Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2016 – 07:45 PM EST

PDB ID	:	5F17
Title	:	Structure of EAV NSP11 K170A mutant at 3.19A
Authors	:	Zhang, M.F.; Chen, Z.Z.
Deposited on	:	2015-11-30
Resolution	:	3.20 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
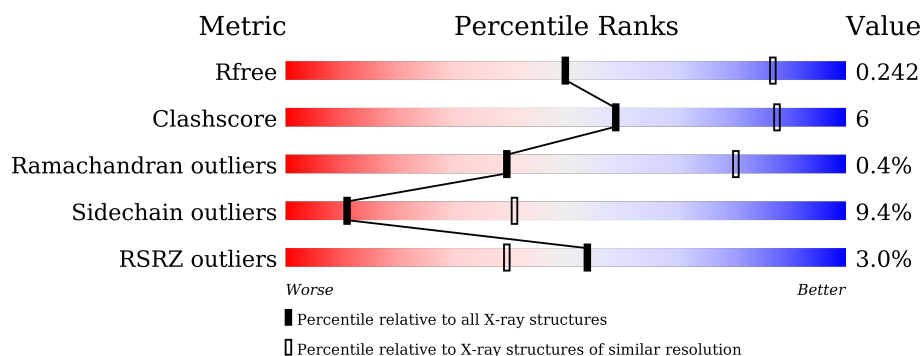with specific help available everywhere you see the (i) symbol.

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 3.20 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	Percentile Ranks	Value
Rfree		0.242
Clashscore		6
Ramachandran outliers		0.4%
Sidechain outliers		9.4%
RSRZ outliers		3.0%

Worse .... *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	219	82% ▕ 16% ▕ •
1	B	219	8% ▕ 83% ▕ 17%
1	C	219	4% ▕ 83% ▕ 15% ▕ •
1	D	219	75% ▕ 16% ▕ 5% ▕ 5%
1	E	219	2% ▕ 71% ▕ 25% ▕ • •
1	F	219	74% ▕ 18% ▕ • ▕ 5%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 9879 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 Non-structural protein 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1690	1088	280	311	11			
1	B	219	Total	C	N	O	S	0	0	0
			1667	1073	277	307	10			
1	C	219	Total	C	N	O	S	0	0	0
			1674	1076	278	309	11			
1	D	209	Total	C	N	O	S	0	0	0
			1609	1040	265	293	11			
1	E	211	Total	C	N	O	S	0	0	0
			1628	1049	270	298	11			
1	F	209	Total	C	N	O	S	0	0	0
			1611	1041	264	296	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	170	ALA	LYS	engineered mutation	UNP P19811
B	170	ALA	LYS	engineered mutation	UNP P19811
C	170	ALA	LYS	engineered mutation	UNP P19811
D	170	ALA	LYS	engineered mutation	UNP P19811
E	170	ALA	LYS	engineered mutation	UNP P19811
F	170	ALA	LYS	engineered mutation	UNP P19811

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: Non-structural protein 11
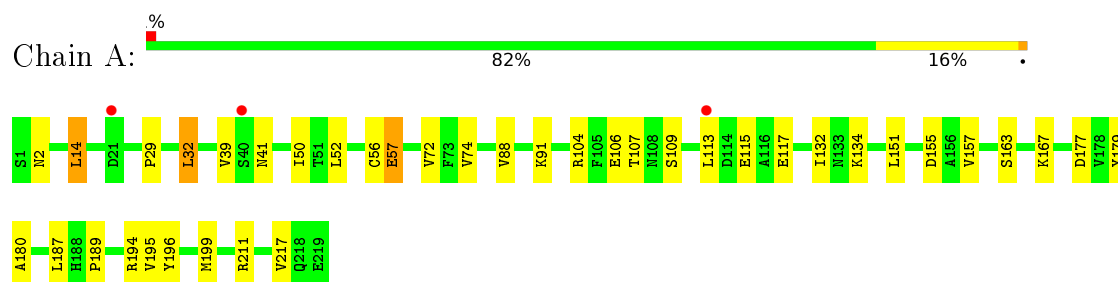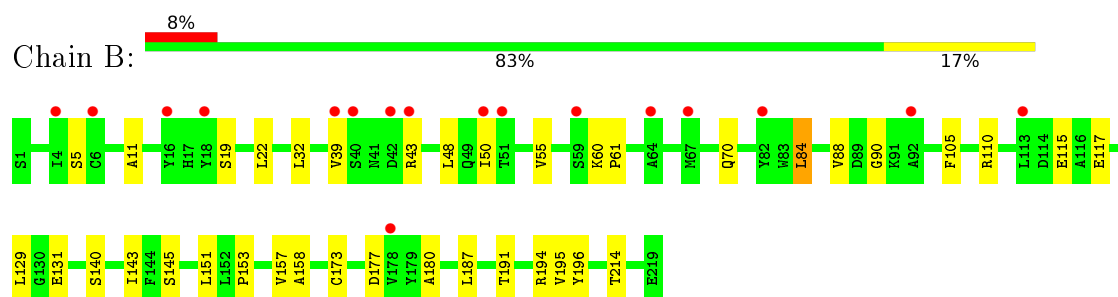
Chain A:

• Molecule 1: Non-structural protein 11

Chain B:

• Molecule 1: Non-structural protein 11

Chain C:

• Molecule 1: Non-structural protein 11

Chain D:

• Molecule 1: Non-structural protein 11

Chain E:

• Molecule 1: Non-structural protein 11

Chain F:
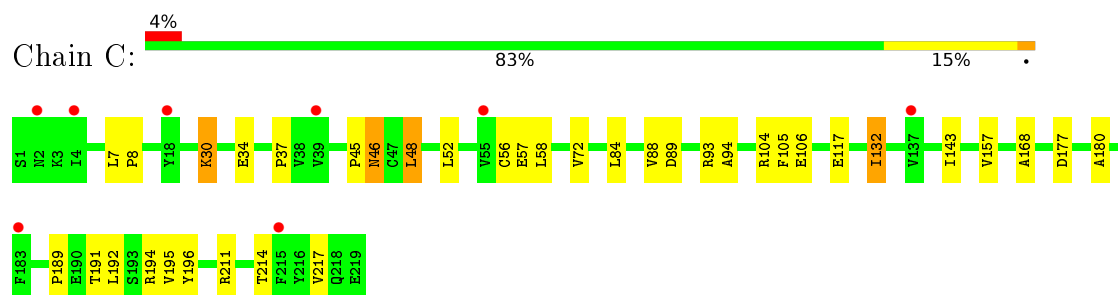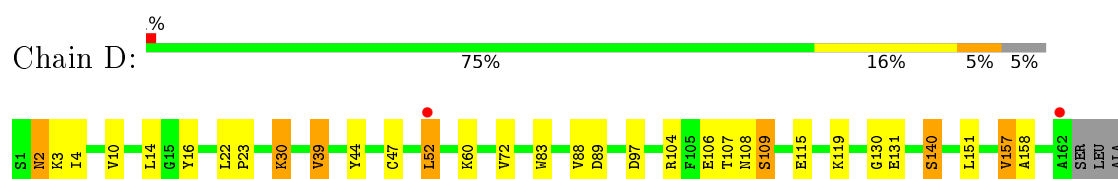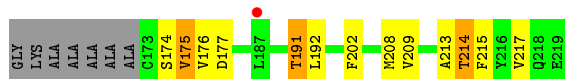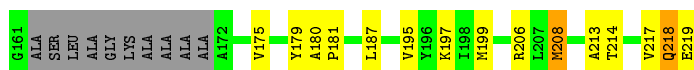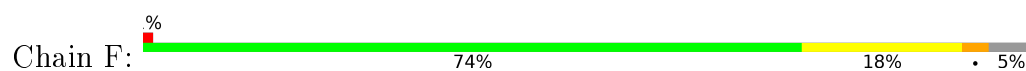
4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	249.18Å 249.18Å 226.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.20 48.72 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-3.20) 99.6 (48.72-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.215 , 0.243 0.211 , 0.242	Depositor DCC
R_{free} test set	2090 reflections (4.71%)	DCC
Wilson B-factor (Å^2)	95.5	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 66.5	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	9879	wwPDB-VP
Average B, all atoms (Å^2)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.24	0/1742	0.44	0/2380
1	B	0.24	0/1718	0.44	0/2352
1	C	0.23	0/1726	0.43	0/2362
1	D	0.26	0/1660	0.47	0/2269
1	E	0.28	0/1678	0.47	0/2291
1	F	0.27	0/1662	0.46	0/2271
All	All	0.25	0/10186	0.45	0/13925

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	1690	0	1634	14	0
1	B	1667	0	1588	12	0
1	C	1674	0	1597	19	0
1	D	1609	0	1522	19	0
1	E	1628	0	1564	27	0
1	F	1611	0	1527	22	0
All	All	9879	0	9432	112	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 (112) 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:D:2:ASN:O	1:D:4:ILE:N	2.22	0.73
1:E:9:ARG:HD3	1:E:160:VAL:HG11	1.70	0.72
1:C:56:CYS:SG	1:C:57:GLU:N	2.66	0.69
1:E:208:MET:HB2	1:E:216:TYR:HB2	1.85	0.59
1:F:9:ARG:NH2	1:F:106:GLU:OE2	2.37	0.57
1:B:11:ALA:HB1	1:B:39:VAL:HG11	1.87	0.57
1:E:13:ASN:HD21	1:E:160:VAL:HG22	1.70	0.57
1:C:189:PRO:HD2	1:C:211:ARG:HG3	1.86	0.57
1:A:117:GLU:HG3	1:A:180:ALA:HB3	1.87	0.56
1:C:132:ILE:HD11	1:C:168:ALA:HB3	1.86	0.56
1:C:88:VAL:HG11	1:C:93:ARG:HH12	1.70	0.56
1:C:117:GLU:HG3	1:C:180:ALA:HB3	1.88	0.56
1:A:72:VAL:HG21	1:A:106:GLU:HG3	1.89	0.55
1:A:163:SER:HB2	1:E:68:VAL:HG21	1.90	0.54
1:A:194:ARG:HG2	1:A:196:TYR:CZ	2.43	0.54
1:F:206:ARG:HB2	1:F:218:GLN:HB3	1.90	0.53
1:F:16:TYR:HB3	1:F:39:VAL:HG22	1.91	0.53
1:F:117:GLU:HG3	1:F:181:PRO:HD3	1.89	0.53
1:E:218:GLN:HG3	1:E:219:GLU:HG3	1.90	0.53
1:D:191:THR:OG1	1:D:192:LEU:N	2.41	0.52
1:F:133:ASN:H	1:F:136:THR:HG22	1.76	0.51
1:C:52:LEU:HD12	1:C:52:LEU:H	1.74	0.51
1:D:131:GLU:H	1:D:140:SER:HB3	1.75	0.51
1:A:104:ARG:HA	1:A:107:THR:HG22	1.92	0.51
1:B:48:LEU:HD11	1:B:84:LEU:HG	1.92	0.51
1:F:131:GLU:HA	1:F:217:VAL:H	1.76	0.50
1:F:99:LEU:N	1:F:199:MET:O	2.34	0.50
1:C:72:VAL:HG21	1:C:106:GLU:HG3	1.93	0.50
1:D:30:LYS:H	1:D:30:LYS:CD	2.24	0.50
1:E:146:GLN:CD	1:E:146:GLN:H	2.16	0.49
1:F:218:GLN:HG3	1:F:219:GLU:HG3	1.94	0.49
1:E:31:GLU:N	1:E:31:GLU:OE2	2.38	0.49
1:E:5:SER:HB2	1:E:22:LEU:HD13	1.95	0.49
1:D:30:LYS:H	1:D:30:LYS:HD3	1.78	0.49
1:E:20:PRO:HD3	1:E:38:VAL:HG21	1.94	0.49
1:D:107:THR:HG22	1:D:109:SER:HB3	1.94	0.48
1:B:19:SER:HB2	1:B:39:VAL:HG23	1.95	0.48
1:A:56:CYS:SG	1:A:57:GLU:N	2.86	0.48
1:F:127:ALA:HA	1:F:214:THR:HG22	1.95	0.48
1:C:194:ARG:HG2	1:C:196:TYR:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:TYR:HB3	1:D:39:VAL:HG22	1.96	0.48
1:D:2:ASN:HD22	1:D:52:LEU:HD13	1.79	0.48
1:B:110:ARG:HD3	1:B:143:ILE:HG12	1.96	0.47
1:E:117:GLU:HG3	1:E:180:ALA:HB3	1.96	0.47
1:F:44:TYR:HB2	1:F:47:CYS:HB3	1.94	0.47
1:F:148:LEU:HD13	1:F:152:LEU:HD21	1.96	0.47
1:F:213:ALA:HB1	1:F:214:THR:HG23	1.97	0.47
1:E:54:GLN:HG3	1:E:59:SER:HB2	1.96	0.47
1:B:5:SER:HB2	1:B:22:LEU:HD22	1.96	0.47
1:D:60:LYS:HE3	1:D:97:ASP:HA	1.97	0.47
1:D:22:LEU:HA	1:D:23:PRO:HD3	1.78	0.46
1:F:113:LEU:HD12	1:F:179:TYR:HD1	1.80	0.46
1:F:64:ALA:HB2	1:F:100:PHE:HB3	1.98	0.46
1:F:36:TRP:CG	1:F:37:PRO:HD2	2.51	0.46
1:A:107:THR:HG23	1:A:109:SER:H	1.80	0.46
1:A:29:PRO:HG2	1:A:32:LEU:HB2	1.98	0.45
1:D:10:VAL:HG13	1:D:202:PHE:HD1	1.81	0.45
1:C:104:ARG:HB3	1:C:143:ILE:HD13	1.99	0.45
1:D:104:ARG:HB2	1:D:177:ASP:OD1	2.15	0.45
1:D:157:VAL:HG23	1:D:174:SER:HA	1.98	0.45
1:C:46:ASN:ND2	1:C:89:ASP:OD1	2.50	0.45
1:D:115:GLU:HG2	1:D:119:LYS:HD3	1.99	0.45
1:E:173:CYS:SG	1:E:174:SER:N	2.90	0.45
1:B:105:PHE:CE1	1:B:177:ASP:HB2	2.52	0.44
1:E:20:PRO:HD3	1:E:38:VAL:CG2	2.46	0.44
1:C:58:LEU:HD22	1:C:94:ALA:HB2	1.98	0.44
1:F:26:CYS:HA	1:F:27:PRO:HD3	1.87	0.44
1:E:113:LEU:HD12	1:E:179:TYR:CD1	2.52	0.44
1:C:88:VAL:HG11	1:C:93:ARG:NH1	2.32	0.44
1:E:206:ARG:HB2	1:E:218:GLN:HB3	1.99	0.44
1:A:74:VAL:HG22	1:A:107:THR:HG21	1.99	0.44
1:A:91:LYS:HB3	1:A:91:LYS:HE2	1.70	0.44
1:A:41:ASN:ND2	1:A:50:ILE:O	2.44	0.43
1:C:34:GLU:O	1:C:45:PRO:HG2	2.18	0.43
1:F:117:GLU:HG3	1:F:180:ALA:HB3	2.01	0.43
1:D:209:VAL:HG12	1:D:215:PHE:HB3	1.99	0.43
1:F:36:TRP:CD2	1:F:37:PRO:HD2	2.54	0.43
1:E:176:VAL:HG12	1:E:178:VAL:H	1.84	0.42
1:C:105:PHE:CE1	1:C:177:ASP:HB2	2.54	0.42
1:B:60:LYS:HA	1:B:61:PRO:HD3	1.89	0.42
1:D:107:THR:O	1:D:108:ASN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:SER:HA	1:B:145:SER:HB3	2.02	0.42
1:D:44:TYR:HB2	1:D:47:CYS:HB3	2.00	0.42
1:E:198:ILE:HD13	1:E:207:LEU:HD22	2.02	0.42
1:F:113:LEU:HD12	1:F:179:TYR:CD1	2.55	0.42
1:E:203:LYS:HA	1:E:204:PRO:HD3	1.91	0.42
1:B:43:ARG:NH2	1:B:90:GLY:O	2.52	0.41
1:E:22:LEU:HD21	1:E:41:ASN:OD1	2.19	0.41
1:D:214:THR:OG1	1:D:215:PHE:N	2.53	0.41
1:B:117:GLU:HG3	1:B:180:ALA:HB3	2.02	0.41
1:C:30:LYS:H	1:C:30:LYS:HE2	1.85	0.41
1:F:208:MET:H	1:F:208:MET:HG2	1.47	0.41
1:A:113:LEU:HD12	1:A:179:TYR:CD1	2.56	0.41
1:A:189:PRO:HD2	1:A:211:ARG:HG3	2.01	0.41
1:B:194:ARG:HG2	1:B:196:TYR:CZ	2.56	0.41
1:C:7:LEU:HA	1:C:8:PRO:HD3	1.91	0.41
1:E:208:MET:H	1:E:208:MET:HG2	1.63	0.41
1:A:14:LEU:HA	1:A:14:LEU:HD12	1.80	0.41
1:F:37:PRO:HA	1:F:46:ASN:O	2.20	0.41
1:E:113:LEU:HD12	1:E:179:TYR:HD1	1.86	0.41
1:E:44:TYR:HB2	1:E:47:CYS:HB3	2.03	0.41
1:F:22:LEU:HA	1:F:23:PRO:HD3	1.72	0.41
1:B:153:PRO:HG2	1:B:158:ALA:HB1	2.03	0.41
1:C:48:LEU:HD11	1:C:84:LEU:HD22	2.02	0.41
1:E:197:LYS:HB2	1:E:197:LYS:HE2	1.95	0.41
1:C:105:PHE:CD2	1:C:143:ILE:HD12	2.56	0.41
1:C:37:PRO:HA	1:C:46:ASN:O	2.21	0.40
1:D:158:ALA:HA	1:D:175:VAL:O	2.21	0.40
1:E:36:TRP:CG	1:E:37:PRO:HD2	2.56	0.40
1:E:110:ARG:NH1	1:E:150:PRO:O	2.55	0.40
1:E:161:GLY:N	1:E:203:LYS:HD2	2.37	0.40
1:E:49:GLN:HG2	1:E:51:THR:HG23	2.04	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	217/219 (99%)	206 (95%)	10 (5%)	1 (0%)	34	78
1	B	217/219 (99%)	205 (94%)	12 (6%)	0	100	100
1	C	217/219 (99%)	205 (94%)	12 (6%)	0	100	100
1	D	205/219 (94%)	190 (93%)	11 (5%)	4 (2%)	9	48
1	E	207/219 (94%)	191 (92%)	16 (8%)	0	100	100
1	F	205/219 (94%)	191 (93%)	14 (7%)	0	100	100
All	All	1268/1314 (96%)	1188 (94%)	75 (6%)	5 (0%)	39	80

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	3	LYS
1	A	134	LYS
1	D	213	ALA
1	D	2	ASN
1	D	130	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	181/184 (98%)	163 (90%)	18 (10%)	10	38
1	B	175/184 (95%)	159 (91%)	16 (9%)	12	42
1	C	177/184 (96%)	167 (94%)	10 (6%)	26	68
1	D	170/184 (92%)	151 (89%)	19 (11%)	7	32
1	E	175/184 (95%)	157 (90%)	18 (10%)	9	36
1	F	170/184 (92%)	153 (90%)	17 (10%)	9	37
All	All	1048/1104 (95%)	950 (91%)	98 (9%)	11	41

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	14	LEU
1	A	32	LEU
1	A	39	VAL
1	A	52	LEU
1	A	57	GLU
1	A	88	VAL
1	A	115	GLU
1	A	132	ILE
1	A	151	LEU
1	A	155	ASP
1	A	157	VAL
1	A	167	LYS
1	A	177	ASP
1	A	187	LEU
1	A	195	VAL
1	A	199	MET
1	A	217	VAL
1	B	32	LEU
1	B	50	ILE
1	B	55	VAL
1	B	70	GLN
1	B	84	LEU
1	B	88	VAL
1	B	115	GLU
1	B	129	LEU
1	B	131	GLU
1	B	151	LEU
1	B	157	VAL
1	B	173	CYS
1	B	187	LEU
1	B	191	THR
1	B	195	VAL
1	B	214	THR
1	C	30	LYS
1	C	46	ASN
1	C	48	LEU
1	C	132	ILE
1	C	157	VAL
1	C	191	THR
1	C	192	LEU
1	C	195	VAL
1	C	214	THR

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Mol	Chain	Res	Type
1	C	217	VAL
1	D	14	LEU
1	D	30	LYS
1	D	39	VAL
1	D	52	LEU
1	D	72	VAL
1	D	83	TRP
1	D	88	VAL
1	D	89	ASP
1	D	106	GLU
1	D	109	SER
1	D	140	SER
1	D	151	LEU
1	D	157	VAL
1	D	175	VAL
1	D	176	VAL
1	D	191	THR
1	D	208	MET
1	D	214	THR
1	D	217	VAL
1	E	1	SER
1	E	7	LEU
1	E	14	LEU
1	E	47	CYS
1	E	48	LEU
1	E	52	LEU
1	E	53	GLN
1	E	72	VAL
1	E	83	TRP
1	E	115	GLU
1	E	129	LEU
1	E	132	ILE
1	E	140	SER
1	E	155	ASP
1	E	157	VAL
1	E	160	VAL
1	E	175	VAL
1	E	187	LEU
1	F	9	ARG
1	F	14	LEU
1	F	39	VAL
1	F	47	CYS

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Mol	Chain	Res	Type
1	F	72	VAL
1	F	83	TRP
1	F	106	GLU
1	F	124	HIS
1	F	129	LEU
1	F	143	ILE
1	F	151	LEU
1	F	175	VAL
1	F	187	LEU
1	F	195	VAL
1	F	197	LYS
1	F	208	MET
1	F	218	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	53	GLN

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 carbohydrates 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(Å²)	Q<0.9
1	A	219/219 (100%)	0.30	3 (1%)	78	65	87, 101, 123, 154	0
1	B	219/219 (100%)	0.52	17 (7%)	16	9	92, 122, 148, 171	0
1	C	219/219 (100%)	0.34	8 (3%)	45	30	95, 118, 145, 163	0
1	D	209/219 (95%)	0.27	3 (1%)	78	65	85, 102, 127, 148	0
1	E	211/219 (96%)	0.30	5 (2%)	62	47	90, 108, 140, 157	0
1	F	209/219 (95%)	0.29	2 (0%)	84	75	84, 108, 139, 179	0
All	All	1286/1314 (97%)	0.34	38 (2%)	54	39	84, 110, 141, 179	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	137	VAL	3.3
1	B	4	ILE	3.2
1	B	50	ILE	3.1
1	C	4	ILE	3.0
1	C	2	ASN	2.8
1	D	162	ALA	2.7
1	C	55	VAL	2.6
1	B	16	TYR	2.6
1	A	40	SER	2.6
1	B	40	SER	2.5
1	F	113	LEU	2.5
1	C	183	PHE	2.5
1	B	42	ASP	2.4
1	F	52	LEU	2.4
1	B	43	ARG	2.3
1	E	187	LEU	2.3
1	C	215	PHE	2.3
1	D	187	LEU	2.3
1	D	52	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	18	TYR	2.2
1	B	51	THR	2.2
1	A	21	ASP	2.2
1	B	39	VAL	2.2
1	A	113	LEU	2.2
1	C	39	VAL	2.2
1	E	142	PHE	2.1
1	B	92	ALA	2.1
1	E	213	ALA	2.1
1	B	6	CYS	2.1
1	B	178	VAL	2.1
1	B	64	ALA	2.1
1	E	192	LEU	2.1
1	B	113	LEU	2.1
1	E	1	SER	2.1
1	C	18	TYR	2.0
1	B	82	TYR	2.0
1	B	67	MET	2.0
1	B	59	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 (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.