



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 2FYZ / pdb_00002fyz
Title : Structural of Mumps virus fusion protein core
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Deposited on : 2006-02-08
Resolution : 2.20 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

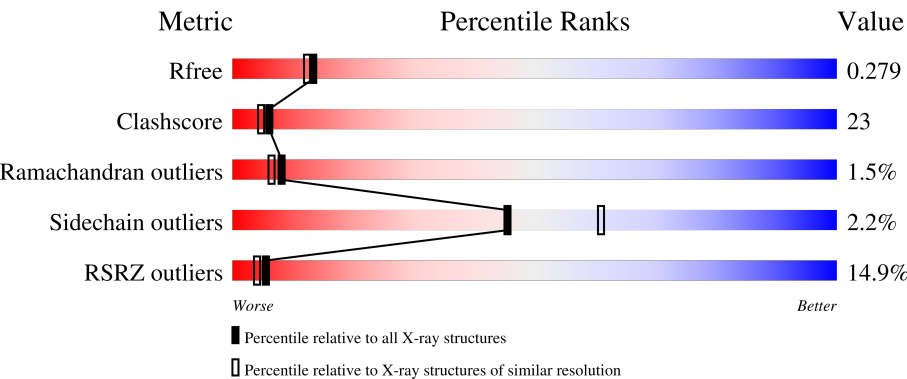
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.20 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.



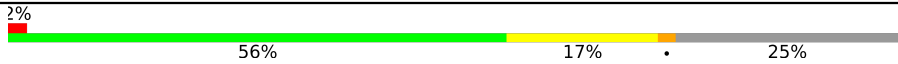
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 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 $\leq 5\%$. 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	63	17% 56% 32% • 10%
1	C	63	22% 62% 29% • 8%
1	E	63	14% 67% 30% ••
2	B	48	4% 52% 12% • 33%
2	D	48	8% 46% 17% • 35%

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Mol	Chain	Length	Quality of chain
2	F	48	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: a small red segment at the beginning labeled '2%', followed by a green segment labeled '56%', a yellow segment labeled '17%', and a grey segment at the end labeled '25%'. A small black dot is located on the boundary between the yellow and grey segments.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2330 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 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	C	N	O	0	0	0
			242	149	42	51			
2	F	36	Total	C	N	O	0	0	0
			273	167	50	56			

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 mutation	UNP P11236
B	478	ILE	ASN	engineered mutation	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 mutation	UNP P11236
D	478	ILE	ASN	engineered mutation	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 mutation	UNP P11236
F	478	ILE	ASN	engineered mutation	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 [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: Fusion glycoprotein F0



- Molecule 1: Fusion glycoprotein F0



- Molecule 1: Fusion glycoprotein F0



- Molecule 2: Fusion glycoprotein F0



- Molecule 2: Fusion glycoprotein F0



- Molecule 2: Fusion glycoprotein F0



4 Data and refinement statistics

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 50.00 – 2.21	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.20) 88.7 (50.00-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.04 (at 2.22Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.231 , 0.278 0.232 , 0.279	Depositor DCC
R_{free} test set	905 reflections (4.88%)	wwPDB-VP
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 , 70.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.40	0/429	0.79	0/580
1	C	0.41	0/427	0.79	1/579 (0.2%)
1	E	0.46	0/454	0.90	1/616 (0.2%)
2	B	0.45	0/247	0.83	0/332
2	D	0.46	0/243	0.81	0/327
2	F	0.43	0/274	0.88	0/367
All	All	0.43	0/2074	0.83	2/2801 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	121	LEU	N-CA-C	-6.24	103.78	112.45
1	C	154	VAL	N-CA-C	-5.03	105.64	110.72

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	428	0	441	32	0
1	C	426	0	435	26	0
1	E	452	0	463	22	0
2	B	246	0	243	14	0
2	D	242	0	242	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	273	0	273	9	0
3	A	50	0	0	3	0
3	B	43	0	0	4	0
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	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 23.

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: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:119:GLY:C	1:E:121:LEU:H	1.96	0.74
1:E:160:ARG:HB2	2:F:456:VAL:HG22	1.71	0.71
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:HE21	2:B:475:GLN:HA	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
1:A:140:MET:HE2	1:E:137:ILE:HG23	1.79	0.65
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:A:123:SER:C	1:A:125:VAL:H	2.05	0.62
1:C:177:ASN:C	1:C:177:ASN:HD22	2.07	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:C:127:LEU:O	1:C:131:GLN:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:THR:HG22	1:A:175:ILE:N	2.19	0.57
1:C:177:ASN:C	1:C:177:ASN:ND2	2.62	0.57
1:A:137:ILE:HG23	1:C:140:MET:HE2	1.87	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
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
2:B:478:ILE:O	2:B:478:ILE:HG22	2.08	0.52
1:A:155:LYS:HZ1	1:A:159:GLN:NE2	2.08	0.52
1:C:160:ARG:NH1	2:D:455:LYS:HB3	2.25	0.51
1:E:127:LEU:C	1:E:127:LEU:HD23	2.36	0.50
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:C:173:ASN:O	1:C:174:THR:C	2.55	0.50
1:A:169:GLN:HA	1:A:169:GLN:OE1	2.12	0.49
1:A:155:LYS:HD3	1:A:155:LYS:C	2.37	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:A:123:SER:C	1:A:125:VAL:N	2.68	0.48
1:C:179:GLN:O	1:C:180:LEU:CG	2.60	0.48
1:A:127:LEU:HD12	3:A:219:HOH:O	2.12	0.48
2:B:460:LEU:O	2:B:463:THR:HB	2.13	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:155:LYS:HZ1	1:A:159:GLN:HE22	1.63	0.45
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:A:140:MET:CE	1:E:137:ILE:HG23	2.45	0.45
1:C:171:HIS:C	1:C:173:ASN:H	2.24	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:HE21	2:B:475:GLN:CA	2.22	0.44
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:C:172:ILE:C	1:C:176:MET:HB2	2.44	0.43
1:E:119:GLY:C	1:E:121:LEU:N	2.66	0.42
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: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:C:171:HIS:C	1:C:173:ASN:N	2.79	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 [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	55/63 (87%)	51 (93%)	2 (4%)	2 (4%)	2	1
1	C	56/63 (89%)	50 (89%)	6 (11%)	0	100	100
1	E	60/63 (95%)	56 (93%)	3 (5%)	1 (2%)	7	5
2	B	30/48 (62%)	28 (93%)	1 (3%)	1 (3%)	3	1
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%)	8	6

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 ⓘ

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%)	44	59
1	E	46/49 (94%)	45 (98%)	1 (2%)	45	61
2	B	29/41 (71%)	29 (100%)	0	100	100
2	D	29/41 (71%)	28 (97%)	1 (3%)	32	44
2	F	31/41 (76%)	29 (94%)	2 (6%)	15	18
All	All	224/270 (83%)	219 (98%)	5 (2%)	45	61

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	177	ASN

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Mol	Chain	Res	Type
2	D	463	THR
1	E	177	ASN
2	F	444	ARG
2	F	462	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	GLN
1	A	159	GLN
1	A	177	ASN
2	B	472	HIS
2	B	475	GLN
1	C	145	GLN
1	C	177	ASN
2	D	457	ASN
2	D	461	GLN
2	D	473	GLN
1	E	131	GLN
1	E	145	GLN
1	E	169	GLN
1	E	171	HIS
1	E	173	ASN
2	F	472	HIS
2	F	473	GLN

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 oligosaccharides 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(Å ²)	Q<0.9
1	A	57/63 (90%)	0.91	11 (19%) 3 2	12, 26, 90, 94	0
1	C	58/63 (92%)	0.88	14 (24%) 2 1	12, 24, 91, 93	0
1	E	62/63 (98%)	0.68	9 (14%) 6 4	11, 23, 84, 99	0
2	B	32/48 (66%)	0.25	2 (6%) 26 23	12, 23, 43, 62	0
2	D	31/48 (64%)	0.56	4 (12%) 7 5	12, 25, 51, 65	0
2	F	36/48 (75%)	0.08	1 (2%) 55 52	12, 20, 29, 39	0
All	All	276/333 (82%)	0.63	41 (14%) 5 4	11, 23, 90, 99	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	175	ILE	8.2
1	E	119	GLY	7.2
1	E	175	ILE	6.1
1	C	175	ILE	5.7
1	A	176	MET	5.0
1	C	176	MET	4.8
1	C	125	VAL	4.8
1	A	178	THR	4.8
1	E	173	ASN	4.8
1	A	179	GLN	4.7
1	A	125	VAL	4.6
1	C	177	ASN	4.5
1	C	179	GLN	4.5
1	C	172	ILE	4.5
1	E	180	LEU	4.5
1	E	176	MET	4.4
1	C	180	LEU	4.3
1	C	174	THR	4.3
1	A	127	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	E	120	PRO	4.2
1	E	179	GLN	4.1
1	A	177	ASN	4.1
1	C	178	THR	4.0
1	C	124	ALA	3.8
1	A	126	SER	3.8
1	C	126	SER	3.8
2	D	478	ILE	3.7
2	D	477	VAL	3.7
1	E	178	THR	3.6
1	A	124	ALA	3.4
2	D	463	THR	3.2
1	A	174	THR	3.1
1	C	123	SER	3.0
2	B	478	ILE	2.8
1	A	171	HIS	2.8
1	C	173	ASN	2.6
1	E	174	THR	2.6
2	F	463	THR	2.4
1	C	127	LEU	2.4
2	D	448	ASP	2.1
2	B	463	THR	2.1

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 oligosaccharides 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.