



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:53 AM UTC

PDB ID : 1QU1 / pdb_00001qu1
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)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

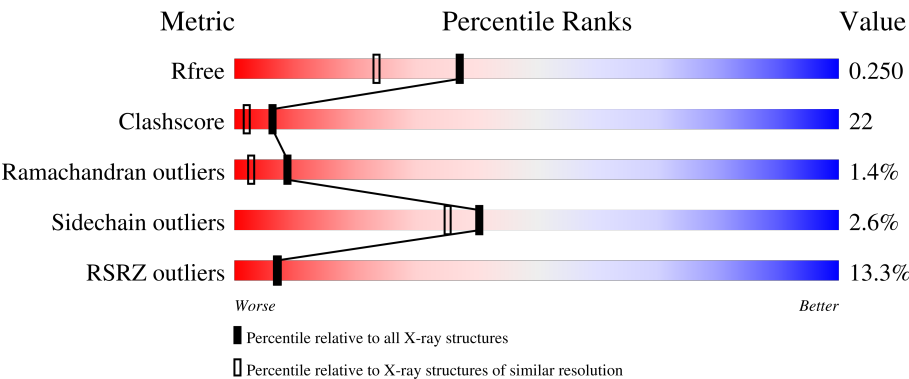
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	155	15% 58%25%14%
1	B	155	17% 58%33%7%
1	C	155	18% 65%26%6%
1	D	155	5% 69%24%6%
1	E	155	13% 70%21%6%

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Mol	Chain	Length	Quality of chain
1	F	155	6% 65% 34%

2 Entry composition

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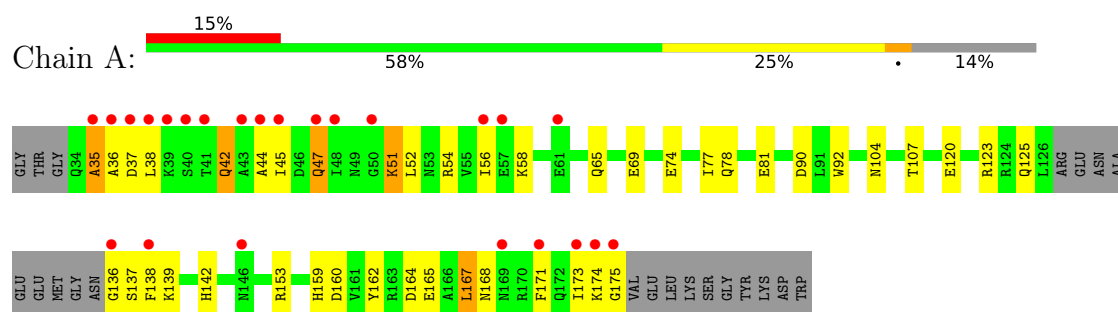
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	162	Total 162	O 162	0	0
2	E	110	Total 110	O 110	0	0
2	F	150	Total 150	O 150	0	0

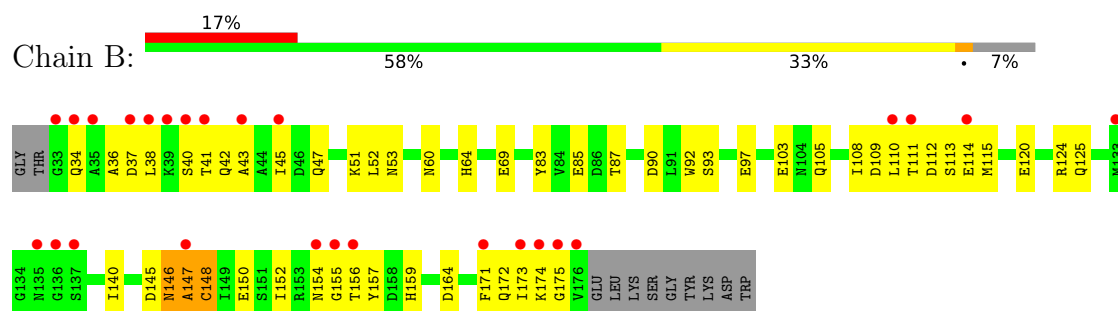
3 Residue-property plots [i](#)

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.

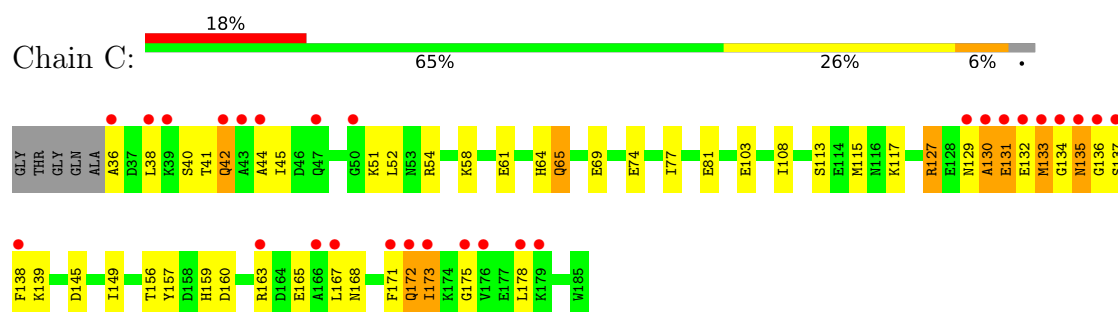
- Molecule 1: PROTEIN (INFLUENZA RECOMBINANT HA2 CHAIN)



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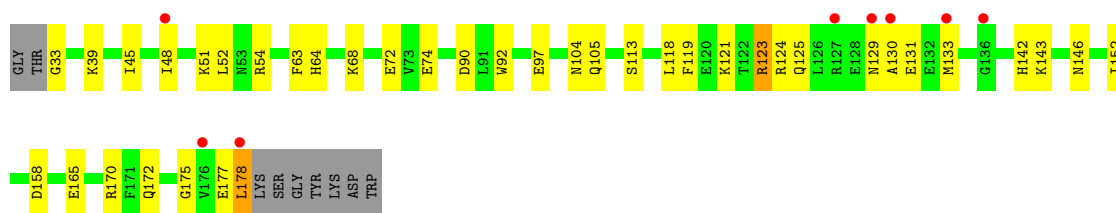


- Molecule 1: PROTEIN (INFLUENZA RECOMBINANT HA2 CHAIN)

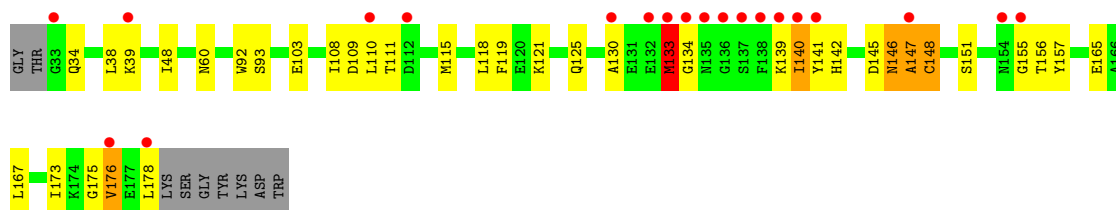


- Molecule 1: PROTEIN (INFLUENZA RECOMBINANT HA2 CHAIN)

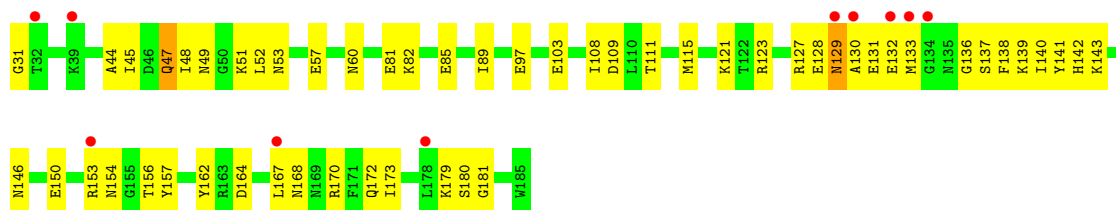




● Molecule 1: PROTEIN (INFLUENZA RECOMBINANT HA2 CHAIN)



● Molecule 1: PROTEIN (INFLUENZA RECOMBINANT HA2 CHAIN)



4 Data and refinement statistics

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 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.3 (20.00-1.90) 95.2 (20.00-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 1.91Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.229 , 0.250 0.229 , 0.250	Depositor DCC
R_{free} test set	5549 reflections (6.22%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.798	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.49	0/1110	0.87	2/1489 (0.1%)
1	B	0.50	0/1193	0.92	2/1601 (0.1%)
1	C	0.50	0/1258	0.94	2/1687 (0.1%)
1	D	0.52	0/1210	0.89	1/1624 (0.1%)
1	E	0.49	0/1210	0.92	3/1624 (0.2%)
1	F	0.59	0/1287	0.92	4/1726 (0.2%)
All	All	0.52	0/7268	0.91	14/9751 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	178	LEU	N-CA-C	-7.66	99.70	110.50
1	E	148	CYS	N-CA-C	-7.51	103.10	111.28
1	D	113	SER	N-CA-C	7.43	120.09	111.02
1	B	146	ASN	N-CA-C	-6.90	100.97	110.35
1	E	146	ASN	N-CA-C	-6.86	101.03	110.35
1	B	148	CYS	N-CA-C	-6.59	104.09	111.28
1	C	113	SER	N-CA-C	5.76	118.02	111.11
1	F	111	THR	N-CA-C	-5.69	106.34	113.28
1	F	129	ASN	N-CA-C	5.65	121.06	113.72
1	A	107	THR	N-CA-C	-5.64	106.53	113.41
1	F	181	GLY	N-CA-C	-5.64	102.89	110.56
1	A	174	LYS	N-CA-C	5.27	116.72	110.97
1	E	176	VAL	N-CA-C	5.20	116.11	109.30
1	F	128	GLU	N-CA-C	5.03	116.45	111.07

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	62	0
1	C	1240	0	1194	80	0
1	D	1195	0	1153	58	0
1	E	1195	0	1153	40	0
1	F	1269	0	1220	71	0
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	20	0
2	E	110	0	0	8	0
2	F	150	0	0	37	0
All	All	7907	0	6919	305	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 (305) 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:B:108:ILE:HD12	1:B:115:MET:HE2	1.45	0.97
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:C:131:GLU:C	1:C:132:GLU:HG3	1.89	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:108:ILE:HD12	1:C:115:MET:HE2	1.50	0.92
1:C:131:GLU:O	1:C:132:GLU:HG3	1.70	0.92
1:C:156:THR:HG23	2:C:283:HOH:O	1.71	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:108:ILE:CD1	1:B:115:MET:HE2	2.10	0.82
1:D:130:ALA:HA	1:D:133:MET:HE2	1.59	0.82
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: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:C:65:GLN:HG2	1:C:160:ASP:HB2	1.67	0.77
1:D:33:GLY:HA2	2:E:269:HOH:O	1.83	0.77
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:F:108:ILE:HD12	1:F:115:MET:HE2	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:119:PHE:CE1	1:D:133:MET:HE1	2.31	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:170:ARG:HH12	1:D:172:GLN:CD	2.05	0.64
1:B:36:ALA:HA	1:C:38:LEU:HD13	1.80	0.64
1:D:68:LYS:HE3	2:D:262:HOH:O	1.96	0.64
1:E:140:ILE:N	2:E:231:HOH:O	2.31	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:A:47:GLN:CD	1:A:168:ASN:HD21	2.07	0.62
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:69:GLU:OE2	1:B:159:HIS:HD2	1.82	0.62
1:F:129:ASN:HB2	2:F:257:HOH:O	2.00	0.62
1:B:108:ILE:HD12	1:B:115:MET:CE	2.27	0.62
1:A:54:ARG:O	1:A:58:LYS:HG3	1.99	0.61
1:C:129:ASN:CG	1:C:130:ALA:H	2.08	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:D:39:LYS:NZ	2:D:334:HOH:O	2.33	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:B:97:GLU:CD	2:B:261:HOH:O	2.44	0.59
1:B:37:ASP:HB3	2:B:260:HOH:O	2.01	0.59
1:A:90:ASP:OD2	1:A:142:HIS:HE1	1.86	0.59
1:D:118:LEU:CG	2:F:335:HOH:O	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:108:ILE:CD1	1:C:115:MET:HE2	2.26	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:B:164:ASP:OD2	1:C:64:HIS:HE1	1.85	0.58
1:E:156:THR:HG21	2:E:279:HOH:O	2.02	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: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:C:156:THR:C	2:C:283:HOH:O	2.47	0.57
1:A:165:GLU:H	1:B:60:ASN:HD21	1.51	0.57
1:B:103:GLU:OE1	1:B:110:LEU:HD12	2.05	0.57
1:C:127:ARG:CG	1:C:132:GLU:OE2	2.42	0.57
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: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:D:130:ALA:HA	1:D:133:MET:CE	2.32	0.56
1:A:160:ASP:CG	2:A:280:HOH:O	2.49	0.56
1:B:103:GLU:CD	1:B:110:LEU:HD12	2.31	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:C:54:ARG:NH1	1:C:165:GLU:OE2	2.40	0.55
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: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:E:110:LEU:HD22	1:E:119:PHE:HB2	1.89	0.55
1:F:108:ILE:CD1	1:F:115:MET:HE2	2.36	0.54
1:E:145:ASP:OD1	1:E:146:ASN:O	2.26	0.54
1:A:44:ALA:HB2	1:A:171:PHE:CD2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:162:TYR:HB3	2:F:330:HOH:O	2.08	0.54
1:F:89:ILE:HG13	1:F:129:ASN:CG	2.32	0.54
1:D:97:GLU:HG2	1:E:118:LEU:HD21	1.90	0.54
1:B:150:GLU:O	1:B:154:ASN:HB2	2.08	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:C:134:GLY:C	1:C:136:GLY:H	2.15	0.54
1:F:180:SER:HB3	2:F:314:HOH:O	2.07	0.54
1:A:167:LEU:HG	1:B:53:ASN:CG	2.33	0.53
1:F:153:ARG:NE	2:F:324:HOH:O	2.41	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:D:92:TRP:CD1	1:D:125:GLN:HG2	2.44	0.53
1:F:44:ALA:C	2:F:287:HOH:O	2.50	0.53
1:D:146:ASN:ND2	2:D:314:HOH:O	2.42	0.52
1:D:172:GLN:OE1	1:D:172:GLN:HA	2.08	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:B:164:ASP:OD2	1:C:64:HIS:CE1	2.62	0.52
1:F:89:ILE:CD1	1:F:129:ASN:CB	2.88	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
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:E:103:GLU:HG3	1:E:110:LEU:HD12	1.92	0.51
1:F:45:ILE:HA	2:F:287:HOH:O	2.09	0.51
1:F:51:LYS:C	2:F:322:HOH:O	2.52	0.51
1:A:173:ILE:HD12	2:B:234:HOH:O	2.09	0.51
1:C:131:GLU:HG2	1:C:132:GLU:N	2.25	0.51
1:E:48:ILE:HD11	1:F:45:ILE:HG23	1.92	0.51
1:F:81:GLU:HB3	2:F:261:HOH:O	2.10	0.51
1:D:170:ARG:NH1	1:D:172:GLN:CD	2.69	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:C:145:ASP:O	1:C:149:ILE:HG13	2.11	0.50
1:D:45:ILE:HG13	1:F:173:ILE:HD11	1.94	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:C:132:GLU:HG2	1:C:138:PHE:HE1	1.77	0.50
1:A:74:GLU:O	1:A:78:GLN:HG2	2.11	0.50
1:B:173:ILE:HG13	1:C:42:GLN:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:133:MET:HE3	1:E:141:TYR:OH	2.12	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:132:GLU:C	1:C:134:GLY:N	2.70	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:E:109:ASP:C	1:E:111:THR:H	2.21	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:E:93:SER:HB2	1:E:140:ILE:HD11	1.95	0.49
1:A:136:GLY:O	1:A:137:SER:HB2	2.13	0.49
1:C:129:ASN:O	1:C:130:ALA:C	2.55	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:F:131:GLU:HG3	1:F:133:MET:SD	2.53	0.48
1:C:131:GLU:O	1:C:138:PHE:CE1	2.67	0.48
1:D:119:PHE:CZ	1:D:133:MET:HE1	2.49	0.48
1:C:131:GLU:OE2	1:C:139:LYS:N	2.42	0.48
1:E:130:ALA:HB2	2:E:249:HOH:O	2.12	0.48
1:F:130:ALA:HB2	1:F:140:ILE:HD13	1.96	0.48
1:F:153:ARG:HB2	1:F:153:ARG:CZ	2.43	0.48
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:A:92:TRP:CE2	1:A:125:GLN:HG3	2.49	0.47
1:A:120:GLU:OE2	1:A:123:ARG:HD3	2.15	0.47
1:C:54:ARG:NH1	1:C:165:GLU:CD	2.72	0.47
1:C:131:GLU:CD	1:C:131:GLU:N	2.73	0.47
1:E:151:SER:O	1:E:155:GLY:HA3	2.14	0.47
1:F:153:ARG:NH2	2:F:324:HOH:O	2.47	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: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:E:115:MET:HE3	1:E:115:MET:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:LEU:HA	1:C:36:ALA:HB2	1.96	0.47
1:A:164:ASP:OD1	1:B:64:HIS:CE1	2.67	0.47
1:E:142:HIS:CD2	2:E:274:HOH:O	2.67	0.47
1:F:97:GLU:C	2:F:335:HOH:O	2.57	0.47
1:D:177:GLU:CG	2:D:268:HOH:O	2.54	0.47
1:A:136:GLY:C	1:A:138:PHE:H	2.23	0.46
1:F:45:ILE:N	2:F:287:HOH:O	2.47	0.46
1:A:74:GLU:HG2	1:C:157:TYR:CD2	2.50	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:B:85:GLU:CD	2:B:220:HOH:O	2.58	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:A:56:ILE:CD1	1:C:51:LYS:HD2	2.46	0.45
1:C:40:SER:OG	1:C:173:ILE:HA	2.16	0.45
1:E:121:LYS:NZ	2:E:278:HOH:O	2.36	0.45
1:E:167:LEU:HD22	1:F:53:ASN:HB3	1.99	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:HE21	1:F:47:GLN:HB3	1.59	0.45
1:E:145:ASP:O	1:E:148:CYS:HB3	2.17	0.45
1:B:92:TRP:CG	1:B:125:GLN:HG3	2.52	0.44
1:F:129:ASN:ND2	1:F:129:ASN:O	2.50	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: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:N	1:C:167:LEU:HD12	2.33	0.43
1:A:173:ILE:CD1	1:B:41:THR:HG22	2.48	0.43
1:A:142:HIS:HD2	2:A:235:HOH:O	2.00	0.43
1:C:172:GLN:HG3	1:C:173:ILE:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:SER:HB2	1:B:140:ILE:HD11	2.01	0.43
1:C:41:THR:O	1:C:45:ILE:HG12	2.19	0.43
1:D:165:GLU:H	1:E:60:ASN:HD21	1.66	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: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: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:132:GLU:O	1:C:133:MET:C	2.63	0.42
1:C:171:PHE:CE2	1:C:172:GLN:HG3	2.54	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:E:167:LEU:HD21	1:F:57:GLU:CG	2.49	0.42
1:F:156:THR:CG2	1:F:157:TYR:H	2.29	0.42
1:A:90:ASP:OD2	1:A:142:HIS:CE1	2.71	0.42
1:E:115:MET:HE3	1:E:115:MET:CA	2.49	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:69:GLU:OE2	1:B:159:HIS:CD2	2.67	0.42
1:C:132:GLU:C	1:C:134:GLY:H	2.27	0.42
1:B:150:GLU:O	1:B:154:ASN:CB	2.67	0.42
1:B:171:PHE:CD1	1:B:171:PHE:C	2.98	0.41
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:D:124:ARG:CB	1:D:124:ARG:HH11	2.33	0.41
1:F:49:ASN:HA	2:F:266:HOH:O	2.20	0.41
1:C:129:ASN:CG	1:C:130:ALA:N	2.76	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:F:85:GLU:O	1:F:89:ILE:HG12	2.20	0.41
1:C:45:ILE:HD13	1:C:45:ILE:HA	1.89	0.41
1:E:133:MET:HB3	1:E:141:TYR:CE2	2.55	0.41
1:F:132:GLU:HA	1:F:137:SER:O	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ILE:HD11	1:C:45:ILE:HD11	2.04	0.40
1:F:129:ASN:CG	1:F:129:ASN:O	2.63	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%)	16	8
1	B	142/155 (92%)	138 (97%)	1 (1%)	3 (2%)	5	1
1	C	148/155 (96%)	138 (93%)	6 (4%)	4 (3%)	4	1
1	D	144/155 (93%)	144 (100%)	0	0	100	100
1	E	144/155 (93%)	134 (93%)	6 (4%)	4 (3%)	4	0
1	F	153/155 (99%)	148 (97%)	5 (3%)	0	100	100
All	All	860/930 (92%)	825 (96%)	23 (3%)	12 (1%)	9	3

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

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Mol	Chain	Res	Type
1	C	135	ASN
1	C	173	ILE
1	E	140	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	120/137 (88%)	115 (96%)	5 (4%)	26	19
1	B	128/137 (93%)	125 (98%)	3 (2%)	44	40
1	C	135/137 (98%)	129 (96%)	6 (4%)	25	17
1	D	130/137 (95%)	128 (98%)	2 (2%)	57	56
1	E	130/137 (95%)	129 (99%)	1 (1%)	73	75
1	F	137/137 (100%)	134 (98%)	3 (2%)	45	42
All	All	780/822 (95%)	760 (97%)	20 (3%)	40	35

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	47	GLN
1	A	51	LYS
1	A	104	ASN
1	A	167	LEU
1	B	47	GLN
1	B	105	GLN
1	B	113	SER
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	123	ARG

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Mol	Chain	Res	Type
1	D	178	LEU
1	E	133	MET
1	F	47	GLN
1	F	142	HIS
1	F	167	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	142	HIS
1	A	159	HIS
1	A	168	ASN
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
1	C	104	ASN
1	C	129	ASN
1	C	146	ASN
1	C	159	HIS
1	D	34	GLN
1	D	64	HIS
1	D	78	GLN
1	D	105	GLN
1	D	116	ASN
1	D	142	HIS
1	D	154	ASN
1	E	34	GLN
1	E	60	ASN
1	F	60	ASN
1	F	64	HIS
1	F	65	GLN
1	F	106	HIS

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Mol	Chain	Res	Type
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 oligosaccharides 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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	133/155 (85%)	0.77	24 (18%)	3 3	13, 36, 68, 76	5 (3%)
1	B	144/155 (92%)	0.88	26 (18%)	3 3	16, 38, 79, 95	4 (2%)
1	C	150/155 (96%)	1.07	28 (18%)	3 3	15, 41, 84, 100	9 (6%)
1	D	146/155 (94%)	0.40	8 (5%)	30 32	16, 33, 56, 73	1 (0%)
1	E	146/155 (94%)	0.71	20 (13%)	6 7	9, 34, 80, 110	7 (4%)
1	F	155/155 (100%)	0.61	10 (6%)	25 26	15, 36, 72, 103	2 (1%)
All	All	874/930 (93%)	0.74	116 (13%)	7 7	9, 36, 75, 110	28 (3%)

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	134	GLY	8.8
1	C	133	MET	5.4
1	B	33	GLY	5.2
1	B	176	VAL	5.2
1	F	129	ASN	4.7
1	D	130	ALA	4.7
1	E	33	GLY	4.7
1	E	39	LYS	4.6
1	E	141	TYR	4.5
1	E	138	PHE	4.4
1	E	136	GLY	4.4
1	B	155	GLY	4.3
1	B	135	ASN	4.2
1	B	35	ALA	4.1
1	B	175	GLY	4.0
1	A	38	LEU	4.0
1	A	175	GLY	4.0
1	E	176	VAL	3.9
1	A	146	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	132	GLU	3.9
1	C	173	ILE	3.8
1	C	137	SER	3.7
1	E	178	LEU	3.7
1	E	137	SER	3.7
1	F	134	GLY	3.7
1	A	136	GLY	3.7
1	E	130	ALA	3.6
1	C	136	GLY	3.5
1	E	134	GLY	3.5
1	C	176	VAL	3.5
1	A	44	ALA	3.5
1	D	136	GLY	3.4
1	B	110	LEU	3.4
1	A	50	GLY	3.3
1	A	35	ALA	3.3
1	C	43	ALA	3.3
1	F	133	MET	3.3
1	E	154	ASN	3.3
1	E	140	ILE	3.2
1	C	167	LEU	3.2
1	A	43	ALA	3.2
1	A	40	SER	3.1
1	A	41	THR	3.1
1	F	130	ALA	3.1
1	B	136	GLY	3.1
1	E	139	LYS	3.0
1	E	135	ASN	3.0
1	D	133	MET	2.9
1	B	154	ASN	2.9
1	E	133	MET	2.9
1	C	36	ALA	2.9
1	C	130	ALA	2.9
1	F	39	LYS	2.9
1	A	48	ILE	2.9
1	C	178	LEU	2.9
1	C	138	PHE	2.9
1	B	133	MET	2.9
1	A	45	ILE	2.9
1	C	39	LYS	2.8
1	F	32	THR	2.8
1	E	112	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	47	GLN	2.8
1	A	173	ILE	2.8
1	A	174	LYS	2.8
1	B	43	ALA	2.8
1	C	171	PHE	2.7
1	C	50	GLY	2.7
1	D	48	ILE	2.7
1	C	163	ARG	2.7
1	A	36	ALA	2.7
1	A	47	GLN	2.7
1	B	34	GLN	2.7
1	A	39	LYS	2.7
1	E	155	GLY	2.7
1	B	41	THR	2.7
1	C	135	ASN	2.7
1	B	171	PHE	2.6
1	D	127	ARG	2.6
1	D	176	VAL	2.6
1	B	137	SER	2.6
1	A	57	GLU	2.5
1	C	129	ASN	2.5
1	C	172	GLN	2.5
1	C	131	GLU	2.4
1	C	166	ALA	2.4
1	B	38	LEU	2.4
1	E	147	ALA	2.4
1	B	39	LYS	2.4
1	B	111	THR	2.4
1	D	129	ASN	2.4
1	F	153	ARG	2.3
1	B	156	THR	2.3
1	A	169	ASN	2.3
1	A	61	GLU	2.3
1	A	56	ILE	2.3
1	F	132	GLU	2.3
1	E	110	LEU	2.3
1	A	37	ASP	2.3
1	C	38	LEU	2.3
1	B	40	SER	2.2
1	B	114	GLU	2.2
1	B	45	ILE	2.2
1	A	138	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	132	GLU	2.2
1	C	175	GLY	2.2
1	B	173	ILE	2.1
1	C	42	GLN	2.1
1	F	178	LEU	2.1
1	B	174	LYS	2.1
1	B	37	ASP	2.1
1	C	179	LYS	2.1
1	D	178	LEU	2.1
1	F	167	LEU	2.1
1	A	171	PHE	2.0
1	B	147	ALA	2.0
1	C	44	ALA	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.