W O R L D W I D E

wwPDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

May 21, 2020 – 04:53 pm BST

PDB ID	:	4JFB
Title	:	Crystal structure of OmpF in C2 with tNCS
Authors	:	Wiseman, B.; Kilburg, A.; Chaptal, V.; Reyes-Meija, G.C.; Sarwan, J.; Falson, P.; Jault, J.M.
Deposited on	:	2013-02-28
Resolution	:	3.80 Å(reported)

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	:	2.11
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)	:	2.11

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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.
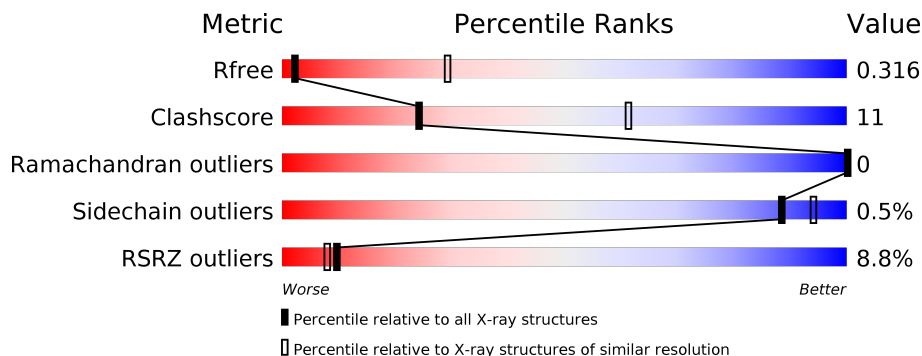
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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 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	340	2% / 79% / 21%
1	B	340	4% / 78% / 22%
1	C	340	5% / 74% / 26%
1	D	340	12% / 76% / 23% •
1	E	340	19% / 75% / 25%
1	F	340	9% / 73% / 27%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 15765 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.
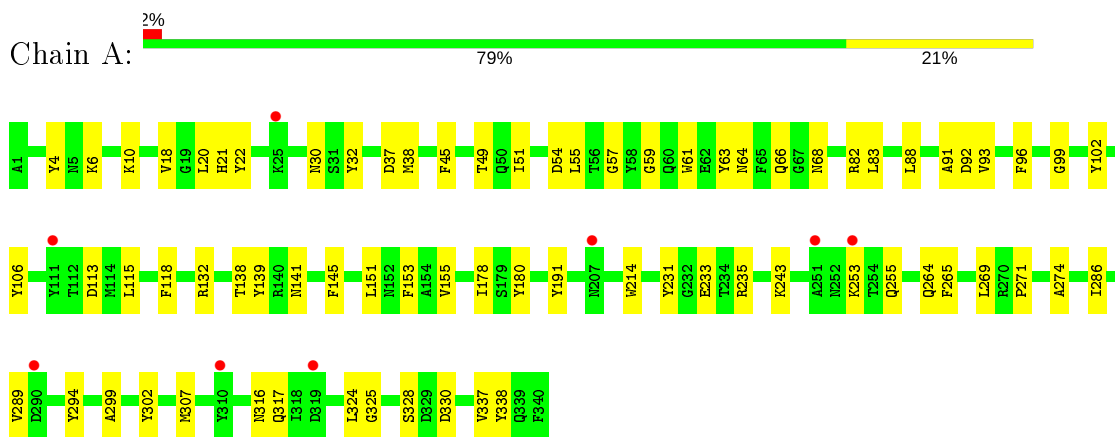
- Molecule 1 is a protein called Outer membrane protein F.

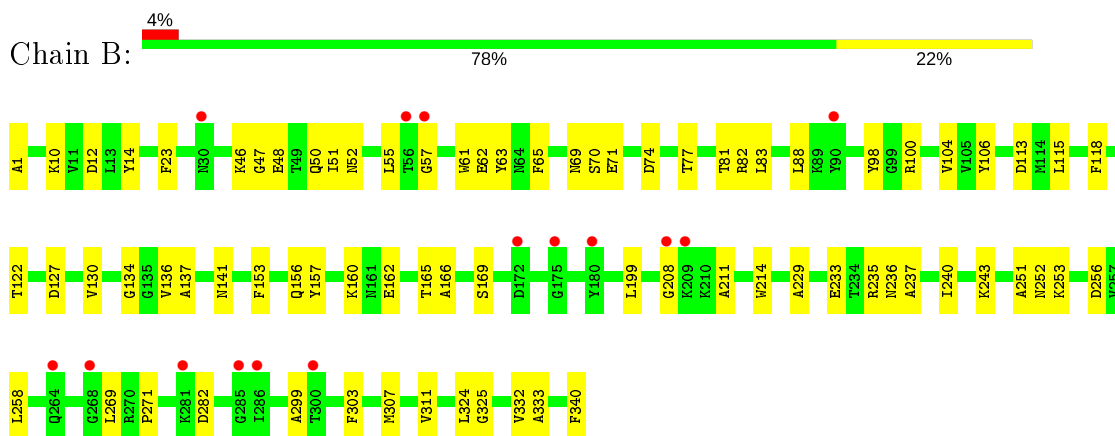| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	B	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	C	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	D	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	E	340	Total	C	N	O	S	0	1	0
			2630	1656	438	533	3			
1	F	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			

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 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.
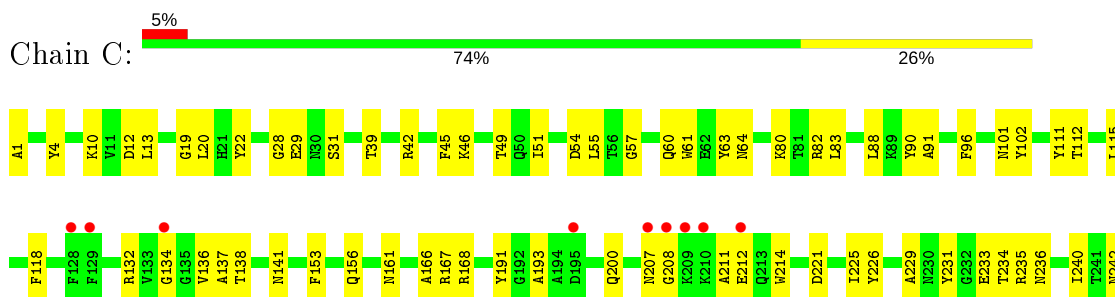
• Molecule 1: Outer membrane protein F

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T247 F250 A251 N252 K253 T254 Q255 D256 V257 L258 L259 V260 Q264 L269 T276 A280 K281 G285 I286 V289 A299 F303 M307 S308 T309 Y310 V311 D312 Y313 L324 D329 V332 A333 Y338 Q339 F340

- Molecule 1: Outer membrane protein F

Chain D:

12%

76%   23%

A1 D12 V18 G19 L20 H21 Y22 F23 S24 K25 G26 N27 G28 S31 Y32 N35 G36 D37 M38 T39 R42 K46 G47 L55 W61 E62 Y63 N64 N68 E71 K80 T81 R82 L83 Y90 G94 N101 Y102 G103 Y106 D107 A108 D113 M114

L115 F118 A123 Y124 V130 R140 N141 F153 D172 I178 S179 Y180 E181 Y182 E183 G184 F185 G186 I187 V188 G189 A190 Y191 D195 N207 G208 K209 K210 A211 W214 A215 T216 G217 Y220 D221 A229 N230 Y231 G232 E233 R235 N236 A237 T238 N242

T247 A251 N252 K253 T254 Q255 Q262 Y263 D266 F267 G268 L269 R270 P271 A274 V283 V289 D290 L291 V292 N293 Y294 F295 E296 Y297 G298 A299 T300 F303 M307 S308 T309 Y310 V311 D312 Y313 I314 Q317 I318 L324 D329 V332 A333 V337 F340
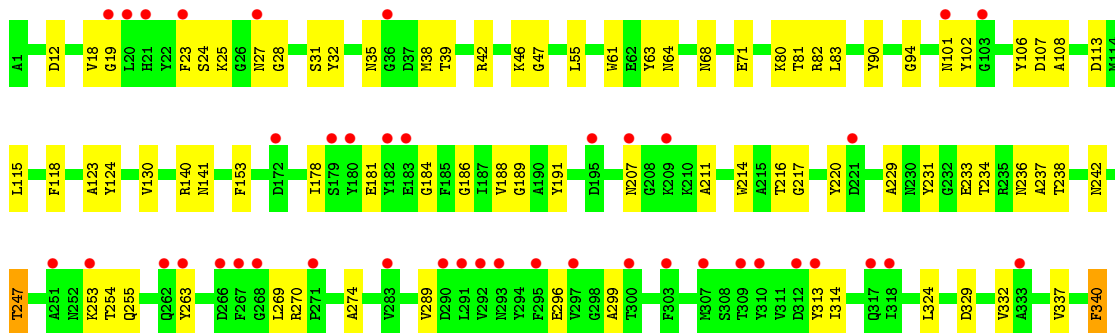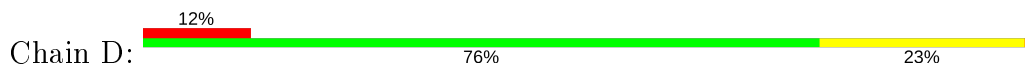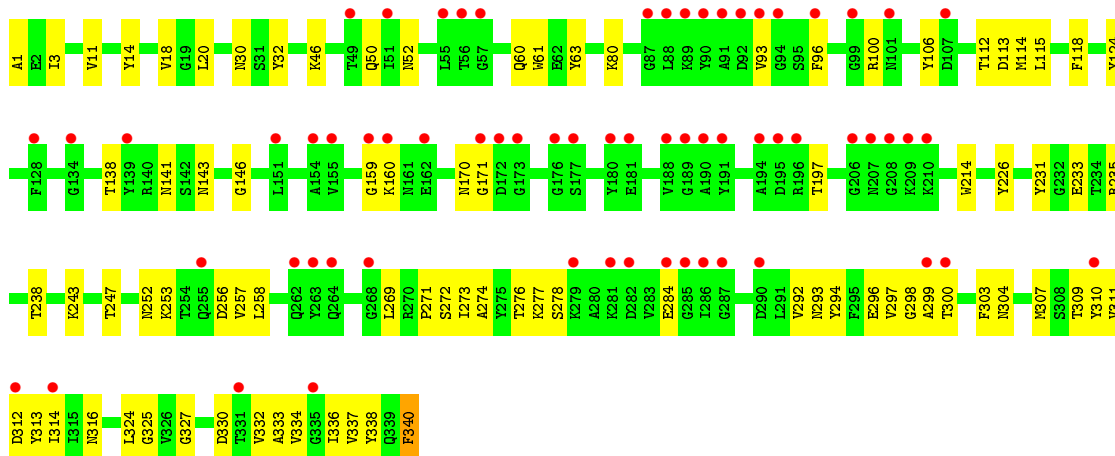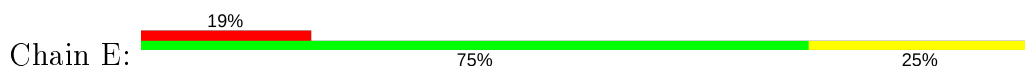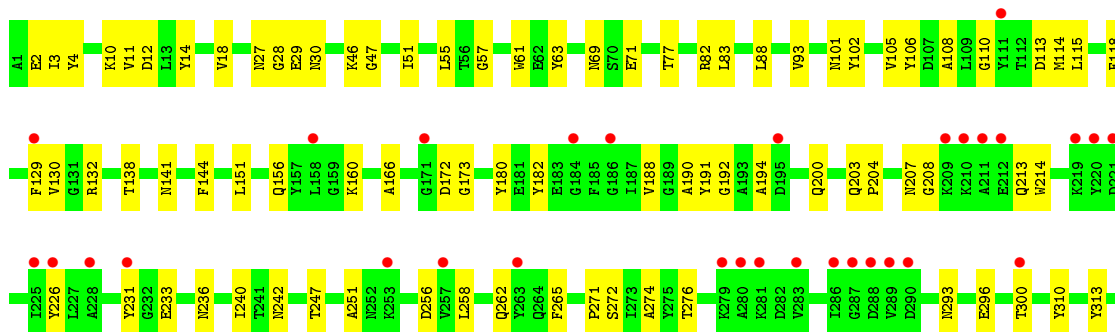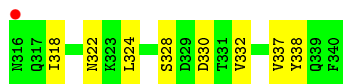
- Molecule 1: Outer membrane protein F

Chain E:

19%

75%   25%

A1 E2 I3 V11 Y14 V18 G19 L20 N30 S31 Y32 K46 T49 Q50 I51 N52 L55 T56 G57 Q60 W61 E62 Y63 K80 G87 L88 K89 Y90 A91 D92 V93 G94 S95 F96 G99 R100 N101 Y106 D107 T112 D113 M114 L115 F118 Y124

F128 G134 T138 Y139 R140 N141 S142 N143 G146 L151 A154 V155 G159 K160 N161 E162 N170 G171 D172 G173 G176 S177 Y180 E181 V188 G189 A190 Y191 A194 D195 R196 T197 G206 N207 G208 K209 K210 W214 Y226 Y231 G232 E233 T234 R235

T238 K243 T247 N252 K253 T254 Q255 D256 V257 L258 Q262 Y263 Q264 G268 L269 R270 P271 S272 I273 A274 Y275 T276 K277 S278 K279 A280 K281 D282 V283 E284 G285 I286 G287 D290 L291 V292 N293 Y294 F295 E296 V297 G298 A299 T300 F303 N304 M307 S308 T309 V310 V311

D312 Y313 I314 I315 N316 L324 G325 V326 G327 T331 V332 A333 V334 G335 I336 V337 Y338 Q339 F340

- Molecule 1: Outer membrane protein F

Chain F:

9%

73%   27%

A1 E2 I3 Y4 K10 V11 D12 L13 Y14 V18 N27 G28 E29 N30 K46 G47 I51 L55 T56 G57 W61 E62 Y63 N69 S70 E71 T77 R82 L83 L88 V93 N101 Y102 V105 Y106 D107 A108 L109 G110 Y111 T112 D113 M114 L115 F118

F129 V130 G131 R132 T138 N141 F144 L151 Q156 Y157 L158 G159 K160 A166 G171 D172 G173 Y180 E181 Y182 E183 G184 F185 G186 I187 V188 G189 A190 Y191 G192 A193 A194 D195 Q200 Q203 P204 N207 G208 K209 K210 A211 E212 Q213 W214 K219 Y220 D221

I225 Y226 L227 A228 Y231 G232 E233 N236 I240 T241 N242 T247 A251 N252 K253 D256 V257 L258 Q262 Y263 Q264 F265 P271 S272 I273 A274 Y275 T276 K279 A280 K281 D282 V283 I286 G287 D288 V289 D290 N293 E296 T300 Y310 Y313

N316 Q317 I318 N322 K323 L324 S328 D329 D330 T331 V332 V337 Y338 Q339 F340

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	161.91Å 110.88Å 226.14Å 90.00° 104.46° 90.00°	Depositor
Resolution (Å)	68.57 – 3.80 78.39 – 3.80	Depositor EDS
% Data completeness (in resolution range)	83.3 (68.57-3.80) 83.6 (78.39-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.41 (at 3.78Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.262 , 0.314 0.262 , 0.316	Depositor DCC
R_{free} test set	1583 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	33.6	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 85.9	EDS
L-test for twinning[2]	$<|L|> = 0.40, <L^2> = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.74	EDS
Total number of atoms	15765	wwPDB-VP
Average B, all atoms (Å^2)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.85 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4444e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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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	0.37	0/2683	0.59	0/3628
1	B	0.36	0/2683	0.59	0/3628
1	C	0.37	0/2683	0.59	0/3628
1	D	0.32	0/2683	0.54	0/3628
1	E	0.32	0/2690	0.53	0/3638
1	F	0.35	0/2683	0.55	0/3628
All	All	0.35	0/16105	0.56	0/21778

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	2627	0	2444	62	0
1	B	2627	0	2444	50	0
1	C	2627	0	2444	67	0
1	D	2627	0	2444	67	0
1	E	2630	0	2447	57	0
1	F	2627	0	2444	60	0
All	All	15765	0	14667	336	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 11.

The worst 5 of 336 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:118:PHE:HD2	1:E:312:ASP:OD2	1.26	1.15
1:E:118:PHE:CD2	1:E:312:ASP:OD2	2.05	1.08
1:D:27:ASN:O	1:D:35:ASN:HB3	1.61	1.01
1:B:100:ARG:HG2	1:B:134:GLY:HA2	1.53	0.89
1:E:309:THR:HG22	1:E:336:ILE:HG12	1.57	0.87

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	338/340 (99%)	321 (95%)	17 (5%)	0	100	100
1	B	338/340 (99%)	319 (94%)	19 (6%)	0	100	100
1	C	338/340 (99%)	320 (95%)	18 (5%)	0	100	100
1	D	338/340 (99%)	321 (95%)	17 (5%)	0	100	100
1	E	339/340 (100%)	323 (95%)	16 (5%)	0	100	100
1	F	338/340 (99%)	322 (95%)	16 (5%)	0	100	100
All	All	2029/2040 (100%)	1926 (95%)	103 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	263/263 (100%)	263 (100%)	0	100	100
1	B	263/263 (100%)	263 (100%)	0	100	100
1	C	263/263 (100%)	261 (99%)	2 (1%)	81	89
1	D	263/263 (100%)	261 (99%)	2 (1%)	81	89
1	E	264/263 (100%)	261 (99%)	3 (1%)	73	85
1	F	263/263 (100%)	262 (100%)	1 (0%)	91	95
All	All	1579/1578 (100%)	1571 (100%)	8 (0%)	88	94

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	340	PHE
1	F	12	ASP
1	E	297	VAL
1	D	247	THR
1	E	247	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	76	GLN
1	F	21	HIS
1	D	68	ASN
1	A	316	ASN
1	D	264	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(Å^2)	Q<0.9
1	A	340/340 (100%)	0.18	8 (2%)	59	50	25, 91, 154, 205	1 (0%)
1	B	340/340 (100%)	0.25	15 (4%)	34	29	18, 97, 153, 214	0
1	C	340/340 (100%)	0.30	18 (5%)	26	23	24, 83, 142, 188	1 (0%)
1	D	340/340 (100%)	0.63	42 (12%)	4	4	53, 136, 193, 246	0
1	E	340/340 (100%)	0.94	65 (19%)	1	1	59, 157, 214, 267	1 (0%)
1	F	340/340 (100%)	0.49	32 (9%)	8	7	51, 112, 175, 209	1 (0%)
All	All	2040/2040 (100%)	0.46	180 (8%)	10	8	18, 109, 190, 267	4 (0%)

The worst 5 of 180 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	57	GLY	11.3
1	E	90	TYR	7.3
1	E	56[A]	THR	7.0
1	E	209	LYS	6.7
1	D	291	LEU	6.2

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.