Full wwPDB X-ray Structure Validation Report ⓘ

Sep 3, 2023 – 08:10 PM EDT

PDB ID	:	3RRT
Title	:	Structure of the RSV F protein in the post-fusion conformation
Authors	:	McLellan, J.S.; Yongping, Y.; Graham, B.S.; Kwong, P.D.
Deposited on	:	2011-04-30
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
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:

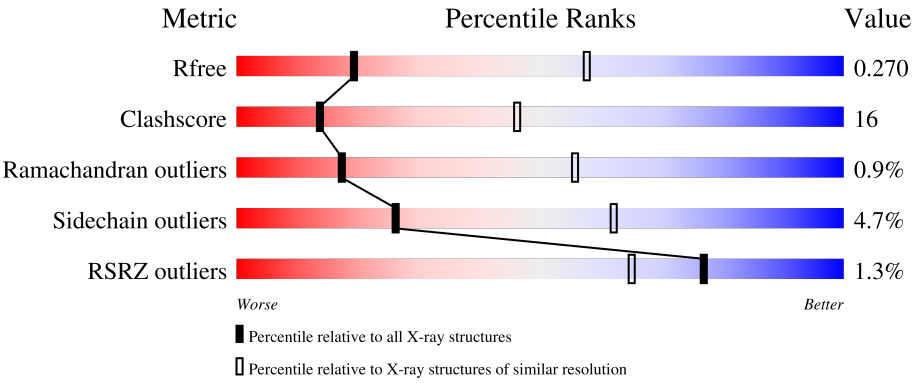
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 <=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	84	2% 70% 13% • 14%
1	C	84	65% 18% • 14%
1	E	84	% 67% 17% • 14%
2	B	374	2% 66% 28% • 5%
2	D	374	% 64% 30% • •

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Mol	Chain	Length	Quality of chain
2	F	374	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 20264 atoms, of which 10200 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	72	Total	C	H	N	O	S	0	0	0
			1152	361	581	93	114	3			
1	C	72	Total	C	H	N	O	S	0	0	0
			1152	361	581	93	114	3			
1	E	72	Total	C	H	N	O	S	0	0	0
			1152	361	581	93	114	3			

- Molecule 2 is a protein called Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	356	Total	C	H	N	O	S	0	0	0
			5545	1738	2790	456	543	18			
2	D	360	Total	C	H	N	O	S	0	0	0
			5605	1757	2821	460	549	18			
2	F	364	Total	C	H	N	O	S	0	0	0
			5658	1772	2846	465	557	18			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	342	TYR	PHE	SEE REMARK 999	UNP Q84850
B	514	GLY	-	expression tag	UNP Q84850
B	515	LEU	-	expression tag	UNP Q84850
B	516	GLU	-	expression tag	UNP Q84850
B	517	VAL	-	expression tag	UNP Q84850
B	518	LEU	-	expression tag	UNP Q84850
B	519	PHE	-	expression tag	UNP Q84850
B	520	GLN	-	expression tag	UNP Q84850
D	342	TYR	PHE	SEE REMARK 999	UNP Q84850
D	514	GLY	-	expression tag	UNP Q84850
D	515	LEU	-	expression tag	UNP Q84850
D	516	GLU	-	expression tag	UNP Q84850

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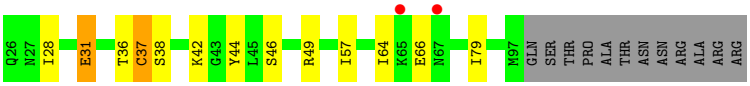
Chain	Residue	Modelled	Actual	Comment	Reference
D	517	VAL	-	expression tag	UNP Q84850
D	518	LEU	-	expression tag	UNP Q84850
D	519	PHE	-	expression tag	UNP Q84850
D	520	GLN	-	expression tag	UNP Q84850
F	342	TYR	PHE	SEE REMARK 999	UNP Q84850
F	514	GLY	-	expression tag	UNP Q84850
F	515	LEU	-	expression tag	UNP Q84850
F	516	GLU	-	expression tag	UNP Q84850
F	517	VAL	-	expression tag	UNP Q84850
F	518	LEU	-	expression tag	UNP Q84850
F	519	PHE	-	expression tag	UNP Q84850
F	520	GLN	-	expression tag	UNP Q84850

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

Chain A:

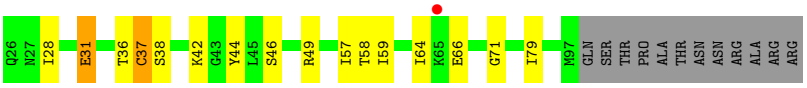


• Molecule 1: Fusion glycoprotein F0

Chain C:

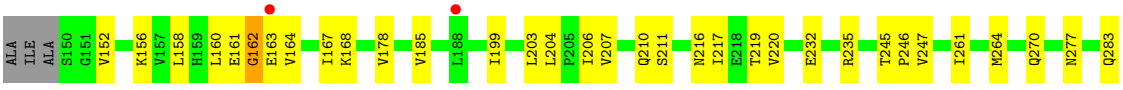
• Molecule 1: Fusion glycoprotein F0

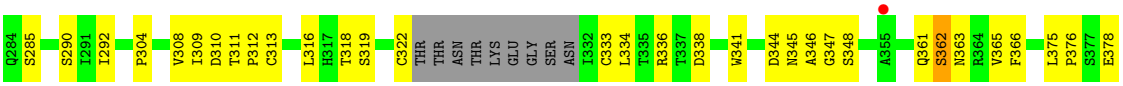
Chain E:

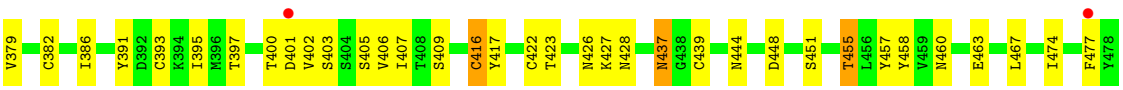


• Molecule 2: Fusion glycoprotein F0

Chain B:

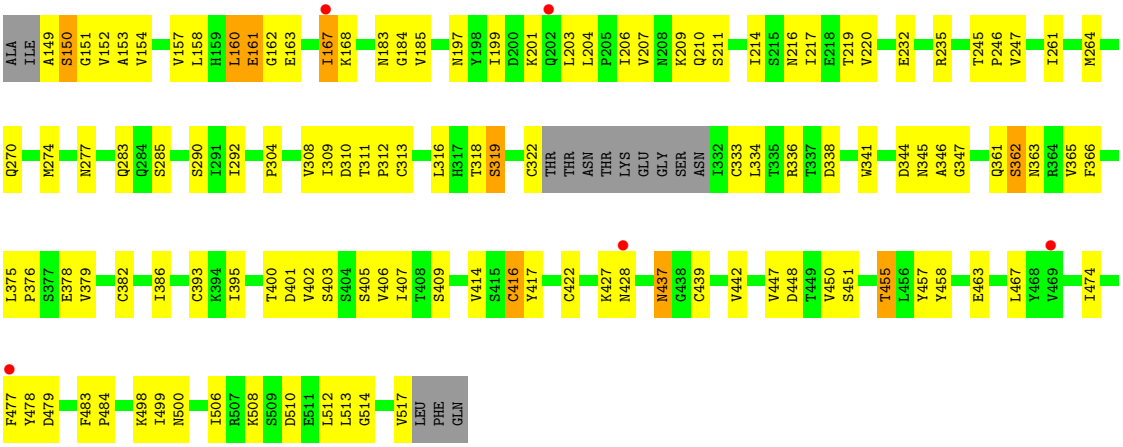






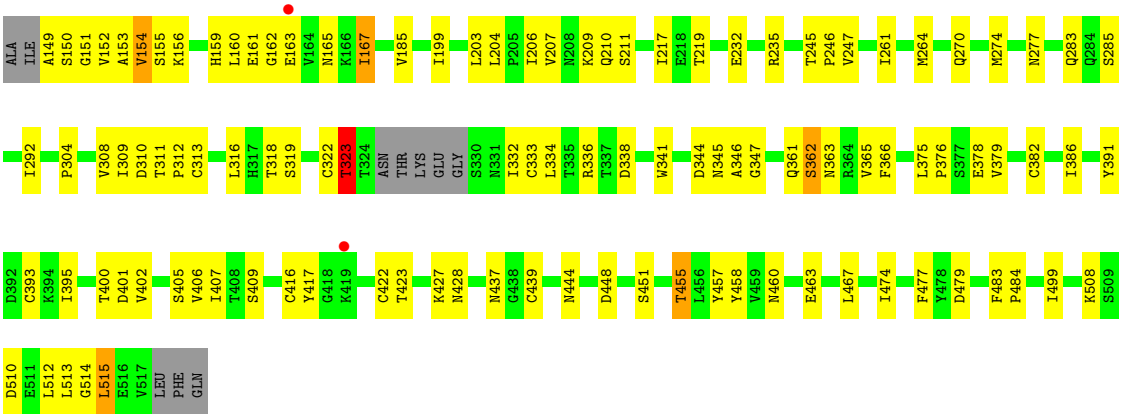
• Molecule 2: Fusion glycoprotein F0

Chain D:



• Molecule 2: Fusion glycoprotein F0

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.02Å 81.88Å 271.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.17 – 3.20 46.17 – 3.15	Depositor EDS
% Data completeness (in resolution range)	91.5 (46.17-3.20) 91.1 (46.17-3.15)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	0.21	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.253 , 0.282 0.239 , 0.270	Depositor DCC
R_{free} test set	1331 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	64.9	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 39.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	20264	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[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	0.39	0/577	0.54	0/777
1	C	0.42	0/577	0.55	0/777
1	E	0.43	0/577	0.56	0/777
2	B	0.41	0/2795	0.54	0/3789
2	D	0.41	0/2824	0.57	1/3829 (0.0%)
2	F	0.45	0/2852	0.57	0/3868
All	All	0.42	0/10202	0.56	1/13817 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	160	LEU	CA-CB-CG	5.63	128.24	115.30

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	571	581	581	18	0
1	C	571	581	581	23	0
1	E	571	581	581	22	0
2	B	2755	2790	2788	103	0
2	D	2784	2821	2819	121	0
2	F	2812	2846	2844	110	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10064	10200	10194	321	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 16.

All (321) 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)
2:F:150:SER:HB2	2:F:154:VAL:HG21	1.53	0.90
2:B:311:THR:HG21	2:B:344:ASP:O	1.81	0.80
2:F:246:PRO:HB3	2:F:283:GLN:HA	1.65	0.78
2:F:510:ASP:O	2:F:514:GLY:HA2	1.84	0.78
1:C:46:SER:HB3	2:D:313:CYS:SG	2.24	0.78
2:D:311:THR:HG21	2:D:344:ASP:O	1.84	0.78
1:E:46:SER:HB3	2:F:313:CYS:SG	2.24	0.78
1:A:46:SER:HB3	2:B:313:CYS:SG	2.24	0.77
2:B:246:PRO:HB3	2:B:283:GLN:HA	1.67	0.76
2:B:311:THR:CG2	2:B:344:ASP:HB2	2.15	0.76
2:B:160:LEU:HD21	2:D:161:GLU:HA	1.68	0.76
1:C:36:THR:HG23	2:D:386:ILE:HD11	1.67	0.76
2:D:311:THR:CG2	2:D:344:ASP:HB2	2.18	0.74
1:E:36:THR:HG23	2:F:386:ILE:HD11	1.67	0.74
2:F:311:THR:CG2	2:F:344:ASP:HB2	2.16	0.74
2:F:311:THR:HG21	2:F:344:ASP:O	1.87	0.74
1:A:36:THR:HG23	2:B:386:ILE:HD11	1.68	0.74
2:D:246:PRO:HB3	2:D:283:GLN:HA	1.70	0.73
2:B:270:GLN:HG2	2:B:309:ILE:HD12	1.72	0.71
2:D:270:GLN:HG2	2:D:309:ILE:HD12	1.71	0.70
2:D:334:LEU:HB3	2:D:395:ILE:HD11	1.74	0.69
2:F:270:GLN:HG2	2:F:309:ILE:HD12	1.75	0.69
2:B:334:LEU:HB3	2:B:395:ILE:HD11	1.74	0.69
2:F:334:LEU:HB3	2:F:395:ILE:HD11	1.74	0.68
2:B:185:VAL:HG12	2:D:499:ILE:HD11	1.76	0.67
2:D:277:ASN:HD22	2:D:366:PHE:HZ	1.42	0.67
1:C:28:ILE:HD11	2:D:363:ASN:HA	1.77	0.66
2:F:277:ASN:HD22	2:F:366:PHE:HZ	1.43	0.66
1:A:28:ILE:HD11	2:B:363:ASN:HA	1.78	0.65
2:D:513:LEU:N	2:D:514:GLY:HA2	2.11	0.65
2:F:161:GLU:O	2:F:165:ASN:OD1	2.14	0.65
2:D:513:LEU:H	2:D:514:GLY:HA2	1.61	0.65
2:D:261:ILE:HG12	2:D:264:MET:HE1	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:277:ASN:HD22	2:B:366:PHE:HZ	1.44	0.63
2:D:160:LEU:O	2:D:161:GLU:C	2.35	0.63
1:E:28:ILE:HD11	2:F:363:ASN:HA	1.81	0.62
2:F:261:ILE:HG12	2:F:264:MET:HE1	1.81	0.62
2:B:316:LEU:HD21	2:B:318:THR:HG23	1.82	0.62
1:A:64:ILE:HD12	1:A:79:ILE:HG23	1.82	0.62
2:D:160:LEU:C	2:D:162:GLY:N	2.50	0.61
2:D:185:VAL:HG12	2:F:499:ILE:HD11	1.80	0.61
2:F:152:VAL:O	2:F:155:SER:HB2	2.01	0.61
2:B:160:LEU:CD2	2:D:161:GLU:HA	2.31	0.60
2:B:311:THR:HG22	2:B:344:ASP:HB2	1.81	0.60
2:F:316:LEU:HD21	2:F:318:THR:HG23	1.83	0.60
2:D:163:GLU:OE2	2:D:163:GLU:HA	2.02	0.60
2:F:161:GLU:HG2	2:F:165:ASN:OD1	2.02	0.60
2:D:311:THR:HG22	2:D:344:ASP:HB2	1.84	0.60
2:F:427:LYS:HG3	2:F:428:ASN:ND2	2.17	0.60
2:F:316:LEU:HD23	2:F:316:LEU:C	2.21	0.60
2:B:199:ILE:HD11	2:F:199:ILE:HD11	1.83	0.60
2:F:150:SER:CB	2:F:154:VAL:HG21	2.29	0.60
2:F:375:LEU:HD13	2:F:379:VAL:HG11	1.84	0.60
2:B:232:GLU:OE2	2:F:235:ARG:NH1	2.35	0.59
2:D:199:ILE:HD11	2:F:199:ILE:HD11	1.84	0.59
2:B:160:LEU:HD21	2:D:161:GLU:CA	2.32	0.59
1:E:64:ILE:HD12	1:E:79:ILE:HG23	1.84	0.59
2:F:316:LEU:HD11	2:F:336:ARG:NH2	2.17	0.59
2:B:161:GLU:O	2:B:164:VAL:N	2.36	0.59
2:D:318:THR:HG21	2:D:336:ARG:HB2	1.84	0.59
1:A:46:SER:OG	2:B:311:THR:HB	2.03	0.58
1:C:36:THR:O	1:C:38:SER:N	2.36	0.58
2:F:152:VAL:HG13	2:F:153:ALA:N	2.17	0.58
2:D:160:LEU:HA	2:D:163:GLU:HB2	1.83	0.58
2:B:167:ILE:HD11	2:D:167:ILE:HG12	1.84	0.58
2:B:167:ILE:HG12	2:F:167:ILE:HD11	1.85	0.58
2:B:400:THR:HG21	2:F:378:GLU:OE2	2.03	0.58
2:D:311:THR:HG23	2:D:312:PRO:HD2	1.86	0.58
2:B:316:LEU:HD11	2:B:336:ARG:NH2	2.19	0.58
1:A:36:THR:O	1:A:38:SER:N	2.37	0.57
2:B:206:ILE:O	2:B:210:GLN:HG3	2.04	0.57
2:D:149:ALA:HB3	2:D:152:VAL:HG12	1.86	0.57
2:B:261:ILE:HG12	2:B:264:MET:HE1	1.84	0.57
2:F:206:ILE:O	2:F:210:GLN:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:386:ILE:O	2:F:393:CYS:SG	2.62	0.57
2:D:149:ALA:O	2:D:152:VAL:HG12	2.04	0.57
2:D:316:LEU:HD21	2:D:318:THR:HG23	1.87	0.57
2:F:510:ASP:HB3	2:F:515:LEU:HB2	1.85	0.57
2:B:499:ILE:HD11	2:F:185:VAL:HG12	1.87	0.57
1:E:46:SER:OG	2:F:311:THR:HB	2.05	0.56
2:B:455:THR:HB	2:F:308:VAL:HB	1.88	0.56
1:C:36:THR:CG2	2:D:386:ILE:HD11	2.36	0.56
2:D:386:ILE:O	2:D:393:CYS:SG	2.63	0.56
2:B:386:ILE:O	2:B:393:CYS:SG	2.64	0.56
2:B:199:ILE:O	2:B:204:LEU:HB2	2.04	0.56
1:C:46:SER:OG	2:D:311:THR:HB	2.06	0.56
1:C:64:ILE:HD12	1:C:79:ILE:HG23	1.88	0.56
2:D:427:LYS:HG3	2:D:428:ASN:ND2	2.21	0.56
2:D:508:LYS:O	2:D:512:LEU:HD13	2.04	0.56
2:F:152:VAL:CG1	2:F:153:ALA:N	2.68	0.56
2:F:311:THR:HG22	2:F:344:ASP:HB2	1.87	0.56
2:B:308:VAL:HB	2:D:455:THR:HB	1.89	0.55
2:B:375:LEU:HD13	2:B:379:VAL:HG11	1.88	0.55
2:F:318:THR:HG21	2:F:336:ARG:HB2	1.89	0.55
1:A:36:THR:CG2	2:B:386:ILE:HD11	2.35	0.55
2:F:379:VAL:O	2:F:382:CYS:HB2	2.05	0.55
2:B:316:LEU:CD2	2:B:318:THR:HG23	2.36	0.55
1:C:79:ILE:HD11	2:D:219:THR:HB	1.89	0.55
1:E:31:GLU:OE2	1:E:42:LYS:HG3	2.07	0.55
2:F:508:LYS:O	2:F:512:LEU:HD13	2.07	0.55
2:B:156:LYS:O	2:B:160:LEU:HB2	2.06	0.55
2:B:311:THR:HG23	2:B:312:PRO:HD2	1.89	0.55
2:D:199:ILE:O	2:D:204:LEU:HB2	2.07	0.55
2:F:199:ILE:O	2:F:204:LEU:HB2	2.06	0.55
1:A:44:TYR:HB2	2:B:313:CYS:HB2	1.89	0.55
2:B:161:GLU:O	2:B:163:GLU:N	2.39	0.54
2:B:199:ILE:HD11	2:D:199:ILE:HD11	1.90	0.54
2:D:316:LEU:HD11	2:D:336:ARG:NH2	2.23	0.54
1:E:36:THR:O	1:E:38:SER:N	2.40	0.54
1:E:36:THR:CG2	2:F:386:ILE:HD11	2.36	0.54
2:F:322:CYS:HB2	2:F:417:TYR:CD1	2.42	0.54
1:E:38:SER:HB3	2:F:318:THR:HG22	1.89	0.54
1:E:79:ILE:HD11	2:F:219:THR:HB	1.90	0.54
2:F:341:TRP:CZ3	2:F:365:VAL:HG21	2.43	0.54
2:B:427:LYS:HG3	2:B:428:ASN:ND2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:375:LEU:HD13	2:D:379:VAL:HG11	1.89	0.54
1:A:38:SER:HB3	2:B:318:THR:HG22	1.90	0.53
2:B:341:TRP:CZ3	2:B:365:VAL:HG21	2.43	0.53
2:F:311:THR:HG23	2:F:312:PRO:HD2	1.90	0.53
2:B:467:LEU:HB2	1:E:57:ILE:HG12	1.91	0.53
2:B:261:ILE:HA	2:B:264:MET:HE2	1.91	0.53
2:D:206:ILE:O	2:D:210:GLN:HG3	2.08	0.53
2:B:318:THR:HG21	2:B:336:ARG:HB2	1.90	0.53
2:B:379:VAL:O	2:B:382:CYS:HB2	2.08	0.53
2:D:168:LYS:HE2	2:F:513:LEU:O	2.09	0.53
2:F:513:LEU:H	2:F:514:GLY:HA2	1.73	0.53
1:E:44:TYR:HB2	2:F:313:CYS:HB2	1.91	0.53
2:D:151:GLY:O	2:D:154:VAL:HG22	2.09	0.52
2:B:508:LYS:O	2:B:512:LEU:HD13	2.10	0.52
1:C:38:SER:HB3	2:D:318:THR:HG22	1.90	0.52
2:D:311:THR:CG2	2:D:312:PRO:HD2	2.39	0.52
2:B:235:ARG:NH1	2:D:232:GLU:OE2	2.42	0.52
2:D:309:ILE:HG22	2:D:310:ASP:CG	2.29	0.52
2:B:160:LEU:HD11	2:D:161:GLU:HA	1.92	0.52
2:B:322:CYS:HB2	2:B:417:TYR:CD1	2.45	0.52
1:A:36:THR:O	1:A:36:THR:HG22	2.10	0.51
2:B:333:CYS:O	2:B:334:LEU:HD23	2.10	0.51
1:A:66:GLU:HB2	1:A:79:ILE:HG21	1.93	0.51
2:D:318:THR:O	2:D:406:VAL:HG21	2.10	0.51
2:D:345:ASN:OD1	2:F:455:THR:HG21	2.11	0.51
2:F:203:LEU:O	2:F:207:VAL:HG23	2.10	0.51
2:F:309:ILE:HG22	2:F:310:ASP:CG	2.29	0.51
2:B:376:PRO:HB2	2:B:378:GLU:HG2	1.92	0.51
2:F:159:HIS:O	2:F:162:GLY:N	2.43	0.51
2:D:322:CYS:HB2	2:D:417:TYR:CD1	2.46	0.51
2:F:345:ASN:O	2:F:347:GLY:N	2.44	0.51
1:A:31:GLU:OE2	1:A:42:LYS:HG3	2.11	0.51
2:D:160:LEU:O	2:D:163:GLU:N	2.44	0.51
2:D:160:LEU:C	2:D:163:GLU:H	2.14	0.51
2:D:379:VAL:O	2:D:382:CYS:HB2	2.10	0.51
1:C:57:ILE:HG12	2:F:467:LEU:HB2	1.92	0.51
2:D:341:TRP:CZ3	2:D:365:VAL:HG21	2.45	0.50
1:C:44:TYR:HB2	2:D:313:CYS:HB2	1.92	0.50
2:B:247:VAL:HG23	2:B:285:SER:HB2	1.94	0.50
1:E:36:THR:O	1:E:36:THR:HG22	2.11	0.50
2:B:309:ILE:HG22	2:B:310:ASP:CG	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:149:ALA:O	2:D:151:GLY:N	2.44	0.50
2:B:217:ILE:HD13	2:D:217:ILE:HG21	1.92	0.50
2:D:308:VAL:HB	2:F:455:THR:HB	1.92	0.50
2:D:407:ILE:HD11	2:D:457:TYR:HB3	1.94	0.50
2:F:376:PRO:HB2	2:F:378:GLU:HG2	1.92	0.50
2:B:311:THR:CG2	2:B:312:PRO:HD2	2.41	0.50
2:D:333:CYS:O	2:D:334:LEU:HD23	2.12	0.50
2:D:345:ASN:O	2:D:347:GLY:N	2.44	0.50
2:B:168:LYS:HE2	2:D:513:LEU:O	2.12	0.49
1:E:66:GLU:HB2	1:E:79:ILE:HG21	1.93	0.49
2:D:235:ARG:NH1	2:F:232:GLU:OE2	2.44	0.49
2:D:508:LYS:O	2:D:512:LEU:CD1	2.60	0.49
2:D:261:ILE:HA	2:D:264:MET:HE2	1.94	0.49
2:F:163:GLU:OE2	2:F:163:GLU:HA	2.12	0.49
1:A:79:ILE:HD11	2:B:219:THR:HB	1.93	0.49
2:B:361:GLN:O	2:B:361:GLN:HG3	2.12	0.49
1:C:66:GLU:HB2	1:C:79:ILE:HG21	1.93	0.49
2:F:159:HIS:C	2:F:162:GLY:H	2.16	0.49
2:B:316:LEU:HD21	2:B:318:THR:CG2	2.41	0.48
2:F:150:SER:HA	2:F:154:VAL:HG22	1.94	0.48
2:F:316:LEU:CD2	2:F:318:THR:HG23	2.42	0.48
2:F:483:PHE:CD1	2:F:484:PRO:HD2	2.47	0.48
1:C:36:THR:O	1:C:36:THR:HG22	2.12	0.48
2:D:203:LEU:O	2:D:207:VAL:HG23	2.13	0.48
2:D:376:PRO:HB2	2:D:378:GLU:HG2	1.95	0.48
2:F:159:HIS:O	2:F:159:HIS:CD2	2.67	0.48
2:F:323:THR:HG21	2:F:332:ILE:HG12	1.95	0.48
2:F:422:CYS:HA	2:F:451:SER:O	2.13	0.48
2:F:232:GLU:HA	2:F:232:GLU:OE1	2.14	0.48
2:F:333:CYS:O	2:F:334:LEU:HD23	2.13	0.48
2:B:345:ASN:O	2:B:347:GLY:N	2.46	0.48
2:D:378:GLU:OE2	2:F:400:THR:HG21	2.14	0.48
2:D:167:ILE:HD11	2:F:167:ILE:HG12	1.96	0.47
1:E:36:THR:HG21	2:F:336:ARG:HD2	1.96	0.47
2:D:361:GLN:O	2:D:361:GLN:HG3	2.14	0.47
2:B:160:LEU:HD23	2:F:160:LEU:HD21	1.95	0.47
2:D:316:LEU:HD23	2:D:316:LEU:C	2.35	0.47
2:B:422:CYS:HA	2:B:451:SER:O	2.15	0.47
1:A:36:THR:O	1:A:37:CYS:C	2.53	0.47
2:B:163:GLU:OE2	2:B:163:GLU:HA	2.14	0.47
1:C:90:VAL:O	1:C:94:GLN:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:316:LEU:CD2	2:D:318:THR:HG23	2.44	0.47
2:B:361:GLN:HE21	2:B:362:SER:HB2	1.80	0.47
2:F:311:THR:CG2	2:F:312:PRO:HD2	2.45	0.47
2:F:160:LEU:HD12	2:F:160:LEU:O	2.15	0.46
2:B:426:ASN:OD1	2:B:427:LYS:N	2.48	0.46
2:B:158:LEU:O	2:B:158:LEU:HG	2.13	0.46
2:B:161:GLU:O	2:B:162:GLY:C	2.53	0.46
2:B:311:THR:CG2	2:B:344:ASP:CB	2.92	0.46
1:C:36:THR:HG21	2:D:336:ARG:HD2	1.97	0.46
2:D:149:ALA:HB3	2:D:152:VAL:CG1	2.44	0.46
2:D:422:CYS:HA	2:D:451:SER:O	2.15	0.46
2:F:318:THR:O	2:F:406:VAL:HG21	2.15	0.46
2:D:483:PHE:CD1	2:D:484:PRO:HD2	2.51	0.46
2:D:361:GLN:HE21	2:D:362:SER:HB2	1.79	0.46
2:F:407:ILE:HD13	2:F:458:TYR:O	2.16	0.46
2:B:407:ILE:HD11	2:B:457:TYR:HB3	1.97	0.46
2:B:316:LEU:C	2:B:316:LEU:HD23	2.36	0.46
2:B:378:GLU:OE2	2:D:400:THR:HG21	2.15	0.46
2:F:508:LYS:O	2:F:512:LEU:CD1	2.63	0.46
2:D:264:MET:HE3	2:D:274:MET:SD	2.56	0.45
1:C:36:THR:O	1:C:37:CYS:C	2.53	0.45
2:F:247:VAL:HG23	2:F:285:SER:HB2	1.97	0.45
2:F:361:GLN:HE21	2:F:362:SER:HB2	1.80	0.45
2:B:152:VAL:HG11	2:D:157:VAL:HG21	1.98	0.45
2:D:157:VAL:HG12	2:D:157:VAL:O	2.15	0.45
2:F:513:LEU:N	2:F:514:GLY:HA2	2.32	0.45
2:F:444:ASN:HB2	2:F:460:ASN:OD1	2.16	0.45
1:E:49:ARG:HG3	2:F:304:PRO:HB2	1.98	0.45
2:F:407:ILE:HD11	2:F:457:TYR:HB3	1.99	0.45
2:B:483:PHE:CD1	2:B:484:PRO:HD2	2.52	0.45
2:F:151:GLY:O	2:F:154:VAL:HG23	2.17	0.45
2:D:217:ILE:HD13	2:F:217:ILE:HG21	1.99	0.44
2:F:156:LYS:O	2:F:159:HIS:HB3	2.17	0.44
2:F:316:LEU:HD21	2:F:318:THR:CG2	2.46	0.44
2:B:160:LEU:CD1	2:D:161:GLU:HA	2.46	0.44
2:D:232:GLU:HA	2:D:232:GLU:OE1	2.15	0.44
2:D:247:VAL:HG23	2:D:285:SER:HB2	1.98	0.44
2:B:163:GLU:O	2:B:167:ILE:HG22	2.18	0.44
2:B:178:VAL:HG11	2:D:506:ILE:HD11	1.99	0.44
2:B:216:ASN:O	2:B:220:VAL:HG23	2.17	0.44
2:B:379:VAL:HG12	2:B:391:TYR:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:152:VAL:O	2:F:155:SER:N	2.49	0.44
2:F:422:CYS:O	2:F:423:THR:HG23	2.18	0.44
2:B:422:CYS:O	2:B:423:THR:HG23	2.17	0.44
2:B:156:LYS:NZ	2:D:161:GLU:HG3	2.32	0.44
2:F:261:ILE:HA	2:F:264:MET:HE2	2.00	0.44
2:B:152:VAL:HG21	2:D:153:ALA:HB1	2.00	0.44
2:B:444:ASN:HB2	2:B:460:ASN:OD1	2.18	0.44
2:D:160:LEU:HD23	2:F:160:LEU:HD23	2.00	0.44
2:D:510:ASP:O	2:D:514:GLY:HA2	2.18	0.44
2:F:361:GLN:O	2:F:361:GLN:HG3	2.16	0.44
2:D:216:ASN:O	2:D:220:VAL:HG23	2.17	0.44
2:B:232:GLU:OE1	2:B:232:GLU:HA	2.18	0.44
2:D:474:ILE:O	2:D:474:ILE:HG13	2.18	0.43
2:F:292:ILE:HG23	2:F:292:ILE:O	2.18	0.43
2:D:407:ILE:HD13	2:D:458:TYR:O	2.18	0.43
2:D:478:TYR:O	2:D:478:TYR:CD2	2.72	0.43
1:A:49:ARG:HG3	2:B:304:PRO:HB2	1.99	0.43
2:D:210:GLN:O	2:D:214:ILE:HG13	2.18	0.43
2:B:416:CYS:O	2:B:437:ASN:HA	2.19	0.43
1:A:36:THR:HG21	2:B:336:ARG:HD2	2.01	0.43
2:B:161:GLU:C	2:B:163:GLU:N	2.72	0.43
2:D:150:SER:HB3	2:F:149:ALA:HA	2.00	0.43
2:B:247:VAL:CG2	2:B:285:SER:HB2	2.49	0.43
1:E:36:THR:O	1:E:37:CYS:C	2.57	0.43
2:D:386:ILE:HG21	2:D:395:ILE:HD12	2.00	0.42
2:F:322:CYS:O	2:F:323:THR:C	2.57	0.42
2:B:164:VAL:HA	2:B:167:ILE:CG2	2.48	0.42
2:B:203:LEU:O	2:B:207:VAL:HG23	2.19	0.42
2:D:292:ILE:HG23	2:D:292:ILE:O	2.19	0.42
2:D:308:VAL:O	2:D:309:ILE:HG13	2.19	0.42
2:B:345:ASN:O	2:B:348:SER:O	2.36	0.42
2:B:474:ILE:O	2:B:474:ILE:HG13	2.19	0.42
2:D:309:ILE:CG2	2:D:310:ASP:N	2.83	0.42
2:F:150:SER:CA	2:F:154:VAL:CG2	2.97	0.42
2:F:246:PRO:CB	2:F:283:GLN:HA	2.43	0.42
2:F:309:ILE:CG2	2:F:310:ASP:N	2.82	0.42
2:F:311:THR:CG2	2:F:344:ASP:CB	2.93	0.42
2:F:379:VAL:HG12	2:F:391:TYR:CE2	2.54	0.42
1:A:57:ILE:HG12	2:D:467:LEU:HB2	2.02	0.42
1:A:64:ILE:CD1	1:A:79:ILE:HG23	2.49	0.42
2:D:158:LEU:HD23	2:D:158:LEU:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:312:PRO:HG2	2:D:344:ASP:OD2	2.19	0.42
2:D:414:VAL:CG2	2:D:450:VAL:HG11	2.49	0.42
2:F:264:MET:HE3	2:F:274:MET:SD	2.60	0.42
2:B:160:LEU:O	2:B:164:VAL:HG23	2.20	0.42
2:B:318:THR:O	2:B:406:VAL:HG21	2.20	0.42
2:B:403:SER:HB3	2:B:417:TYR:H	1.85	0.42
2:D:183:ASN:O	2:D:184:GLY:C	2.59	0.41
2:F:477:PHE:CE2	2:F:479:ASP:HB2	2.54	0.41
2:D:442:VAL:CG1	2:D:447:VAL:HB	2.49	0.41
2:D:477:PHE:CE2	2:D:479:ASP:HB2	2.55	0.41
2:B:312:PRO:HG2	2:B:344:ASP:OD2	2.21	0.41
1:E:36:THR:HG21	2:F:336:ARG:CD	2.50	0.41
2:B:292:ILE:HG23	2:B:292:ILE:O	2.20	0.41
2:D:264:MET:CE	2:D:274:MET:SD	3.09	0.41
1:C:31:GLU:OE2	1:C:42:LYS:HG3	2.20	0.41
2:D:316:LEU:HD21	2:D:318:THR:CG2	2.49	0.41
2:D:403:SER:HB3	2:D:417:TYR:H	1.85	0.41
2:F:308:VAL:O	2:F:309:ILE:HG13	2.21	0.41
2:F:427:LYS:HG3	2:F:428:ASN:HD22	1.83	0.41
1:C:36:THR:HG21	2:D:336:ARG:CD	2.51	0.41
1:C:71:GLY:O	2:D:209:LYS:HB3	2.20	0.41
2:D:261:ILE:HG23	2:D:264:MET:CE	2.50	0.41
2:B:477:PHE:CE2	2:B:479:ASP:HB2	2.55	0.41
2:D:319:SER:OG	2:D:406:VAL:HG23	2.21	0.41
1:E:71:GLY:O	2:F:209:LYS:HB3	2.21	0.41
1:C:33:TYR:CD2	1:C:33:TYR:N	2.89	0.41
2:D:197:ASN:O	2:D:201:LYS:HG2	2.21	0.41
2:B:498:LYS:HD3	2:B:498:LYS:HA	1.89	0.40
1:E:58:THR:C	1:E:59:ILE:HG13	2.40	0.40
2:D:427:LYS:HG3	2:D:428:ASN:HD22	1.86	0.40
2:F:163:GLU:O	2:F:167:ILE:HG22	2.22	0.40
2:B:379:VAL:HG12	2:B:391:TYR:CZ	2.55	0.40
1:C:36:THR:CG2	2:D:336:ARG:HD2	2.51	0.40
2:B:334:LEU:CD2	2:B:397:THR:HG22	2.52	0.40
2:B:474:ILE:HD11	1:E:64:ILE:HG22	2.02	0.40
1:C:49:ARG:HG3	2:D:304:PRO:HB2	2.02	0.40
1:C:64:ILE:HG22	2:F:474:ILE:HG12	2.04	0.40
2:D:498:LYS:HA	2:D:498:LYS:HD3	1.95	0.40
1:E:36:THR:CG2	2:F:336:ARG:HD2	2.52	0.40
2:F:422:CYS:O	2:F:423:THR:CG2	2.69	0.40
2:B:407:ILE:HD13	2:B:458:TYR:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:416:CYS:O	2:D:437:ASN:HA	2.21	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	70/84 (83%)	67 (96%)	2 (3%)	1 (1%)	11	46
1	C	70/84 (83%)	67 (96%)	2 (3%)	1 (1%)	11	46
1	E	70/84 (83%)	67 (96%)	2 (3%)	1 (1%)	11	46
2	B	352/374 (94%)	329 (94%)	20 (6%)	3 (1%)	17	56
2	D	356/374 (95%)	336 (94%)	17 (5%)	3 (1%)	19	58
2	F	360/374 (96%)	341 (95%)	16 (4%)	3 (1%)	19	58
All	All	1278/1374 (93%)	1207 (94%)	59 (5%)	12 (1%)	17	56

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	346	ALA
2	D	346	ALA
2	F	346	ALA
1	A	37	CYS
2	B	162	GLY
1	C	37	CYS
1	E	37	CYS
2	F	323	THR
2	B	362	SER
2	D	150	SER
2	D	362	SER
2	F	362	SER

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	65/75 (87%)	64 (98%)	1 (2%)	65	85
1	C	65/75 (87%)	64 (98%)	1 (2%)	65	85
1	E	65/75 (87%)	64 (98%)	1 (2%)	65	85
2	B	329/344 (96%)	313 (95%)	16 (5%)	25	61
2	D	332/344 (96%)	313 (94%)	19 (6%)	20	56
2	F	336/344 (98%)	318 (95%)	18 (5%)	22	58
All	All	1192/1257 (95%)	1136 (95%)	56 (5%)	26	62

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLU
2	B	211	SER
2	B	245	THR
2	B	290	SER
2	B	319	SER
2	B	338	ASP
2	B	401	ASP
2	B	402	VAL
2	B	405	SER
2	B	409	SER
2	B	416	CYS
2	B	437	ASN
2	B	439	CYS
2	B	448	ASP
2	B	455	THR
2	B	463	GLU
2	B	500	ASN
1	C	31	GLU
2	D	161	GLU
2	D	167	ILE
2	D	211	SER
2	D	245	THR

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Mol	Chain	Res	Type
2	D	290	SER
2	D	319	SER
2	D	338	ASP
2	D	401	ASP
2	D	402	VAL
2	D	405	SER
2	D	409	SER
2	D	416	CYS
2	D	437	ASN
2	D	439	CYS
2	D	448	ASP
2	D	455	THR
2	D	463	GLU
2	D	500	ASN
2	D	517	VAL
1	E	31	GLU
2	F	154	VAL
2	F	167	ILE
2	F	211	SER
2	F	245	THR
2	F	319	SER
2	F	323	THR
2	F	338	ASP
2	F	401	ASP
2	F	402	VAL
2	F	405	SER
2	F	409	SER
2	F	416	CYS
2	F	437	ASN
2	F	439	CYS
2	F	448	ASP
2	F	455	THR
2	F	463	GLU
2	F	515	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
2	B	202	GLN
2	B	270	GLN
2	B	276	ASN

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Mol	Chain	Res	Type
2	B	277	ASN
2	B	361	GLN
2	B	380	ASN
2	B	383	ASN
2	B	428	ASN
2	B	437	ASN
1	C	34	GLN
2	D	202	GLN
2	D	276	ASN
2	D	361	GLN
2	D	380	ASN
2	D	383	ASN
2	D	428	ASN
2	D	437	ASN
1	E	34	GLN
2	F	159	HIS
2	F	202	GLN
2	F	270	GLN
2	F	276	ASN
2	F	361	GLN
2	F	380	ASN
2	F	383	ASN
2	F	428	ASN
2	F	437	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

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

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	72/84 (85%)	0.30	2 (2%) 53 37	44, 76, 128, 176	0
1	C	72/84 (85%)	0.11	0 100 100	45, 72, 135, 164	0
1	E	72/84 (85%)	0.14	1 (1%) 75 63	47, 73, 138, 157	0
2	B	356/374 (95%)	0.19	7 (1%) 65 51	39, 73, 116, 178	0
2	D	360/374 (96%)	0.19	5 (1%) 75 63	28, 73, 112, 162	0
2	F	364/374 (97%)	0.14	2 (0%) 91 86	37, 68, 104, 132	0
All	All	1296/1374 (94%)	0.17	17 (1%) 77 65	28, 72, 114, 178	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	65	LYS	5.1
2	D	477	PHE	3.6
2	B	477	PHE	3.4
2	F	419	LYS	2.9
1	A	67	ASN	2.7
2	F	163	GLU	2.7
2	B	163	GLU	2.5
2	B	355	ALA	2.5
2	D	202	GLN	2.5
2	D	428	ASN	2.3
1	E	65	LYS	2.3
2	B	401	ASP	2.2
2	B	496	ASN	2.2
2	B	492	ILE	2.1
2	D	469	VAL	2.1
2	D	167	ILE	2.1
2	B	188	LEU	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 monosaccharides 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.