



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:15 PM UTC

PDB ID : 6IGF / pdb_00006igf
Title : Crystal structure of Human Papillomavirus type 52 pentamer
Authors : Li, Z.H.; Song, S.; He, M.Z.; Gu, Y.; Li, S.W.
Deposited on : 2018-09-25
Resolution : 2.75 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

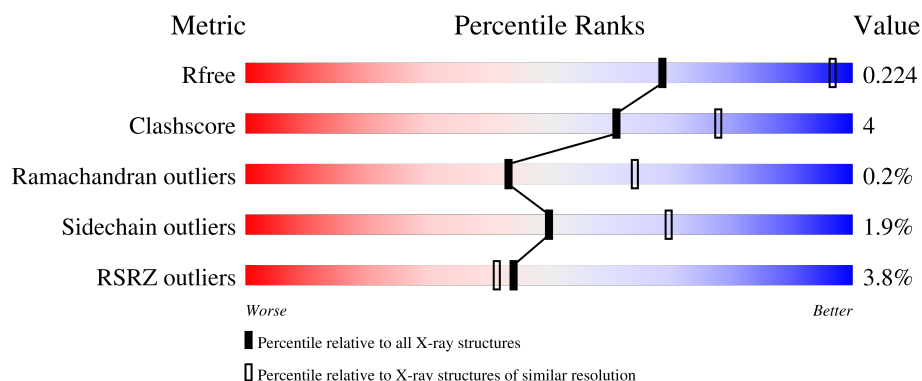
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	529	4% 69% 9% 22%
1	B	529	4% 72% 7% 20%
1	C	529	2% 72% 8% 19%
1	D	529	2% 68% 9% 22%
1	E	529	2% 74% 8% 19%

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Mol	Chain	Length	Quality of chain
1	F	529	4% 69%10%21%
1	G	529	3% 68%10%21%
1	H	529	3% 68%10%21%
1	I	529	2% 70%8%21%
1	J	529	3% 70%9%21%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 33255 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.

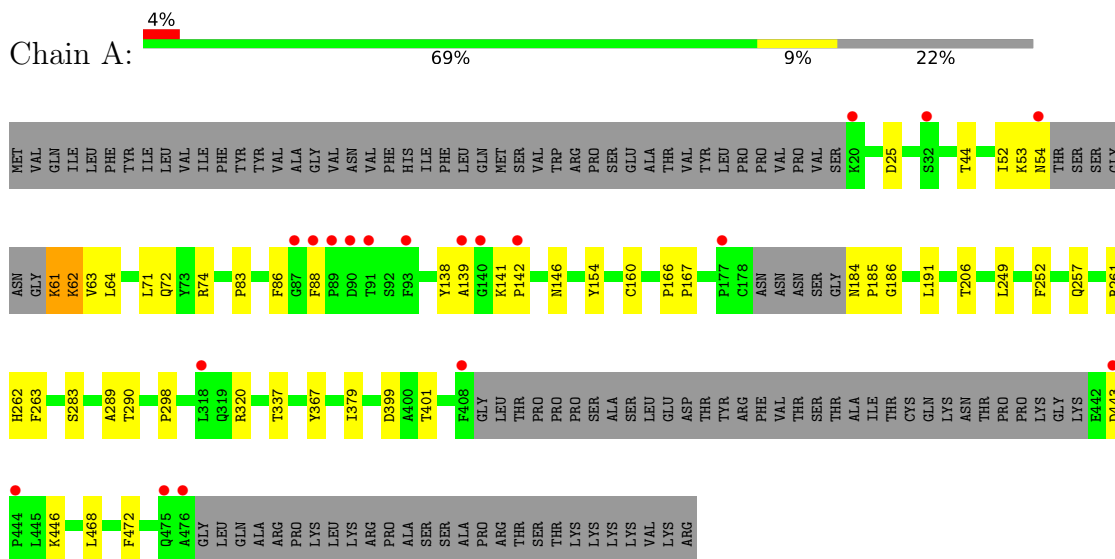
- Molecule 1 is a protein called Major capsid protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	1	0
			3293	2105	544	621	23			
1	B	421	Total	C	N	O	S	0	1	0
			3344	2139	552	631	22			
1	C	427	Total	C	N	O	S	0	0	0
			3377	2149	562	644	22			
1	D	414	Total	C	N	O	S	0	0	0
			3291	2103	545	621	22			
1	E	429	Total	C	N	O	S	0	1	0
			3400	2168	567	642	23			
1	F	417	Total	C	N	O	S	0	1	0
			3316	2119	548	626	23			
1	G	418	Total	C	N	O	S	0	1	0
			3322	2120	550	630	22			
1	H	416	Total	C	N	O	S	0	0	0
			3305	2111	547	625	22			
1	I	416	Total	C	N	O	S	0	0	0
			3300	2108	547	623	22			
1	J	417	Total	C	N	O	S	0	0	0
			3307	2113	548	625	21			

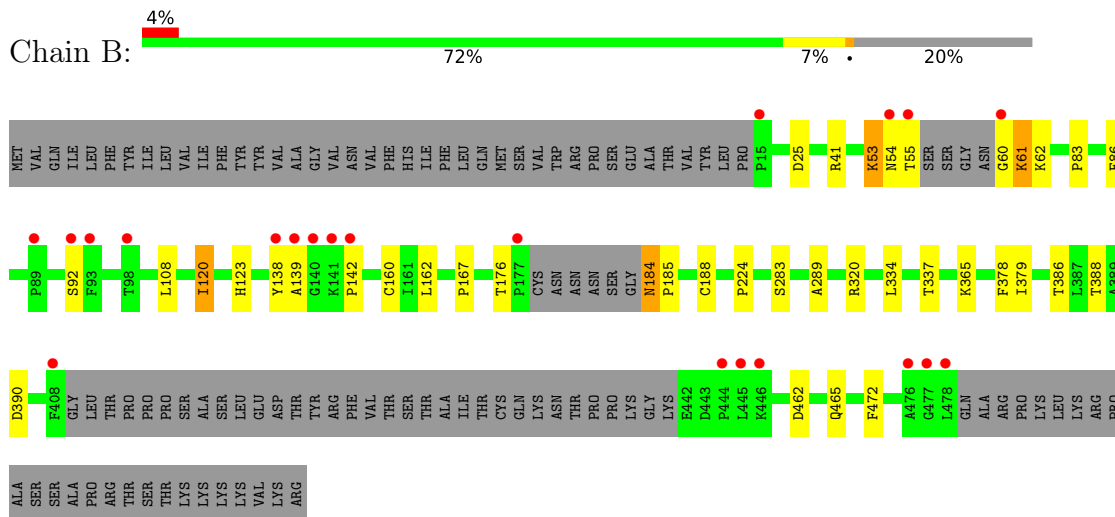
3 Residue-property plots

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: Major capsid protein L1

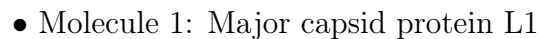


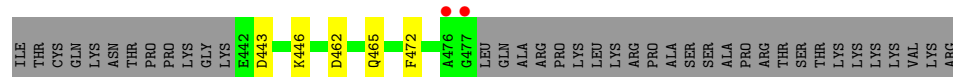
- Molecule 1: Major capsid protein L1



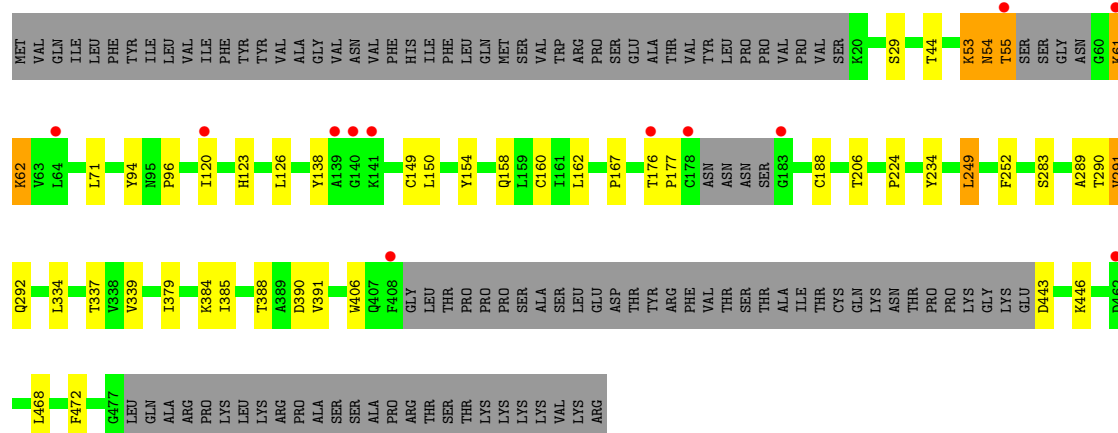
- Molecule 1: Major capsid protein L1



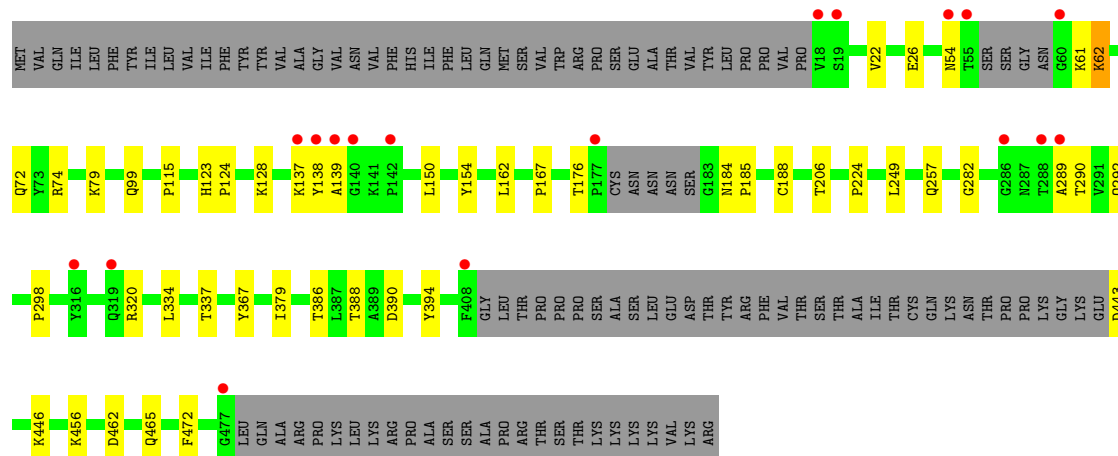




• Molecule 1: Major capsid protein L1



• Molecule 1: Major capsid protein L1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	306.77Å 105.07Å 196.90Å 90.00° 125.80° 90.00°	Depositor
Resolution (Å)	42.95 – 2.75 42.95 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (42.95-2.75) 99.8 (42.95-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.187 , 0.235 (Not available) , 0.224	Depositor DCC
R_{free} test set	6708 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	43.8	Xtriage
Anisotropy	0.865	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	33255	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.30	1/3381 (0.0%)	0.53	1/4578 (0.0%)
1	B	0.29	0/3434	0.50	0/4652
1	C	0.25	0/3464	0.50	0/4693
1	D	0.30	0/3376	0.53	0/4571
1	E	0.31	0/3491	0.51	0/4730
1	F	0.28	0/3404	0.50	0/4609
1	G	0.32	0/3411	0.56	1/4620 (0.0%)
1	H	0.28	0/3390	0.50	0/4590
1	I	0.30	0/3385	0.54	1/4583 (0.0%)
1	J	0.32	0/3392	0.56	0/4593
All	All	0.30	1/34128 (0.0%)	0.52	3/46219 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	166	PRO	CA-C	-7.72	1.47	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	PRO	O-C-N	-8.35	117.22	121.15
1	I	53	LYS	N-CA-C	6.33	113.97	108.78
1	G	71	LEU	CA-CB-CG	-5.18	98.16	116.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	139	ALA	Peptide

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	3293	0	3191	32	0
1	B	3344	0	3248	27	1
1	C	3377	0	3262	24	0
1	D	3291	0	3188	35	1
1	E	3400	0	3300	23	0
1	F	3316	0	3215	39	1
1	G	3322	0	3216	38	0
1	H	3305	0	3199	42	0
1	I	3300	0	3196	33	0
1	J	3307	0	3205	31	1
All	All	33255	0	32220	275	2

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 4.

All (275) 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:A:54:ASN:HB2	1:A:64:LEU:HD12	1.54	0.89
1:J:79:LYS:HE2	1:J:456:LYS:HE3	1.56	0.87
1:B:120:ILE:HD12	1:E:298:PRO:HB3	1.54	0.87
1:A:25:ASP:OD2	1:A:320:ARG:NH1	2.11	0.84
1:G:443:ASP:HB3	1:G:446:LYS:HG3	1.61	0.82
1:F:142:PRO:O	1:F:146:ASN:ND2	2.18	0.77
1:F:72:GLN:OE1	1:F:74:ARG:NH2	2.18	0.76
1:G:286:GLY:O	1:G:288:THR:N	2.19	0.75
1:J:388:THR:OG1	1:J:390:ASP:OD1	2.05	0.74
1:D:25:ASP:OD2	1:D:320:ARG:NH1	2.22	0.73
1:E:379:ILE:HD13	1:E:472:PHE:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:54:ASN:HD22	1:I:55:THR:H	1.35	0.72
1:I:388:THR:OG1	1:I:390:ASP:OD1	2.08	0.72
1:B:54:ASN:OD1	1:B:55:THR:N	2.23	0.71
1:I:162:LEU:HD11	1:I:334:LEU:HD12	1.71	0.71
1:E:79:LYS:HE2	1:E:456:LYS:HE3	1.73	0.70
1:C:370:HIS:NE2	1:C:372:GLU:OE2	2.25	0.69
1:B:162:LEU:HD11	1:B:334:LEU:HD12	1.74	0.69
1:H:162:LEU:HD21	1:H:334:LEU:HD12	1.74	0.67
1:C:162:LEU:HD11	1:C:334:LEU:HD12	1.77	0.67
1:C:443:ASP:HB3	1:C:446:LYS:HG3	1.77	0.66
1:H:443:ASP:HB3	1:H:446:LYS:HG3	1.78	0.65
1:F:298:PRO:HB3	1:H:120:ILE:HD12	1.78	0.65
1:B:379:ILE:HD13	1:B:472:PHE:HB2	1.79	0.65
1:F:120:ILE:HD12	1:G:298:PRO:HB3	1.79	0.64
1:G:379:ILE:HD13	1:G:472:PHE:HB2	1.80	0.64
1:D:79:LYS:HE2	1:D:456:LYS:HE3	1.79	0.63
1:C:388:THR:OG1	1:C:390:ASP:OD1	2.19	0.61
1:H:283:SER:O	1:H:289:ALA:HB2	2.01	0.60
1:D:236:ASP:OD2	1:E:41:ARG:NH2	2.35	0.60
1:F:260:VAL:HG11	1:H:120:ILE:HD11	1.83	0.60
1:I:443:ASP:HB3	1:I:446:LYS:HE3	1.82	0.60
1:B:365:LYS:HG2	1:E:269:THR:OG1	2.01	0.60
1:A:443:ASP:HB3	1:A:446:LYS:HG3	1.85	0.59
1:B:120:ILE:HD11	1:E:260:VAL:HG11	1.84	0.58
1:C:379:ILE:HD13	1:C:472:PHE:HB2	1.85	0.58
1:D:54:ASN:CA	1:D:64:LEU:HD11	2.32	0.58
1:J:22:VAL:HG22	1:J:394:TYR:CE2	2.39	0.58
1:J:184:ASN:HB2	1:J:185:PRO:HD2	1.85	0.57
1:H:370:HIS:NE2	1:H:372:GLU:OE2	2.37	0.57
1:G:146:ASN:O	1:J:137:LYS:HE2	2.04	0.57
1:G:146:ASN:HB3	1:J:137:LYS:NZ	2.20	0.57
1:D:176:THR:HG22	1:D:177:PRO:HD2	1.87	0.56
1:F:167:PRO:HG3	1:F:337:THR:OG1	2.05	0.56
1:F:298:PRO:HB3	1:H:120:ILE:CD1	2.35	0.56
1:J:379:ILE:HD13	1:J:472:PHE:HB2	1.88	0.56
1:I:379:ILE:HD13	1:I:472:PHE:HB2	1.89	0.55
1:E:283:SER:O	1:E:289:ALA:HB2	2.06	0.55
1:A:72:GLN:OE1	1:A:74:ARG:NH2	2.40	0.55
1:A:53:LYS:HD3	1:A:61:LYS:HG2	1.89	0.55
1:A:184:ASN:HB2	1:A:185:PRO:HD3	1.89	0.55
1:J:167:PRO:HG3	1:J:337:THR:OG1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:ASN:OD1	1:D:55:THR:N	2.41	0.54
1:C:108:LEU:HD22	1:C:162:LEU:HD22	1.90	0.54
1:I:126:LEU:HD23	1:I:150:LEU:HD12	1.90	0.54
1:A:186:GLY:O	1:C:367:TYR:OH	2.25	0.54
1:G:71:LEU:HD22	1:G:206:THR:HG22	1.90	0.54
1:B:462:ASP:OD2	1:B:465:GLN:HG2	2.09	0.53
1:D:167:PRO:HG3	1:D:337:THR:OG1	2.08	0.53
1:H:390:ASP:OD1	1:H:391:VAL:N	2.41	0.53
1:J:22:VAL:HB	1:J:26:GLU:OE1	2.07	0.53
1:C:160:CYS:HA	1:C:337:THR:O	2.09	0.53
1:C:113:GLY:HA3	1:C:373:GLU:CD	2.34	0.53
1:F:22:VAL:HG22	1:F:394:TYR:CE2	2.44	0.53
1:G:167:PRO:HG3	1:G:337:THR:OG1	2.08	0.53
1:F:25:ASP:OD2	1:F:320:ARG:NH1	2.39	0.52
1:D:269:THR:OG1	1:E:365:LYS:HG2	2.09	0.52
1:A:298:PRO:HB3	1:C:120:ILE:HD12	1.92	0.52
1:F:108:LEU:HD22	1:F:162:LEU:HD22	1.92	0.52
1:F:188:CYS:HB2	1:H:367:TYR:CD2	2.45	0.52
1:F:120:ILE:HD11	1:G:263:PHE:CD2	2.45	0.52
1:H:298:PRO:HB3	1:I:120:ILE:CD1	2.40	0.52
1:H:379:ILE:HD13	1:H:472:PHE:HB2	1.91	0.52
1:D:138:TYR:CE2	1:D:292:GLN:HG3	2.45	0.51
1:G:146:ASN:HB3	1:J:137:LYS:HZ1	1.74	0.51
1:J:154:TYR:CD1	1:J:206:THR:HB	2.46	0.51
1:A:52:ILE:HG22	1:A:54:ASN:ND2	2.26	0.51
1:D:144:ILE:HD11	1:E:360:LYS:HG2	1.92	0.51
1:D:443:ASP:HB3	1:D:446:LYS:HE3	1.93	0.51
1:F:54:ASN:HB2	1:F:62:LYS:HB3	1.93	0.51
1:A:167:PRO:HG3	1:A:337:THR:OG1	2.11	0.50
1:H:54:ASN:HD21	1:H:61:LYS:HB2	1.76	0.50
1:D:54:ASN:CB	1:D:64:LEU:HD11	2.40	0.50
1:F:154:TYR:CD1	1:F:206:THR:HB	2.46	0.50
1:H:388:THR:OG1	1:H:390:ASP:OD1	2.29	0.50
1:C:154:TYR:CD1	1:C:206:THR:HB	2.47	0.50
1:H:136:ASN:ND2	1:I:149:CYS:HB3	2.26	0.50
1:H:162:LEU:HD13	1:H:250:PHE:HD2	1.77	0.50
1:I:283:SER:O	1:I:289:ALA:HB2	2.11	0.50
1:I:167:PRO:HG3	1:I:337:THR:OG1	2.12	0.50
1:F:379:ILE:HD13	1:F:472:PHE:HB2	1.95	0.49
1:A:249:LEU:HD21	1:A:252:PHE:HB3	1.94	0.49
1:C:123:HIS:HB2	1:C:224:PRO:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:41:ARG:NH2	1:G:236:ASP:OD2	2.46	0.49
1:F:443:ASP:HB3	1:F:446:LYS:HE3	1.94	0.49
1:D:462:ASP:OD2	1:D:465:GLN:HG2	2.12	0.49
1:F:317:TRP:NE1	1:F:475:GLN:OE1	2.46	0.49
1:A:257:GLN:HA	1:C:305:VAL:O	2.13	0.49
1:G:469:GLY:HA2	1:G:472:PHE:HB3	1.94	0.48
1:C:77:ARG:NH2	1:C:443:ASP:OD2	2.43	0.48
1:H:125:LEU:HD13	1:H:147:ARG:NH2	2.28	0.48
1:I:154:TYR:CD1	1:I:206:THR:HB	2.47	0.48
1:J:22:VAL:HG22	1:J:394:TYR:CZ	2.48	0.48
1:I:54:ASN:HD22	1:I:55:THR:N	2.09	0.48
1:I:62:LYS:HE2	1:I:62:LYS:HA	1.96	0.48
1:G:54:ASN:HD21	1:G:62:LYS:HD2	1.79	0.48
1:H:154:TYR:CD1	1:H:206:THR:HB	2.48	0.48
1:H:462:ASP:OD2	1:H:465:GLN:HG2	2.13	0.48
1:I:94:TYR:CZ	1:I:96:PRO:HG3	2.48	0.48
1:F:443:ASP:HB3	1:F:446:LYS:HG3	1.95	0.48
1:A:160[A]:CYS:HA	1:A:337:THR:O	2.13	0.48
1:E:379:ILE:HD13	1:E:472:PHE:CB	2.43	0.48
1:A:138:TYR:HA	1:A:139:ALA:HA	1.61	0.48
1:E:388:THR:OG1	1:E:390:ASP:OD1	2.26	0.48
1:J:282:GLY:HA3	1:J:289:ALA:HB3	1.94	0.48
1:A:142:PRO:O	1:A:146:ASN:ND2	2.40	0.47
1:F:116:LEU:HD22	1:G:256:GLU:HB2	1.96	0.47
1:D:22:VAL:HG22	1:D:394:TYR:CE2	2.49	0.47
1:J:162:LEU:HD11	1:J:334:LEU:HD21	1.95	0.47
1:B:54:ASN:HB3	1:B:62:LYS:HB3	1.96	0.47
1:G:184:ASN:HB2	1:G:187:ASP:OD1	2.15	0.47
1:I:291:VAL:HG12	1:J:124:PRO:HB2	1.96	0.47
1:D:54:ASN:HA	1:D:64:LEU:HD21	1.97	0.47
1:F:256:GLU:HB2	1:H:116:LEU:HD22	1.97	0.47
1:G:154:TYR:CD1	1:G:206:THR:HB	2.49	0.47
1:B:167:PRO:HG3	1:B:337:THR:OG1	2.14	0.47
1:E:123:HIS:HB3	1:E:126:LEU:HB2	1.96	0.47
1:E:162:LEU:HD11	1:E:334:LEU:HD21	1.97	0.47
1:F:191:LEU:HD11	1:H:349:LEU:HD11	1.95	0.47
1:J:462:ASP:OD2	1:J:465:GLN:HG2	2.15	0.47
1:D:160:CYS:HA	1:D:337:THR:O	2.14	0.47
1:I:390:ASP:OD1	1:I:391:VAL:N	2.48	0.47
1:A:71:LEU:HG	1:A:154:TYR:HD2	1.80	0.46
1:D:29:SER:HB2	1:D:384:LYS:HG3	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:ASN:HA	1:D:64:LEU:HD11	1.97	0.46
1:H:138:TYR:HA	1:H:139:ALA:HA	1.70	0.46
1:D:53:LYS:HA	1:D:62:LYS:O	2.14	0.46
1:D:54:ASN:HB2	1:D:64:LEU:HD11	1.98	0.46
1:B:53:LYS:HZ2	1:B:61:LYS:HE2	1.80	0.46
1:F:61:LYS:HD2	1:F:61:LYS:O	2.15	0.46
1:E:72:GLN:OE1	1:E:74:ARG:NH2	2.49	0.46
1:J:54:ASN:HD22	1:J:62:LYS:HG2	1.81	0.46
1:A:263:PHE:CD2	1:C:120:ILE:HD11	2.51	0.46
1:G:148:GLU:OE2	1:J:137:LYS:HE3	2.16	0.46
1:C:167:PRO:HG3	1:C:337:THR:OG1	2.15	0.46
1:H:61:LYS:HB2	1:H:62:LYS:H	1.57	0.46
1:A:160[B]:CYS:HA	1:A:337:THR:O	2.16	0.46
1:B:138:TYR:HA	1:B:139:ALA:HA	1.55	0.46
1:J:72:GLN:OE1	1:J:74:ARG:NH2	2.48	0.46
1:A:141:LYS:HB3	1:A:142:PRO:HD2	1.98	0.45
1:B:83:PRO:HA	1:B:86:PHE:HB2	1.98	0.45
1:B:160[A]:CYS:HA	1:B:337:THR:O	2.17	0.45
1:B:283:SER:O	1:B:289:ALA:HB2	2.16	0.45
1:F:305:VAL:O	1:G:257:GLN:HA	2.16	0.45
1:H:160:CYS:HA	1:H:337:THR:O	2.16	0.45
1:D:123:HIS:HB2	1:D:224:PRO:HA	1.98	0.45
1:G:55:THR:HA	1:G:56:SER:HA	1.65	0.45
1:H:108:LEU:HD22	1:H:162:LEU:HG	1.98	0.45
1:C:162:LEU:HD13	1:C:336:VAL:HG22	1.99	0.45
1:C:284:ASN:O	1:C:285:SER:OG	2.25	0.45
1:F:138:TYR:HA	1:F:139:ALA:HA	1.60	0.45
1:F:263:PHE:CD2	1:H:120:ILE:HD13	2.51	0.45
1:F:283:SER:O	1:F:289:ALA:HB2	2.15	0.45
1:B:25:ASP:OD2	1:B:320:ARG:NH1	2.33	0.45
1:E:71:LEU:HG	1:E:154:TYR:HD2	1.80	0.45
1:G:138:TYR:CE2	1:G:292:GLN:HG3	2.51	0.45
1:B:53:LYS:NZ	1:B:61:LYS:HE2	2.32	0.45
1:H:162:LEU:HD13	1:H:250:PHE:CD2	2.52	0.45
1:I:123:HIS:HB2	1:I:224:PRO:HA	1.98	0.45
1:I:160:CYS:HA	1:I:337:THR:O	2.16	0.45
1:G:120:ILE:CD1	1:J:298:PRO:HB3	2.47	0.45
1:H:136:ASN:HD22	1:I:149:CYS:HB3	1.81	0.45
1:I:249:LEU:HD21	1:I:252:PHE:HB3	1.99	0.45
1:C:129:PHE:HE1	1:C:146:ASN:HD22	1.65	0.45
1:D:379:ILE:HD12	1:D:468:LEU:HG	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:ALA:HB1	1:D:455:LEU:HD13	1.98	0.44
1:A:83:PRO:HA	1:A:86:PHE:HB2	1.98	0.44
1:A:379:ILE:HD12	1:A:468:LEU:HG	1.99	0.44
1:H:385:ILE:HD12	1:H:406:TRP:CH2	2.53	0.44
1:J:138:TYR:HA	1:J:139:ALA:HA	1.63	0.44
1:E:138:TYR:HA	1:E:139:ALA:HA	1.60	0.44
1:H:123:HIS:HB2	1:H:224:PRO:HA	1.98	0.44
1:H:240:MET:O	1:H:243:GLU:HG2	2.18	0.44
1:J:99:GLN:HG2	1:J:386:THR:HA	1.99	0.44
1:A:261:ARG:HG3	1:A:262:HIS:CD2	2.52	0.44
1:F:257:GLN:HA	1:H:305:VAL:O	2.17	0.44
1:H:385:ILE:HD12	1:H:406:TRP:HH2	1.83	0.44
1:I:29:SER:HB2	1:I:384:LYS:HG3	1.99	0.44
1:J:443:ASP:HA	1:J:446:LYS:HE3	1.99	0.44
1:G:54:ASN:HB3	1:G:58:GLY:HA3	1.98	0.44
1:I:234:TYR:CD1	1:J:115:PRO:HB3	2.52	0.44
1:I:62:LYS:HA	1:I:62:LYS:CE	2.47	0.44
1:J:184:ASN:HB2	1:J:185:PRO:CD	2.48	0.44
1:G:42:LEU:HB2	1:G:374:PHE:HB2	2.00	0.44
1:G:83:PRO:HA	1:G:86:PHE:HB2	1.99	0.44
1:H:176:THR:N	1:H:177:PRO:CD	2.81	0.44
1:G:161:ILE:HB	1:G:337:THR:HB	2.00	0.43
1:J:123:HIS:HB2	1:J:224:PRO:HA	2.00	0.43
1:B:41:ARG:NH2	1:E:236:ASP:OD2	2.52	0.43
1:G:291:VAL:HG12	1:G:292:GLN:O	2.18	0.43
1:B:54:ASN:ND2	1:B:62:LYS:H	2.16	0.43
1:H:167:PRO:HG3	1:H:337:THR:OG1	2.18	0.43
1:H:298:PRO:HB3	1:I:120:ILE:HD12	2.01	0.43
1:B:386:THR:HG22	1:B:388:THR:HG23	2.00	0.43
1:G:184:ASN:N	1:G:185:PRO:HD3	2.34	0.43
1:G:126:LEU:HD23	1:G:150:LEU:HD12	2.01	0.43
1:G:379:ILE:CD1	1:G:468:LEU:HG	2.49	0.43
1:F:30:ARG:HB3	1:F:381:GLN:NE2	2.33	0.43
1:G:43:LEU:HD23	1:G:43:LEU:HA	1.84	0.43
1:B:184:ASN:HA	1:B:185:PRO:HD3	1.91	0.43
1:C:217:GLN:HA	1:D:350:CYS:HB3	2.01	0.43
1:D:35:TYR:CZ	1:D:461:ALA:HB2	2.54	0.43
1:C:54:ASN:OD1	1:C:62:LYS:HD3	2.18	0.42
1:D:249:LEU:HD21	1:D:252:PHE:HB3	2.01	0.42
1:D:379:ILE:HD13	1:D:472:PHE:HB2	2.00	0.42
1:F:124:PRO:HB2	1:G:291:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:188:CYS:HB2	1:H:367:TYR:CE2	2.55	0.42
1:H:174:LYS:HG2	1:H:175:GLY:O	2.19	0.42
1:A:64:LEU:HD23	1:A:64:LEU:HA	1.85	0.42
1:B:60:GLY:O	1:B:61:LYS:HD2	2.19	0.42
1:D:129:PHE:CZ	1:D:142:PRO:HA	2.55	0.42
1:A:191:LEU:HD23	1:A:191:LEU:HA	1.91	0.42
1:B:388:THR:OG1	1:B:390:ASP:OD1	2.35	0.42
1:D:199:GLN:NE2	1:D:448:TYR:HD1	2.18	0.42
1:G:305:VAL:O	1:J:257:GLN:HA	2.19	0.42
1:I:379:ILE:HD11	1:I:468:LEU:O	2.19	0.42
1:A:399:ASP:OD1	1:A:401:THR:HG22	2.19	0.42
1:D:154:TYR:CD1	1:D:206:THR:HB	2.55	0.42
1:D:261:ARG:HG3	1:D:262:HIS:CD2	2.54	0.42
1:F:146:ASN:HD22	1:H:361:ASN:HD21	1.68	0.42
1:H:30:ARG:HB3	1:H:381:GLN:NE2	2.35	0.42
1:I:61:LYS:HB3	1:I:61:LYS:HE2	1.85	0.42
1:B:120:ILE:CD1	1:E:298:PRO:HB3	2.36	0.42
1:E:154:TYR:CD1	1:E:206:THR:HB	2.55	0.42
1:F:37:ALA:HB1	1:F:455:LEU:HD13	2.02	0.42
1:F:249:LEU:HD21	1:F:252:PHE:HB3	2.02	0.42
1:B:379:ILE:CD1	1:B:472:PHE:HB2	2.49	0.41
1:C:257:GLN:HA	1:D:305:VAL:O	2.19	0.41
1:E:100:ARG:HD3	1:E:100:ARG:HA	1.93	0.41
1:E:379:ILE:HD12	1:E:468:LEU:HG	2.02	0.41
1:H:128:LYS:HD2	1:H:150:LEU:HD11	2.02	0.41
1:B:123:HIS:HB2	1:B:224:PRO:HA	2.01	0.41
1:C:379:ILE:HD11	1:C:468:LEU:O	2.20	0.41
1:G:24:THR:HA	1:G:27:TYR:CE1	2.55	0.41
1:G:379:ILE:HD12	1:G:468:LEU:HG	2.01	0.41
1:I:138:TYR:CE2	1:I:292:GLN:HG3	2.54	0.41
1:D:64:LEU:CD1	1:D:64:LEU:N	2.84	0.41
1:I:71:LEU:HG	1:I:154:TYR:HD2	1.85	0.41
1:A:71:LEU:HD13	1:A:71:LEU:HA	1.93	0.41
1:J:138:TYR:CZ	1:J:292:GLN:HG3	2.56	0.41
1:A:86:PHE:O	1:A:88:PHE:N	2.53	0.41
1:A:283:SER:O	1:A:289:ALA:HB2	2.20	0.41
1:F:271:GLY:HA3	1:H:367:TYR:CE2	2.56	0.41
1:G:249:LEU:HD21	1:G:252:PHE:HB3	2.03	0.41
1:G:367:TYR:CD2	1:J:188:CYS:HB2	2.56	0.41
1:A:62:LYS:HB2	1:A:62:LYS:HE3	1.57	0.41
1:A:367:TYR:CD2	1:B:188:CYS:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:349:LEU:HD22	1:G:216:LEU:HB3	2.02	0.41
1:I:158:GLN:HA	1:I:339:VAL:O	2.20	0.41
1:I:188:CYS:HB2	1:J:367:TYR:CD2	2.56	0.41
1:A:154:TYR:CD1	1:A:206:THR:HB	2.56	0.41
1:A:379:ILE:HD13	1:A:472:PHE:HB2	2.02	0.41
1:F:360:LYS:HG2	1:G:144:ILE:HD12	2.02	0.40
1:I:123:HIS:HB3	1:I:126:LEU:HB2	2.01	0.40
1:B:108:LEU:HD13	1:B:378:PHE:CE2	2.55	0.40
1:F:162:LEU:HD11	1:F:334:LEU:HD21	2.02	0.40
1:H:177:PRO:HD2	1:H:190:PRO:CG	2.52	0.40
1:I:385:ILE:HD12	1:I:406:TRP:HH2	1.85	0.40
1:E:160[B]:CYS:HA	1:E:337:THR:O	2.21	0.40
1:J:128:LYS:HD2	1:J:150:LEU:HD11	2.04	0.40
1:C:80:LEU:HD11	1:C:334:LEU:HD22	2.04	0.40
1:D:77:ARG:HD3	1:D:452:GLU:OE1	2.20	0.40
1:D:257:GLN:HA	1:E:305:VAL:O	2.22	0.40
1:F:394:TYR:CD1	1:F:394:TYR:C	3.00	0.40
1:I:176:THR:HG22	1:I:177:PRO:HD2	2.04	0.40

All (2) 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:D:284:ASN:ND2	1:F:94:TYR:O[3_555]	1.95	0.25
1:B:92:SER:OG	1:J:320:ARG:NH2[2_556]	2.16	0.04

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	406/529 (77%)	391 (96%)	15 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	414/529 (78%)	401 (97%)	12 (3%)	1 (0%)	43	64
1	C	423/529 (80%)	404 (96%)	19 (4%)	0	100	100
1	D	406/529 (77%)	392 (97%)	14 (3%)	0	100	100
1	E	424/529 (80%)	405 (96%)	18 (4%)	1 (0%)	43	64
1	F	410/529 (78%)	395 (96%)	15 (4%)	0	100	100
1	G	413/529 (78%)	393 (95%)	17 (4%)	3 (1%)	18	34
1	H	408/529 (77%)	391 (96%)	15 (4%)	2 (0%)	24	43
1	I	408/529 (77%)	392 (96%)	16 (4%)	0	100	100
1	J	409/529 (77%)	394 (96%)	15 (4%)	0	100	100
All	All	4121/5290 (78%)	3958 (96%)	156 (4%)	7 (0%)	43	64

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	287	ASN
1	H	177	PRO
1	B	142	PRO
1	E	177	PRO
1	H	176	THR
1	G	142	PRO
1	G	286	GLY

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	368/469 (78%)	363 (99%)	5 (1%)	59	75
1	B	374/469 (80%)	369 (99%)	5 (1%)	61	76
1	C	377/469 (80%)	367 (97%)	10 (3%)	39	62
1	D	367/469 (78%)	358 (98%)	9 (2%)	42	64
1	E	380/469 (81%)	372 (98%)	8 (2%)	47	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	370/469 (79%)	364 (98%)	6 (2%)	55	73
1	G	371/469 (79%)	362 (98%)	9 (2%)	43	65
1	H	368/469 (78%)	363 (99%)	5 (1%)	59	75
1	I	367/469 (78%)	358 (98%)	9 (2%)	42	64
1	J	368/469 (78%)	363 (99%)	5 (1%)	59	75
All	All	3710/4690 (79%)	3639 (98%)	71 (2%)	50	70

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	THR
1	A	61	LYS
1	A	62	LYS
1	A	63	VAL
1	A	290	THR
1	B	53	LYS
1	B	61	LYS
1	B	120	ILE
1	B	176	THR
1	B	184	ASN
1	C	20	LYS
1	C	53	LYS
1	C	54	ASN
1	C	55	THR
1	C	120	ILE
1	C	176	THR
1	C	182	SER
1	C	249	LEU
1	C	269	THR
1	C	290	THR
1	D	44	THR
1	D	53	LYS
1	D	55	THR
1	D	61	LYS
1	D	62	LYS
1	D	64	LEU
1	D	176	THR
1	D	249	LEU
1	D	401	THR
1	E	15	PRO

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Mol	Chain	Res	Type
1	E	61	LYS
1	E	62	LYS
1	E	249	LEU
1	E	284	ASN
1	E	290	THR
1	E	479	GLN
1	E	481	ARG
1	F	44	THR
1	F	61	LYS
1	F	64	LEU
1	F	120	ILE
1	F	184	ASN
1	F	401	THR
1	G	56	SER
1	G	59	ASN
1	G	71	LEU
1	G	78	ILE
1	G	249	LEU
1	G	269	THR
1	G	318	LEU
1	G	345	THR
1	G	474	LEU
1	H	44	THR
1	H	53	LYS
1	H	61	LYS
1	H	162	LEU
1	H	291	VAL
1	I	44	THR
1	I	53	LYS
1	I	54	ASN
1	I	55	THR
1	I	61	LYS
1	I	62	LYS
1	I	249	LEU
1	I	290	THR
1	I	291	VAL
1	J	61	LYS
1	J	62	LYS
1	J	176	THR
1	J	249	LEU
1	J	290	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	B	136	ASN
1	B	184	ASN
1	B	292	GLN
1	C	54	ASN
1	C	361	ASN
1	D	156	GLN
1	D	184	ASN
1	D	333	GLN
1	E	156	GLN
1	E	192	GLN
1	F	54	ASN
1	F	156	GLN
1	F	199	GLN
1	F	257	GLN
1	G	156	GLN
1	G	239	GLN
1	H	136	ASN
1	H	156	GLN
1	H	239	GLN
1	H	292	GLN
1	H	332	ASN
1	H	361	ASN
1	I	136	ASN
1	I	199	GLN
1	I	239	GLN
1	I	465	GLN
1	J	171	HIS

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	413/529 (78%)	0.17	19 (4%) 37 36	28, 55, 113, 200	1 (0%)
1	B	421/529 (79%)	0.04	21 (4%) 34 34	25, 47, 104, 163	1 (0%)
1	C	427/529 (80%)	0.11	11 (2%) 57 55	33, 53, 112, 170	0
1	D	414/529 (78%)	-0.06	13 (3%) 51 49	27, 47, 96, 195	0
1	E	429/529 (81%)	-0.21	13 (3%) 52 50	20, 39, 98, 154	1 (0%)
1	F	417/529 (78%)	0.17	22 (5%) 32 31	25, 51, 111, 166	1 (0%)
1	G	418/529 (79%)	-0.15	16 (3%) 44 41	17, 38, 97, 154	1 (0%)
1	H	416/529 (78%)	0.14	16 (3%) 44 41	29, 53, 105, 151	0
1	I	416/529 (78%)	-0.11	12 (2%) 53 52	24, 43, 93, 169	0
1	J	417/529 (78%)	-0.25	18 (4%) 40 38	20, 36, 92, 150	0
All	All	4188/5290 (79%)	-0.01	161 (3%) 44 41	17, 47, 103, 200	5 (0%)

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	478	LEU	6.8
1	B	478	LEU	6.6
1	F	478	LEU	5.9
1	I	408	PHE	5.8
1	G	286	GLY	5.5
1	J	408	PHE	5.4
1	D	89	PRO	5.0
1	F	139	ALA	4.8
1	D	60	GLY	4.7
1	G	185	PRO	4.6
1	J	289	ALA	4.6
1	F	60	GLY	4.4
1	F	55	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	F	476	ALA	4.3
1	G	285	SER	4.3
1	F	140	GLY	4.2
1	B	55	THR	4.2
1	J	55	THR	4.2
1	A	476	ALA	4.1
1	A	54	ASN	4.1
1	I	139	ALA	4.0
1	J	18	VAL	4.0
1	I	140	GLY	3.9
1	G	177	PRO	3.8
1	B	89	PRO	3.8
1	E	408	PHE	3.8
1	F	178	CYS	3.8
1	D	178	CYS	3.7
1	J	139	ALA	3.7
1	F	477	GLY	3.7
1	H	176	THR	3.7
1	I	55	THR	3.7
1	J	138	TYR	3.7
1	D	183	GLY	3.6
1	H	178	CYS	3.6
1	B	477	GLY	3.6
1	A	88	PHE	3.6
1	D	55	THR	3.5
1	I	183	GLY	3.5
1	F	177	PRO	3.5
1	F	138	TYR	3.4
1	J	177	PRO	3.4
1	J	288	THR	3.4
1	E	318	LEU	3.4
1	B	93	PHE	3.4
1	E	177	PRO	3.3
1	H	60	GLY	3.3
1	H	139	ALA	3.3
1	D	61	LYS	3.2
1	C	55	THR	3.2
1	E	60	GLY	3.2
1	J	142	PRO	3.2
1	B	92	SER	3.2
1	E	142	PRO	3.1
1	B	177	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	287	ASN	3.1
1	A	139	ALA	3.1
1	B	15	PRO	3.0
1	B	476	ALA	3.0
1	E	139	ALA	3.0
1	A	142	PRO	2.9
1	F	20	LYS	2.9
1	J	137	LYS	2.9
1	A	89	PRO	2.9
1	B	140	GLY	2.9
1	H	177	PRO	2.9
1	G	284	ASN	2.9
1	J	140	GLY	2.9
1	A	20	LYS	2.9
1	E	285	SER	2.8
1	H	476	ALA	2.8
1	F	408	PHE	2.8
1	D	177	PRO	2.8
1	A	177	PRO	2.7
1	B	142	PRO	2.7
1	D	142	PRO	2.7
1	A	90	ASP	2.7
1	C	476	ALA	2.7
1	F	318	LEU	2.7
1	F	142	PRO	2.7
1	A	475	GLN	2.6
1	A	140	GLY	2.6
1	J	286	GLY	2.6
1	B	446	LYS	2.6
1	A	93	PHE	2.6
1	B	445	LEU	2.6
1	G	143	GLY	2.5
1	A	444	PRO	2.5
1	B	54	ASN	2.5
1	G	476	ALA	2.5
1	I	141	LYS	2.5
1	B	60	GLY	2.5
1	G	184	ASN	2.5
1	A	87	GLY	2.5
1	J	316	TYR	2.5
1	H	408	PHE	2.5
1	C	140	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	444	PRO	2.4
1	G	316	TYR	2.4
1	F	93	PHE	2.4
1	H	20	LYS	2.4
1	B	139	ALA	2.4
1	I	176	THR	2.4
1	A	318	LEU	2.4
1	B	98	THR	2.4
1	A	443	ASP	2.4
1	H	477	GLY	2.4
1	F	92	SER	2.3
1	G	444	PRO	2.3
1	H	142	PRO	2.3
1	A	91	THR	2.3
1	F	176	THR	2.3
1	H	184	ASN	2.3
1	B	444	PRO	2.3
1	G	20	LYS	2.3
1	H	61	LYS	2.3
1	F	86	PHE	2.3
1	I	64	LEU	2.3
1	H	93	PHE	2.3
1	H	55	THR	2.2
1	C	180	ASN	2.2
1	C	285	SER	2.2
1	B	408	PHE	2.2
1	E	55	THR	2.2
1	C	444	PRO	2.2
1	A	408	PHE	2.2
1	E	178	CYS	2.2
1	F	97	GLU	2.2
1	I	178	CYS	2.2
1	E	140	GLY	2.2
1	H	79	LYS	2.2
1	J	477	GLY	2.2
1	G	176	THR	2.2
1	D	444	PRO	2.2
1	I	61	LYS	2.2
1	A	32	SER	2.2
1	G	56	SER	2.2
1	D	141	LYS	2.1
1	G	55	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	60	GLY	2.1
1	F	393	THR	2.1
1	D	475	GLN	2.1
1	J	319	GLN	2.1
1	F	391	VAL	2.1
1	G	283	SER	2.1
1	J	19	SER	2.1
1	E	481	ARG	2.1
1	E	444	PRO	2.1
1	E	319	GLN	2.1
1	I	120	ILE	2.1
1	I	462	ASP	2.0
1	D	20	LYS	2.0
1	H	137	LYS	2.0
1	C	445	LEU	2.0
1	C	120	ILE	2.0
1	C	477	GLY	2.0
1	B	138	TYR	2.0
1	D	90	ASP	2.0
1	B	141	LYS	2.0
1	C	60	GLY	2.0
1	J	54	ASN	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.