WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 03:44 PM GMT

PDB ID	:	2FYZ
Title	:	Structural of Mumps virus fusion protein core
Authors	:	Lou, Z.; Xu, Y.; Liu, Y.; Rao, Z.
Deposited on	:	2006-02-08
Resolution	:	2.20 Å(reported)

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

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1   Overall quality at a glance ⓘ

The reported resolution of this entry is 2.20 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		0.287
Clashscore		21
Ramachandran outliers		1.5%
Sidechain outliers		1.3%
RSRZ outliers		12.3%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
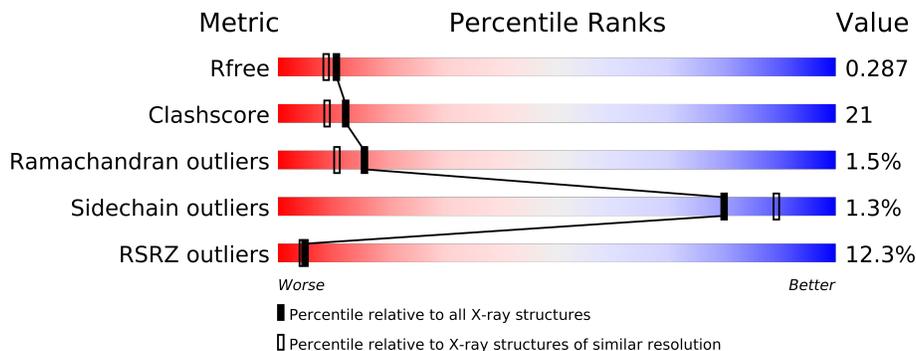
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	63	
1	C	63	
1	E	63	
2	B	48	
2	D	48	
2	F	48	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2330 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	57	Total	C	N	O	S	0	0	0
			428	261	82	83	2			
1	C	58	Total	C	N	O	S	0	0	0
			426	262	79	83	2			
1	E	62	Total	C	N	O	S	0	0	0
			452	278	86	87	1			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	GLY	-	CLONING ARTIFACT	UNP P11236
A	120	PRO	-	CLONING ARTIFACT	UNP P11236
A	121	LEU	-	CLONING ARTIFACT	UNP P11236
A	122	GLY	-	CLONING ARTIFACT	UNP P11236
A	123	SER	-	CLONING ARTIFACT	UNP P11236
C	119	GLY	-	CLONING ARTIFACT	UNP P11236
C	120	PRO	-	CLONING ARTIFACT	UNP P11236
C	121	LEU	-	CLONING ARTIFACT	UNP P11236
C	122	GLY	-	CLONING ARTIFACT	UNP P11236
C	123	SER	-	CLONING ARTIFACT	UNP P11236
E	119	GLY	-	CLONING ARTIFACT	UNP P11236
E	120	PRO	-	CLONING ARTIFACT	UNP P11236
E	121	LEU	-	CLONING ARTIFACT	UNP P11236
E	122	GLY	-	CLONING ARTIFACT	UNP P11236
E	123	SER	-	CLONING ARTIFACT	UNP P11236

- Molecule 2 is a protein called Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	32	Total	C	N	O	0	0	0
			246	151	43	52			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	31	Total 242	C 149	N 42	O 51	0	0	0
2	F	36	Total 273	C 167	N 50	O 56	0	0	0

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	438	ASN	-	CLONING ARTIFACT	UNP P11236
B	439	MET	-	CLONING ARTIFACT	UNP P11236
B	440	SER	-	CLONING ARTIFACT	UNP P11236
B	441	SER	-	CLONING ARTIFACT	UNP P11236
B	442	GLY	-	CLONING ARTIFACT	UNP P11236
B	443	GLY	-	CLONING ARTIFACT	UNP P11236
B	444	ARG	-	CLONING ARTIFACT	UNP P11236
B	445	GLY	-	CLONING ARTIFACT	UNP P11236
B	446	GLY	-	CLONING ARTIFACT	UNP P11236
B	463	THR	ALA	ENGINEERED	UNP P11236
B	478	ILE	ASN	ENGINEERED	UNP P11236
D	438	ASN	-	CLONING ARTIFACT	UNP P11236
D	439	MET	-	CLONING ARTIFACT	UNP P11236
D	440	SER	-	CLONING ARTIFACT	UNP P11236
D	441	SER	-	CLONING ARTIFACT	UNP P11236
D	442	GLY	-	CLONING ARTIFACT	UNP P11236
D	443	GLY	-	CLONING ARTIFACT	UNP P11236
D	444	ARG	-	CLONING ARTIFACT	UNP P11236
D	445	GLY	-	CLONING ARTIFACT	UNP P11236
D	446	GLY	-	CLONING ARTIFACT	UNP P11236
D	463	THR	ALA	ENGINEERED	UNP P11236
D	478	ILE	ASN	ENGINEERED	UNP P11236
F	438	ASN	-	CLONING ARTIFACT	UNP P11236
F	439	MET	-	CLONING ARTIFACT	UNP P11236
F	440	SER	-	CLONING ARTIFACT	UNP P11236
F	441	SER	-	CLONING ARTIFACT	UNP P11236
F	442	GLY	-	CLONING ARTIFACT	UNP P11236
F	443	GLY	-	CLONING ARTIFACT	UNP P11236
F	444	ARG	-	CLONING ARTIFACT	UNP P11236
F	445	GLY	-	CLONING ARTIFACT	UNP P11236
F	446	GLY	-	CLONING ARTIFACT	UNP P11236
F	463	THR	ALA	ENGINEERED	UNP P11236
F	478	ILE	ASN	ENGINEERED	UNP P11236

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	50	Total 50	O 50	0	0
3	B	43	Total 43	O 43	0	0
3	C	44	Total 44	O 44	0	0
3	D	43	Total 43	O 43	0	0
3	E	36	Total 36	O 36	0	0
3	F	47	Total 47	O 47	0	0

3   Residue-property plots ⓘ

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: Fusion glycoprotein F0
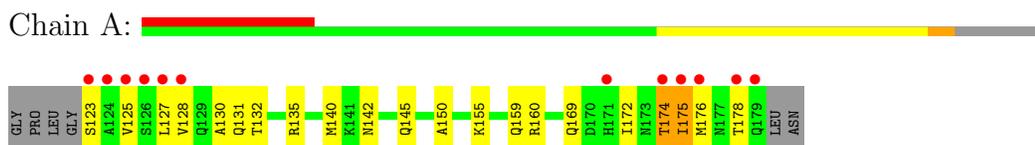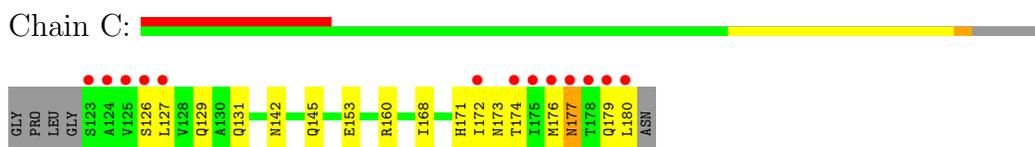
Chain A:

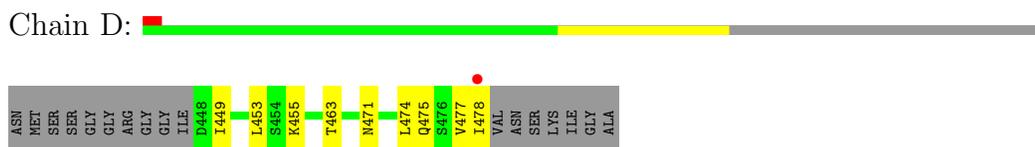
- Molecule 1: Fusion glycoprotein F0
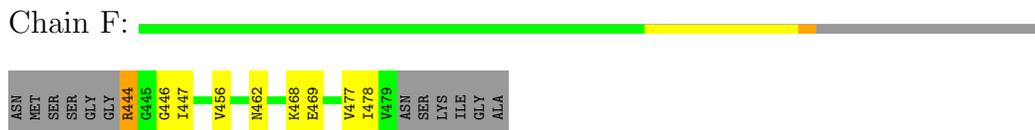
Chain C:

- Molecule 1: Fusion glycoprotein F0

Chain E:

- Molecule 2: Fusion glycoprotein F0

Chain B:

- Molecule 2: Fusion glycoprotein F0

Chain D:

- Molecule 2: Fusion glycoprotein F0

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	161.17Å 60.81Å 40.15Å 90.00° 98.36° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 40.02 – 2.21	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.20) 88.9 (40.02-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.04 (at 2.22Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.231 , 0.278 0.237 , 0.287	Depositor DCC
R_{free} test set	851 reflections (4.95%)	DCC
Wilson B-factor (Å^2)	18.3	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 54.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	0 of 18557 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	2330	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.25% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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	0.30	0/429	0.47	0/580
1	C	0.32	0/427	0.47	0/579
1	E	0.35	0/454	0.54	0/616
2	B	0.35	0/247	0.54	0/332
2	D	0.34	0/243	0.50	0/327
2	F	0.33	0/274	0.52	0/367
All	All	0.33	0/2074	0.50	0/2801

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2   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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	428	0	441	31	0
1	C	426	0	435	22	0
1	E	452	0	463	21	0
2	B	246	0	243	14	0
2	D	242	0	242	9	0
2	F	273	0	273	9	0
3	A	50	0	0	3	0
3	B	43	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	44	0	0	3	0
3	D	43	0	0	0	0
3	E	36	0	0	0	0
3	F	47	0	0	2	0
All	All	2330	0	2097	89	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

All (89) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:119:GLY:O	1:E:121:LEU:N	2.01	0.92
1:A:150:ALA:HA	3:B:162:HOH:O	1.74	0.87
2:B:463:THR:HA	3:B:162:HOH:O	1.77	0.84
1:E:156:GLU:O	1:E:160:ARG:HG2	1.81	0.80
2:F:444:ARG:HG2	2:F:447:ILE:H	1.47	0.78
1:C:179:GLN:O	1:C:180:LEU:HG	1.83	0.77
1:A:142:ASN:HA	1:A:145:GLN:HE21	1.50	0.76
1:E:160:ARG:HB2	2:F:456:VAL:HG22	1.71	0.71
1:E:119:GLY:C	1:E:121:LEU:H	1.96	0.69
1:A:142:ASN:HA	1:A:145:GLN:NE2	2.07	0.69
1:A:172:ILE:O	1:A:176:MET:HB2	1.92	0.69
2:B:475:GLN:HA	2:B:475:GLN:HE21	1.58	0.69
1:A:127:LEU:O	1:A:131:GLN:HG3	1.94	0.67
2:B:478:ILE:HD11	1:E:138:ALA:HA	1.76	0.66
2:B:457:ASN:HB3	3:B:267:HOH:O	1.98	0.64
1:A:174:THR:HG22	1:A:175:ILE:HG13	1.80	0.64
2:B:466:TYR:HD1	3:B:162:HOH:O	1.80	0.63
1:C:160:ARG:HH11	2:D:455:LYS:HB3	1.63	0.63
2:F:444:ARG:HE	2:F:446:GLY:HA3	1.63	0.63
1:A:128:VAL:HA	1:A:131:GLN:OE1	1.99	0.62
1:E:169:GLN:NE2	1:E:173:ASN:HD21	1.99	0.61
1:C:172:ILE:HG22	1:C:172:ILE:O	2.01	0.60
1:A:123:SER:C	1:A:125:VAL:H	2.05	0.58
1:C:127:LEU:O	1:C:131:GLN:HG3	2.04	0.58
1:C:177:ASN:HD22	1:C:177:ASN:C	2.07	0.58
1:A:174:THR:HG22	1:A:175:ILE:N	2.19	0.57
1:E:169:GLN:NE2	1:E:173:ASN:ND2	2.53	0.56
2:F:444:ARG:HG3	2:F:446:GLY:H	1.71	0.56
1:A:155:LYS:NZ	1:A:159:GLN:NE2	2.54	0.56
1:C:142:ASN:HA	1:C:145:GLN:HE21	1.71	0.55
1:A:174:THR:HG22	1:A:175:ILE:H	1.72	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:475:GLN:HA	2:B:475:GLN:NE2	2.22	0.54
2:D:471:ASN:O	2:D:475:GLN:HG2	2.09	0.53
1:A:130:ALA:HB3	3:A:219:HOH:O	2.08	0.53
2:D:477:VAL:O	2:D:478:ILE:HB	2.08	0.53
2:F:477:VAL:O	2:F:478:ILE:HD13	2.09	0.53
1:C:173:ASN:O	1:C:177:ASN:HB3	2.08	0.52
1:C:177:ASN:ND2	1:C:177:ASN:C	2.62	0.52
2:B:478:ILE:O	2:B:478:ILE:HG22	2.08	0.52
1:C:160:ARG:NH1	2:D:455:LYS:HB3	2.25	0.51
2:F:444:ARG:HG3	2:F:446:GLY:N	2.27	0.50
1:C:145:GLN:HG2	3:C:191:HOH:O	2.11	0.50
1:A:169:GLN:HA	1:A:169:GLN:OE1	2.12	0.49
1:C:172:ILE:HA	1:C:176:MET:CG	2.42	0.49
1:C:171:HIS:O	1:C:176:MET:HG2	2.12	0.49
1:A:155:LYS:NZ	1:A:159:GLN:HE22	2.11	0.49
1:C:179:GLN:O	1:C:180:LEU:CG	2.60	0.48
2:B:460:LEU:O	2:B:463:THR:HB	2.13	0.48
1:A:127:LEU:HD12	3:A:219:HOH:O	2.12	0.48
1:A:145:GLN:HG3	2:D:474:LEU:HD21	1.95	0.47
2:B:478:ILE:HD11	1:E:138:ALA:CA	2.44	0.47
1:A:132:THR:HA	1:A:135:ARG:NH1	2.29	0.47
1:A:169:GLN:NE2	2:D:449:ILE:HD12	2.30	0.47
1:A:123:SER:C	1:A:125:VAL:N	2.68	0.47
1:E:171:HIS:CD2	1:E:175:ILE:HB	2.49	0.47
1:C:168:ILE:O	1:C:172:ILE:HG13	2.15	0.47
2:F:468:LYS:HB2	3:F:283:HOH:O	2.15	0.47
1:E:135:ARG:HG2	1:E:135:ARG:HH11	1.80	0.46
1:A:178:THR:HG22	1:A:178:THR:O	2.14	0.46
1:A:140:MET:CE	1:E:137:ILE:HG23	2.45	0.46
1:A:140:MET:HE2	1:E:137:ILE:HG23	1.97	0.46
1:A:176:MET:CE	1:E:172:ILE:HG23	2.45	0.46
1:C:153:GLU:HB2	2:D:463:THR:OG1	2.16	0.46
1:E:127:LEU:C	1:E:127:LEU:HD23	2.36	0.46
1:C:172:ILE:HA	1:C:176:MET:HG3	1.98	0.46
2:F:469:GLU:HG3	3:F:108:HOH:O	2.15	0.46
1:A:175:ILE:O	1:A:176:MET:HG2	2.16	0.45
2:B:478:ILE:HD11	1:E:138:ALA:CB	2.45	0.45
1:C:173:ASN:O	1:C:174:THR:C	2.55	0.45
1:A:155:LYS:HD3	1:A:155:LYS:C	2.37	0.45
2:B:457:ASN:OD1	1:E:159:GLN:NE2	2.46	0.44
1:C:172:ILE:O	1:C:176:MET:HB2	2.17	0.44
2:B:475:GLN:CA	2:B:475:GLN:HE21	2.22	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:133:ASN:O	1:E:137:ILE:HG13	2.18	0.43
1:C:177:ASN:HA	3:C:222:HOH:O	2.17	0.43
2:D:477:VAL:O	2:D:478:ILE:CB	2.65	0.43
1:A:155:LYS:HZ1	1:A:159:GLN:NE2	2.16	0.43
1:E:160:ARG:HB2	2:F:456:VAL:CG2	2.43	0.42
2:B:460:LEU:HB3	1:E:155:LYS:HE2	2.02	0.42
1:A:131:GLN:O	1:A:135:ARG:HG3	2.21	0.41
1:C:127:LEU:HD12	3:C:196:HOH:O	2.19	0.41
1:E:135:ARG:HG2	1:E:135:ARG:NH1	2.35	0.41
1:E:147:THR:O	1:E:151:VAL:HG23	2.21	0.41
1:A:155:LYS:HZ3	1:A:159:GLN:NE2	2.18	0.41
1:A:174:THR:CG2	1:A:175:ILE:H	2.28	0.40
3:A:219:HOH:O	1:C:126:SER:HA	2.21	0.40
2:D:453:LEU:HD23	2:D:453:LEU:HA	1.89	0.40
1:A:160:ARG:HD3	2:B:455:LYS:HB3	2.03	0.40
1:A:130:ALA:HB1	1:C:129:GLN:HG3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

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	55/63 (87%)	51 (93%)	2 (4%)	2 (4%)	5	2
1	C	56/63 (89%)	50 (89%)	6 (11%)	0	100	100
1	E	60/63 (95%)	56 (93%)	3 (5%)	1 (2%)	14	8
2	B	30/48 (62%)	28 (93%)	1 (3%)	1 (3%)	6	2
2	D	29/48 (60%)	29 (100%)	0	0	100	100
2	F	34/48 (71%)	33 (97%)	1 (3%)	0	100	100
All	All	264/333 (79%)	247 (94%)	13 (5%)	4 (2%)	15	10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	THR
2	B	478	ILE
1	E	120	PRO
1	A	175	ILE

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	45/49 (92%)	45 (100%)	0	100	100
1	C	44/49 (90%)	43 (98%)	1 (2%)	63	74
1	E	46/49 (94%)	46 (100%)	0	100	100
2	B	29/41 (71%)	29 (100%)	0	100	100
2	D	29/41 (71%)	29 (100%)	0	100	100
2	F	31/41 (76%)	29 (94%)	2 (6%)	24	25
All	All	224/270 (83%)	221 (99%)	3 (1%)	80	89

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	177	ASN
2	F	444	ARG
2	F	462	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	GLN
1	A	159	GLN
1	A	177	ASN
2	B	475	GLN
1	C	145	GLN
1	C	177	ASN
2	D	457	ASN
2	D	461	GLN

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Mol	Chain	Res	Type
2	D	472	HIS
1	E	131	GLN
1	E	145	GLN
1	E	169	GLN
1	E	171	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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, 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	57/63 (90%)	0.60	12 (21%)	1	1	12, 26, 90, 94	0
1	C	58/63 (92%)	0.54	13 (22%)	1	1	12, 24, 91, 93	0
1	E	62/63 (98%)	0.25	8 (12%)	4	4	11, 23, 84, 99	0
2	B	32/48 (66%)	-0.21	0	100	100	12, 23, 43, 62	0
2	D	31/48 (64%)	-0.10	1 (3%)	45	46	12, 25, 51, 65	0
2	F	36/48 (75%)	-0.31	0	100	100	12, 20, 29, 39	0
All	All	276/333 (82%)	0.22	34 (12%)	5	4	11, 23, 90, 99	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	175	ILE	8.9
1	A	175	ILE	8.0
1	A	125	VAL	7.4
1	E	119	GLY	6.9
1	E	175	ILE	6.7
1	E	178	THR	6.4
1	A	176	MET	5.5
1	E	180	LEU	5.4
1	C	123	SER	4.9
1	C	126	SER	4.7
1	C	174	THR	4.7
1	C	179	GLN	4.3
1	A	124	ALA	4.3
1	C	176	MET	4.2
1	A	179	GLN	4.0
1	A	126	SER	3.8
1	C	178	THR	3.4
1	E	173	ASN	3.4
1	C	177	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	127	LEU	3.1
1	E	179	GLN	3.0
1	C	124	ALA	2.9
1	C	180	LEU	2.8
1	A	123	SER	2.7
1	C	125	VAL	2.7
1	C	172	ILE	2.7
1	A	171	HIS	2.4
1	E	120	PRO	2.2
1	A	178	THR	2.2
1	A	128	VAL	2.2
1	A	174	THR	2.1
2	D	478	ILE	2.1
1	C	127	LEU	2.1
1	E	176	MET	2.0

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

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

6.3 Carbohydrates ⓘ

There are no 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.