



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 02:10 am BST

PDB ID : 4LO7
Title : HA70(D3)-HA17-HA33
Authors : Lee, K.; Gu, S.; Jin, L.; Le, T.T.; Cheng, L.W.; Strotmeier, J.; Kruel, A.M.; Yao, G.; Perry, K.; Rummel, A.; Jin, R.
Deposited on : 2013-07-12
Resolution : 3.73 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

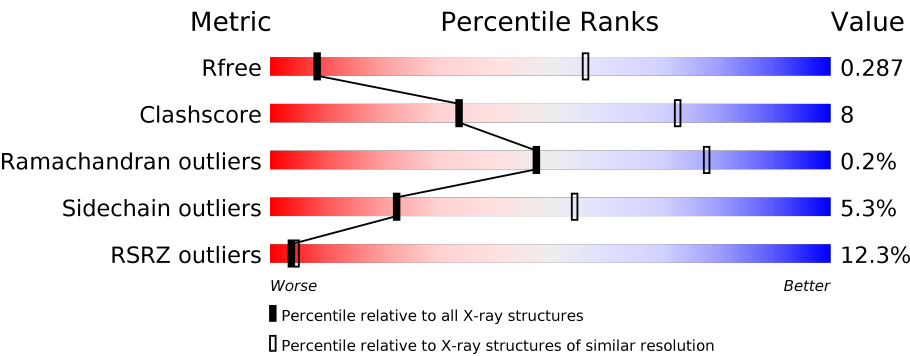
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.73 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	1001 (3.90-3.58)
Clashscore	141614	1063 (3.90-3.58)
Ramachandran outliers	138981	1027 (3.90-3.58)
Sidechain outliers	138945	1023 (3.90-3.58)
RSRZ outliers	127900	1006 (3.92-3.56)

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 $\leq 5\%$. 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	254	<div><div>14%</div><div><div></div><div></div><div></div><div></div></div><div>72%15%•10%</div></div>
1	E	254	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>76%13%•10%</div></div>
2	B	296	<div><div>5%</div><div><div></div><div></div><div></div><div></div></div><div>84%11%••</div></div>
2	D	296	<div><div>22%</div><div><div></div><div></div><div></div><div></div></div><div>78%16%••</div></div>
2	F	296	<div><div>11%</div><div><div></div><div></div><div></div><div></div></div><div>85%10%••</div></div>
2	H	296	<div><div>23%</div><div><div></div><div></div><div></div><div></div></div><div>76%18%••</div></div>

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Mol	Chain	Length	Quality of chain
3	C	147	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>79%</div><div>15%</div><div>• 5%</div></div></div>
3	G	147	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>80%</div><div>14%</div><div>• 5%</div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15326 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 HA-70.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	12	0	0
			1852	1171	315	365	1			
1	E	229	Total	C	N	O	S	12	0	0
			1860	1177	316	366	1			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	373	GLY	-	EXPRESSION TAG	UNP Q8KHU9
A	374	PRO	-	EXPRESSION TAG	UNP Q8KHU9
A	375	LEU	-	EXPRESSION TAG	UNP Q8KHU9
A	376	GLY	-	EXPRESSION TAG	UNP Q8KHU9
A	377	SER	-	EXPRESSION TAG	UNP Q8KHU9
E	373	GLY	-	EXPRESSION TAG	UNP Q8KHU9
E	374	PRO	-	EXPRESSION TAG	UNP Q8KHU9
E	375	LEU	-	EXPRESSION TAG	UNP Q8KHU9
E	376	GLY	-	EXPRESSION TAG	UNP Q8KHU9
E	377	SER	-	EXPRESSION TAG	UNP Q8KHU9

- Molecule 2 is a protein called HA-33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	286	Total	C	N	O	S	0	1	0
			2334	1477	399	455	3			
2	D	286	Total	C	N	O	S	0	1	0
			2334	1477	399	455	3			
2	F	286	Total	C	N	O	S	0	1	0
			2334	1477	399	455	3			
2	H	286	Total	C	N	O	S	0	1	0
			2334	1477	399	455	3			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	294	PRO	-	EXPRESSION TAG	UNP Q45871
B	295	GLY	-	EXPRESSION TAG	UNP Q45871
B	296	SER	-	EXPRESSION TAG	UNP Q45871
B	297	ALA	-	EXPRESSION TAG	UNP Q45871
D	294	PRO	-	EXPRESSION TAG	UNP Q45871
D	295	GLY	-	EXPRESSION TAG	UNP Q45871
D	296	SER	-	EXPRESSION TAG	UNP Q45871
D	297	ALA	-	EXPRESSION TAG	UNP Q45871
F	294	PRO	-	EXPRESSION TAG	UNP Q45871
F	295	GLY	-	EXPRESSION TAG	UNP Q45871
F	296	SER	-	EXPRESSION TAG	UNP Q45871
F	297	ALA	-	EXPRESSION TAG	UNP Q45871
H	294	PRO	-	EXPRESSION TAG	UNP Q45871
H	295	GLY	-	EXPRESSION TAG	UNP Q45871
H	296	SER	-	EXPRESSION TAG	UNP Q45871
H	297	ALA	-	EXPRESSION TAG	UNP Q45871

- Molecule 3 is a protein called HA-17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	139	Total	C	N	O	S	0	0	0
			1139	735	181	218	5			
3	G	139	Total	C	N	O	S	0	0	0
			1139	735	181	218	5			

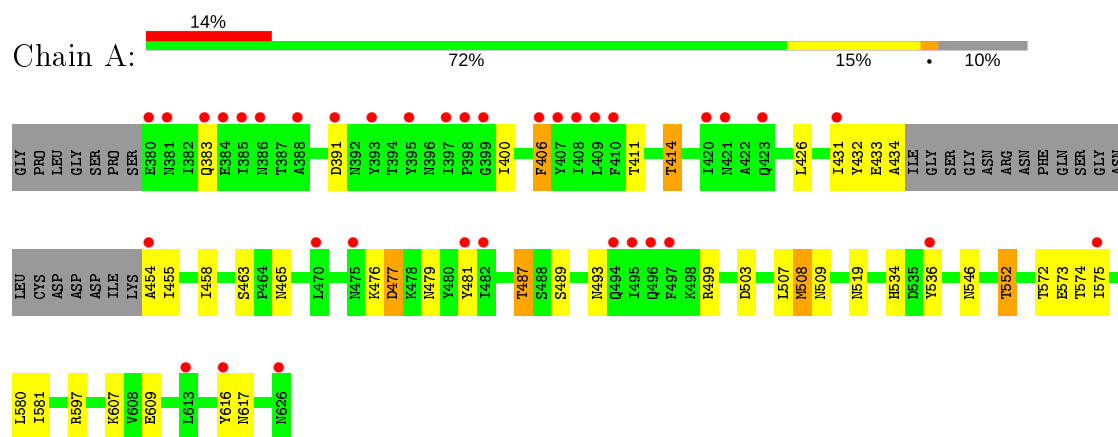
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	GLY	-	EXPRESSION TAG	UNP Q45878
C	1	PRO	-	EXPRESSION TAG	UNP Q45878
G	0	GLY	-	EXPRESSION TAG	UNP Q45878
G	1	PRO	-	EXPRESSION TAG	UNP Q45878

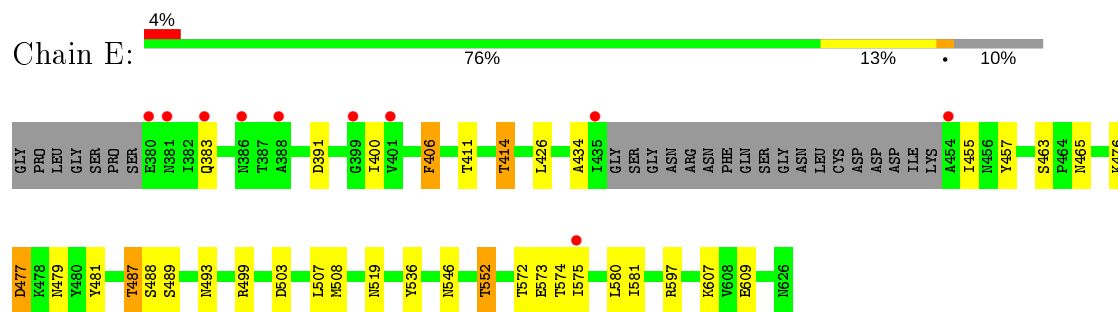
3 Residue-property plots [i](#)

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.

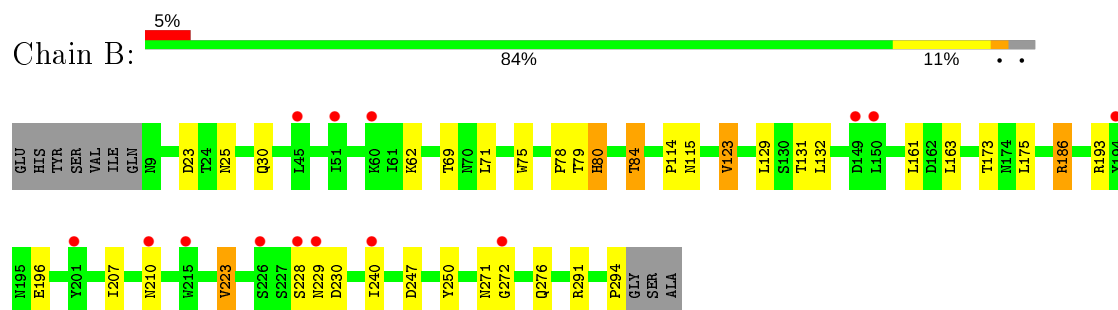
• Molecule 1: HA-70



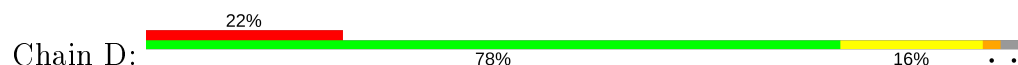
• Molecule 1: HA-70

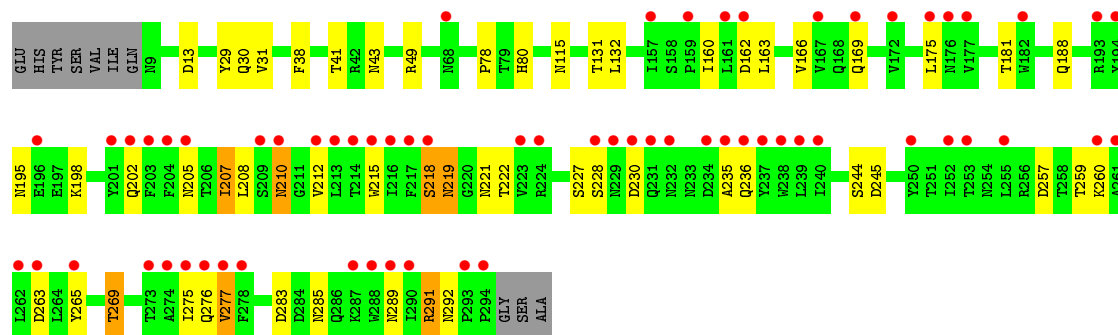


• Molecule 2: HA-33

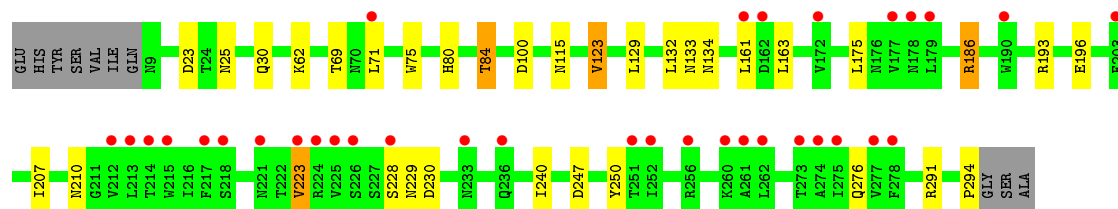
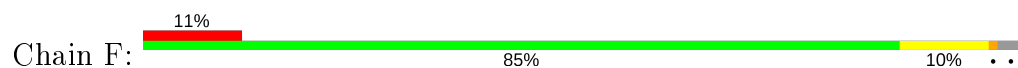


• Molecule 2: HA-33

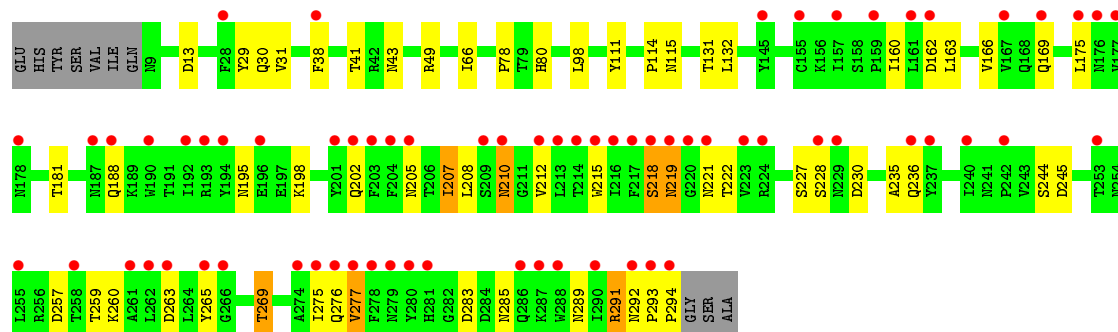
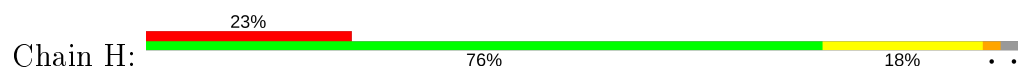




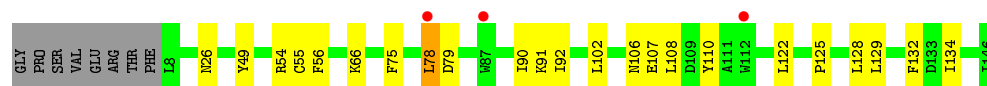
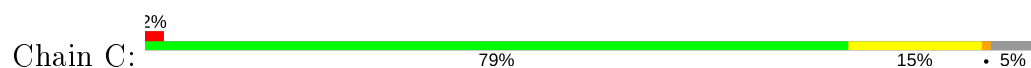
• Molecule 2: HA-33



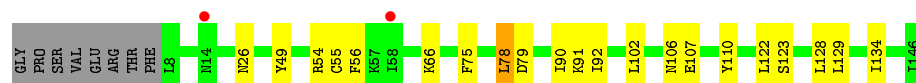
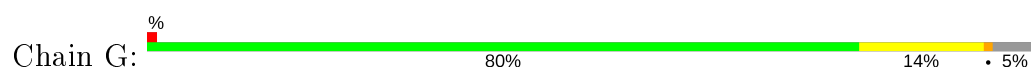
• Molecule 2: HA-33



• Molecule 3: HA-17



• Molecule 3: HA-17



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	159.59 Å 187.49 Å 120.43 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.20 – 3.73 49.20 – 3.73	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.20-3.73) 99.5 (49.20-3.73)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.77 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.268 , 0.293 0.263 , 0.287	Depositor DCC
R_{free} test set	1907 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	111.9	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 97.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	15326	wwPDB-VP
Average B, all atoms (Å ²)	169.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.24	0/1886	0.45	0/2570
1	E	0.24	0/1894	0.45	0/2581
2	B	0.49	0/2393	0.59	1/3267 (0.0%)
2	D	0.46	0/2393	0.61	1/3267 (0.0%)
2	F	0.49	0/2393	0.59	1/3267 (0.0%)
2	H	0.47	0/2393	0.61	1/3267 (0.0%)
3	C	0.50	0/1168	0.62	0/1587
3	G	0.50	0/1168	0.62	0/1587
All	All	0.44	0/15688	0.57	4/21393 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	230	ASP	CB-CG-OD2	5.20	122.98	118.30
2	F	230	ASP	CB-CG-OD2	5.20	122.97	118.30
2	D	230	ASP	CB-CG-OD2	5.18	122.97	118.30
2	B	230	ASP	CB-CG-OD2	5.16	122.94	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1852	0	1807	61	9

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1860	0	1818	59	4
2	B	2334	0	2250	46	7
2	D	2334	0	2250	35	3
2	F	2334	0	2250	41	0
2	H	2334	0	2250	42	3
3	C	1139	0	1097	57	0
3	G	1139	0	1097	50	0
All	All	15326	0	14819	255	13

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 8.

All (255) 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:575:ILE:HG12	3:G:49:TYR:CE1	1.62	1.33
1:E:575:ILE:HD13	3:G:56:PHE:CZ	1.65	1.31
1:A:575:ILE:HG12	3:C:49:TYR:CE1	1.74	1.22
2:B:294:PRO:HB3	2:F:23:ASP:OD2	1.40	1.17
1:E:575:ILE:CG1	3:G:49:TYR:CE1	2.27	1.16
1:E:573:GLU:O	3:G:91:LYS:N	1.88	1.05
1:E:575:ILE:HG21	3:G:54:ARG:O	1.54	1.05
1:A:573:GLU:O	3:C:91:LYS:N	1.89	1.04
2:B:294:PRO:O	2:F:25:ASN:ND2	1.91	1.04
1:E:575:ILE:HD13	3:G:56:PHE:HZ	0.99	1.03
1:A:573:GLU:O	3:C:91:LYS:CB	2.09	0.99
2:B:294:PRO:CB	2:F:23:ASP:OD2	2.10	0.99
1:A:573:GLU:N	3:C:91:LYS:O	1.95	0.98
1:A:574:THR:HG22	3:C:90:ILE:HA	1.45	0.98
1:A:572:THR:HB	3:C:91:LYS:O	1.64	0.97
1:A:581:ILE:CD1	3:C:134:ILE:HD11	1.94	0.96
2:B:23:ASP:OD2	2:F:294:PRO:HB3	1.63	0.96
1:A:572:THR:HG22	3:C:92:ILE:HA	1.46	0.96
1:A:573:GLU:O	3:C:91:LYS:HB3	1.66	0.93
1:A:575:ILE:HD13	3:C:56:PHE:HZ	1.28	0.93
1:E:572:THR:HB	3:G:91:LYS:O	1.74	0.88
1:A:575:ILE:CG1	3:C:49:TYR:CE1	2.56	0.88
2:B:25:ASN:ND2	2:F:294:PRO:O	2.06	0.87
1:E:572:THR:HG22	3:G:92:ILE:HA	1.58	0.86
2:F:134:ASN:OD1	2:H:114:PRO:HG3	1.74	0.86
1:A:581:ILE:HD12	3:C:134:ILE:HD11	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:ILE:HD13	3:C:56:PHE:CZ	2.11	0.85
1:E:573:GLU:N	3:G:91:LYS:O	2.09	0.85
1:E:575:ILE:HG12	3:G:49:TYR:CD1	2.11	0.85
1:E:575:ILE:HB	3:G:56:PHE:HE1	1.42	0.85
2:B:291:ARG:NH1	2:F:123:VAL:HG23	1.93	0.84
1:E:575:ILE:CG1	3:G:49:TYR:HE1	1.78	0.84
1:E:573:GLU:HB3	3:G:91:LYS:HB3	1.57	0.84
1:E:575:ILE:HG12	3:G:49:TYR:HE1	1.09	0.84
1:E:574:THR:HG22	3:G:90:ILE:HA	1.61	0.83
2:D:212:VAL:HG13	2:D:228:SER:HB2	1.59	0.82
2:B:23:ASP:OD2	2:F:294:PRO:CB	2.27	0.82
2:H:212:VAL:HG13	2:H:228:SER:HB2	1.59	0.82
1:A:572:THR:CB	3:C:91:LYS:O	2.28	0.82
1:A:572:THR:CA	3:C:91:LYS:O	2.28	0.81
1:E:575:ILE:CD1	3:G:56:PHE:CZ	2.59	0.80
1:A:575:ILE:HG12	3:C:49:TYR:HE1	1.40	0.80
1:E:572:THR:CA	3:G:91:LYS:O	2.30	0.80
2:B:294:PRO:CB	2:F:23:ASP:CG	2.50	0.80
2:F:134:ASN:CG	2:H:114:PRO:HG3	2.03	0.79
1:A:581:ILE:HD11	3:C:134:ILE:CD1	2.11	0.79
2:B:80:HIS:HB3	3:C:132:PHE:CD2	2.18	0.79
2:F:62:LYS:NZ	2:F:69:THR:O	2.15	0.77
1:A:573:GLU:CA	3:C:91:LYS:HB3	2.15	0.77
2:D:212:VAL:CG1	2:D:228:SER:HB2	2.14	0.76
1:E:573:GLU:O	3:G:91:LYS:CB	2.34	0.76
2:H:212:VAL:CG1	2:H:228:SER:HB2	2.14	0.76
1:E:572:THR:CB	3:G:91:LYS:O	2.34	0.75
1:A:573:GLU:C	3:C:91:LYS:HB3	2.07	0.75
1:A:575:ILE:HG12	3:C:49:TYR:CD1	2.22	0.75
2:B:132:LEU:N	2:D:115:ASN:OD1	2.18	0.75
1:E:575:ILE:HG13	3:G:49:TYR:CE1	2.21	0.73
1:E:573:GLU:CA	3:G:91:LYS:HB3	2.19	0.72
1:A:573:GLU:HB3	3:C:91:LYS:HB3	1.72	0.71
2:B:62:LYS:NZ	2:B:69:THR:O	2.15	0.71
1:E:573:GLU:CB	3:G:91:LYS:HB3	2.20	0.71
1:A:573:GLU:O	3:C:91:LYS:CA	2.41	0.69
1:E:400:ILE:O	1:E:400:ILE:HG22	1.93	0.68
2:F:132:LEU:N	2:H:115:ASN:OD1	2.27	0.68
1:E:573:GLU:O	3:G:91:LYS:HB3	1.94	0.68
1:A:400:ILE:O	1:A:400:ILE:HG22	1.93	0.67
1:E:575:ILE:HB	3:G:56:PHE:CE1	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:291:ARG:HH12	2:F:123:VAL:HG23	1.61	0.66
2:B:80:HIS:HB3	3:C:132:PHE:CG	2.31	0.66
1:A:572:THR:HG21	3:C:92:ILE:HG22	1.76	0.66
1:E:573:GLU:HB3	3:G:91:LYS:CB	2.25	0.65
1:A:575:ILE:HB	3:C:56:PHE:HE1	1.62	0.65
1:E:572:THR:HA	3:G:91:LYS:O	1.96	0.64
2:B:294:PRO:HB3	2:F:23:ASP:CG	2.14	0.64
1:A:573:GLU:CB	3:C:91:LYS:HB3	2.28	0.64
2:B:78:PRO:HA	3:C:108:LEU:CD2	2.27	0.64
2:H:215:TRP:HB3	2:H:235:ALA:HB1	1.80	0.64
1:A:572:THR:CG2	3:C:92:ILE:HA	2.23	0.64
2:D:215:TRP:HB3	2:D:235:ALA:HB1	1.80	0.64
1:A:575:ILE:HG21	3:C:54:ARG:O	1.98	0.63
1:A:572:THR:HG22	3:C:92:ILE:CA	2.24	0.63
2:H:38:PHE:HE2	2:H:41:THR:CG2	2.12	0.62
2:D:38:PHE:HE2	2:D:41:THR:CG2	2.12	0.62
2:H:269:THR:O	2:H:269:THR:OG1	2.14	0.62
2:B:80:HIS:HB3	3:C:132:PHE:CE2	2.36	0.61
2:D:163:LEU:O	2:D:291:ARG:NH2	2.33	0.61
2:H:163:LEU:O	2:H:291:ARG:NH2	2.34	0.60
2:H:162:ASP:HB2	2:H:269:THR:HB	1.84	0.60
2:H:66:ILE:HG22	2:H:66:ILE:O	2.02	0.59
2:B:131:THR:HB	2:D:115:ASN:OD1	2.02	0.59
1:A:572:THR:CG2	3:C:92:ILE:HG22	2.33	0.58
2:D:162:ASP:HB2	2:D:269:THR:HB	1.84	0.58
2:B:291:ARG:NH1	2:F:123:VAL:CG2	2.66	0.58
2:D:269:THR:OG1	2:D:269:THR:O	2.14	0.58
2:B:161:LEU:HD22	1:E:597:ARG:HE	1.69	0.58
2:B:294:PRO:CA	2:F:23:ASP:OD2	2.50	0.58
2:H:218:SER:OG	2:H:219:ASN:OD1	2.21	0.57
2:H:207:ILE:HG23	2:H:208:LEU:HD12	1.87	0.57
1:A:575:ILE:HB	3:C:56:PHE:CE1	2.39	0.57
2:D:218:SER:OG	2:D:219:ASN:OD1	2.21	0.57
2:F:134:ASN:CG	2:H:114:PRO:CG	2.73	0.57
2:D:207:ILE:HG23	2:D:208:LEU:HD12	1.87	0.57
2:B:223:VAL:HG13	2:B:276:GLN:HA	1.86	0.56
2:F:134:ASN:ND2	2:H:111:TYR:O	2.39	0.56
2:B:196:GLU:CD	2:B:196:GLU:H	2.09	0.56
2:F:223:VAL:HG13	2:F:276:GLN:HA	1.86	0.56
1:A:581:ILE:HD11	3:C:134:ILE:HD11	1.66	0.55
2:F:196:GLU:H	2:F:196:GLU:CD	2.09	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:THR:C	3:C:91:LYS:O	2.45	0.55
2:F:115:ASN:ND2	2:H:132:LEU:O	2.40	0.55
2:D:221:ASN:O	2:D:276:GLN:HB2	2.07	0.55
2:H:221:ASN:O	2:H:276:GLN:HB2	2.07	0.55
2:B:210:ASN:ND2	2:B:229:ASN:OD1	2.40	0.54
1:A:572:THR:HA	3:C:91:LYS:O	2.04	0.54
1:E:581:ILE:CD1	3:G:134:ILE:HD11	2.36	0.54
2:F:210:ASN:ND2	2:F:229:ASN:OD1	2.40	0.54
3:G:123:SER:O	2:H:78:PRO:HB3	2.08	0.54
3:G:75:PHE:CG	2:H:80:HIS:NE2	2.76	0.53
1:A:391:ASP:HA	1:A:499:ARG:HB2	1.90	0.53
1:E:391:ASP:HA	1:E:499:ARG:HB2	1.90	0.53
1:E:573:GLU:C	3:G:91:LYS:HB3	2.28	0.53
1:A:400:ILE:CG2	1:A:400:ILE:O	2.57	0.53
1:A:503:ASP:HB3	1:A:580:LEU:HB2	1.91	0.52
1:E:552:THR:HG22	1:E:597:ARG:HH11	1.75	0.52
1:A:573:GLU:H	3:C:91:LYS:C	2.05	0.52
2:D:38:PHE:CE2	2:D:41:THR:CG2	2.92	0.52
1:E:573:GLU:O	3:G:91:LYS:CA	2.55	0.52
1:A:581:ILE:CD1	3:C:134:ILE:CD1	2.70	0.52
1:E:503:ASP:HB3	1:E:580:LEU:HB2	1.91	0.52
1:E:573:GLU:N	3:G:91:LYS:HB3	2.25	0.52
1:A:552:THR:HG22	1:A:597:ARG:HH11	1.74	0.52
2:D:169:GLN:HE22	2:D:208:LEU:HD13	1.75	0.52
2:H:169:GLN:HE22	2:H:208:LEU:HD13	1.76	0.51
1:A:573:GLU:HB3	3:C:91:LYS:CB	2.38	0.51
2:H:38:PHE:CE2	2:H:41:THR:CG2	2.92	0.51
1:E:573:GLU:HB3	3:G:91:LYS:HD3	1.93	0.51
2:H:66:ILE:CG2	2:H:66:ILE:O	2.58	0.51
2:B:131:THR:HG21	3:C:129:LEU:HD13	1.93	0.51
2:B:114:PRO:HB2	2:D:132:LEU:HB3	1.94	0.50
2:B:161:LEU:HD22	1:E:597:ARG:NE	2.26	0.50
1:E:400:ILE:CG2	1:E:400:ILE:O	2.57	0.50
2:F:133:ASN:C	2:H:114:PRO:HG2	2.32	0.50
2:B:291:ARG:HH11	2:F:123:VAL:HG23	1.73	0.50
1:A:581:ILE:HD11	3:C:134:ILE:HD13	1.91	0.50
3:C:125:PRO:HB3	2:D:78:PRO:O	2.12	0.50
1:E:487:THR:C	1:E:489:SER:H	2.15	0.49
1:A:487:THR:C	1:A:489:SER:H	2.15	0.49
1:E:414:THR:HA	1:E:476:LYS:HE2	1.94	0.49
2:F:134:ASN:ND2	2:H:114:PRO:HG3	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:575:ILE:CG1	3:G:49:TYR:CD1	2.83	0.49
1:A:383:GLN:HG3	1:A:406:PHE:HE2	1.77	0.49
3:C:75:PHE:CG	2:D:80:HIS:NE2	2.81	0.49
1:E:575:ILE:CD1	3:G:49:TYR:CD1	2.96	0.49
1:A:573:GLU:HB3	3:C:91:LYS:HD3	1.95	0.48
1:A:414:THR:HA	1:A:476:LYS:HE2	1.94	0.48
1:E:383:GLN:HG3	1:E:406:PHE:HE2	1.77	0.48
3:G:55:CYS:SG	3:G:102:LEU:HD13	2.53	0.48
3:C:55:CYS:SG	3:C:102:LEU:HD13	2.53	0.48
2:B:23:ASP:CG	2:F:294:PRO:CB	2.81	0.48
1:A:476:LYS:HG3	1:A:477:ASP:OD1	2.13	0.48
2:D:166:VAL:HG11	2:D:188:GLN:HB3	1.96	0.48
2:D:215:TRP:HD1	2:D:222:THR:O	1.97	0.48
2:H:215:TRP:HD1	2:H:222:THR:O	1.97	0.48
2:D:38:PHE:HE2	2:D:41:THR:HG22	1.79	0.47
2:B:294:PRO:HA	2:F:23:ASP:OD2	2.15	0.47
2:D:210:ASN:OD1	2:D:228:SER:HB3	2.14	0.47
2:H:166:VAL:HG11	2:H:188:GLN:HB3	1.96	0.47
1:A:573:GLU:N	3:C:91:LYS:HB3	2.29	0.47
1:E:476:LYS:HG3	1:E:477:ASP:OD1	2.14	0.47
2:H:38:PHE:HE2	2:H:41:THR:HG22	1.79	0.47
1:A:573:GLU:O	3:C:91:LYS:HB2	2.07	0.47
1:E:536:TYR:CE1	1:E:609:GLU:HB2	2.49	0.47
2:H:210:ASN:OD1	2:H:228:SER:HB3	2.15	0.47
2:D:195:ASN:ND2	2:D:198:LYS:HG3	2.30	0.47
2:B:123:VAL:HG23	2:F:291:ARG:NH1	2.30	0.47
2:H:195:ASN:ND2	2:H:198:LYS:HG3	2.30	0.47
1:A:536:TYR:CE1	1:A:609:GLU:HB2	2.49	0.46
2:B:78:PRO:HA	3:C:108:LEU:HD21	1.96	0.46
2:D:218:SER:OG	2:D:219:ASN:N	2.48	0.46
2:F:163:LEU:O	2:F:291:ARG:NH2	2.49	0.46
1:E:572:THR:CG2	3:G:92:ILE:HA	2.40	0.46
1:E:575:ILE:HD11	3:G:49:TYR:CD1	2.51	0.46
2:F:132:LEU:O	2:H:115:ASN:ND2	2.48	0.46
2:H:218:SER:OG	2:H:219:ASN:N	2.48	0.46
2:B:163:LEU:O	2:B:291:ARG:NH2	2.49	0.45
2:B:294:PRO:CA	2:F:23:ASP:CG	2.84	0.45
3:C:75:PHE:CD1	2:D:80:HIS:NE2	2.84	0.45
1:A:508:MET:HA	1:A:509:ASN:HA	1.70	0.45
1:E:536:TYR:CD1	1:E:607:LYS:HE2	2.51	0.45
1:A:536:TYR:CD1	1:A:607:LYS:HE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:ALA:HB3	1:A:479:ASN:HB2	1.99	0.45
2:D:263:ASP:OD2	2:D:285:ASN:ND2	2.50	0.45
2:H:263:ASP:OD2	2:H:285:ASN:ND2	2.50	0.45
1:A:573:GLU:HB3	3:C:91:LYS:CG	2.47	0.44
2:D:13:ASP:OD1	2:D:49:ARG:HD3	2.17	0.44
1:E:434:ALA:HB3	1:E:479:ASN:HB2	1.99	0.44
2:F:207:ILE:HD12	2:F:207:ILE:HA	1.85	0.44
2:F:71:LEU:HB3	2:F:84:THR:HB	1.99	0.44
2:H:13:ASP:OD1	2:H:49:ARG:HD3	2.17	0.44
2:B:291:ARG:HH12	2:F:123:VAL:CG2	2.28	0.44
2:H:293:PRO:HA	2:H:294:PRO:HD3	1.89	0.44
1:E:552:THR:HG21	1:E:597:ARG:HD3	2.00	0.44
2:H:215:TRP:CD1	2:H:277:VAL:HG11	2.53	0.44
1:E:581:ILE:HD12	3:G:134:ILE:HD11	1.98	0.44
2:B:114:PRO:HB2	2:D:132:LEU:C	2.37	0.44
1:E:572:THR:C	3:G:91:LYS:O	2.56	0.44
2:B:71:LEU:HB3	2:B:84:THR:HB	1.99	0.43
2:D:215:TRP:CD1	2:D:277:VAL:HG11	2.53	0.43
3:G:66:LYS:HB3	3:G:78:LEU:HD22	2.00	0.43
2:D:257:ASP:OD1	2:D:259:THR:OG1	2.36	0.43
2:B:207:ILE:HD12	2:B:207:ILE:HA	1.85	0.43
2:B:23:ASP:OD2	2:F:294:PRO:CA	2.67	0.43
2:D:202:GLN:HG2	2:D:236:GLN:O	2.19	0.43
2:D:260:LYS:HD3	2:D:277:VAL:HG23	2.00	0.43
2:B:186:ARG:HB2	2:B:207:ILE:HD13	2.01	0.43
2:B:80:HIS:N	3:C:132:PHE:CD1	2.86	0.43
3:C:66:LYS:HB3	3:C:78:LEU:HD22	2.00	0.43
2:H:260:LYS:HD3	2:H:277:VAL:HG23	2.00	0.43
2:F:100:ASP:HA	2:H:98:LEU:HD23	2.00	0.43
2:H:202:GLN:HG2	2:H:236:GLN:O	2.19	0.43
1:A:552:THR:HG21	1:A:597:ARG:HD3	2.00	0.43
1:E:573:GLU:H	3:G:91:LYS:HB3	1.83	0.43
2:H:257:ASP:OD1	2:H:259:THR:OG1	2.36	0.43
2:F:186:ARG:HB2	2:F:207:ILE:HD13	2.01	0.42
3:G:106:ASN:O	3:G:107:GLU:HG2	2.19	0.42
3:C:106:ASN:O	3:C:107:GLU:HG2	2.19	0.42
3:G:129:LEU:HD21	2:H:131:THR:HG21	2.02	0.42
1:A:477:ASP:OD1	1:A:477:ASP:N	2.52	0.42
2:D:219:ASN:OD1	2:D:219:ASN:N	2.52	0.42
3:G:78:LEU:HD23	3:G:78:LEU:HA	1.88	0.42
1:A:383:GLN:HG3	1:A:406:PHE:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:205:ASN:OD1	2:D:207:ILE:HG22	2.19	0.42
1:E:383:GLN:HG3	1:E:406:PHE:CE2	2.55	0.42
2:D:212:VAL:HG11	2:D:228:SER:HB2	2.00	0.42
2:H:205:ASN:OD1	2:H:207:ILE:HG22	2.20	0.42
2:H:219:ASN:N	2:H:219:ASN:OD1	2.52	0.42
2:B:79:THR:C	3:C:132:PHE:CE1	2.93	0.42
1:A:597:ARG:HE	2:F:161:LEU:HD22	1.85	0.41
2:B:240:ILE:HG22	2:B:250:TYR:CD1	2.55	0.41
2:B:78:PRO:CA	3:C:108:LEU:CD2	2.96	0.41
3:C:110:TYR:HB3	3:C:128:LEU:HG	2.02	0.41
2:B:75:TRP:CE2	2:B:129:LEU:HD12	2.56	0.41
1:E:477:ASP:N	1:E:477:ASP:OD1	2.52	0.41
2:B:294:PRO:HB2	2:F:23:ASP:CG	2.35	0.41
2:B:115:ASN:ND2	2:D:131:THR:HB	2.36	0.41
1:E:581:ILE:HD11	3:G:134:ILE:HD11	2.02	0.41
3:G:110:TYR:HB3	3:G:128:LEU:HG	2.01	0.41
1:A:431:ILE:HG23	1:A:458:ILE:HB	2.03	0.41
1:A:433:GLU:HB2	1:A:458:ILE:HD11	2.02	0.41
1:E:572:THR:HG21	3:G:92:ILE:HG22	2.03	0.41
1:A:432:TYR:HB2	1:A:481:TYR:HB2	2.03	0.40
2:F:75:TRP:CE2	2:F:129:LEU:HD12	2.56	0.40
1:E:581:ILE:HD11	3:G:134:ILE:CD1	2.52	0.40
1:E:573:GLU:HB3	3:G:91:LYS:CG	2.51	0.40
2:F:240:ILE:HG22	2:F:250:TYR:CD1	2.56	0.40

All (13) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:616:TYR:CB	2:B:272:GLY:O[3_456]	1.30	0.90
1:A:616:TYR:CD2	2:B:272:GLY:CA[3_456]	1.34	0.86
2:B:173:THR:O	1:E:481:TYR:OH[4_546]	1.55	0.65
1:A:455:ILE:O	1:E:455:ILE:O[2_455]	1.65	0.55
1:A:616:TYR:CB	2:B:272:GLY:C[3_456]	1.86	0.34
1:A:616:TYR:CG	2:B:272:GLY:CA[3_456]	1.86	0.34
2:D:43:ASN:ND2	2:H:31:VAL:CG1[1_554]	2.05	0.15
2:D:29:TYR:OH	2:H:29:TYR:OH[1_554]	2.05	0.15
1:A:534:HIS:CE1	1:E:477:ASP:OD2[2_455]	2.06	0.14
2:D:31:VAL:CG1	2:H:43:ASN:ND2[1_554]	2.07	0.13
1:A:454:ALA:CB	1:E:457:TYR:N[2_455]	2.11	0.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:616:TYR:CG	2:B:272:GLY:O[3_456]	2.19	0.01
1:A:617:ASN:OD1	2:B:271:ASN:O[3_456]	2.19	0.01

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	224/254 (88%)	212 (95%)	12 (5%)	0	100	100
1	E	225/254 (89%)	213 (95%)	11 (5%)	1 (0%)	34	69
2	B	285/296 (96%)	276 (97%)	9 (3%)	0	100	100
2	D	285/296 (96%)	269 (94%)	15 (5%)	1 (0%)	34	69
2	F	285/296 (96%)	277 (97%)	8 (3%)	0	100	100
2	H	285/296 (96%)	270 (95%)	14 (5%)	1 (0%)	34	69
3	C	137/147 (93%)	133 (97%)	4 (3%)	0	100	100
3	G	137/147 (93%)	133 (97%)	4 (3%)	0	100	100
All	All	1863/1986 (94%)	1783 (96%)	77 (4%)	3 (0%)	47	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	265	TYR
2	H	265	TYR
1	E	488	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	211/232 (91%)	197 (93%)	14 (7%)	16	48
1	E	212/232 (91%)	198 (93%)	14 (7%)	16	48
2	B	263/270 (97%)	253 (96%)	10 (4%)	33	61
2	D	263/270 (97%)	245 (93%)	18 (7%)	16	47
2	F	263/270 (97%)	253 (96%)	10 (4%)	33	61
2	H	263/270 (97%)	245 (93%)	18 (7%)	16	47
3	C	130/138 (94%)	126 (97%)	4 (3%)	40	65
3	G	130/138 (94%)	126 (97%)	4 (3%)	40	65
All	All	1735/1820 (95%)	1643 (95%)	92 (5%)	22	54

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	406	PHE
1	A	411	THR
1	A	414	THR
1	A	426	LEU
1	A	463	SER
1	A	465	ASN
1	A	477	ASP
1	A	487	THR
1	A	493	ASN
1	A	507	LEU
1	A	508	MET
1	A	519	ASN
1	A	546	ASN
1	A	552	THR
2	B	30	GLN
2	B	80	HIS
2	B	84	THR
2	B	123	VAL
2	B	175	LEU
2	B	186	ARG
2	B	193	ARG
2	B	223	VAL
2	B	228	SER
2	B	247	ASP

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Mol	Chain	Res	Type
3	C	26	ASN
3	C	78	LEU
3	C	79	ASP
3	C	122	LEU
2	D	30	GLN
2	D	160	ILE
2	D	175	LEU
2	D	181	THR
2	D	207	ILE
2	D	210	ASN
2	D	218	SER
2	D	219	ASN
2	D	227	SER
2	D	244	SER
2	D	245	ASP
2	D	269	THR
2	D	275	ILE
2	D	277	VAL
2	D	283	ASP
2	D	289	ASN
2	D	291	ARG
2	D	292	ASN
1	E	406	PHE
1	E	411	THR
1	E	414	THR
1	E	426	LEU
1	E	463	SER
1	E	465	ASN
1	E	477	ASP
1	E	487	THR
1	E	493	ASN
1	E	507	LEU
1	E	508	MET
1	E	519	ASN
1	E	546	ASN
1	E	552	THR
2	F	30	GLN
2	F	80	HIS
2	F	84	THR
2	F	123	VAL
2	F	175	LEU
2	F	186	ARG

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Mol	Chain	Res	Type
2	F	193	ARG
2	F	223	VAL
2	F	228	SER
2	F	247	ASP
3	G	26	ASN
3	G	78	LEU
3	G	79	ASP
3	G	122	LEU
2	H	30	GLN
2	H	160	ILE
2	H	175	LEU
2	H	181	THR
2	H	207	ILE
2	H	210	ASN
2	H	218	SER
2	H	219	ASN
2	H	227	SER
2	H	244	SER
2	H	245	ASP
2	H	269	THR
2	H	275	ILE
2	H	277	VAL
2	H	283	ASP
2	H	289	ASN
2	H	291	ARG
2	H	292	ASN

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	392	ASN
1	A	534	HIS
2	B	115	ASN
2	D	86	GLN
1	E	392	ASN
2	H	86	GLN

5.3.3 RNA ⓘ

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 ⓘ

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	228/254 (89%)	0.81	36 (15%) 2 2	99, 151, 222, 268	3 (1%)
1	E	229/254 (90%)	0.22	10 (4%) 34 29	101, 147, 213, 274	3 (1%)
2	B	286/296 (96%)	0.48	14 (4%) 29 26	85, 132, 183, 234	0
2	D	286/296 (96%)	1.15	64 (22%) 0 0	99, 207, 325, 398	0
2	F	286/296 (96%)	0.61	34 (11%) 4 5	93, 145, 203, 256	0
2	H	286/296 (96%)	1.09	69 (24%) 0 0	94, 195, 353, 422	0
3	C	139/147 (94%)	0.18	3 (2%) 62 55	107, 154, 194, 221	0
3	G	139/147 (94%)	0.19	2 (1%) 75 70	109, 147, 192, 208	0
All	All	1879/1986 (94%)	0.66	232 (12%) 4 4	85, 153, 303, 422	6 (0%)

All (232) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	202	GLN	15.5
2	D	215	TRP	8.5
2	D	237	TYR	7.6
1	A	381	ASN	7.6
2	H	169	GLN	7.6
2	H	255	LEU	7.0
2	D	277	VAL	7.0
1	E	454	ALA	6.9
2	D	203	PHE	6.8
2	D	261	ALA	6.6
2	H	175	LEU	6.6
2	H	277	VAL	6.5
2	D	265	TYR	6.5
2	H	275	ILE	6.3
2	H	218	SER	6.3
2	H	162	ASP	6.3

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Mol	Chain	Res	Type	RSRZ
2	B	228	SER	6.2
2	D	201	TYR	6.1
2	D	161	LEU	5.9
2	H	216	ILE	5.9
1	E	575	ILE	5.9
1	A	399	GLY	5.9
2	H	274	ALA	5.8
1	A	496	GLN	5.8
2	H	262	LEU	5.8
2	H	261	ALA	5.8
2	H	161	LEU	5.8
2	D	167	VAL	5.7
2	H	204	PHE	5.7
2	H	203	PHE	5.7
1	E	435	ILE	5.7
2	D	169	GLN	5.7
2	D	255	LEU	5.6
2	D	262	LEU	5.5
2	D	214	THR	5.5
2	D	223	VAL	5.4
2	H	228	SER	5.4
2	H	213	LEU	5.4
2	D	194	TYR	5.4
2	H	276	GLN	5.3
2	H	167	VAL	5.2
2	D	236	GLN	5.2
2	H	190	TRP	5.2
2	D	176	ASN	4.9
2	F	277	VAL	4.9
2	D	175	LEU	4.8
2	D	228	SER	4.8
2	D	276	GLN	4.7
2	H	194	TYR	4.6
2	H	279	ASN	4.6
1	A	495	ILE	4.6
2	D	294	PRO	4.5
2	H	210	ASN	4.5
2	D	253	THR	4.5
2	D	218	SER	4.5
2	D	288	TRP	4.4
2	D	157	ILE	4.3
2	H	229	ASN	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	497	PHE	4.3
2	D	216	ILE	4.3
2	H	280	TYR	4.3
2	F	215	TRP	4.2
2	H	157	ILE	4.2
2	H	193	ARG	4.2
2	F	274	ALA	4.1
2	F	71	LEU	4.1
2	H	258	THR	4.1
2	H	159	PRO	4.1
2	H	221	ASN	4.1
2	H	266	GLY	4.1
2	B	272	GLY	4.0
2	H	265	TYR	4.0
2	D	238	TRP	4.0
2	H	281	HIS	4.0
2	D	240	ILE	4.0
1	A	406	PHE	3.9
2	D	274	ALA	3.9
2	H	219	ASN	3.9
2	D	231	GLN	3.9
2	H	294	PRO	3.9
2	H	202	GLN	3.8
1	A	395	TYR	3.8
1	A	616	TYR	3.8
2	D	229	ASN	3.8
2	D	275	ILE	3.8
2	H	209	SER	3.8
1	A	454	ALA	3.8
1	E	383	GLN	3.7
2	D	217	PHE	3.7
2	B	229	ASN	3.7
1	A	385	ILE	3.7
1	E	386	ASN	3.7
2	H	215	TRP	3.6
2	D	204	PHE	3.6
2	H	214	THR	3.6
1	E	388	ALA	3.6
1	A	393	TYR	3.6
2	H	288	TRP	3.6
1	A	575	ILE	3.5
1	A	408	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	383	GLN	3.5
2	D	196	GLU	3.5
2	F	262	LEU	3.5
2	H	240	ILE	3.5
3	G	14	ASN	3.4
2	D	224	ARG	3.4
2	H	205	ASN	3.4
2	D	177	VAL	3.4
2	F	161	LEU	3.4
2	F	213	LEU	3.4
1	A	423	GLN	3.4
1	A	494	GLN	3.4
1	A	421	ASN	3.3
2	F	224	ARG	3.3
2	H	278	PHE	3.2
2	D	293	PRO	3.2
2	F	221	ASN	3.2
1	A	397	ILE	3.2
2	H	38	PHE	3.2
2	F	217	PHE	3.2
2	H	224	ARG	3.1
2	D	278	PHE	3.1
2	H	293	PRO	3.1
1	E	380	GLU	3.1
2	F	228	SER	3.1
1	A	410	PHE	3.0
2	D	289	ASN	3.0
2	F	226	SER	3.0
1	A	482	ILE	3.0
2	H	212	VAL	3.0
2	F	275	ILE	3.0
2	H	263	ASP	3.0
2	D	159	PRO	3.0
2	D	68	ASN	3.0
2	F	225	VAL	2.9
2	D	193	ARG	2.9
1	A	386	ASN	2.9
2	D	290	ILE	2.9
2	H	237	TYR	2.9
2	F	261	ALA	2.9
1	A	407	TYR	2.9
2	D	162	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
2	H	217	PHE	2.8
2	H	176	ASN	2.8
2	H	177	VAL	2.8
1	E	399	GLY	2.8
2	D	234	ASP	2.8
1	A	420	ILE	2.8
2	D	210	ASN	2.8
2	H	155	CYS	2.8
2	H	178	ASN	2.8
2	B	51	ILE	2.7
2	D	263	ASP	2.7
1	A	391	ASP	2.7
2	H	236	GLN	2.7
2	F	190	TRP	2.7
2	H	287	LYS	2.7
2	H	196	GLU	2.7
2	D	172	VAL	2.6
2	B	149	ASP	2.6
2	H	242	PRO	2.6
2	D	273	THR	2.6
2	H	286	GLN	2.6
2	D	209	SER	2.6
3	C	78	LEU	2.5
2	F	178	ASN	2.5
3	C	112	TRP	2.5
2	F	162	ASP	2.5
2	F	251	THR	2.5
2	F	218	SER	2.5
1	A	388	ALA	2.5
2	D	287	LYS	2.5
2	D	213	LEU	2.5
2	H	192	ILE	2.5
2	F	212	VAL	2.5
2	D	205	ASN	2.5
2	H	28	PHE	2.5
2	D	212	VAL	2.4
1	A	626	ASN	2.4
2	F	260	LYS	2.4
2	H	292	ASN	2.4
2	H	290	ILE	2.4
2	F	233	ASN	2.4
2	F	278	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	230	ASP	2.4
1	A	536	TYR	2.4
2	B	210	ASN	2.4
1	A	398	PRO	2.4
2	D	252	ILE	2.4
2	F	214	THR	2.4
3	C	87	TRP	2.3
2	F	256	ARG	2.3
1	A	409	LEU	2.3
2	B	201	TYR	2.3
2	D	239	LEU	2.3
1	A	613	LEU	2.3
2	H	201	TYR	2.3
1	A	470	LEU	2.3
2	D	232	ASN	2.3
2	F	236	GLN	2.3
2	H	145	TYR	2.2
1	E	401	VAL	2.2
2	H	253	THR	2.2
1	A	380	GLU	2.2
2	F	179	LEU	2.2
2	F	273	THR	2.2
2	F	223	VAL	2.2
2	D	260	LYS	2.2
1	E	381	ASN	2.2
2	B	226	SER	2.2
2	H	220	GLY	2.1
2	B	194	TYR	2.1
1	A	481	TYR	2.1
1	A	475	ASN	2.1
3	G	58	ILE	2.1
2	H	188	GLN	2.1
2	F	252	ILE	2.1
1	A	384	GLU	2.1
2	D	182	TRP	2.1
2	B	60	LYS	2.1
2	B	215	TRP	2.1
2	H	187	ASN	2.1
2	F	203	PHE	2.1
2	H	223	VAL	2.1
2	F	172	VAL	2.1
2	B	240	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	235	ALA	2.1
2	D	250	TYR	2.0
2	F	177	VAL	2.0
1	A	431	ILE	2.0
2	B	45	LEU	2.0
2	B	150	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 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.