



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:58 PM UTC

PDB ID : 4LO7 / pdb_00004lo7
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 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:

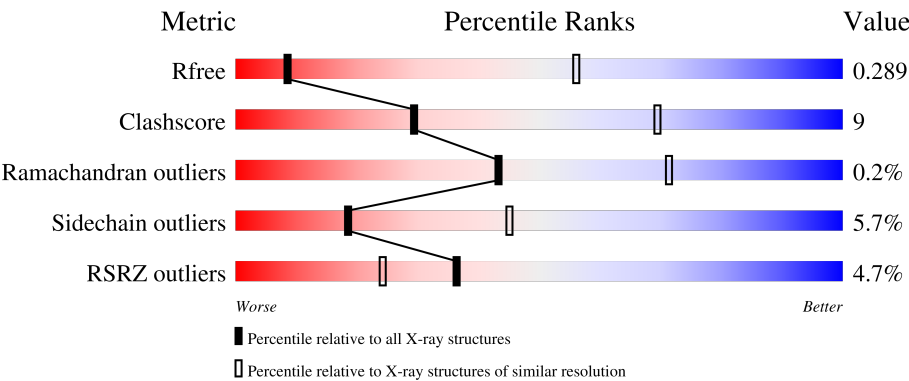
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 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}	180053	1234 (3.88-3.60)
Clashscore	190562	1274 (3.88-3.60)
Ramachandran outliers	187476	1226 (3.88-3.60)
Sidechain outliers	187428	1221 (3.88-3.60)
RSRZ outliers	180081	1233 (3.88-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	254	5% 72%15%•10%
1	E	254	8% 75%13%•10%
2	B	296	6% 84%10%••
2	D	296	4% 78%15%••
2	F	296	% 85%9%••

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Mol	Chain	Length	Quality of chain
2	H	296	7% 77% 17% • •
3	C	147	78% 16% • 5%
3	G	147	% 80% 14% • 5%

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			

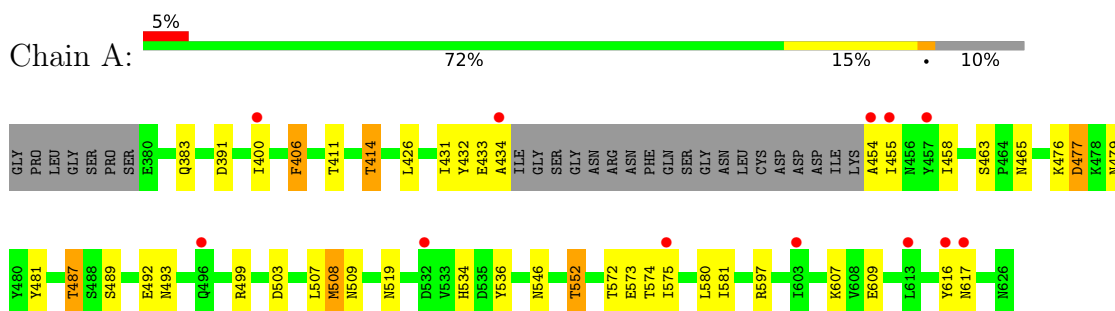
There are 4 discrepancies between the modelled and reference sequences:

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

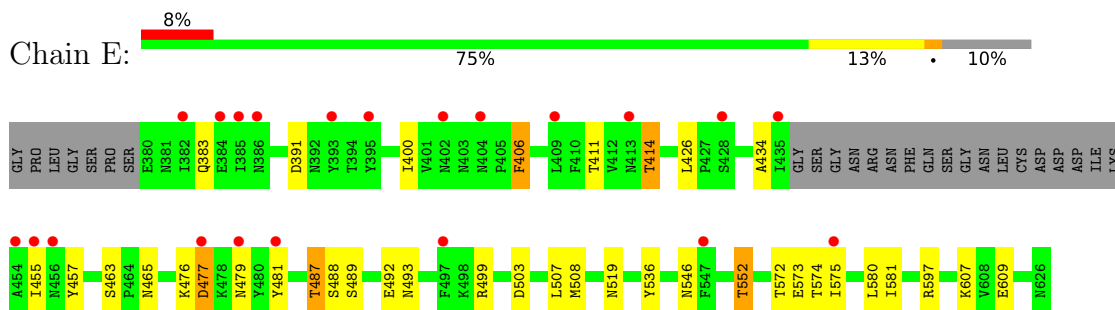
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

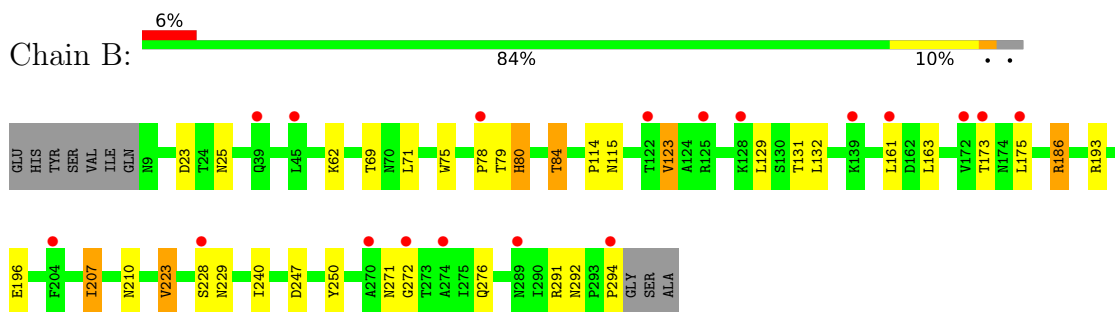
• Molecule 1: HA-70



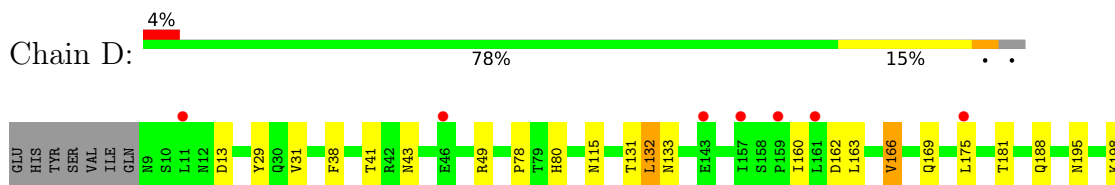
• Molecule 1: HA-70

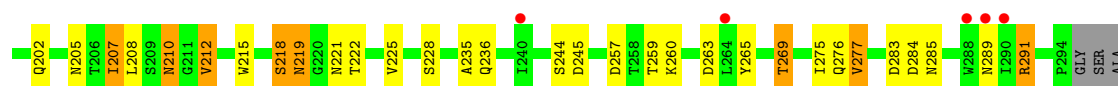


• Molecule 2: HA-33

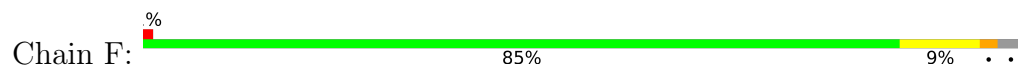


• Molecule 2: HA-33

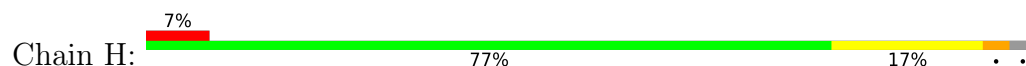




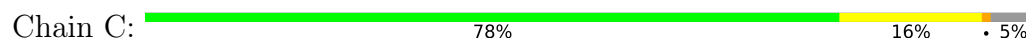
• Molecule 2: HA-33



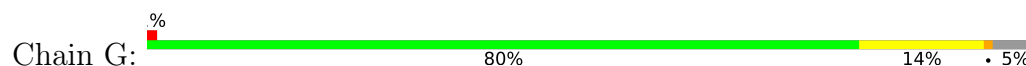
• Molecule 2: HA-33



• 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	159.59Å 187.49Å 120.43Å 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) 99.4 (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 3.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.268 , 0.293 0.261 , 0.289	Depositor DCC
R_{free} test set	1907 reflections (4.97%)	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)	0.32 , 130.0	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	0.89	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	0.28	0/1886	0.72	0/2570
1	E	0.28	0/1894	0.72	0/2581
2	B	0.56	0/2393	0.80	0/3267
2	D	0.54	0/2393	0.82	1/3267 (0.0%)
2	F	0.56	0/2393	0.79	0/3267
2	H	0.55	0/2393	0.82	1/3267 (0.0%)
3	C	0.60	1/1168 (0.1%)	0.85	0/1587
3	G	0.60	1/1168 (0.1%)	0.85	0/1587
All	All	0.51	2/15688 (0.0%)	0.79	2/21393 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	93	ALA	C-O	-5.44	1.19	1.24
3	C	93	ALA	C-O	-5.41	1.19	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	284	ASP	N-CA-C	5.67	119.71	112.34
2	H	284	ASP	N-CA-C	5.66	119.70	112.34

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
1	E	1860	0	1818	60	4
2	B	2334	0	2250	47	7
2	D	2334	0	2250	36	3
2	F	2334	0	2250	41	0
2	H	2334	0	2250	42	3
3	C	1139	0	1097	58	0
3	G	1139	0	1097	52	0
All	All	15326	0	14819	259	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 9.

All (259) 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
1:A:572:THR:HG22	3:C:92:ILE:HA	1.46	0.96
2:B:23:ASP:OD2	2:F:294:PRO:HB3	1.63	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
2:B:294:PRO:CB	2:F:23:ASP:CG	2.50	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
2:F:134:ASN:CG	2:H:114:PRO:HG3	2.03	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:573:GLU:C	3:C:91:LYS:HB3	2.07	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
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: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
2:B:294:PRO:HB3	2:F:23:ASP:CG	2.14	0.69
1:E:400:ILE:O	1:E:400:ILE:HG22	1.93	0.68
1:E:573:GLU:O	3:G:91:LYS:HB3	1.94	0.68
2:F:132:LEU:N	2:H:115:ASN:OD1	2.27	0.68
1:A:400:ILE:HG22	1:A:400:ILE:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:575:ILE:HB	3:G:56:PHE:CE1	2.26	0.67
1:A:572:THR:HG21	3:C:92:ILE:HG22	1.76	0.66
2:B:80:HIS:HB3	3:C:132:PHE:CG	2.31	0.66
2:B:291:ARG:HH12	2:F:123:VAL:HG23	1.61	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
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:OG1	2:H:269:THR:O	2.14	0.62
2:F:134:ASN:CG	2:H:114:PRO:CG	2.73	0.61
2:B:80:HIS:HB3	3:C:132:PHE:CE2	2.36	0.61
1:A:573:GLU:H	3:C:91:LYS:C	2.05	0.61
2:D:163:LEU:O	2:D:291:ARG:NH2	2.33	0.61
2:B:196:GLU:CD	2:B:196:GLU:H	2.09	0.60
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
1:A:572:THR:C	3:C:91:LYS:O	2.45	0.60
2:H:66:ILE:HG22	2:H:66:ILE:O	2.02	0.59
2:F:196:GLU:CD	2:F:196:GLU:H	2.09	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:O	2:D:269:THR:OG1	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
1:E:573:GLU:C	3:G:91:LYS:HB3	2.28	0.57
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:134:ASN:ND2	2:H:111:TYR:O	2.39	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: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:F:133:ASN:C	2:H:114:PRO:HG2	2.32	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:487:THR:C	1:E:489:SER:H	2.15	0.54
1:E:581:ILE:CD1	3:G:134:ILE:HD11	2.36	0.54
1:A:487:THR:C	1:A:489:SER:H	2.15	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
2:B:23:ASP:CG	2:F:294:PRO:CB	2.81	0.53
1:E:391:ASP:HA	1:E:499:ARG:HB2	1.90	0.53
1:A:400:ILE:O	1:A:400:ILE:CG2	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:E:573:GLU:H	3:G:91:LYS:C	2.16	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:O	2:H:66:ILE:CG2	2.58	0.51
2:B:131:THR:HG21	3:C:129:LEU:HD13	1.93	0.51
2:B:294:PRO:CA	2:F:23:ASP:CG	2.84	0.50
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:O	1:E:400:ILE:CG2	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:125:PRO:HB3	2:D:78:PRO:O	2.12	0.50
1:E:414:THR:HA	1:E:476:LYS:HE2	1.94	0.49
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
2:B:294:PRO:HB2	2:F:23:ASP:CG	2.35	0.48
1:A:414:THR:HA	1:A:476:LYS:HE2	1.94	0.48
2:B:114:PRO:HB2	2:D:132:LEU:C	2.37	0.48
1:E:383:GLN:HG3	1:E:406:PHE:HE2	1.77	0.48
2:F:134:ASN:ND2	2:H:114:PRO:HG3	2.26	0.48
1:E:572:THR:C	3:G:91:LYS:O	2.56	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
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:79:THR:C	3:C:132:PHE:CE1	2.93	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
1:E:572:THR:CG2	3:G:92:ILE:HA	2.40	0.46
2:F:163:LEU:O	2:F:291:ARG:NH2	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:LEU:O	2:B:291:ARG:NH2	2.49	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
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:71:LEU:HB3	2:F:84:THR:HB	1.99	0.44
2:F:207:ILE:HD12	2:F:207:ILE:HA	1.85	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: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:B:114:PRO:HG2	2:D:133:ASN:C	2.44	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:80:HIS:N	3:C:132:PHE:CD1	2.86	0.43
2:B:186:ARG:HB2	2:B:207:ILE:HD13	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:106:ASN:C	3:C:107:GLU:HG2	2.44	0.42
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:OD1	2:H:219:ASN:N	2.52	0.42
3:G:106:ASN:C	3:G:107:GLU:HG2	2.44	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:OD1	1:E:477:ASP:N	2.52	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:29:TYR:OH	2:H:29:TYR:OH[1_554]	2.05	0.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:43:ASN:ND2	2:H:31:VAL:CG1[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
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

5.3.1 Protein backbone

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%)	30	60
2	B	285/296 (96%)	276 (97%)	9 (3%)	0	100	100
2	D	285/296 (96%)	269 (94%)	15 (5%)	1 (0%)	30	60
2	F	285/296 (96%)	277 (97%)	8 (3%)	0	100	100
2	H	285/296 (96%)	270 (95%)	14 (5%)	1 (0%)	30	60
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%)	43	71

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 ⓘ

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%)	196 (93%)	15 (7%)	13	40
1	E	212/232 (91%)	197 (93%)	15 (7%)	13	40
2	B	263/270 (97%)	252 (96%)	11 (4%)	26	51
2	D	263/270 (97%)	244 (93%)	19 (7%)	13	40
2	F	263/270 (97%)	252 (96%)	11 (4%)	26	51
2	H	263/270 (97%)	244 (93%)	19 (7%)	13	40
3	C	130/138 (94%)	126 (97%)	4 (3%)	35	57
3	G	130/138 (94%)	126 (97%)	4 (3%)	35	57
All	All	1735/1820 (95%)	1637 (94%)	98 (6%)	18	45

All (98) 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	492	GLU
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	80	HIS
2	B	84	THR
2	B	123	VAL
2	B	175	LEU

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Mol	Chain	Res	Type
2	B	186	ARG
2	B	193	ARG
2	B	207	ILE
2	B	223	VAL
2	B	228	SER
2	B	247	ASP
2	B	292	ASN
3	C	18	ILE
3	C	26	ASN
3	C	78	LEU
3	C	122	LEU
2	D	132	LEU
2	D	160	ILE
2	D	166	VAL
2	D	175	LEU
2	D	181	THR
2	D	207	ILE
2	D	210	ASN
2	D	212	VAL
2	D	218	SER
2	D	219	ASN
2	D	225	VAL
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
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	492	GLU
1	E	493	ASN
1	E	507	LEU
1	E	508	MET

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Mol	Chain	Res	Type
1	E	519	ASN
1	E	546	ASN
1	E	552	THR
2	F	80	HIS
2	F	84	THR
2	F	123	VAL
2	F	175	LEU
2	F	186	ARG
2	F	193	ARG
2	F	207	ILE
2	F	223	VAL
2	F	228	SER
2	F	247	ASP
2	F	292	ASN
3	G	18	ILE
3	G	26	ASN
3	G	78	LEU
3	G	122	LEU
2	H	132	LEU
2	H	160	ILE
2	H	166	VAL
2	H	175	LEU
2	H	181	THR
2	H	207	ILE
2	H	210	ASN
2	H	212	VAL
2	H	218	SER
2	H	219	ASN
2	H	225	VAL
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	392	ASN

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Mol	Chain	Res	Type
1	A	534	HIS
1	A	579	ASN
1	A	588	HIS
2	B	115	ASN
2	B	152	ASN
2	B	202	GLN
2	B	236	GLN
2	B	289	ASN
3	C	95	ASN
3	C	131	ASN
3	C	138	ASN
2	D	86	GLN
2	D	134	ASN
2	D	279	ASN
1	E	392	ASN
1	E	421	ASN
1	E	496	GLN
1	E	519	ASN
1	E	524	HIS
1	E	588	HIS
2	F	152	ASN
2	F	202	GLN
2	F	236	GLN
2	F	289	ASN
3	G	95	ASN
3	G	131	ASN
3	G	138	ASN
2	H	86	GLN
2	H	279	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.38	12 (5%)	32 22	99, 150, 221, 268	3 (1%)
1	E	229/254 (90%)	0.49	21 (9%)	14 13	86, 146, 212, 274	3 (1%)
2	B	286/296 (96%)	0.38	18 (6%)	26 18	85, 131, 183, 234	0
2	D	286/296 (96%)	0.31	12 (4%)	40 26	99, 207, 325, 398	0
2	F	286/296 (96%)	0.05	4 (1%)	73 48	93, 145, 203, 256	0
2	H	286/296 (96%)	0.40	20 (6%)	22 17	94, 195, 353, 422	0
3	C	139/147 (94%)	-0.04	0	100 100	107, 154, 194, 221	0
3	G	139/147 (94%)	-0.16	2 (1%)	73 48	109, 147, 192, 208	0
All	All	1879/1986 (94%)	0.27	89 (4%)	36 24	85, 152, 303, 422	6 (0%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	454	ALA	7.1
1	E	575	ILE	5.4
2	B	272	GLY	5.0
2	B	274	ALA	4.9
2	H	157	ILE	4.7
2	H	167	VAL	4.5
1	E	435	ILE	4.4
1	A	616	TYR	4.2
2	B	173	THR	3.9
2	H	114	PRO	3.8
2	H	190	TRP	3.7
2	B	172	VAL	3.7
1	E	382	ILE	3.6
1	A	457	TYR	3.6
1	E	481	TYR	3.4
2	H	175	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	454	ALA	3.2
1	A	496	GLN	3.2
1	E	384	GLU	3.2
2	H	143	GLU	3.1
2	B	122	THR	3.1
1	E	455	ILE	3.1
2	B	39	GLN	3.1
1	A	575	ILE	3.1
2	H	264	LEU	3.0
2	D	157	ILE	2.9
2	B	270	ALA	2.9
2	H	203	PHE	2.9
2	F	20	CYS	2.9
1	E	386	ASN	2.9
1	E	477	ASP	2.8
2	B	228	SER	2.8
2	B	45	LEU	2.8
2	D	175	LEU	2.8
2	B	161	LEU	2.8
2	H	240	ILE	2.8
2	H	241	ASN	2.7
2	B	289	ASN	2.6
2	D	290	ILE	2.6
1	A	613	LEU	2.6
1	E	393	TYR	2.5
1	E	456	ASN	2.5
2	D	289	ASN	2.5
2	B	78	PRO	2.5
1	E	479	ASN	2.5
3	G	106	ASN	2.5
2	D	264	LEU	2.5
2	F	249	THR	2.5
1	A	532	ASP	2.4
2	B	139	LYS	2.4
2	B	294	PRO	2.4
1	E	409	LEU	2.4
2	D	143	GLU	2.4
1	A	617	ASN	2.3
2	H	41	THR	2.3
1	E	497	PHE	2.3
2	H	242	PRO	2.3
2	H	28	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	159	PRO	2.3
2	H	159	PRO	2.3
2	H	194	TYR	2.2
2	H	10	SER	2.2
2	H	32	ALA	2.2
2	H	172	VAL	2.2
2	F	29	TYR	2.2
2	D	46	GLU	2.2
1	A	400	ILE	2.1
2	B	204	PHE	2.1
2	D	11	LEU	2.1
1	E	413	ASN	2.1
3	G	94	VAL	2.1
1	E	395	TYR	2.1
2	D	240	ILE	2.1
2	F	292	ASN	2.1
1	E	402	ASN	2.1
2	B	125	ARG	2.1
1	E	385	ILE	2.1
2	H	155	CYS	2.1
2	B	175	LEU	2.1
2	H	177	VAL	2.1
2	D	288	TRP	2.0
1	A	455	ILE	2.0
1	A	603	ILE	2.0
1	A	434	ALA	2.0
1	E	547	PHE	2.0
2	D	161	LEU	2.0
1	E	404	ASN	2.0
2	B	128	LYS	2.0
1	E	428	SER	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.