Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:50 PM GMT

PDB ID	:	1QU1
Title	:	CRYSTAL STRUCTURE OF EHA2 (23-185)
Authors	:	Chen, J.; Skehel, J.J.; Wiley, D.C.
Deposited on	:	1999-07-05
Resolution	:	1.90 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.90 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.
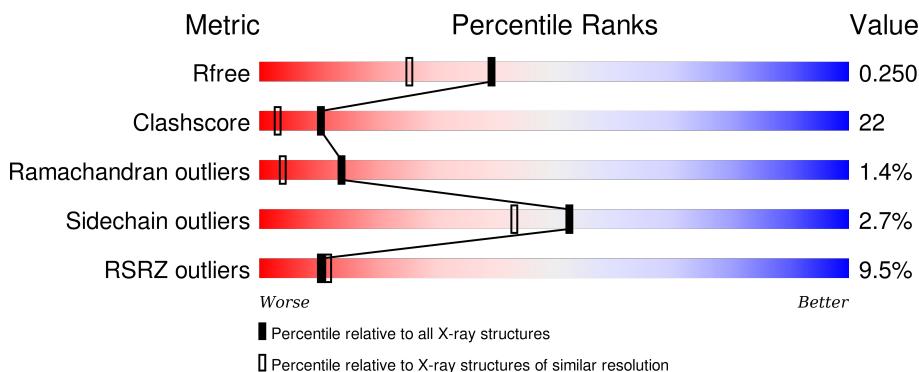
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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. 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	155	8% / 59% / 25% / • / 14%
1	B	155	12% / 57% / 34% / • / 7%
1	C	155	12% / 66% / 25% / 5% • •
1	D	155	6% / 70% / 23% / • / 6%
1	E	155	12% / 71% / 21% / •• / 6%
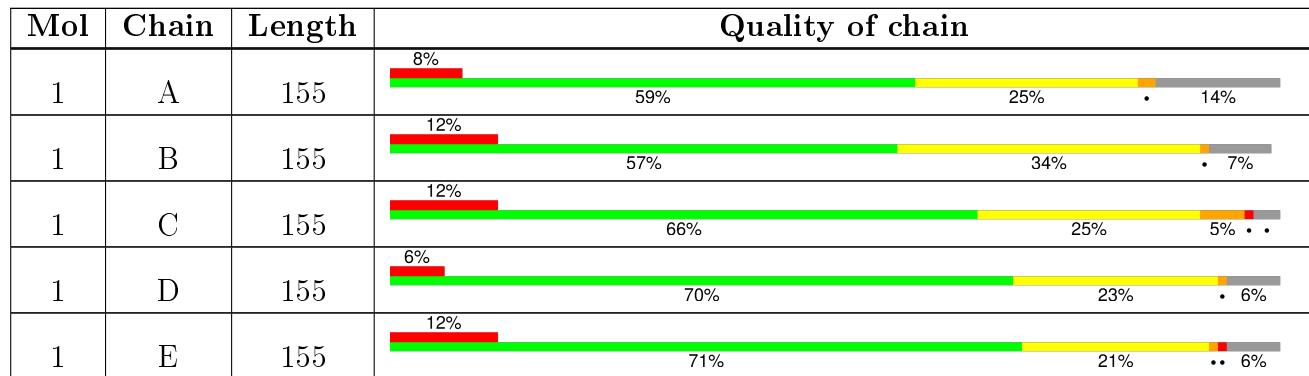
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Mol	Chain	Length	Quality of chain
1	F	155	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7907 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 PROTEIN (INFLUENZA RECOMBINANT HA2 CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	133	Total	C	N	O	S	27	0	0
			1096	681	193	219	3			
1	B	144	Total	C	N	O	S	22	0	0
			1178	727	209	238	4			
1	C	150	Total	C	N	O	S	49	0	0
			1240	769	217	250	4			
1	D	146	Total	C	N	O	S	5	0	0
			1195	738	211	242	4			
1	E	146	Total	C	N	O	S	37	0	0
			1195	738	211	242	4			
1	F	155	Total	C	N	O	S	13	0	0
			1269	785	223	257	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	137	SER	CYS	CONFLICT	UNP P03437
B	137	SER	CYS	CONFLICT	UNP P03437
C	137	SER	CYS	CONFLICT	UNP P03437
D	137	SER	CYS	CONFLICT	UNP P03437
E	137	SER	CYS	CONFLICT	UNP P03437
F	137	SER	CYS	CONFLICT	UNP P03437

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	115	Total	O	0	0
			115	115		
2	B	98	Total	O	0	0
			98	98		
2	C	99	Total	O	0	0
			99	99		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	162	Total 162	O 162	0	0
2	E	110	Total 110	O 110	0	0
2	F	150	Total 150	O 150	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: PROTEIN (INFLUENZA RECOMBINANT HA2 CHAIN)
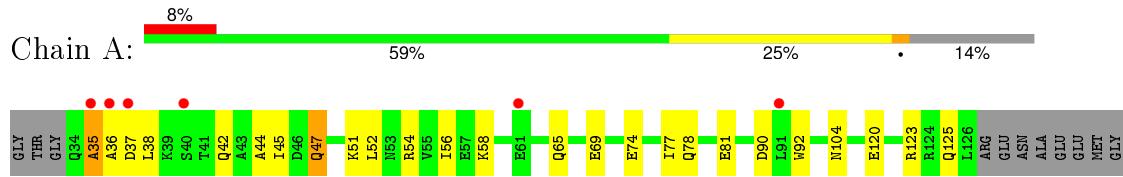
- Molecule 1: PROTEIN (INFLUENZA RECOMBINANT HA2 CHAIN)
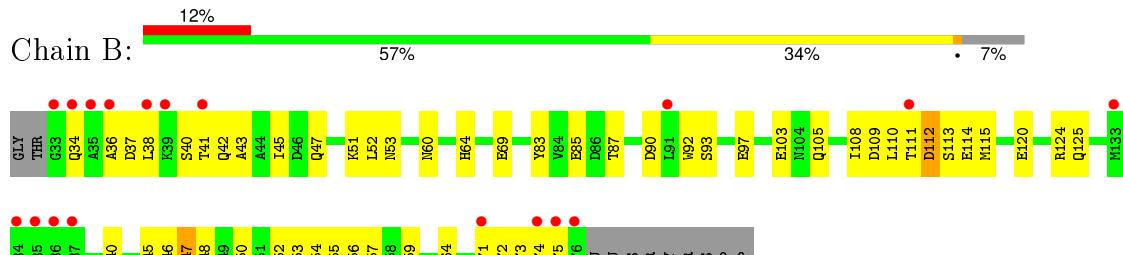
- Molecule 1: PROTEIN (INFLUENZA RECOMBINANT HA2 CHAIN)
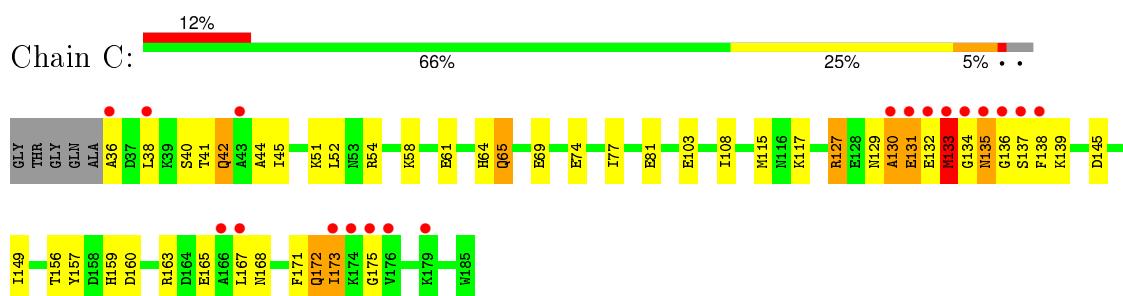
- Molecule 1: PROTEIN (INFLUENZA RECOMBINANT HA2 CHAIN)
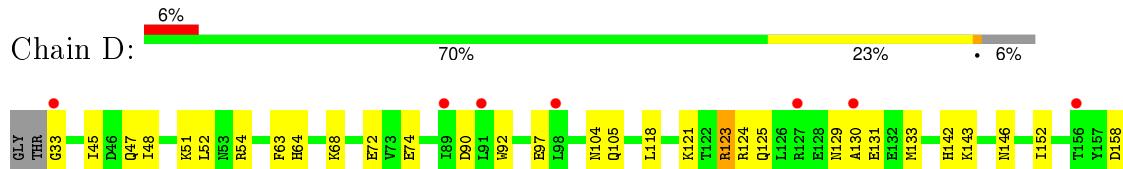
● Molecule 1: PROTEIN (INFLUENZA RECOMBINANT HA2 CHAIN)
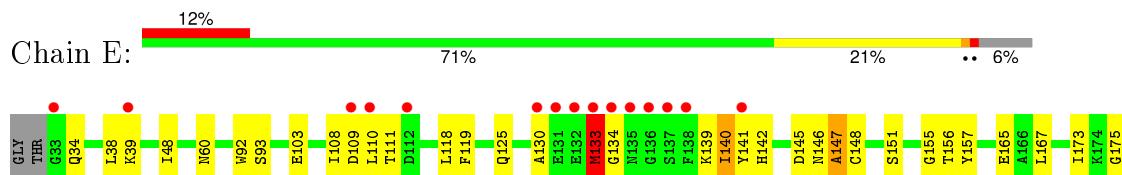
Chain E:

● Molecule 1: PROTEIN (INFLUENZA RECOMBINANT HA2 CHAIN)

Chain F:
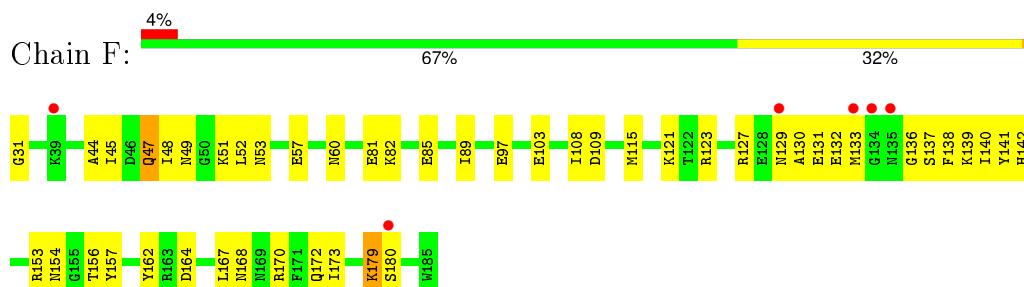
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	113.24Å 48.88Å 221.30Å 90.00° 103.26° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90	Depositor
	30.70 – 1.90	EDS
% Data completeness	94.3 (20.00-1.90)	Depositor
(in resolution range)	95.2 (30.70-1.90)	EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 1.91Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.229 , 0.250	Depositor
	0.229 , 0.250	DCC
R_{free} test set	5547 reflections (6.22%)	DCC
Wilson B-factor (Å^2)	25.9	Xtriage
Anisotropy	0.798	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 61.5	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning [2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Outliers	2 of 89222 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7907	wwPDB-VP
Average B, all atoms (Å^2)	40.0	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 23.39 % 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 4.7092e-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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.40	0/1110	0.59	0/1489
1	B	0.41	0/1193	0.64	0/1601
1	C	0.44	0/1258	0.67	1/1687 (0.1%)
1	D	0.41	0/1210	0.64	0/1624
1	E	0.39	0/1210	0.63	0/1624
1	F	0.45	0/1287	0.64	0/1726
All	All	0.42	0/7268	0.64	1/9751 (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})
1	C	133	MET	CG-SD-CE	6.12	110.00	100.20

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	1096	0	1063	48	0
1	B	1178	0	1136	63	0
1	C	1240	0	1194	78	0
1	D	1195	0	1153	55	0
1	E	1195	0	1153	36	0
1	F	1269	0	1220	69	0

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PROTEIN DATA BANK

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	115	0	0	11	0
2	B	98	0	0	14	0
2	C	99	0	0	5	0
2	D	162	0	0	19	0
2	E	110	0	0	7	0
2	F	150	0	0	37	0
All	All	7907	0	6919	295	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 22.

All (295) 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:D:333:HOH:O	1:E:60:ASN:HB3	1.47	1.13
1:A:65:GLN:HG3	2:A:280:HOH:O	1.56	1.04
1:D:52:LEU:HD21	2:F:322:HOH:O	1.57	1.03
1:C:127:ARG:HG3	1:C:132:GLU:OE2	1.58	1.01
1:D:51:LYS:HB2	2:D:316:HOH:O	1.62	0.99
1:D:118:LEU:HD11	2:F:335:HOH:O	1.62	0.99
1:C:129:ASN:ND2	1:C:130:ALA:H	1.63	0.97
1:D:118:LEU:HD21	2:F:335:HOH:O	1.66	0.94
1:F:146:ASN:HB3	2:F:310:HOH:O	1.65	0.94
1:D:143:LYS:HE3	2:D:225:HOH:O	1.67	0.93
1:C:131:GLU:O	1:C:132:GLU:HG3	1.70	0.92
1:C:131:GLU:C	1:C:132:GLU:HG3	1.89	0.90
1:D:130:ALA:HA	1:D:133:MET:HE2	1.53	0.89
1:C:156:THR:HG23	2:C:283:HOH:O	1.71	0.89
1:D:92:TRP:NE1	1:D:125:GLN:HG2	1.89	0.88
1:B:87:THR:HA	2:B:249:HOH:O	1.73	0.88
1:A:52:LEU:HA	2:A:292:HOH:O	1.72	0.87
1:F:48:ILE:HG22	2:F:266:HOH:O	1.74	0.87
1:F:179:LYS:HG3	2:F:333:HOH:O	1.75	0.86
1:B:90:ASP:HB2	2:B:249:HOH:O	1.74	0.86
2:A:292:HOH:O	1:B:52:LEU:HD11	1.75	0.85
1:C:131:GLU:O	1:C:132:GLU:CG	2.24	0.84
1:F:109:ASP:HA	2:F:296:HOH:O	1.82	0.80
1:E:156:THR:HG22	1:E:157:TYR:H	1.47	0.80
1:D:92:TRP:CE2	1:D:125:GLN:HG2	2.16	0.80
1:D:63:PHE:CD1	2:D:310:HOH:O	2.35	0.79
1:B:108:ILE:HD12	1:B:115:MET:HE2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:ASN:O	1:E:147:ALA:HB3	1.81	0.79
1:B:42:GLN:HB2	2:B:234:HOH:O	1.83	0.79
1:E:156:THR:HG22	1:E:157:TYR:N	2.00	0.77
1:A:36:ALA:HA	1:A:175:GLY:HA2	1.66	0.77
1:D:33:GLY:HA2	2:E:269:HOH:O	1.83	0.77
1:C:65:GLN:HG2	1:C:160:ASP:HB2	1.67	0.77
1:F:108:ILE:HD12	1:F:115:MET:HE2	1.67	0.76
1:D:68:LYS:HG2	2:D:262:HOH:O	1.86	0.75
1:B:173:ILE:N	1:C:42:GLN:HE21	1.85	0.75
1:D:177:GLU:HG3	2:D:268:HOH:O	1.87	0.75
1:B:173:ILE:N	1:C:42:GLN:NE2	2.35	0.74
1:C:129:ASN:HD22	1:C:130:ALA:H	1.34	0.74
1:B:152:ILE:HG13	2:B:255:HOH:O	1.87	0.73
1:C:65:GLN:HG2	1:C:160:ASP:CB	2.19	0.73
1:F:108:ILE:HD12	1:F:115:MET:CE	2.20	0.72
1:B:146:ASN:O	1:B:147:ALA:HB3	1.88	0.72
1:B:172:GLN:HG3	1:C:42:GLN:HE22	1.55	0.71
1:F:156:THR:HG22	1:F:157:TYR:H	1.56	0.71
1:B:146:ASN:O	1:B:147:ALA:CB	2.38	0.71
1:E:146:ASN:O	1:E:147:ALA:CB	2.39	0.70
1:C:132:GLU:O	1:C:134:GLY:N	2.24	0.70
1:A:153:ARG:NH2	2:A:219:HOH:O	2.23	0.69
1:A:38:LEU:HD22	1:C:175:GLY:HA3	1.72	0.69
1:C:77:ILE:O	1:C:81:GLU:HG3	1.92	0.69
1:D:177:GLU:O	1:F:180:SER:CB	2.40	0.69
1:F:52:LEU:N	2:F:322:HOH:O	2.25	0.68
1:B:109:ASP:OD1	1:B:111:THR:HG23	1.94	0.68
1:C:117:LYS:HD3	2:C:274:HOH:O	1.93	0.67
1:C:132:GLU:HG2	1:C:138:PHE:CE1	2.30	0.67
1:B:83:TYR:HB2	2:B:255:HOH:O	1.94	0.67
1:F:89:ILE:CD1	1:F:129:ASN:HB3	2.24	0.66
1:D:105:GLN:HE22	1:E:108:ILE:HG22	1.59	0.66
1:B:175:GLY:HA3	1:C:38:LEU:HD21	1.77	0.66
1:C:108:ILE:HD12	1:C:115:MET:HE2	1.78	0.66
2:D:323:HOH:O	1:F:31:GLY:HA3	1.96	0.65
1:B:173:ILE:H	1:C:42:GLN:NE2	1.92	0.65
1:D:64:HIS:CD2	2:F:330:HOH:O	2.50	0.65
1:D:45:ILE:HD12	2:F:287:HOH:O	1.96	0.65
1:D:68:LYS:HE3	2:D:262:HOH:O	1.96	0.64
1:B:36:ALA:HA	1:C:38:LEU:HD13	1.80	0.64
1:E:140:ILE:N	2:E:231:HOH:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:GLU:C	1:C:132:GLU:CG	2.65	0.63
1:A:173:ILE:HB	2:B:234:HOH:O	1.97	0.63
1:F:89:ILE:HD12	1:F:129:ASN:HB3	1.79	0.63
1:F:150:GLU:OE2	1:F:154:ASN:HB2	1.99	0.63
1:D:118:LEU:CD2	2:F:335:HOH:O	2.36	0.62
1:D:123:ARG:HE	1:D:129:ASN:HA	1.63	0.62
1:B:108:ILE:HD12	1:B:115:MET:CE	2.27	0.62
1:F:129:ASN:HB2	2:F:257:HOH:O	2.00	0.62
1:B:69:GLU:OE2	1:B:159:HIS:HD2	1.82	0.62
1:A:54:ARG:O	1:A:58:LYS:HG3	1.99	0.61
1:C:171:PHE:CD2	1:C:172:GLN:HG3	2.36	0.61
1:D:90:ASP:OD2	1:D:142:HIS:HE1	1.84	0.61
2:A:300:HOH:O	1:C:167:LEU:HD11	2.01	0.61
1:F:103:GLU:HG3	2:F:296:HOH:O	2.00	0.60
1:F:156:THR:HG22	1:F:157:TYR:N	2.15	0.60
1:F:141:TYR:N	2:F:326:HOH:O	2.30	0.60
1:D:158:ASP:CB	2:D:262:HOH:O	2.49	0.60
1:D:170:ARG:HH12	1:D:172:GLN:CD	2.05	0.60
1:B:37:ASP:HB3	2:B:260:HOH:O	2.01	0.59
1:D:118:LEU:CG	2:F:335:HOH:O	2.50	0.59
1:A:90:ASP:OD2	1:A:142:HIS:HE1	1.86	0.59
1:B:140:ILE:HA	2:B:247:HOH:O	2.01	0.59
1:A:137:SER:HA	2:A:277:HOH:O	2.02	0.59
1:B:173:ILE:H	1:C:42:GLN:HE21	1.47	0.59
2:A:240:HOH:O	1:B:114:GLU:HG3	2.03	0.58
1:C:69:GLU:OE1	1:C:159:HIS:HD2	1.85	0.58
1:B:120:GLU:O	1:B:124:ARG:HB2	2.03	0.58
1:D:121:LYS:NZ	2:D:344:HOH:O	2.35	0.58
1:E:167:LEU:HD21	1:F:57:GLU:HG3	1.85	0.58
1:E:156:THR:HG21	2:E:279:HOH:O	2.02	0.58
1:B:164:ASP:OD2	1:C:64:HIS:HE1	1.85	0.58
1:C:131:GLU:HG2	1:C:133:MET:HG3	1.86	0.58
1:C:135:ASN:OD1	1:C:137:SER:HB2	2.03	0.58
1:A:69:GLU:OE2	1:A:159:HIS:HD2	1.86	0.58
1:A:47:GLN:CD	1:A:168:ASN:HD21	2.07	0.58
1:D:52:LEU:CD2	2:F:322:HOH:O	2.33	0.57
1:D:118:LEU:CD1	2:F:335:HOH:O	2.34	0.57
1:D:158:ASP:HB2	2:D:262:HOH:O	2.03	0.57
1:A:165:GLU:H	1:B:60:ASN:HD21	1.51	0.57
1:C:127:ARG:CG	1:C:132:GLU:OE2	2.42	0.57
1:B:103:GLU:OE1	1:B:110:LEU:HD12	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:GLU:O	1:C:138:PHE:CD1	2.56	0.57
1:F:47:GLN:OE1	1:F:168:ASN:ND2	2.37	0.57
1:A:45:ILE:HG13	1:C:173:ILE:HD11	1.85	0.56
1:D:177:GLU:O	1:F:180:SER:OG	2.22	0.56
1:F:130:ALA:HB1	1:F:139:LYS:O	2.05	0.56
1:C:129:ASN:CG	1:C:130:ALA:H	2.08	0.56
1:A:136:GLY:HA3	1:A:139:LYS:HB3	1.86	0.56
1:F:132:GLU:OE1	1:F:136:GLY:HA2	2.06	0.56
1:B:175:GLY:HA3	1:C:38:LEU:CD2	2.36	0.56
1:E:156:THR:CG2	1:E:157:TYR:N	2.69	0.56
1:D:104:ASN:HB2	2:D:271:HOH:O	2.04	0.56
1:D:178:LEU:HA	2:F:280:HOH:O	2.07	0.55
1:E:109:ASP:OD1	1:E:111:THR:HB	2.05	0.55
1:C:54:ARG:NH1	1:C:165:GLU:OE2	2.40	0.55
1:A:42:GLN:NE2	1:C:172:GLN:O	2.40	0.55
1:A:42:GLN:HE21	1:C:173:ILE:HG13	1.70	0.55
1:E:156:THR:CG2	1:E:157:TYR:H	2.16	0.55
1:B:97:GLU:CD	2:B:261:HOH:O	2.44	0.55
1:E:110:LEU:HD22	1:E:119:PHE:HB2	1.89	0.55
1:E:145:ASP:OD1	1:E:146:ASN:O	2.26	0.54
1:F:162:TYR:HB3	2:F:330:HOH:O	2.08	0.54
1:A:44:ALA:HB2	1:A:171:PHE:CD2	2.43	0.54
1:D:97:GLU:HG2	1:E:118:LEU:HD21	1.90	0.54
1:F:180:SER:HB3	2:F:314:HOH:O	2.07	0.54
1:C:54:ARG:NH1	1:C:165:GLU:OE1	2.41	0.54
1:C:61:GLU:HG3	2:C:258:HOH:O	2.08	0.54
1:B:150:GLU:O	1:B:154:ASN:HB2	2.08	0.54
1:F:153:ARG:NE	2:F:324:HOH:O	2.41	0.53
1:D:92:TRP:CD1	1:D:125:GLN:HG2	2.44	0.53
1:A:37:ASP:H	1:A:175:GLY:HA2	1.73	0.53
1:B:37:ASP:CB	2:B:260:HOH:O	2.56	0.53
1:C:156:THR:C	2:C:283:HOH:O	2.47	0.53
1:D:172:GLN:HA	1:D:172:GLN:OE1	2.08	0.53
1:D:146:ASN:ND2	2:D:314:HOH:O	2.42	0.52
1:E:176:VAL:O	1:E:178:LEU:HD12	2.09	0.52
1:C:131:GLU:O	1:C:132:GLU:HG2	2.07	0.52
1:D:130:ALA:HA	1:D:133:MET:CE	2.32	0.52
1:F:89:ILE:CD1	1:F:129:ASN:CB	2.88	0.52
1:B:164:ASP:OD2	1:C:64:HIS:CE1	2.62	0.52
1:A:56:ILE:HD11	1:C:51:LYS:HD2	1.91	0.52
1:A:42:GLN:HE21	1:C:173:ILE:CG1	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:LYS:CA	2:D:316:HOH:O	2.58	0.51
2:E:289:HOH:O	1:F:121:LYS:HE3	2.09	0.51
1:F:45:ILE:HA	2:F:287:HOH:O	2.09	0.51
1:E:103:GLU:HG3	1:E:110:LEU:HD12	1.92	0.51
1:C:131:GLU:HG2	1:C:132:GLU:N	2.25	0.51
1:A:173:ILE:HD12	2:B:234:HOH:O	2.09	0.51
1:E:48:ILE:HD11	1:F:45:ILE:HG23	1.92	0.51
1:A:160:ASP:CG	2:A:280:HOH:O	2.49	0.51
1:B:103:GLU:CD	1:B:110:LEU:HD12	2.31	0.51
1:F:81:GLU:HB3	2:F:261:HOH:O	2.10	0.51
1:D:45:ILE:O	1:D:48:ILE:HG12	2.11	0.50
1:E:165:GLU:H	1:F:60:ASN:HD21	1.58	0.50
1:D:45:ILE:HG13	1:F:173:ILE:HD11	1.94	0.50
1:C:145:ASP:O	1:C:149:ILE:HG13	2.11	0.50
1:C:132:GLU:HG2	1:C:138:PHE:HE1	1.77	0.50
1:A:51:LYS:HG2	1:B:52:LEU:HD21	1.92	0.50
1:B:155:GLY:O	1:B:156:THR:HB	2.11	0.50
1:B:173:ILE:HG13	1:C:42:GLN:HG3	1.94	0.50
1:A:74:GLU:O	1:A:78:GLN:HG2	2.11	0.50
1:B:109:ASP:HB3	1:B:112:ASP:OD1	2.12	0.49
1:F:108:ILE:CD1	1:F:115:MET:CE	2.90	0.49
1:C:108:ILE:HD12	1:C:115:MET:CE	2.43	0.49
1:F:89:ILE:HG13	1:F:129:ASN:CG	2.32	0.49
1:F:131:GLU:O	1:F:138:PHE:HA	2.12	0.49
1:A:45:ILE:HD11	1:C:45:ILE:CD1	2.43	0.49
1:D:177:GLU:O	1:F:180:SER:HB3	2.10	0.49
1:F:123:ARG:HG2	2:F:269:HOH:O	2.12	0.49
1:D:54:ARG:HD3	1:D:165:GLU:OE1	2.11	0.49
1:C:134:GLY:C	1:C:136:GLY:H	2.15	0.49
1:E:93:SER:HB2	1:E:140:ILE:HD11	1.95	0.49
1:D:68:LYS:CD	2:D:262:HOH:O	2.61	0.49
1:F:89:ILE:HG13	1:F:129:ASN:ND2	2.28	0.49
1:A:136:GLY:O	1:A:137:SER:HB2	2.13	0.49
1:F:131:GLU:HG3	1:F:133:MET:SD	2.53	0.48
1:A:167:LEU:HG	1:B:53:ASN:CG	2.33	0.48
1:C:131:GLU:O	1:C:138:PHE:CE1	2.67	0.48
1:F:44:ALA:C	2:F:287:HOH:O	2.50	0.48
1:C:131:GLU:OE2	1:C:139:LYS:N	2.42	0.48
1:F:130:ALA:HB2	1:F:140:ILE:HD13	1.96	0.48
1:E:130:ALA:HB2	2:E:249:HOH:O	2.12	0.48
1:F:153:ARG:CZ	1:F:153:ARG:HB2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:TYR:CE2	1:C:74:GLU:HG2	2.48	0.48
1:A:42:GLN:HA	1:C:173:ILE:HD12	1.94	0.48
1:E:39:LYS:HG3	2:E:196:HOH:O	2.13	0.48
1:E:34:GLN:NE2	1:E:175:GLY:HA3	2.28	0.48
1:A:51:LYS:HD2	1:A:168:ASN:HB2	1.95	0.47
1:B:92:TRP:CD2	1:B:125:GLN:HG3	2.49	0.47
1:F:51:LYS:HB3	2:F:322:HOH:O	2.13	0.47
1:F:45:ILE:HD13	2:F:287:HOH:O	2.13	0.47
1:F:153:ARG:NH2	2:F:324:HOH:O	2.47	0.47
1:A:120:GLU:OE2	1:A:123:ARG:HD3	2.15	0.47
1:E:151:SER:O	1:E:155:GLY:HA3	2.14	0.47
1:A:92:TRP:CE2	1:A:125:GLN:HG3	2.49	0.47
1:D:63:PHE:N	2:D:310:HOH:O	2.48	0.47
1:D:64:HIS:CE1	1:F:164:ASP:OD1	2.68	0.47
1:C:51:LYS:HG2	1:C:168:ASN:HB2	1.97	0.47
1:C:58:LYS:NZ	1:C:163:ARG:O	2.48	0.47
1:A:38:LEU:HA	1:C:36:ALA:HB2	1.96	0.47
1:E:142:HIS:CD2	2:E:274:HOH:O	2.67	0.47
1:A:164:ASP:OD1	1:B:64:HIS:CE1	2.67	0.47
1:D:177:GLU:CG	2:D:268:HOH:O	2.54	0.47
1:F:45:ILE:N	2:F:287:HOH:O	2.47	0.46
1:D:170:ARG:NH1	1:D:172:GLN:CD	2.69	0.46
1:A:74:GLU:HG2	1:C:157:TYR:CD2	2.50	0.46
1:B:108:ILE:CD1	1:B:115:MET:CE	2.92	0.46
1:A:173:ILE:HD11	1:B:45:ILE:HG13	1.97	0.46
1:C:172:GLN:O	1:C:173:ILE:HB	2.16	0.46
1:D:68:LYS:O	1:D:72:GLU:HG3	2.16	0.46
1:D:170:ARG:NH1	1:D:172:GLN:OE1	2.49	0.45
1:F:53:ASN:O	1:F:57:GLU:HG3	2.16	0.45
1:F:51:LYS:C	2:F:322:HOH:O	2.52	0.45
1:B:159:HIS:HE1	2:C:222:HOH:O	1.99	0.45
1:A:74:GLU:HG2	1:C:157:TYR:CE2	2.52	0.45
1:B:157:TYR:CD2	1:C:74:GLU:HG2	2.52	0.45
1:A:47:GLN:OE1	1:A:168:ASN:ND2	2.50	0.45
1:C:40:SER:OG	1:C:173:ILE:HA	2.16	0.45
1:E:167:LEU:HD22	1:F:53:ASN:HB3	1.99	0.45
1:A:56:ILE:CD1	1:C:51:LYS:HD2	2.46	0.45
1:F:82:LYS:HG2	1:F:143:LYS:NZ	2.31	0.45
1:B:145:ASP:O	1:B:148:CYS:HB3	2.17	0.45
1:D:74:GLU:HG2	1:F:157:TYR:CE2	2.52	0.45
1:F:47:GLN:HB3	1:F:47:GLN:HE21	1.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:GLU:C	1:C:134:GLY:N	2.70	0.45
1:E:145:ASP:O	1:E:148:CYS:HB3	2.17	0.45
1:F:129:ASN:O	1:F:129:ASN:ND2	2.50	0.44
1:B:92:TRP:CG	1:B:125:GLN:HG3	2.52	0.44
1:B:42:GLN:CB	2:B:234:HOH:O	2.55	0.44
1:D:152:ILE:O	2:D:324:HOH:O	2.21	0.44
1:E:109:ASP:C	1:E:111:THR:H	2.21	0.44
1:C:129:ASN:O	1:C:130:ALA:C	2.55	0.44
1:C:172:GLN:CG	1:C:173:ILE:H	2.31	0.44
1:E:133:MET:HB3	1:E:134:GLY:H	1.50	0.44
1:C:44:ALA:HB2	1:C:171:PHE:CD2	2.53	0.44
1:A:52:LEU:CA	2:A:292:HOH:O	2.48	0.44
1:F:89:ILE:HD11	1:F:129:ASN:CB	2.48	0.44
1:B:171:PHE:HE2	2:B:268:HOH:O	2.00	0.43
1:C:167:LEU:HD12	1:C:167:LEU:N	2.33	0.43
1:A:173:ILE:CD1	1:B:41:THR:HG22	2.48	0.43
1:C:172:GLN:HG3	1:C:173:ILE:H	1.84	0.43
1:A:142:HIS:HD2	2:A:235:HOH:O	2.00	0.43
1:B:93:SER:HB2	1:B:140:ILE:HD11	2.01	0.43
1:D:165:GLU:H	1:E:60:ASN:HD21	1.66	0.43
1:C:41:THR:O	1:C:45:ILE:HG12	2.19	0.43
1:F:172:GLN:NE2	2:F:331:HOH:O	2.51	0.43
1:D:129:ASN:OD1	1:D:131:GLU:HB3	2.18	0.43
1:C:131:GLU:CD	1:C:131:GLU:N	2.73	0.43
1:A:162:TYR:HE2	1:B:60:ASN:HD22	1.66	0.43
1:E:92:TRP:CD2	1:E:125:GLN:HG3	2.54	0.43
1:F:97:GLU:C	2:F:335:HOH:O	2.57	0.43
1:D:68:LYS:CE	2:D:262:HOH:O	2.61	0.43
1:F:123:ARG:O	1:F:127:ARG:HG3	2.19	0.42
1:C:171:PHE:CE2	1:C:172:GLN:HG3	2.54	0.42
1:C:54:ARG:NH1	1:C:165:GLU:CD	2.72	0.42
1:F:132:GLU:HG3	2:F:299:HOH:O	2.19	0.42
1:B:145:ASP:OD1	1:B:146:ASN:O	2.38	0.42
1:F:156:THR:CG2	1:F:157:TYR:H	2.29	0.42
1:E:167:LEU:HD21	1:F:57:GLU:CG	2.49	0.42
1:A:90:ASP:OD2	1:A:142:HIS:CE1	2.71	0.42
1:A:36:ALA:HB2	1:B:38:LEU:HA	2.02	0.42
1:F:45:ILE:CA	2:F:287:HOH:O	2.68	0.42
1:F:127:ARG:HG2	2:F:299:HOH:O	2.19	0.42
1:F:153:ARG:CZ	2:F:324:HOH:O	2.68	0.42
1:B:108:ILE:CD1	1:B:115:MET:HE1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:GLU:OE2	1:B:159:HIS:CD2	2.67	0.42
1:B:150:GLU:O	1:B:154:ASN:CB	2.67	0.42
1:A:136:GLY:C	1:A:138:PHE:H	2.23	0.42
1:B:172:GLN:HA	1:C:42:GLN:NE2	2.35	0.41
1:D:178:LEU:HD22	1:E:176:VAL:HG11	2.02	0.41
1:F:170:ARG:NH1	1:F:172:GLN:HG2	2.35	0.41
1:B:108:ILE:HD13	1:B:115:MET:HE1	2.02	0.41
1:D:124:ARG:HH11	1:D:124:ARG:CB	2.33	0.41
1:F:49:ASN:HA	2:F:266:HOH:O	2.20	0.41
1:F:85:GLU:O	1:F:89:ILE:HG12	2.20	0.41
1:A:35:ALA:HA	1:B:36:ALA:O	2.20	0.41
1:D:175:GLY:HA3	1:E:38:LEU:HD22	2.03	0.41
1:C:45:ILE:HD13	1:C:45:ILE:HA	1.89	0.41
1:F:132:GLU:HA	1:F:137:SER:O	2.20	0.41
1:E:133:MET:HB3	1:E:141:TYR:CE2	2.55	0.41
1:E:173:ILE:HD11	1:F:45:ILE:HG13	2.03	0.41
1:A:51:LYS:NZ	2:A:293:HOH:O	2.55	0.40
1:B:40:SER:O	1:B:43:ALA:HB3	2.20	0.40
1:B:51:LYS:CG	1:C:52:LEU:HD21	2.52	0.40
1:B:85:GLU:CD	2:B:220:HOH:O	2.58	0.40
1:B:45:ILE:HD11	1:C:45:ILE:HD11	2.04	0.40
1:A:77:ILE:O	1:A:81:GLU:HG3	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	129/155 (83%)	123 (95%)	5 (4%)	1 (1%)	24	11
1	B	142/155 (92%)	138 (97%)	1 (1%)	3 (2%)	9	1
1	C	148/155 (96%)	138 (93%)	6 (4%)	4 (3%)	6	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	144/155 (93%)	144 (100%)	0	0	100	100
1	E	144/155 (93%)	134 (93%)	6 (4%)	4 (3%)	6	1
1	F	153/155 (99%)	148 (97%)	5 (3%)	0	100	100
All	All	860/930 (92%)	825 (96%)	23 (3%)	12 (1%)	14	4

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	147	ALA
1	C	130	ALA
1	C	133	MET
1	E	139	LYS
1	A	35	ALA
1	B	34	GLN
1	E	133	MET
1	E	147	ALA
1	B	174	LYS
1	C	135	ASN
1	C	173	ILE
1	E	140	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	120/137 (88%)	117 (98%)	3 (2%)	55	47
1	B	128/137 (93%)	123 (96%)	5 (4%)	39	27
1	C	135/137 (98%)	129 (96%)	6 (4%)	35	22
1	D	130/137 (95%)	128 (98%)	2 (2%)	72	69
1	E	130/137 (95%)	129 (99%)	1 (1%)	86	86
1	F	137/137 (100%)	133 (97%)	4 (3%)	50	40
All	All	780/822 (95%)	759 (97%)	21 (3%)	52	43

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	104	ASN
1	A	167	LEU
1	B	47	GLN
1	B	105	GLN
1	B	112	ASP
1	B	113	SER
1	B	153	ARG
1	C	42	GLN
1	C	65	GLN
1	C	103	GLU
1	C	127	ARG
1	C	131	GLU
1	C	172	GLN
1	D	47	GLN
1	D	123	ARG
1	E	133	MET
1	F	47	GLN
1	F	142	HIS
1	F	167	LEU
1	F	179	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	78	GLN
1	A	142	HIS
1	A	159	HIS
1	B	47	GLN
1	B	60	ASN
1	B	64	HIS
1	B	95	ASN
1	B	105	GLN
1	B	135	ASN
1	B	154	ASN
1	B	159	HIS
1	C	42	GLN
1	C	60	ASN
1	C	64	HIS
1	C	95	ASN

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Mol	Chain	Res	Type
1	C	104	ASN
1	C	129	ASN
1	C	159	HIS
1	D	47	GLN
1	D	64	HIS
1	D	78	GLN
1	D	105	GLN
1	D	125	GLN
1	D	142	HIS
1	D	154	ASN
1	D	168	ASN
1	E	34	GLN
1	E	60	ASN
1	F	60	ASN
1	F	64	HIS
1	F	129	ASN
1	F	142	HIS

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	133/155 (85%)	0.53	13 (9%)	10	11	16, 37, 68, 76	5 (3%)
1	B	144/155 (92%)	0.79	18 (12%)	5	5	17, 39, 79, 95	4 (2%)
1	C	150/155 (96%)	0.67	19 (12%)	5	5	20, 44, 84, 100	9 (6%)
1	D	146/155 (94%)	0.34	9 (6%)	24	27	16, 33, 56, 73	1 (0%)
1	E	146/155 (94%)	0.63	18 (12%)	5	6	17, 34, 85, 110	7 (4%)
1	F	155/155 (100%)	0.18	6 (3%)	43	47	18, 36, 72, 103	2 (1%)
All	All	874/930 (93%)	0.52	83 (9%)	10	12	16, 37, 76, 110	28 (3%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	176	VAL	18.3
1	C	134	GLY	15.2
1	E	137	SER	12.9
1	C	133	MET	12.9
1	E	178	LEU	10.4
1	E	134	GLY	9.8
1	B	135	ASN	9.5
1	E	136	GLY	8.7
1	B	33	GLY	7.4
1	F	133	MET	6.9
1	E	135	ASN	6.5
1	B	175	GLY	6.4
1	E	138	PHE	6.4
1	E	133	MET	5.9
1	E	177	GLU	5.5
1	D	33	GLY	5.5
1	C	135	ASN	5.2
1	B	133	MET	5.1
1	A	35	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	132	GLU	4.4
1	E	39	LYS	4.4
1	E	176	VAL	4.4
1	C	137	SER	4.3
1	B	34	GLN	4.3
1	C	131	GLU	4.2
1	F	129	ASN	4.1
1	C	136	GLY	4.0
1	C	173	ILE	4.0
1	B	134	GLY	3.9
1	C	175	GLY	3.7
1	C	130	ALA	3.6
1	A	175	GLY	3.6
1	A	171	PHE	3.6
1	E	141	TYR	3.4
1	B	137	SER	3.4
1	B	174	LYS	3.3
1	F	180	SER	3.3
1	A	40	SER	3.3
1	A	174	LYS	3.2
1	E	109	ASP	3.1
1	A	146	ASN	3.1
1	D	163	ARG	3.0
1	F	134	GLY	3.0
1	B	41	THR	3.0
1	B	136	GLY	2.9
1	D	91	LEU	2.9
1	D	127	ARG	2.9
1	B	111	THR	2.8
1	D	89	ILE	2.8
1	B	35	ALA	2.8
1	A	36	ALA	2.7
1	B	38	LEU	2.7
1	C	167	LEU	2.7
1	D	178	LEU	2.7
1	A	172	GLN	2.7
1	D	130	ALA	2.6
1	B	36	ALA	2.6
1	A	173	ILE	2.6
1	C	179	LYS	2.6
1	A	169	ASN	2.4
1	B	39	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	156	THR	2.4
1	E	33	GLY	2.4
1	A	37	ASP	2.3
1	A	91	LEU	2.3
1	C	176	VAL	2.3
1	B	171	PHE	2.3
1	F	39	LYS	2.3
1	B	91	LEU	2.2
1	C	38	LEU	2.2
1	E	131	GLU	2.2
1	C	43	ALA	2.2
1	E	112	ASP	2.2
1	E	110	LEU	2.2
1	C	166	ALA	2.2
1	E	132	GLU	2.2
1	C	36	ALA	2.1
1	E	130	ALA	2.1
1	D	98	LEU	2.1
1	F	135	ASN	2.1
1	A	61	GLU	2.1
1	C	138	PHE	2.0
1	C	174	LYS	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.