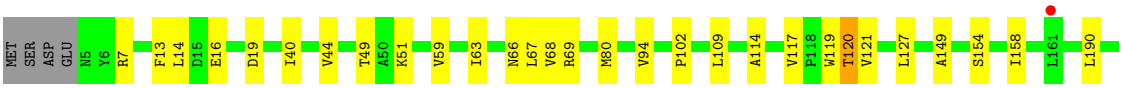
Chain D:

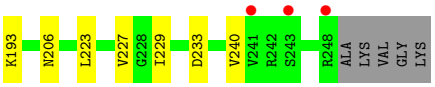




• Molecule 1: Nucleoprotein

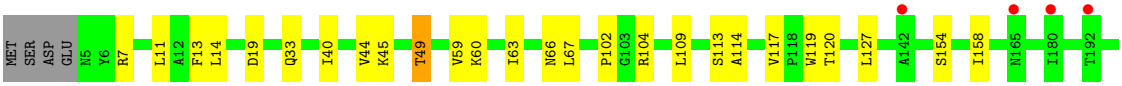
Chain E:

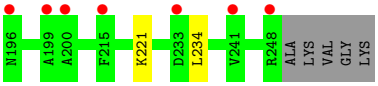




• Molecule 1: Nucleoprotein

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	50.35Å 93.75Å 95.52Å 67.92° 85.94° 87.95°	Depositor
Resolution (Å)	50.22 – 2.75 50.22 – 2.75	Depositor EDS
% Data completeness (in resolution range)	95.2 (50.22-2.75) 95.2 (50.22-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.77Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.8.0, BUSTER 2.10	Depositor
R, R_{free}	0.219 , 0.238 0.240 , 0.248	Depositor DCC
R_{free} test set	2022 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	52.5	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 41.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.020 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11238	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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 (i)

5.1 Standard geometry (i)

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	0.45	0/1900	0.60	0/2565
1	B	0.45	0/1902	0.61	0/2569
1	C	0.45	0/1905	0.59	0/2573
1	D	0.45	0/1905	0.60	0/2573
1	E	0.45	0/1905	0.58	0/2573
1	F	0.45	0/1895	0.59	0/2562
All	All	0.45	0/11412	0.60	0/15415

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 (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	1869	0	1908	16	0
1	B	1870	0	1911	19	0
1	C	1873	0	1912	16	0
1	D	1873	0	1912	20	0
1	E	1873	0	1912	19	0
1	F	1863	0	1890	15	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	3	0	0	0	0
2	F	4	0	0	0	0
All	All	11238	0	11445	94	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 4.

All (94) 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:A:117:VAL:HA	1:A:120:THR:HG22	1.51	0.92
1:B:117:VAL:HA	1:B:120:THR:HG22	1.51	0.92
1:F:117:VAL:HA	1:F:120:THR:HG22	1.53	0.88
1:D:117:VAL:HA	1:D:120:THR:CG2	2.07	0.84
1:D:117:VAL:HA	1:D:120:THR:HG22	1.63	0.77
1:C:117:VAL:HA	1:C:120:THR:HG22	1.65	0.77
1:C:40:ILE:HD11	1:C:115:ALA:HB2	1.66	0.77
1:C:117:VAL:HA	1:C:120:THR:CG2	2.19	0.71
1:E:117:VAL:HA	1:E:120:THR:CG2	2.23	0.68
1:B:66:ASN:HB2	1:B:109:LEU:HB3	1.77	0.65
1:F:66:ASN:HB2	1:F:109:LEU:HB3	1.78	0.65
1:A:117:VAL:HA	1:A:120:THR:CG2	2.27	0.63
1:B:117:VAL:HA	1:B:120:THR:CG2	2.27	0.63
1:F:117:VAL:HA	1:F:120:THR:CG2	2.28	0.63
1:B:71:ASN:HD21	1:B:108:THR:HB	1.65	0.61
1:E:63:ILE:HG21	1:E:120:THR:HB	1.84	0.60
1:C:114:ALA:HA	1:C:154:SER:HB2	1.83	0.60
1:E:227:VAL:HG23	1:E:229:ILE:HG12	1.83	0.59
1:F:114:ALA:HA	1:F:154:SER:HB2	1.85	0.58
1:A:108:THR:OG1	1:A:111:ARG:HD2	2.03	0.58
1:A:158:ILE:HD11	1:A:223:LEU:HD12	1.86	0.58
1:E:66:ASN:HB2	1:E:109:LEU:HB3	1.84	0.58
1:D:66:ASN:HB2	1:D:109:LEU:HB3	1.86	0.58
1:A:66:ASN:HB2	1:A:109:LEU:HB3	1.86	0.57
1:F:221:LYS:HE3	1:F:234:LEU:HD21	1.86	0.56
1:F:45:LYS:O	1:F:49:THR:HB	2.04	0.56
1:A:229:ILE:HG23	1:A:240:VAL:HG21	1.87	0.56
1:D:28:ASN:HB3	1:D:213:ARG:HH12	1.72	0.55
1:C:190:LEU:HA	1:C:193:LYS:HD3	1.90	0.54
1:E:114:ALA:HA	1:E:154:SER:HB2	1.89	0.54
1:B:114:ALA:HA	1:B:154:SER:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:LYS:HD3	1:C:34:GLY:HA2	1.90	0.53
1:A:119:TRP:CZ3	1:A:123:ALA:HB2	2.45	0.52
1:D:114:ALA:HA	1:D:154:SER:HB2	1.91	0.52
1:E:190:LEU:HA	1:E:193:LYS:HG3	1.92	0.51
1:C:224:LEU:HB3	1:C:230:ILE:HG12	1.93	0.51
1:A:71:ASN:ND2	1:A:110:SER:H	2.10	0.50
1:E:119:TRP:HB2	1:F:13:PHE:HB3	1.93	0.50
1:A:114:ALA:HA	1:A:154:SER:HB2	1.93	0.49
1:A:225:ILE:HA	1:A:230:ILE:O	2.12	0.49
1:C:119:TRP:HB2	1:D:13:PHE:HB3	1.94	0.49
1:E:229:ILE:HG23	1:E:240:VAL:HG21	1.94	0.49
1:D:60:LYS:NZ	1:E:16:GLU:HG3	2.28	0.49
1:F:44:VAL:HG11	1:F:59:VAL:CG1	2.43	0.48
1:A:44:VAL:HG11	1:A:59:VAL:CG1	2.43	0.48
1:A:43:LEU:HB3	1:A:107:ILE:HD11	1.95	0.48
1:E:44:VAL:HG11	1:E:59:VAL:CG1	2.44	0.48
1:F:33:GLN:OE1	1:F:104:ARG:HD3	2.13	0.48
1:C:80:MET:O	1:D:104:ARG:NE	2.46	0.48
1:B:71:ASN:O	1:B:73:PRO:HD3	2.13	0.48
1:B:44:VAL:HG11	1:B:59:VAL:CG1	2.44	0.47
1:D:51:LYS:HD2	1:D:94:VAL:HG22	1.97	0.47
1:B:119:TRP:HB2	1:C:13:PHE:HB3	1.96	0.47
1:C:40:ILE:CD1	1:C:115:ALA:HB2	2.40	0.47
1:D:119:TRP:HB2	1:E:13:PHE:HB3	1.97	0.47
1:C:44:VAL:HG11	1:C:59:VAL:CG1	2.45	0.46
1:B:223:LEU:HD21	1:C:11:LEU:HD23	1.97	0.46
1:B:232:GLU:CD	1:B:232:GLU:H	2.19	0.46
1:D:44:VAL:HG11	1:D:59:VAL:CG1	2.46	0.46
1:B:121:VAL:HG22	1:B:149:ALA:HB1	1.99	0.45
1:D:190:LEU:HD21	1:D:201:THR:HG21	1.99	0.44
1:D:224:LEU:HB3	1:D:230:ILE:HG12	1.99	0.44
1:E:117:VAL:HA	1:E:120:THR:HG22	1.98	0.43
1:D:121:VAL:HG22	1:D:149:ALA:HB1	2.00	0.43
1:D:227:VAL:HG23	1:D:229:ILE:HG12	2.00	0.43
1:A:121:VAL:HG22	1:A:149:ALA:HB1	2.00	0.43
1:F:67:LEU:HD13	1:F:127:LEU:HD11	2.00	0.43
1:D:225:ILE:HG13	1:D:230:ILE:HG13	2.01	0.43
1:B:68:VAL:HG13	1:B:69:ARG:HG2	2.01	0.42
1:E:63:ILE:CG2	1:E:120:THR:HB	2.49	0.42
1:B:190:LEU:HA	1:B:193:LYS:HG3	2.02	0.42
1:D:173:ASP:OD2	1:D:248:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:LYS:HD3	1:B:34:GLY:HA2	2.00	0.42
1:E:51:LYS:HG3	1:E:94:VAL:HG13	2.02	0.42
1:C:60:LYS:HG2	1:C:119:TRP:CE2	2.55	0.42
1:E:67:LEU:HD13	1:E:127:LEU:HD11	2.02	0.41
1:F:63:ILE:HG12	1:F:113:SER:HA	2.01	0.41
1:B:67:LEU:HD13	1:B:127:LEU:HD11	2.00	0.41
1:D:67:LEU:HD13	1:D:127:LEU:HD11	2.03	0.41
1:B:224:LEU:HB3	1:B:230:ILE:HG12	2.01	0.41
1:E:223:LEU:HD21	1:F:11:LEU:HD23	2.01	0.41
1:D:68:VAL:HG13	1:D:69:ARG:HG2	2.03	0.41
1:C:66:ASN:HB2	1:C:109:LEU:HB3	2.02	0.41
1:C:67:LEU:HD13	1:C:127:LEU:HD11	2.02	0.41
1:B:117:VAL:CA	1:B:120:THR:HG22	2.37	0.41
1:E:80:MET:O	1:F:104:ARG:NE	2.53	0.41
1:B:225:ILE:HA	1:B:230:ILE:O	2.21	0.40
1:A:67:LEU:HD13	1:A:127:LEU:HD11	2.04	0.40
1:F:60:LYS:HG2	1:F:119:TRP:CE2	2.57	0.40
1:D:113:SER:O	1:D:120:THR:HG21	2.21	0.40
1:E:121:VAL:HG22	1:E:149:ALA:HB1	2.04	0.40
1:A:51:LYS:HG3	1:A:94:VAL:HG13	2.03	0.40
1:E:68:VAL:HG13	1:E:69:ARG:HG2	2.03	0.40
1:F:117:VAL:CA	1:F:120:THR:HG22	2.39	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	239/253 (94%)	226 (95%)	11 (5%)	2 (1%)	19 34
1	B	242/253 (96%)	231 (96%)	10 (4%)	1 (0%)	34 53
1	C	242/253 (96%)	230 (95%)	11 (4%)	1 (0%)	34 53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	242/253 (96%)	231 (96%)	10 (4%)	1 (0%)	34	53
1	E	242/253 (96%)	234 (97%)	7 (3%)	1 (0%)	34	53
1	F	242/253 (96%)	233 (96%)	8 (3%)	1 (0%)	34	53
All	All	1449/1518 (96%)	1385 (96%)	57 (4%)	7 (0%)	29	47

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	232	GLU
1	A	102	PRO
1	B	102	PRO
1	C	102	PRO
1	D	102	PRO
1	E	102	PRO
1	F	102	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	198/206 (96%)	188 (95%)	10 (5%)	24	41
1	B	197/206 (96%)	189 (96%)	8 (4%)	30	50
1	C	198/206 (96%)	192 (97%)	6 (3%)	41	61
1	D	198/206 (96%)	188 (95%)	10 (5%)	24	41
1	E	198/206 (96%)	189 (96%)	9 (4%)	27	46
1	F	196/206 (95%)	190 (97%)	6 (3%)	40	60
All	All	1185/1236 (96%)	1136 (96%)	49 (4%)	30	50

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG

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Mol	Chain	Res	Type
1	A	14	LEU
1	A	19	ASP
1	A	40	ILE
1	A	49	THR
1	A	71	ASN
1	A	108	THR
1	A	158	ILE
1	A	231	ASP
1	A	236	LEU
1	B	7	ARG
1	B	14	LEU
1	B	19	ASP
1	B	40	ILE
1	B	49	THR
1	B	71	ASN
1	B	158	ILE
1	B	235	VAL
1	C	7	ARG
1	C	14	LEU
1	C	19	ASP
1	C	49	THR
1	C	206	ASN
1	C	236	LEU
1	D	7	ARG
1	D	14	LEU
1	D	19	ASP
1	D	40	ILE
1	D	49	THR
1	D	138	MET
1	D	158	ILE
1	D	223	LEU
1	D	238	SER
1	D	248	ARG
1	E	7	ARG
1	E	14	LEU
1	E	19	ASP
1	E	40	ILE
1	E	49	THR
1	E	120	THR
1	E	158	ILE
1	E	206	ASN
1	E	233	ASP

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Mol	Chain	Res	Type
1	F	7	ARG
1	F	14	LEU
1	F	19	ASP
1	F	40	ILE
1	F	49	THR
1	F	158	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	71	ASN
1	B	71	ASN
1	C	66	ASN
1	D	66	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	243/253 (96%)	0.14	5 (2%) 63 72	40, 80, 145, 240	0
1	B	244/253 (96%)	0.01	2 (0%) 86 90	34, 78, 131, 205	0
1	C	244/253 (96%)	0.42	22 (9%) 9 11	42, 86, 179, 229	0
1	D	244/253 (96%)	-0.11	0 100 100	32, 65, 108, 142	0
1	E	244/253 (96%)	-0.02	4 (1%) 72 79	30, 76, 138, 178	0
1	F	244/253 (96%)	0.06	11 (4%) 33 39	28, 70, 152, 233	0
All	All	1463/1518 (96%)	0.08	44 (3%) 50 59	28, 76, 150, 240	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	196	ASN	7.7
1	C	142	ALA	3.8
1	C	237	ALA	3.7
1	E	248	ARG	3.6
1	A	165	ASN	3.6
1	F	248	ARG	3.4
1	C	230	ILE	3.4
1	F	241	VAL	3.4
1	C	165	ASN	3.3
1	C	246	LYS	3.1
1	A	192	THR	3.0
1	A	234	LEU	2.9
1	A	198	VAL	2.9
1	C	227	VAL	2.8
1	C	193	LYS	2.8
1	A	186	ILE	2.8
1	C	194	GLN	2.7
1	F	199	ALA	2.7
1	F	196	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	236	LEU	2.7
1	C	240	VAL	2.6
1	E	161	LEU	2.6
1	C	199	ALA	2.6
1	C	167	ALA	2.4
1	F	165	ASN	2.4
1	C	232	GLU	2.4
1	F	142	ALA	2.4
1	B	202	PHE	2.4
1	F	180	ILE	2.3
1	F	215	PHE	2.3
1	C	235	VAL	2.3
1	C	241	VAL	2.3
1	F	200	ALA	2.2
1	F	192	THR	2.2
1	C	170	THR	2.2
1	E	243	SER	2.2
1	F	233	ASP	2.2
1	C	192	THR	2.1
1	C	229	ILE	2.1
1	C	242	ARG	2.1
1	C	231	ASP	2.1
1	B	97	LEU	2.1
1	C	171	ILE	2.0
1	E	241	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.