Full wwPDB X-ray Structure Validation Report ⓘ

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)

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

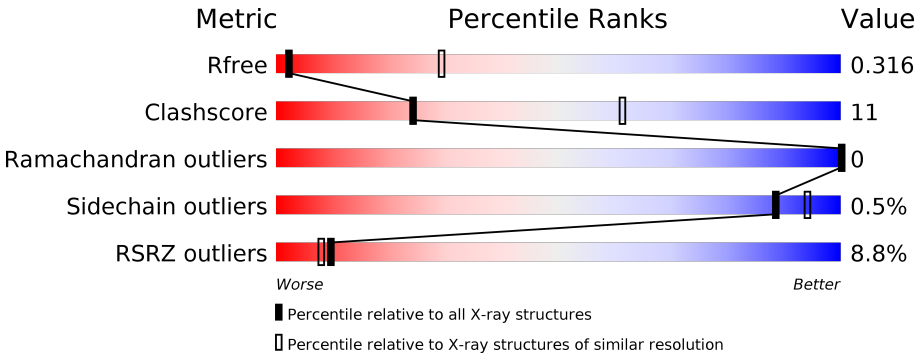
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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.

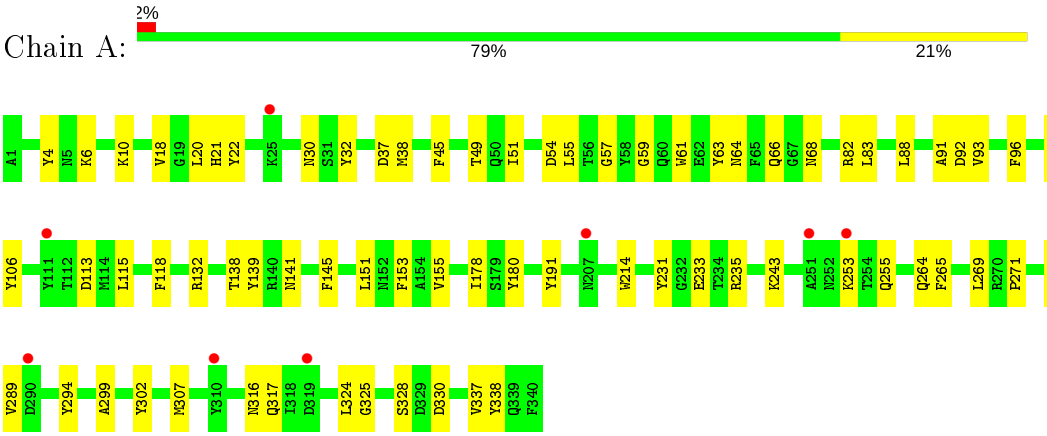
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	B	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	C	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	D	340	Total	C	N	O	S	0	0	0
			2627	1654	438	532	3			
1	E	340	Total	C	N	O	S	0	1	0
			2630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

3 Residue-property plots (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 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.

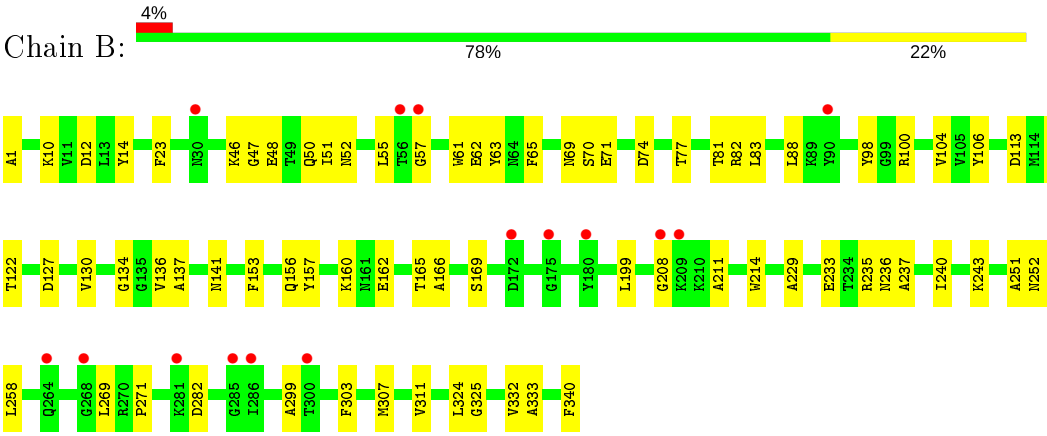
- Molecule 1: Outer membrane protein F

Chain A:



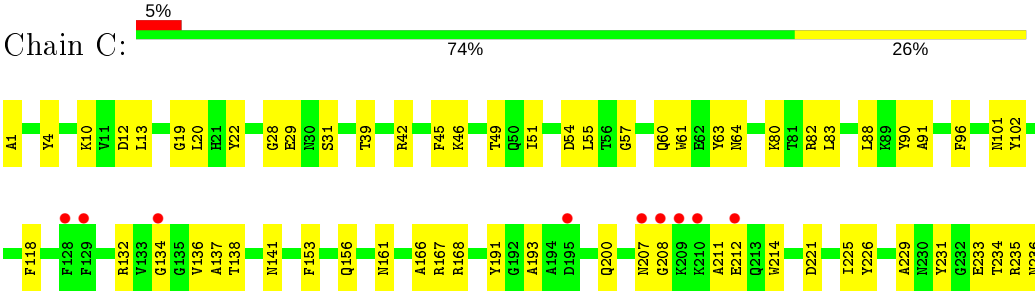
- Molecule 1: Outer membrane protein F

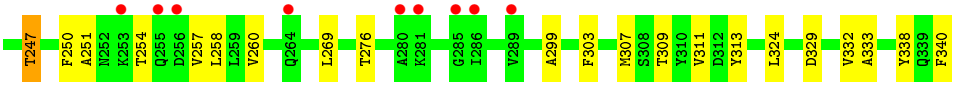
Chain B:



- Molecule 1: Outer membrane protein F

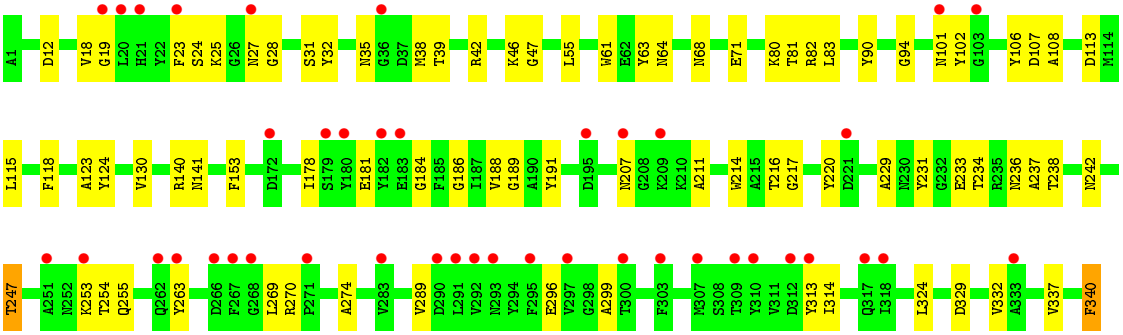
Chain C:





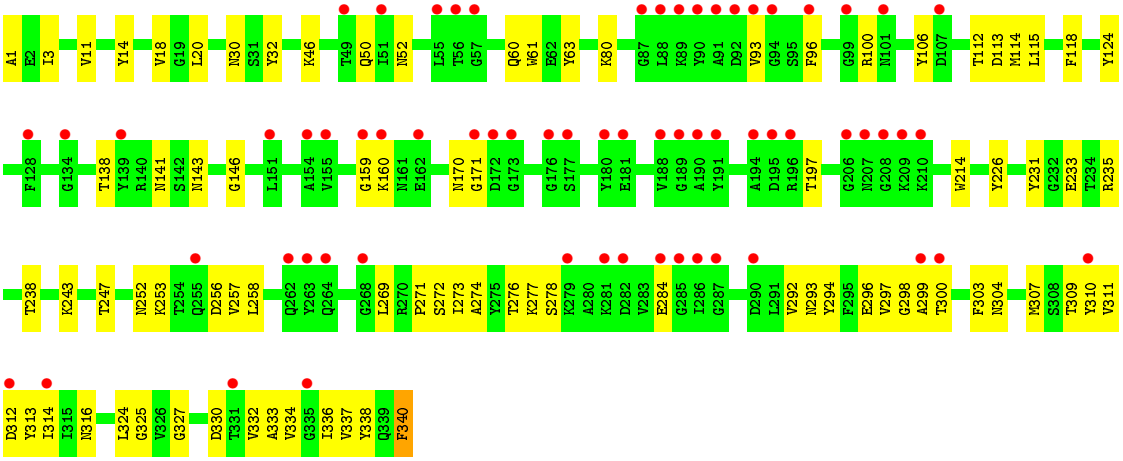
• Molecule 1: Outer membrane protein F

Chain D:



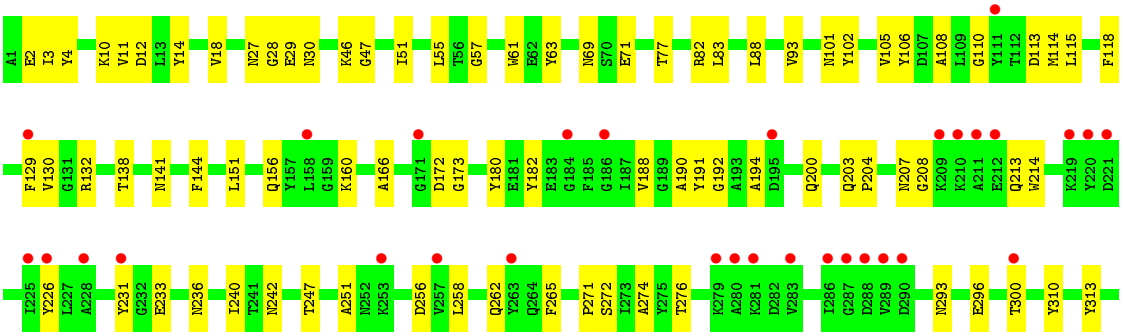
• Molecule 1: Outer membrane protein F

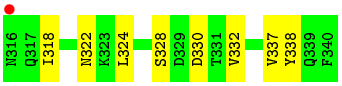
Chain E:



• Molecule 1: Outer membrane protein F

Chain F:




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.*

[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

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	0.37	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

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.

All (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
1:A:99:GLY:HA2	1:C:39:THR:HG21	1.58	0.86
1:E:160:LYS:HG3	1:E:171:GLY:HA2	1.57	0.85
1:D:27:ASN:O	1:D:35:ASN:CB	2.25	0.85
1:D:27:ASN:C	1:D:35:ASN:HB3	1.98	0.84
1:D:25:LYS:HD2	1:D:329:ASP:CG	1.99	0.83
1:D:25:LYS:HD2	1:D:329:ASP:OD2	1.77	0.83
1:D:27:ASN:N	1:D:28:GLY:HA2	1.95	0.79
1:F:27:ASN:HB2	1:F:29:GLU:H	1.47	0.79
1:D:27:ASN:O	1:D:35:ASN:N	2.17	0.78
1:B:23:PHE:HB2	1:B:332:VAL:HB	1.66	0.76
1:D:27:ASN:O	1:D:35:ASN:CA	2.34	0.76
1:E:309:THR:CG2	1:E:336:ILE:HG12	2.17	0.74
1:B:69:ASN:ND2	1:B:77:THR:O	2.17	0.71
1:E:93:VAL:O	1:E:141:ASN:ND2	2.24	0.70
1:A:151:LEU:HD13	1:A:180:TYR:CE2	2.27	0.70
1:A:64:ASN:HB2	1:A:82:ARG:HD2	1.72	0.69
1:B:166:ALA:HB2	1:B:199:LEU:HG	1.75	0.68
1:B:141:ASN:ND2	1:B:153:PHE:CZ	2.53	0.68
1:C:29:GLU:C	1:C:31:SER:H	1.97	0.67
1:C:54:ASP:HB3	1:C:91:ALA:HB2	1.74	0.67
1:F:207:ASN:O	1:F:236:ASN:ND2	2.27	0.67
1:A:191:TYR:HD1	1:A:214:TRP:HB3	1.61	0.66
1:D:269:LEU:HD11	1:D:299:ALA:HB1	1.76	0.65
1:C:313:TYR:CD1	1:C:332:VAL:HG22	2.32	0.65
1:F:242:ASN:HB3	1:F:247:THR:HG22	1.78	0.65
1:E:272:SER:N	1:E:298:GLY:O	2.25	0.64
1:F:69:ASN:ND2	1:F:77:THR:O	2.21	0.64
1:A:64:ASN:ND2	1:A:66:GLN:OE1	2.30	0.64
1:D:141:ASN:HB3	1:D:153:PHE:CE1	2.34	0.63
1:C:83:LEU:HD11	1:C:102:TYR:HE1	1.63	0.63
1:A:269:LEU:HG	1:A:271:PRO:HD3	1.80	0.63
1:A:141:ASN:HB3	1:A:153:PHE:CE1	2.33	0.62
1:A:286:ILE:HG21	1:A:289:VAL:HG21	1.81	0.62
1:A:253:LYS:HE3	1:A:255:GLN:HE21	1.64	0.62
1:C:64:ASN:HB2	1:C:82:ARG:HD2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:269:LEU:HD11	1:E:299:ALA:HB1	1.82	0.62
1:E:14:TYR:CE1	1:E:46:LYS:HG3	2.35	0.61
1:C:141:ASN:HB3	1:C:153:PHE:CE1	2.36	0.60
1:A:93:VAL:O	1:A:141:ASN:ND2	2.34	0.60
1:C:234:THR:OG1	1:C:254:THR:OG1	2.17	0.60
1:F:27:ASN:N	1:F:28:GLY:HA2	2.16	0.60
1:F:27:ASN:HB2	1:F:29:GLU:N	2.14	0.60
1:A:307:MET:HG2	1:B:88:LEU:HD21	1.84	0.60
1:C:31:SER:HA	1:C:329:ASP:HB2	1.83	0.59
1:B:1:ALA:HB1	1:C:4:TYR:CD1	2.37	0.59
1:C:28:GLY:O	1:C:31:SER:OG	2.16	0.59
1:D:24:SER:HB2	1:D:35:ASN:HB2	1.83	0.59
1:D:38:MET:HA	1:D:68:ASN:HD22	1.67	0.59
1:F:93:VAL:O	1:F:141:ASN:ND2	2.35	0.59
1:B:106:TYR:OH	1:B:113:ASP:OD2	2.18	0.59
1:E:300:THR:HG23	1:E:310:TYR:HB3	1.85	0.59
1:E:3:ILE:HG21	1:F:3:ILE:HD12	1.85	0.59
1:D:274:ALA:HB3	1:D:296:GLU:HB3	1.85	0.58
1:C:1:ALA:N	1:C:12:ASP:OD1	2.32	0.58
1:D:25:LYS:CD	1:D:329:ASP:OD2	2.49	0.58
1:C:19:GLY:HA2	1:C:39:THR:HG22	1.84	0.57
1:F:106:TYR:O	1:F:110:GLY:N	2.35	0.57
1:A:49:THR:HG21	1:C:307:MET:HB2	1.86	0.57
1:D:12:ASP:OD1	1:D:46:LYS:HB3	2.05	0.57
1:A:51:ILE:HD12	1:A:55:LEU:HG	1.86	0.57
1:E:274:ALA:HB3	1:E:296:GLU:HB3	1.86	0.57
1:E:214:TRP:NE1	1:E:233:GLU:HB2	2.20	0.57
1:E:277:LYS:HA	1:E:292:VAL:O	2.04	0.57
1:A:4:TYR:CE1	1:A:6:LYS:HB3	2.39	0.57
1:B:70:SER:OG	1:B:74:ASP:OD1	2.11	0.56
1:E:313:TYR:CD1	1:E:332:VAL:HG22	2.40	0.56
1:F:160:LYS:N	1:F:172:ASP:OD1	2.38	0.56
1:C:101:ASN:OD1	1:C:102:TYR:N	2.37	0.56
1:D:106:TYR:OH	1:D:113:ASP:OD2	2.17	0.56
1:F:27:ASN:H	1:F:28:GLY:HA2	1.69	0.56
1:F:313:TYR:CD1	1:F:332:VAL:HG22	2.39	0.56
1:C:29:GLU:C	1:C:31:SER:N	2.59	0.56
1:C:55:LEU:HD13	1:C:90:TYR:HD1	1.69	0.56
1:D:63:TYR:HD1	1:D:81:THR:HA	1.71	0.56
1:B:141:ASN:HD22	1:B:153:PHE:HZ	1.44	0.55
1:E:269:LEU:HG	1:E:271:PRO:HD3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:ASN:C	1:D:35:ASN:CB	2.70	0.55
1:E:124:TYR:HE2	1:E:238:THR:HG23	1.72	0.55
1:F:300:THR:HG23	1:F:310:TYR:HB3	1.88	0.55
1:C:212:GLU:HB2	1:C:235:ARG:HB2	1.88	0.55
1:E:316:ASN:N	1:E:330:ASP:OD1	2.38	0.55
1:A:37:ASP:OD1	1:B:98:TYR:OH	2.23	0.55
1:C:28:GLY:O	1:C:31:SER:CB	2.54	0.55
1:B:1:ALA:HB1	1:C:4:TYR:CG	2.41	0.55
1:D:80:LYS:HD3	1:F:71:GLU:HB3	1.88	0.55
1:D:24:SER:N	1:D:35:ASN:OD1	2.25	0.54
1:D:340:PHE:CD2	1:E:11:VAL:HG21	2.42	0.54
1:E:114:MET:HG3	1:E:226:TYR:CE2	2.43	0.54
1:A:57:GLY:HA2	1:A:88:LEU:HD23	1.89	0.54
1:A:32:TYR:HB2	1:A:316:ASN:HD21	1.71	0.54
1:E:231:TYR:HD1	1:E:257:VAL:HG22	1.73	0.54
1:B:269:LEU:HD11	1:B:299:ALA:HB1	1.89	0.54
1:A:59:GLY:HA3	1:C:338:TYR:HB3	1.90	0.54
1:D:101:ASN:OD1	1:D:102:TYR:N	2.39	0.54
1:D:42:ARG:NE	1:D:64:ASN:OD1	2.38	0.54
1:F:274:ALA:HB3	1:F:296:GLU:HB3	1.89	0.54
1:C:207:ASN:O	1:C:236:ASN:ND2	2.40	0.53
1:D:253:LYS:HE3	1:D:255:GLN:HE21	1.73	0.53
1:C:12:ASP:HB3	1:C:46:LYS:HB2	1.89	0.53
1:B:57:GLY:HA2	1:B:88:LEU:HD23	1.91	0.53
1:B:63:TYR:HD2	1:B:65:PHE:CE2	2.27	0.53
1:F:83:LEU:HD11	1:F:102:TYR:HE1	1.73	0.53
1:C:214:TRP:NE1	1:C:233:GLU:HB2	2.23	0.53
1:E:106:TYR:OH	1:E:113:ASP:OD2	2.24	0.53
1:D:207:ASN:O	1:D:236:ASN:ND2	2.41	0.53
1:A:30:ASN:ND2	1:A:328:SER:OG	2.42	0.53
1:B:214:TRP:NE1	1:B:233:GLU:HB2	2.23	0.53
1:E:159:GLY:O	1:E:170:ASN:ND2	2.43	0.52
1:B:307:MET:HB2	1:C:49:THR:HG21	1.92	0.52
1:E:256:ASP:OD1	1:E:278:SER:OG	2.19	0.52
1:E:61:TRP:CZ2	1:E:63:TYR:HB2	2.45	0.52
1:A:139:TYR:HD2	1:A:155:VAL:HG12	1.74	0.52
1:B:50:GLN:NE2	1:B:52:ASN:O	2.33	0.52
1:B:208:GLY:HA3	1:B:236:ASN:ND2	2.25	0.52
1:C:61:TRP:CZ2	1:C:63:TYR:HB2	2.45	0.52
1:D:189:GLY:HA2	1:D:216:THR:HG22	1.91	0.51
1:F:114:MET:HG3	1:F:226:TYR:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:18:VAL:HG22	1:F:337:VAL:HG22	1.92	0.51
1:A:115:LEU:HD21	1:A:274:ALA:HB2	1.91	0.51
1:B:160:LYS:NZ	1:B:162:GLU:OE2	2.25	0.51
1:F:138:THR:OG1	1:F:156:GLN:NE2	2.40	0.51
1:D:61:TRP:CZ2	1:D:63:TYR:HB2	2.46	0.51
1:E:303:PHE:HB2	1:E:307:MET:HB3	1.93	0.51
1:A:286:ILE:CG2	1:A:289:VAL:HG21	2.39	0.51
1:A:45:PHE:CD1	1:C:340:PHE:HE2	2.28	0.51
1:B:340:PHE:HE2	1:C:45:PHE:CD1	2.29	0.51
1:D:27:ASN:N	1:D:28:GLY:CA	2.73	0.51
1:E:311:VAL:HA	1:E:333:ALA:O	2.11	0.51
1:D:108:ALA:HA	1:D:188:VAL:HG11	1.93	0.50
1:E:18:VAL:HG13	1:E:337:VAL:HG22	1.93	0.50
1:D:18:VAL:HG13	1:D:337:VAL:HG22	1.93	0.50
1:A:83:LEU:HD11	1:A:102:TYR:HE1	1.77	0.50
1:C:115:LEU:HB2	1:C:118:PHE:O	2.11	0.50
1:D:211:ALA:HB1	1:D:237:ALA:HB2	1.94	0.50
1:F:101:ASN:OD1	1:F:102:TYR:N	2.40	0.50
1:A:286:ILE:CG2	1:A:289:VAL:CG2	2.89	0.50
1:A:61:TRP:HZ2	1:A:63:TYR:HD2	1.60	0.50
1:E:243:LYS:HD2	1:E:325:GLY:O	2.12	0.50
1:D:47:GLY:HA3	1:F:338:TYR:CE2	2.46	0.50
1:E:160:LYS:HE2	1:E:197:THR:HG22	1.93	0.50
1:A:253:LYS:HE3	1:A:255:GLN:NE2	2.25	0.49
1:A:30:ASN:O	1:A:328:SER:N	2.44	0.49
1:F:57:GLY:HA2	1:F:88:LEU:HD23	1.93	0.49
1:E:235:ARG:HD3	1:E:253:LYS:HG2	1.94	0.49
1:E:112:THR:HG21	1:E:258:LEU:HB2	1.94	0.49
1:E:273:ILE:HA	1:E:296:GLU:O	2.12	0.49
1:B:243:LYS:HD2	1:B:325:GLY:O	2.13	0.49
1:D:82:ARG:HA	1:F:71:GLU:OE2	2.12	0.49
1:A:38:MET:HA	1:A:68:ASN:HD22	1.77	0.49
1:C:20:LEU:H	1:C:39:THR:HG22	1.78	0.49
1:A:264:GLN:HE22	1:A:302:TYR:HD2	1.59	0.49
1:F:214:TRP:NE1	1:F:233:GLU:HB2	2.28	0.49
1:A:243:LYS:HD2	1:A:325:GLY:O	2.12	0.49
1:A:338:TYR:CE2	1:B:47:GLY:HA3	2.47	0.49
1:D:231:TYR:OH	1:D:233:GLU:OE2	2.29	0.49
1:A:235:ARG:HE	1:A:253:LYS:HG3	1.77	0.48
1:B:165:THR:O	1:B:169:SER:OG	2.20	0.48
1:E:46:LYS:HG2	1:E:60:GLN:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:ASN:HA	1:C:324:LEU:HD22	1.95	0.48
1:B:252:ASN:HB3	1:B:282:ASP:HB2	1.94	0.48
1:F:115:LEU:HB2	1:F:118:PHE:O	2.14	0.48
1:E:340:PHE:CD2	1:F:11:VAL:HG21	2.48	0.48
1:C:111:TYR:O	1:C:226:TYR:OH	2.23	0.48
1:D:83:LEU:HD21	1:D:102:TYR:CD1	2.49	0.48
1:D:83:LEU:HD21	1:D:102:TYR:CE1	2.48	0.48
1:D:289:VAL:HG21	1:D:324:LEU:HG	1.96	0.48
1:D:253:LYS:HE3	1:D:255:GLN:NE2	2.29	0.48
1:A:18:VAL:HG12	1:A:20:LEU:HB2	1.95	0.48
1:A:269:LEU:HD11	1:A:299:ALA:HB1	1.96	0.48
1:F:105:VAL:HA	1:F:190:ALA:HB1	1.95	0.47
1:B:51:ILE:HD12	1:B:55:LEU:HG	1.96	0.47
1:D:18:VAL:HG22	1:D:337:VAL:HG22	1.95	0.47
1:E:115:LEU:HB2	1:E:118:PHE:O	2.15	0.47
1:C:311:VAL:HA	1:C:333:ALA:O	2.14	0.47
1:A:51:ILE:HD13	1:C:303:PHE:HB3	1.96	0.47
1:E:143:ASN:HB2	1:E:146:GLY:HA2	1.96	0.47
1:D:80:LYS:HB2	1:F:71:GLU:HG2	1.96	0.47
1:F:313:TYR:OH	1:F:330:ASP:OD2	2.31	0.47
1:C:242:ASN:HB3	1:C:247:THR:HG22	1.97	0.47
1:D:191:TYR:HD1	1:D:214:TRP:HB3	1.78	0.47
1:F:166:ALA:HB1	1:F:200:GLN:HG2	1.97	0.47
1:A:22:TYR:CD1	1:A:38:MET:HG3	2.50	0.47
1:F:129:PHE:CD2	1:F:192:GLY:HA3	2.50	0.47
1:B:14:TYR:CE1	1:B:46:LYS:HG3	2.50	0.46
1:C:45:PHE:O	1:C:60:GLN:HG3	2.15	0.46
1:E:307:MET:SD	1:F:57:GLY:HA3	2.55	0.46
1:C:102:TYR:HA	1:C:132:ARG:HA	1.97	0.46
1:C:96:PHE:CZ	1:C:137:ALA:HB1	2.50	0.46
1:B:115:LEU:HB2	1:B:118:PHE:O	2.16	0.46
1:C:96:PHE:HA	1:C:138:THR:O	2.15	0.46
1:F:51:ILE:HD12	1:F:55:LEU:HG	1.97	0.46
1:C:208:GLY:HA3	1:C:236:ASN:ND2	2.30	0.46
1:C:82:ARG:O	1:C:132:ARG:HD2	2.15	0.46
1:B:303:PHE:HB2	1:B:307:MET:HB3	1.98	0.46
1:D:32:TYR:HE2	1:D:118:PHE:CD1	2.34	0.46
1:A:289:VAL:HG11	1:A:324:LEU:HG	1.98	0.46
1:B:235:ARG:HD3	1:B:253:LYS:HG2	1.98	0.46
1:B:61:TRP:HA	1:B:83:LEU:O	2.16	0.46
1:F:318:ILE:HD12	1:F:322:ASN:ND2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:TYR:HE2	1:C:340:PHE:HD2	1.63	0.46
1:C:240:ILE:HD13	1:C:251:ALA:HB2	1.98	0.45
1:F:108:ALA:HA	1:F:188:VAL:HG11	1.97	0.45
1:A:243:LYS:HB2	1:A:325:GLY:HA3	1.98	0.45
1:B:63:TYR:HD1	1:B:81:THR:HA	1.82	0.45
1:C:51:ILE:HD12	1:C:55:LEU:HG	1.99	0.45
1:F:208:GLY:HA3	1:F:236:ASN:ND2	2.32	0.45
1:B:104:VAL:N	1:B:156:GLN:OE1	2.46	0.45
1:D:32:TYR:CE2	1:D:314:ILE:HG13	2.52	0.45
1:E:96:PHE:HA	1:E:138:THR:O	2.16	0.45
1:F:144:PHE:N	1:F:151:LEU:O	2.49	0.45
1:B:269:LEU:HG	1:B:271:PRO:HD3	1.98	0.45
1:D:242:ASN:HB3	1:D:247:THR:HG22	1.99	0.45
1:E:294:TYR:CE1	1:E:314:ILE:HD12	2.51	0.45
1:A:22:TYR:HE2	1:A:118:PHE:CE1	2.35	0.45
1:B:1:ALA:N	1:B:12:ASP:OD1	2.35	0.45
1:C:83:LEU:HD11	1:C:102:TYR:CE1	2.48	0.45
1:D:31:SER:HA	1:D:329:ASP:HB2	1.98	0.45
1:F:166:ALA:HB1	1:F:200:GLN:HA	1.99	0.45
1:B:127:ASP:O	1:B:130:VAL:HG22	2.17	0.44
1:D:181:GLU:HG2	1:D:186:GLY:HA2	1.99	0.44
1:A:92:ASP:O	1:A:145:PHE:HA	2.17	0.44
1:A:294:TYR:HA	1:A:317:GLN:HG2	1.98	0.44
1:D:107:ASP:CG	1:D:140:ARG:HH12	2.21	0.44
1:D:42:ARG:HD3	1:D:64:ASN:HA	1.98	0.44
1:F:30:ASN:O	1:F:328:SER:N	2.50	0.44
1:C:231:TYR:HD1	1:C:257:VAL:HG22	1.82	0.44
1:C:258:LEU:HG	1:C:276:THR:HG23	1.98	0.44
1:B:324:LEU:HD23	1:B:324:LEU:HA	1.83	0.44
1:F:106:TYR:OH	1:F:113:ASP:OD2	2.35	0.44
1:F:265:PHE:HE2	1:F:271:PRO:HG3	1.81	0.44
1:F:231:TYR:HA	1:F:256:ASP:O	2.17	0.44
1:F:61:TRP:CZ2	1:F:63:TYR:HB2	2.52	0.44
1:D:27:ASN:O	1:D:35:ASN:O	2.35	0.44
1:A:265:PHE:HE2	1:A:271:PRO:HG3	1.81	0.44
1:E:252:ASN:ND2	1:E:284:GLU:OE2	2.50	0.43
1:A:10:LYS:HB3	1:A:10:LYS:HE2	1.86	0.43
1:E:338:TYR:OH	1:F:47:GLY:HA3	2.18	0.43
1:E:258:LEU:HG	1:E:276:THR:HG23	2.00	0.43
1:E:276:THR:O	1:E:293:ASN:HA	2.18	0.43
1:F:262:GLN:HG2	1:F:272:SER:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ARG:O	1:A:132:ARG:HD2	2.19	0.43
1:B:160:LYS:HE2	1:B:162:GLU:HG3	2.01	0.43
1:C:42:ARG:HD3	1:C:64:ASN:HA	1.99	0.43
1:D:313:TYR:HD1	1:D:332:VAL:HG22	1.83	0.43
1:E:309:THR:HG22	1:E:336:ILE:CG1	2.40	0.43
1:D:217:GLY:HA2	1:D:229:ALA:O	2.19	0.43
1:D:313:TYR:CD1	1:D:332:VAL:HG22	2.53	0.43
1:D:71:GLU:HG3	1:E:100:ARG:NH2	2.33	0.43
1:F:82:ARG:O	1:F:132:ARG:HD2	2.19	0.43
1:A:307:MET:SD	1:A:338:TYR:HB2	2.58	0.43
1:D:18:VAL:HG22	1:D:337:VAL:HG13	2.00	0.43
1:E:50:GLN:NE2	1:E:52:ASN:O	2.37	0.43
1:A:4:TYR:HE1	1:A:6:LYS:HB3	1.84	0.43
1:F:105:VAL:HA	1:F:190:ALA:CB	2.49	0.43
1:B:62:GLU:O	1:B:82:ARG:N	2.47	0.43
1:D:141:ASN:HB3	1:D:153:PHE:HE1	1.79	0.43
1:B:61:TRP:CZ2	1:B:63:TYR:HB2	2.53	0.42
1:C:191:TYR:HD1	1:C:214:TRP:HB3	1.84	0.42
1:C:20:LEU:HD21	1:C:22:TYR:HE1	1.84	0.42
1:F:180:TYR:CE2	1:F:182:TYR:HB2	2.54	0.42
1:A:286:ILE:HG22	1:A:289:VAL:CG2	2.49	0.42
1:A:54:ASP:HB3	1:A:91:ALA:HB2	2.01	0.42
1:D:184:GLY:O	1:D:220:TYR:HA	2.19	0.42
1:D:234:THR:OG1	1:D:254:THR:OG1	2.19	0.42
1:D:123:ALA:HA	1:D:130:VAL:O	2.20	0.42
1:C:134:GLY:O	1:C:161:ASN:ND2	2.52	0.42
1:C:138:THR:OG1	1:C:156:GLN:NE2	2.52	0.42
1:F:130:VAL:HG13	1:F:213:GLN:CD	2.39	0.42
1:B:71:GLU:HB2	1:C:168:ARG:HH12	1.84	0.42
1:E:324:LEU:HA	1:E:324:LEU:HD23	1.94	0.42
1:A:316:ASN:HD22	1:A:330:ASP:HA	1.84	0.42
1:D:55:LEU:HD13	1:D:90:TYR:HD1	1.85	0.42
1:E:304:ASN:ND2	1:F:51:ILE:HA	2.34	0.42
1:D:115:LEU:HB2	1:D:118:PHE:O	2.19	0.42
1:E:309:THR:HG22	1:E:336:ILE:HG23	2.02	0.42
1:B:122:THR:HG21	1:B:256:ASP:HB3	2.01	0.42
1:E:311:VAL:HG22	1:E:334:VAL:HG22	2.00	0.42
1:A:106:TYR:OH	1:A:113:ASP:OD2	2.33	0.42
1:B:311:VAL:HA	1:B:333:ALA:O	2.20	0.42
1:C:193:ALA:HA	1:C:211:ALA:O	2.20	0.42
1:D:124:TYR:HE2	1:D:238:THR:HG23	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:LEU:HD11	1:C:299:ALA:HB1	2.02	0.42
1:C:1:ALA:O	1:C:13:LEU:N	2.53	0.41
1:C:57:GLY:HA2	1:C:88:LEU:HD23	2.02	0.41
1:F:2:GLU:OE1	1:F:10:LYS:HD2	2.20	0.41
1:A:21:HIS:HD2	1:A:22:TYR:O	2.02	0.41
1:A:32:TYR:HE2	1:A:118:PHE:CD1	2.38	0.41
1:D:19:GLY:HA2	1:D:39:THR:HG23	2.01	0.41
1:D:263:TYR:O	1:D:270:ARG:HA	2.20	0.41
1:E:32:TYR:HE2	1:E:118:PHE:CD1	2.38	0.41
1:F:191:TYR:HD1	1:F:214:TRP:HB3	1.84	0.41
1:F:324:LEU:HD23	1:F:324:LEU:HA	1.92	0.41
1:F:258:LEU:HG	1:F:276:THR:HG23	2.02	0.41
1:B:137:ALA:HB3	1:B:157:TYR:HB3	2.01	0.41
1:C:166:ALA:HB1	1:C:200:GLN:HA	2.02	0.41
1:C:4:TYR:O	1:C:10:LYS:HA	2.20	0.41
1:A:153:PHE:HB2	1:A:178:ILE:HG12	2.03	0.41
1:A:231:TYR:OH	1:A:233:GLU:OE2	2.39	0.41
1:E:80:LYS:HE2	1:E:80:LYS:HB3	1.93	0.41
1:F:14:TYR:CE1	1:F:46:LYS:HG3	2.55	0.41
1:A:18:VAL:HG22	1:A:337:VAL:HG22	2.02	0.41
1:B:229:ALA:HA	1:B:258:LEU:O	2.21	0.41
1:A:18:VAL:HG13	1:A:337:VAL:HG22	2.02	0.41
1:D:63:TYR:CD1	1:D:81:THR:HA	2.54	0.41
1:D:94:GLY:CA	1:D:141:ASN:HD22	2.34	0.41
1:E:294:TYR:CD1	1:E:314:ILE:HG23	2.55	0.41
1:A:96:PHE:HA	1:A:138:THR:O	2.21	0.41
1:B:136:VAL:HA	1:B:157:TYR:O	2.20	0.41
1:C:221:ASP:HA	1:C:225:ILE:O	2.21	0.41
1:F:173:GLY:HA3	1:F:194:ALA:HB2	2.02	0.41
1:C:229:ALA:HA	1:C:258:LEU:O	2.21	0.41
1:B:71:GLU:HB3	1:C:80:LYS:HD2	2.02	0.41
1:E:1:ALA:HB1	1:F:4:TYR:CD2	2.55	0.41
1:A:21:HIS:HD2	1:A:22:TYR:N	2.19	0.40
1:B:211:ALA:HB1	1:B:237:ALA:HB2	2.03	0.40
1:F:240:ILE:HD13	1:F:251:ALA:HB2	2.01	0.40
1:C:112:THR:O	1:C:260:VAL:HG21	2.22	0.40
1:A:45:PHE:CE1	1:C:340:PHE:HE2	2.39	0.40
1:D:153:PHE:HB2	1:D:178:ILE:HG12	2.03	0.40
1:E:30:ASN:OD1	1:E:327:GLY:HA2	2.21	0.40
1:F:203:GLN:HA	1:F:204:PRO:HD3	1.90	0.40
1:C:167:ARG:HA	1:C:250:PHE:CZ	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:TYR:C	1:C:338:TYR:CD2	2.92	0.40
1:D:23:PHE:HB2	1:D:332:VAL:HB	2.03	0.40
1:A:32:TYR:CB	1:A:316:ASN:HD21	2.32	0.40
1:A:32:TYR:HB2	1:A:316:ASN:ND2	2.34	0.40
1:B:240:ILE:HD13	1:B:251:ALA:HB2	2.03	0.40
1:B:10:LYS:HG2	1:B:48:GLU:O	2.21	0.40
1:C:136:VAL:HG23	1:C:136:VAL:O	2.21	0.40
1:F:276:THR:O	1:F:293:ASN:HA	2.22	0.40
1:E:20:LEU:HD13	1:E:310:TYR:OH	2.22	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	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

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	247	THR
1	C	309	THR
1	D	247	THR
1	D	340	PHE
1	E	247	THR
1	E	297	VAL
1	E	340	PHE
1	F	12	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	255	GLN
1	A	316	ASN
1	C	76	GLN
1	D	68	ASN
1	D	264	GLN
1	F	21	HIS

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 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, 95^{th} 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%)

All (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
1	E	285	GLY	5.2
1	E	180	TYR	5.1
1	E	128	PHE	4.9
1	D	290	ASP	4.7
1	E	282	ASP	4.7
1	E	139	TYR	4.6
1	E	173	GLY	4.3
1	A	319	ASP	4.2
1	F	289	VAL	4.2
1	E	172	ASP	4.2
1	E	287	GLY	4.2
1	E	94	GLY	4.1
1	C	209	LYS	4.0
1	F	210	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	F	220	TYR	4.0
1	D	310	TYR	4.0
1	C	253	LYS	4.0
1	A	251	ALA	3.9
1	E	55	LEU	3.9
1	E	195	ASP	3.9
1	F	209	LYS	3.9
1	E	51	ILE	3.8
1	E	300	THR	3.8
1	D	317	GLN	3.7
1	E	196	ARG	3.6
1	E	207	ASN	3.6
1	D	182	TYR	3.6
1	E	210	LYS	3.5
1	E	281	LYS	3.5
1	D	318	ILE	3.5
1	E	206	GLY	3.5
1	E	171	GLY	3.5
1	F	280	ALA	3.4
1	C	264	GLN	3.4
1	D	309	THR	3.4
1	C	210	LYS	3.4
1	D	20	LEU	3.4
1	B	285	GLY	3.4
1	F	253	LYS	3.3
1	D	207	ASN	3.3
1	D	209	LYS	3.3
1	E	176	GLY	3.3
1	E	93	VAL	3.3
1	E	89	LYS	3.3
1	E	314	ILE	3.2
1	A	290	ASP	3.2
1	E	312	ASP	3.2
1	F	219	LYS	3.2
1	E	208	GLY	3.2
1	F	186	GLY	3.1
1	D	266	ASP	3.1
1	D	101	ASN	3.1
1	B	264	GLN	3.1
1	E	155	VAL	3.0
1	F	212	GLU	3.0
1	E	159	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	303	PHE	3.0
1	F	281	LYS	3.0
1	D	23	PHE	2.9
1	D	300	THR	2.9
1	E	88	LEU	2.9
1	C	280	ALA	2.9
1	C	255	GLN	2.9
1	F	287	GLY	2.9
1	E	181	GLU	2.9
1	D	313	TYR	2.9
1	E	255	GLN	2.8
1	F	290	ASP	2.8
1	D	36	GLY	2.8
1	B	90	TYR	2.8
1	C	285	GLY	2.8
1	E	49	THR	2.8
1	C	212	GLU	2.8
1	B	268	GLY	2.8
1	D	297	VAL	2.8
1	F	283	VAL	2.8
1	E	99	GLY	2.7
1	A	310	TYR	2.7
1	D	103	GLY	2.7
1	E	299	ALA	2.7
1	F	228	ALA	2.7
1	C	208	GLY	2.7
1	C	256	ASP	2.7
1	D	19	GLY	2.7
1	E	189	GLY	2.7
1	D	180	TYR	2.6
1	C	134	GLY	2.6
1	F	286	ILE	2.6
1	D	312	ASP	2.6
1	E	96	PHE	2.6
1	F	129	PHE	2.6
1	D	293	ASN	2.6
1	F	279	LYS	2.6
1	E	263	TYR	2.6
1	D	179	SER	2.5
1	B	180	TYR	2.5
1	F	195	ASP	2.5
1	D	263	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	281	LYS	2.5
1	F	300	THR	2.5
1	E	162	GLU	2.5
1	F	231	TYR	2.5
1	F	111	TYR	2.5
1	B	281	LYS	2.4
1	B	209	LYS	2.4
1	E	268	GLY	2.4
1	D	253	LYS	2.4
1	E	160	LYS	2.4
1	D	307	MET	2.4
1	A	25	LYS	2.4
1	E	264	GLN	2.4
1	F	158	LEU	2.4
1	F	316	ASN	2.4
1	D	21	HIS	2.4
1	E	101	ASN	2.4
1	E	154	ALA	2.4
1	E	107	ASP	2.3
1	F	288	ASP	2.3
1	E	191	TYR	2.3
1	E	151	LEU	2.3
1	D	292	VAL	2.3
1	E	194	ALA	2.3
1	E	92	ASP	2.3
1	B	208	GLY	2.3
1	F	225	ILE	2.3
1	D	221	ASP	2.3
1	E	290	ASP	2.3
1	E	262	GLN	2.3
1	E	87	GLY	2.3
1	D	172	ASP	2.3
1	C	289	VAL	2.3
1	F	184	GLY	2.3
1	B	175	GLY	2.2
1	F	263	TYR	2.2
1	F	171	GLY	2.2
1	C	286	ILE	2.2
1	B	30	ASN	2.2
1	D	267	PHE	2.2
1	E	134	GLY	2.2
1	E	279	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	283	VAL	2.2
1	E	177	SER	2.2
1	D	183	GLU	2.2
1	D	251	ALA	2.2
1	F	211	ALA	2.2
1	C	128	PHE	2.2
1	A	207	ASN	2.2
1	D	333	ALA	2.2
1	B	300	THR	2.2
1	D	268	GLY	2.2
1	D	195	ASP	2.2
1	E	190	ALA	2.2
1	D	262	GLN	2.2
1	E	188	VAL	2.2
1	E	91	ALA	2.1
1	D	295	PHE	2.1
1	E	310	TYR	2.1
1	A	111	TYR	2.1
1	A	253	LYS	2.1
1	F	226	TYR	2.1
1	B	286	ILE	2.1
1	F	221	ASP	2.1
1	F	257	VAL	2.1
1	C	207	ASN	2.1
1	B	172	ASP	2.1
1	C	195	ASP	2.1
1	D	27	ASN	2.1
1	B	57	GLY	2.1
1	C	129	PHE	2.1
1	E	335	GLY	2.1
1	B	56	THR	2.0
1	E	284	GLU	2.0
1	D	271	PRO	2.0
1	E	331	THR	2.0
1	E	286	ILE	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.