



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:40 PM UTC

PDB ID : 5AZ4 / pdb_00005az4
Title : Crystal structure of a 79KDa fragment of FlgE, the hook protein from *Campylobacter jejuni*
Authors : Samatey, F.A.; Kido, Y.
Deposited on : 2015-09-25
Resolution : 2.45 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

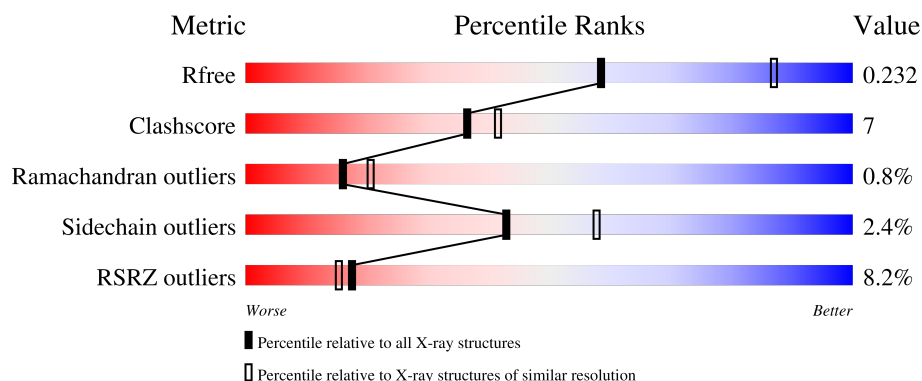
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	741	3% 84% 13% ..
1	B	741	7% 82% 14% ..
1	C	741	12% 81% 15% ..
1	D	741	11% 77% 20% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23180 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 Flagellar hook subunit protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	0	0
			5428	3348	949	1123	8			
1	B	726	Total	C	N	O	S	0	0	0
			5428	3348	949	1123	8			
1	C	726	Total	C	N	O	S	0	0	0
			5428	3348	949	1123	8			
1	D	726	Total	C	N	O	S	0	0	0
			5428	3348	949	1123	8			

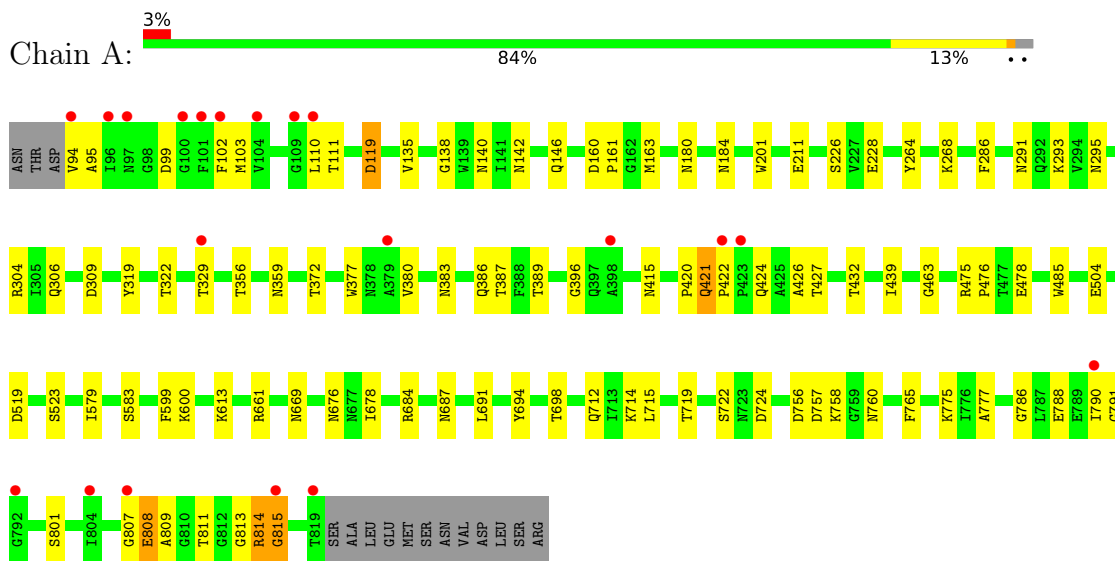
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	372	Total	O	0	0
			372	372		
2	B	417	Total	O	0	0
			417	417		
2	C	388	Total	O	0	0
			388	388		
2	D	291	Total	O	0	0
			291	291		

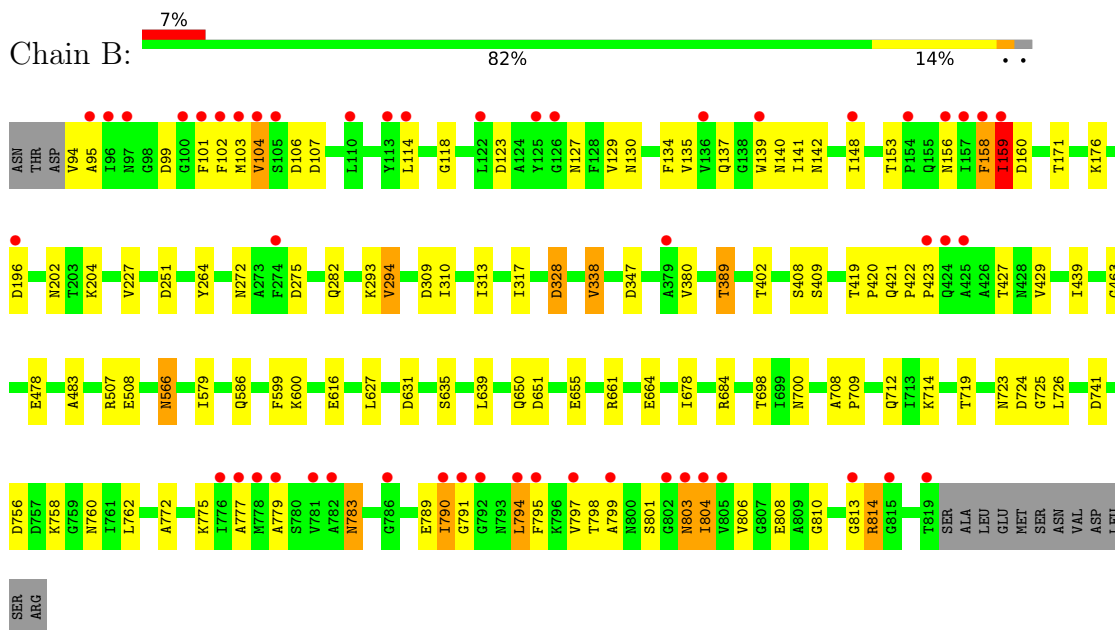
3 Residue-property plots [i](#)

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.

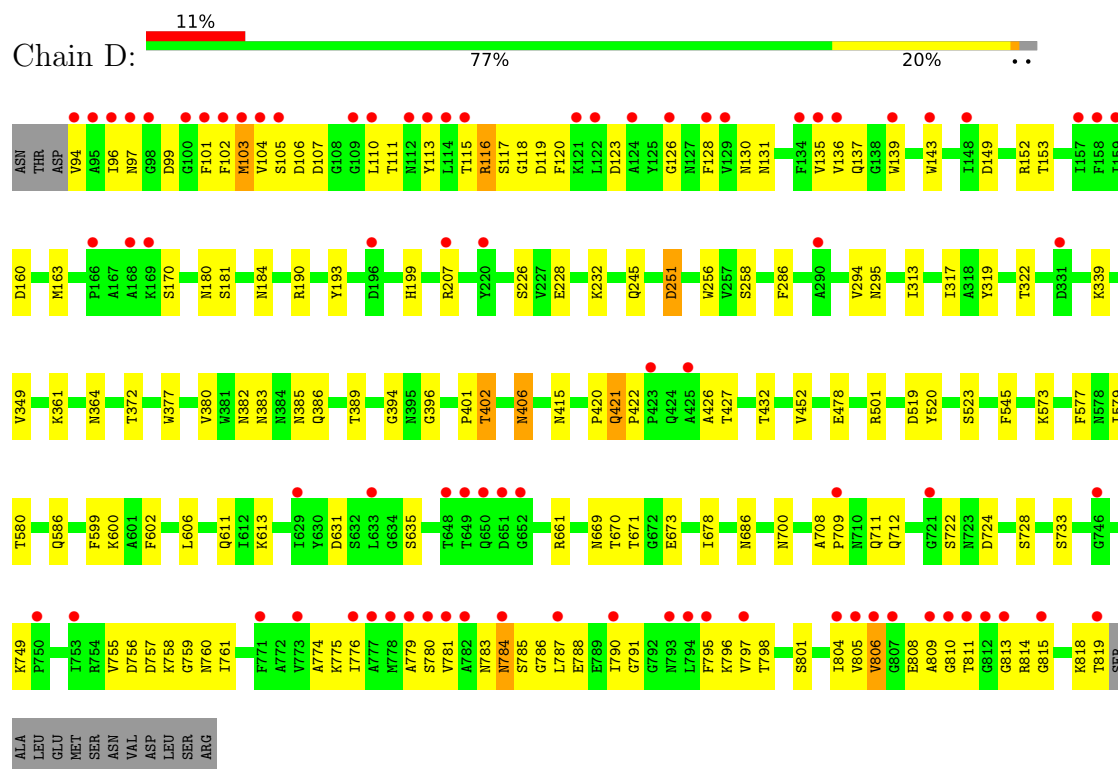
- Molecule 1: Flagellar hook subunit protein



- Molecule 1: Flagellar hook subunit protein



- Molecule 1: Flagellar hook subunit protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.46Å 173.54Å 147.09Å 90.00° 102.66° 90.00°	Depositor
Resolution (Å)	24.96 – 2.45 24.96 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.7 (24.96-2.45) 94.4 (24.96-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 2.45Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.202 , 0.229 0.203 , 0.232	Depositor DCC
R_{free} test set	7994 reflections (5.99%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23180	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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	0.31	0/5527	0.75	6/7533 (0.1%)
1	B	0.31	0/5527	0.72	5/7533 (0.1%)
1	C	0.35	0/5527	0.80	11/7533 (0.1%)
1	D	0.34	0/5527	0.79	10/7533 (0.1%)
All	All	0.33	0/22108	0.77	32/30132 (0.1%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	785	SER	N-CA-C	7.95	123.16	113.38
1	D	422	PRO	N-CA-C	6.94	119.17	110.70
1	C	422	PRO	N-CA-C	6.93	119.15	110.70
1	C	135	VAL	N-CA-C	6.78	118.34	108.58
1	A	815	GLY	N-CA-C	6.55	118.72	112.04
1	A	422	PRO	N-CA-C	6.34	118.44	110.70
1	C	421	GLN	CA-C-N	6.32	126.89	120.38
1	C	421	GLN	C-N-CA	6.32	126.89	120.38
1	A	478	GLU	CA-C-N	6.30	125.79	119.24
1	A	478	GLU	C-N-CA	6.30	125.79	119.24
1	D	478	GLU	CA-C-N	6.26	125.76	119.24
1	D	478	GLU	C-N-CA	6.26	125.76	119.24
1	D	421	GLN	CA-C-N	6.12	126.68	120.38
1	D	421	GLN	C-N-CA	6.12	126.68	120.38
1	C	749	LYS	CA-C-N	5.99	125.47	119.24
1	C	749	LYS	C-N-CA	5.99	125.47	119.24
1	D	749	LYS	CA-C-N	5.84	125.98	119.32
1	D	749	LYS	C-N-CA	5.84	125.98	119.32
1	C	478	GLU	CA-C-N	5.80	125.28	119.24
1	C	478	GLU	C-N-CA	5.80	125.28	119.24
1	A	421	GLN	CA-C-N	5.58	126.13	120.38
1	A	421	GLN	C-N-CA	5.58	126.13	120.38
1	B	422	PRO	N-CA-C	5.47	117.37	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	478	GLU	CA-C-N	5.37	124.83	119.24
1	B	478	GLU	C-N-CA	5.37	124.83	119.24
1	C	134	PHE	N-CA-C	5.37	117.99	109.24
1	D	116	ARG	N-CA-C	-5.31	106.58	113.16
1	C	101	PHE	N-CA-C	5.26	118.79	109.96
1	C	110	LEU	CB-CA-C	-5.21	109.59	115.79
1	B	463	GLY	CA-C-N	5.20	125.49	119.93
1	B	463	GLY	C-N-CA	5.20	125.49	119.93
1	D	784	ASN	N-CA-C	5.18	121.84	110.80

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	5428	0	5168	59	0
1	B	5428	0	5168	66	0
1	C	5428	0	5168	82	1
1	D	5428	0	5168	104	1
2	A	372	0	0	9	0
2	B	417	0	0	7	0
2	C	388	0	0	10	0
2	D	291	0	0	13	0
All	All	23180	0	20672	306	1

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 7.

All (306) 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:D:758:LYS:O	1:D:775:LYS:NZ	2.09	0.85
1:C:757:ASP:HA	1:C:816:GLU:HB3	1.59	0.82
1:D:117:SER:OG	1:D:119:ASP:OD1	2.01	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:GLN:NE2	1:B:156:ASN:OD1	2.19	0.74
1:D:779:ALA:HA	1:D:806:VAL:HA	1.70	0.74
1:A:712:GLN:NE2	1:D:686:ASN:OD1	2.21	0.73
1:C:141:ILE:HG12	1:C:148:ILE:HG12	1.70	0.73
1:C:95:ALA:HB2	1:C:754:ARG:HH22	1.55	0.72
1:D:119:ASP:OD2	1:D:131:ASN:ND2	2.22	0.72
1:B:655:GLU:HG3	1:B:684:ARG:HG2	1.72	0.71
1:B:650:GLN:NE2	2:B:908:HOH:O	2.24	0.71
1:B:798:THR:H	1:B:801:SER:HB3	1.56	0.71
1:D:787:LEU:HD12	1:D:788:GLU:H	1.56	0.70
1:A:758:LYS:O	1:A:775:LYS:NZ	2.22	0.68
1:C:754:ARG:O	1:C:762:LEU:N	2.26	0.68
1:D:797:VAL:HG11	1:D:804:ILE:HD11	1.73	0.68
1:B:483:ALA:O	2:B:901:HOH:O	2.11	0.68
1:B:664:GLU:OE1	2:B:902:HOH:O	2.12	0.67
1:C:141:ILE:HD11	1:C:773:VAL:HA	1.77	0.67
1:A:684:ARG:NH2	2:A:910:HOH:O	2.26	0.67
1:D:780:SER:N	1:D:805:VAL:O	2.22	0.67
1:C:138:GLY:O	1:C:155:GLN:N	2.21	0.67
1:A:613:LYS:NZ	2:A:913:HOH:O	2.28	0.66
1:B:130:ASN:HD21	1:B:134:PHE:HB2	1.58	0.66
1:B:803:ASN:OD1	1:B:803:ASN:N	2.29	0.66
1:B:328:ASP:N	1:B:328:ASP:OD1	2.28	0.65
1:C:729:SER:OG	2:C:902:HOH:O	2.14	0.65
1:C:519:ASP:OD1	2:C:901:HOH:O	2.13	0.65
1:D:245:GLN:OE1	2:D:901:HOH:O	2.14	0.65
1:B:176:LYS:NZ	1:B:723:ASN:O	2.30	0.65
1:B:655:GLU:OE2	1:B:684:ARG:NH1	2.29	0.64
1:C:104:VAL:HG23	1:C:136:VAL:HG13	1.78	0.64
1:D:104:VAL:HG23	1:D:137:GLN:HB2	1.80	0.64
1:D:733:SER:O	2:D:903:HOH:O	2.15	0.64
1:A:295:ASN:H	1:A:372:THR:HG1	1.44	0.64
1:B:579:ILE:O	1:B:600:LYS:NZ	2.30	0.64
1:B:700:ASN:OD1	1:B:712:GLN:NE2	2.30	0.64
1:D:611:GLN:OE1	2:D:902:HOH:O	2.15	0.64
1:B:758:LYS:O	1:B:775:LYS:NZ	2.30	0.63
1:A:226:SER:OG	1:A:228:GLU:OE2	2.16	0.63
1:A:788:GLU:N	1:A:788:GLU:OE1	2.32	0.63
1:B:798:THR:OG1	1:B:799:ALA:N	2.30	0.63
1:D:787:LEU:HD21	1:D:795:PHE:HB3	1.80	0.62
1:B:783:ASN:ND2	1:B:801:SER:O	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:ASP:OD1	1:D:119:ASP:N	2.32	0.62
1:A:291:ASN:OD1	1:B:99:ASP:HB2	1.99	0.62
1:D:579:ILE:O	1:D:600:LYS:NZ	2.32	0.61
1:D:251:ASP:OD2	2:D:905:HOH:O	2.16	0.61
1:A:790:ILE:HG13	1:A:791:GLY:H	1.65	0.61
1:B:227:VAL:O	1:B:661:ARG:NH1	2.31	0.61
1:B:421:GLN:HB3	1:B:423:PRO:HG2	1.83	0.61
1:C:749:LYS:HG3	1:C:752:ALA:HB3	1.83	0.60
1:C:415:ASN:HB2	1:C:432:THR:HB	1.84	0.60
1:B:293:LYS:HD3	1:B:309:ASP:HA	1.84	0.60
1:B:698:THR:HG22	1:B:714:LYS:HA	1.84	0.59
1:B:275:ASP:O	1:B:282:GLN:NE2	2.33	0.59
1:C:140:ASN:ND2	1:C:155:GLN:OE1	2.36	0.59
1:D:670:THR:HG23	1:D:671:THR:HG23	1.84	0.59
1:D:94:VAL:HA	1:D:120:PHE:H	1.67	0.58
1:D:180:ASN:ND2	1:D:184:ASN:O	2.36	0.58
1:A:95:ALA:O	1:A:103:MET:HE1	2.04	0.58
1:C:753:ILE:HD11	1:C:761:ILE:HD11	1.85	0.58
1:C:101:PHE:HB3	1:C:102:PHE:HD2	1.68	0.58
1:A:383:ASN:O	1:A:386:GLN:NE2	2.35	0.58
1:A:519:ASP:OD1	2:A:901:HOH:O	2.17	0.58
1:C:136:VAL:O	1:C:157:ILE:HG12	2.04	0.58
1:C:232:LYS:HZ2	1:C:657:GLN:CD	2.11	0.58
1:D:102:PHE:CD1	1:D:116:ARG:HA	2.39	0.57
1:D:102:PHE:HB3	1:D:115:THR:O	2.05	0.57
1:A:814:ARG:NH2	2:A:924:HOH:O	2.33	0.57
1:D:319:TYR:O	1:D:322:THR:OG1	2.20	0.57
1:C:385:ASN:ND2	2:C:923:HOH:O	2.35	0.57
1:C:759:GLY:O	1:C:776:ILE:N	2.30	0.57
1:A:268:LYS:NZ	2:A:936:HOH:O	2.37	0.56
1:C:113:TYR:HE1	1:C:134:PHE:CE2	2.22	0.56
1:D:415:ASN:HB2	1:D:432:THR:HB	1.86	0.56
1:D:519:ASP:OD1	2:D:904:HOH:O	2.18	0.56
1:A:579:ILE:O	1:A:600:LYS:NZ	2.39	0.56
1:D:761:ILE:HD12	1:D:774:ALA:HB3	1.87	0.56
1:C:700:ASN:OD1	1:C:712:GLN:NE2	2.39	0.55
1:C:224:LYS:NZ	2:C:911:HOH:O	2.30	0.55
1:D:94:VAL:N	1:D:819:THR:O	2.39	0.55
1:C:787:LEU:HD12	1:C:788:GLU:H	1.70	0.55
1:D:96:ILE:HA	1:D:118:GLY:HA3	1.89	0.55
1:D:190:ARG:NH2	2:D:938:HOH:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:669:ASN:ND2	1:D:673:GLU:O	2.28	0.55
1:B:159:ILE:HG12	1:B:160:ASP:H	1.72	0.54
1:B:789:GLU:HG3	1:B:795:PHE:HE1	1.72	0.54
1:B:566:ASN:ND2	2:B:934:HOH:O	2.41	0.54
1:C:501:ARG:NH2	2:C:930:HOH:O	2.37	0.53
1:B:264:TYR:HB2	1:B:439:ILE:HG13	1.89	0.53
1:D:286:PHE:HB3	1:D:377:TRP:CD1	2.44	0.53
1:C:428:ASN:ND2	2:C:912:HOH:O	2.30	0.53
1:D:139:TRP:NE1	1:D:152:ARG:O	2.30	0.53
1:D:501:ARG:NH1	2:D:913:HOH:O	2.33	0.53
1:D:380:VAL:HB	1:D:389:THR:HG23	1.90	0.53
1:C:107:ASP:HB2	1:C:134:PHE:CZ	2.44	0.53
1:B:579:ILE:HG13	1:B:599:PHE:O	2.09	0.52
1:A:786:GLY:O	1:A:801:SER:HB3	2.10	0.52
1:D:143:TRP:HH2	1:D:163:MET:SD	2.31	0.52
1:B:380:VAL:HB	1:B:389:THR:HG22	1.92	0.52
1:A:694:TYR:OH	1:A:715:LEU:O	2.19	0.52
1:B:141:ILE:HA	1:B:148:ILE:HG12	1.91	0.52
1:D:586:GLN:N	1:D:586:GLN:OE1	2.43	0.52
1:A:415:ASN:HB3	1:A:432:THR:HB	1.92	0.51
1:D:788:GLU:OE1	1:D:788:GLU:N	2.43	0.51
1:B:724:ASP:OD1	1:B:724:ASP:N	2.43	0.51
1:A:722:SER:OG	1:A:724:ASP:OD1	2.26	0.51
1:A:811:THR:O	1:A:814:ARG:NE	2.31	0.51
1:A:356:THR:HG1	1:A:583:SER:HG	1.59	0.51
1:B:408:SER:OG	1:B:409:SER:N	2.43	0.51
1:C:579:ILE:HG13	1:C:599:PHE:O	2.10	0.51
1:C:606:LEU:HD13	1:C:613:LYS:HG2	1.91	0.51
1:D:103:MET:HG3	1:D:136:VAL:HG13	1.91	0.51
1:C:128:PHE:H	1:C:157:ILE:HD12	1.76	0.51
1:C:319:TYR:O	1:C:322:THR:OG1	2.22	0.51
1:B:616:GLU:OE1	2:B:903:HOH:O	2.19	0.50
1:C:105:SER:HB3	1:C:134:PHE:CD2	2.46	0.50
1:A:163:MET:HE3	1:A:765:PHE:HZ	1.75	0.50
1:A:523:SER:OG	2:A:901:HOH:O	2.15	0.50
1:C:286:PHE:HB3	1:C:377:TRP:CD1	2.46	0.50
1:D:790:ILE:HG13	1:D:791:GLY:H	1.76	0.50
1:A:99:ASP:OD1	1:A:99:ASP:N	2.41	0.49
1:B:148:ILE:HD11	1:B:772:ALA:O	2.12	0.49
1:C:796:LYS:NZ	1:C:797:VAL:O	2.42	0.49
1:D:722:SER:OG	1:D:724:ASP:OD1	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:THR:HG21	1:B:101:PHE:HZ	1.76	0.49
1:A:163:MET:HE3	1:A:765:PHE:CZ	2.48	0.49
1:D:160:ASP:HB3	1:D:163:MET:SD	2.52	0.49
1:D:170:SER:O	1:D:711:GLN:NE2	2.35	0.49
1:A:286:PHE:HB3	1:A:377:TRP:CD1	2.47	0.49
1:C:769:LYS:HD3	1:C:771:PHE:HE2	1.78	0.49
1:D:226:SER:OG	1:D:228:GLU:OE2	2.31	0.49
1:D:579:ILE:HG13	1:D:599:PHE:O	2.12	0.49
1:A:160:ASP:HB3	1:A:163:MET:HB2	1.94	0.49
1:C:358:ASP:OD2	1:C:585:LYS:NZ	2.44	0.49
1:D:394:GLY:HA3	1:D:401:PRO:O	2.13	0.49
1:B:313:ILE:O	1:B:317:ILE:HG12	2.12	0.49
1:D:809:ALA:HA	1:D:814:ARG:HD2	1.93	0.49
1:D:102:PHE:CE1	1:D:116:ARG:HG3	2.48	0.48
1:D:123:ASP:OD1	1:D:126:GLY:N	2.45	0.48
1:B:272:ASN:ND2	2:B:947:HOH:O	2.45	0.48
1:D:199:HIS:NE2	2:D:926:HOH:O	2.35	0.48
1:D:756:ASP:OD1	1:D:760:ASN:N	2.41	0.48
1:B:95:ALA:O	1:B:118:GLY:HA3	2.13	0.48
1:B:114:LEU:HD11	1:B:804:ILE:HD11	1.94	0.48
1:C:141:ILE:HG22	1:C:142:ASN:C	2.38	0.48
1:A:712:GLN:OE1	2:A:902:HOH:O	2.20	0.48
1:B:420:PRO:HD3	1:B:427:THR:HG23	1.96	0.48
1:C:380:VAL:HB	1:C:389:THR:HG23	1.96	0.48
1:C:694:TYR:OH	1:C:715:LEU:O	2.22	0.48
1:C:114:LEU:HD21	1:C:780:SER:HA	1.96	0.48
1:D:117:SER:OG	1:D:130:ASN:HB2	2.14	0.48
1:D:420:PRO:HD2	1:D:426:ALA:HA	1.94	0.48
1:B:114:LEU:O	1:B:794:LEU:HA	2.14	0.48
1:C:103:MET:N	1:C:115:THR:O	2.47	0.48
1:D:520:TYR:CG	1:D:573:LYS:HD2	2.49	0.48
1:A:293:LYS:HD3	1:A:309:ASP:HA	1.96	0.47
1:B:106:ASP:OD1	1:B:107:ASP:N	2.47	0.47
1:D:96:ILE:HG22	1:D:97:ASN:H	1.79	0.47
1:A:698:THR:HG22	1:A:714:LYS:HA	1.96	0.47
1:D:606:LEU:HD13	1:D:613:LYS:HG2	1.96	0.47
1:A:661:ARG:HG2	1:A:678:ILE:HG12	1.96	0.47
1:B:631:ASP:OD2	1:B:635:SER:HB2	2.14	0.47
1:C:94:VAL:O	1:C:818:LYS:NZ	2.36	0.47
1:C:228:GLU:HB3	2:C:924:HOH:O	2.15	0.47
1:B:756:ASP:OD1	1:B:760:ASN:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:ARG:NH1	1:C:209:GLU:OE2	2.39	0.47
1:C:264:TYR:HB2	1:C:439:ILE:HG13	1.96	0.47
1:A:201:TRP:CD2	1:A:463:GLY:HA2	2.49	0.47
1:C:755:VAL:HA	1:C:761:ILE:HA	1.97	0.47
1:A:119:ASP:N	1:A:119:ASP:OD1	2.48	0.47
1:B:129:VAL:HG12	1:B:135:VAL:HA	1.96	0.47
1:C:157:ILE:HG13	1:C:157:ILE:O	2.15	0.46
1:B:294:VAL:HG23	1:B:310:ILE:HB	1.98	0.46
1:D:295:ASN:H	1:D:372:THR:HG1	1.60	0.46
1:D:545:PHE:HB3	1:D:602:PHE:HZ	1.80	0.46
1:A:319:TYR:O	1:A:322:THR:OG1	2.24	0.46
1:C:787:LEU:HG	1:C:795:PHE:CD1	2.51	0.46
1:B:708:ALA:HA	1:B:709:PRO:HD3	1.82	0.46
1:B:810:GLY:N	1:B:814:ARG:O	2.30	0.46
1:C:631:ASP:OD1	1:C:635:SER:N	2.41	0.46
1:D:396:GLY:HA2	1:D:402:THR:HG22	1.98	0.46
1:C:113:TYR:HE1	1:C:134:PHE:HE2	1.62	0.46
1:C:182:GLY:HA3	1:C:730:ASN:OD1	2.16	0.46
1:C:135:VAL:HG23	1:C:157:ILE:HD11	1.97	0.46
1:C:791:GLY:HA3	1:C:794:LEU:HB2	1.98	0.46
1:C:755:VAL:HB	1:C:761:ILE:HA	1.98	0.45
1:D:143:TRP:CH2	1:D:163:MET:SD	3.08	0.45
1:D:787:LEU:HD11	1:D:796:LYS:H	1.82	0.45
1:A:304:ARG:NH2	1:A:306:GLN:OE1	2.50	0.45
1:D:382:ASN:OD1	1:D:385:ASN:N	2.38	0.45
1:A:579:ILE:HG13	1:A:599:PHE:O	2.17	0.45
1:D:97:ASN:ND2	1:D:99:ASP:O	2.50	0.45
1:D:758:LYS:HD2	1:D:810:GLY:HA3	1.99	0.45
1:B:661:ARG:HG2	1:B:678:ILE:HG12	1.99	0.45
1:D:106:ASP:OD1	1:D:107:ASP:N	2.49	0.45
1:D:120:PHE:HB3	1:D:128:PHE:CZ	2.51	0.45
1:D:775:LYS:HE3	1:D:808:GLU:OE1	2.17	0.45
1:D:787:LEU:HD12	1:D:788:GLU:N	2.28	0.45
1:A:475:ARG:HG3	1:A:485:TRP:CD1	2.51	0.45
1:C:171:THR:OG1	1:C:741:ASP:OD2	2.23	0.45
1:C:724:ASP:OD1	1:C:724:ASP:N	2.50	0.45
1:D:94:VAL:HA	1:D:120:PHE:N	2.31	0.45
1:D:102:PHE:CZ	1:D:116:ARG:HG3	2.52	0.45
2:C:928:HOH:O	1:D:207:ARG:HD3	2.17	0.44
1:D:631:ASP:OD1	1:D:635:SER:N	2.45	0.44
1:D:661:ARG:HG2	1:D:678:ILE:HG12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:789:GLU:CD	1:C:789:GLU:H	2.24	0.44
1:D:103:MET:H	1:D:103:MET:HE2	1.82	0.44
1:C:184:ASN:ND2	2:C:955:HOH:O	2.49	0.44
1:D:452:VAL:N	2:D:963:HOH:O	2.50	0.44
1:A:807:GLY:HA3	1:A:814:ARG:NH1	2.32	0.44
1:C:94:VAL:HA	1:C:120:PHE:H	1.83	0.44
1:D:523:SER:OG	2:D:904:HOH:O	2.16	0.44
1:A:140:ASN:ND2	2:A:964:HOH:O	2.51	0.44
1:A:138:GLY:HA2	1:A:777:ALA:HB2	2.00	0.44
1:B:106:ASP:HB3	1:B:137:GLN:NE2	2.33	0.44
1:D:313:ILE:O	1:D:317:ILE:HG12	2.18	0.44
1:C:119:ASP:OD1	1:C:119:ASP:N	2.47	0.43
1:C:196:ASP:N	1:C:231:GLU:OE2	2.40	0.43
1:B:202:ASN:OD1	1:B:204:LYS:HG2	2.17	0.43
1:C:749:LYS:HA	1:C:750:PRO:HD3	1.78	0.43
1:D:105:SER:O	1:D:113:TYR:N	2.47	0.43
1:D:755:VAL:HG22	1:D:761:ILE:HG12	2.01	0.43
1:A:211:GLU:HB2	1:A:504:GLU:HG2	1.98	0.43
1:A:691:LEU:HD21	1:A:694:TYR:HD1	1.83	0.43
1:B:123:ASP:OD2	1:B:127:ASN:HB2	2.18	0.43
1:C:818:LYS:HG2	1:C:819:THR:H	1.81	0.43
1:B:176:LYS:HD2	1:B:725:GLY:O	2.18	0.43
1:B:627:LEU:HB2	1:B:639:LEU:HB2	2.01	0.43
1:B:507:ARG:NH2	1:B:508:GLU:OE1	2.50	0.43
1:C:201:TRP:CE2	1:C:463:GLY:HA2	2.54	0.43
1:C:757:ASP:OD1	1:C:757:ASP:N	2.51	0.43
1:A:142:ASN:O	1:A:146:GLN:N	2.51	0.43
1:C:756:ASP:OD1	1:C:760:ASN:HB2	2.18	0.43
1:D:420:PRO:HD2	1:D:427:THR:H	1.82	0.43
1:C:507:ARG:NH2	1:C:508:GLU:OE1	2.52	0.43
1:D:798:THR:H	1:D:801:SER:HB3	1.84	0.43
1:A:809:ALA:HB1	1:A:815:GLY:HA2	2.01	0.43
1:B:142:ASN:OD1	2:B:904:HOH:O	2.21	0.43
1:A:775:LYS:HE2	1:A:808:GLU:CD	2.44	0.42
1:C:313:ILE:O	1:C:317:ILE:HG12	2.19	0.42
1:A:264:TYR:HB2	1:A:439:ILE:HG13	2.01	0.42
1:C:631:ASP:OD2	1:C:635:SER:HB2	2.18	0.42
1:C:661:ARG:HG2	1:C:678:ILE:HG12	2.01	0.42
1:A:669:ASN:O	1:A:676:ASN:HA	2.20	0.42
1:A:756:ASP:OD2	1:A:760:ASN:HB2	2.19	0.42
1:C:110:LEU:HB2	1:C:111:THR:H	1.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:ASN:ND2	2:A:942:HOH:O	2.41	0.42
1:B:338:VAL:HG12	1:B:347:ASP:HB2	2.02	0.42
1:C:115:THR:HG22	1:C:794:LEU:HG	2.02	0.42
1:D:294:VAL:HG12	1:D:377:TRP:CZ2	2.54	0.42
1:D:364:ASN:OD1	2:D:906:HOH:O	2.21	0.42
1:D:700:ASN:OD1	1:D:712:GLN:NE2	2.53	0.42
1:D:724:ASP:OD1	1:D:724:ASP:N	2.49	0.42
1:A:475:ARG:HA	1:A:476:PRO:HD3	1.86	0.42
1:C:558:PRO:O	1:D:207:ARG:NH2	2.52	0.42
1:A:724:ASP:OD1	1:A:724:ASP:N	2.49	0.42
1:C:106:ASP:O	1:C:135:VAL:HG13	2.20	0.42
1:D:258:SER:O	1:D:577:PHE:HA	2.20	0.42
1:D:818:LYS:HG2	1:D:819:THR:H	1.85	0.42
1:B:130:ASN:ND2	1:B:134:PHE:HB2	2.31	0.42
1:B:402:THR:HG22	1:B:427:THR:O	2.20	0.42
1:B:779:ALA:HB2	1:B:806:VAL:HG23	2.02	0.42
1:C:278:LEU:HG	1:C:280:GLN:HG2	2.02	0.41
1:B:139:TRP:CZ3	1:B:777:ALA:HA	2.55	0.41
1:B:775:LYS:HD3	1:B:808:GLU:HG2	2.03	0.41
1:D:193:TYR:CE2	1:D:232:LYS:HD3	2.55	0.41
1:D:256:TRP:HB2	1:D:580:THR:OG1	2.20	0.41
1:D:759:GLY:O	1:D:776:ILE:HG12	2.20	0.41
1:D:96:ILE:HG22	1:D:97:ASN:N	2.36	0.41
1:D:149:ASP:OD2	1:D:152:ARG:HG2	2.20	0.41
1:D:708:ALA:HA	1:D:709:PRO:HD3	1.91	0.41
1:D:787:LEU:CD2	1:D:795:PHE:HB3	2.48	0.41
1:A:420:PRO:HD2	1:A:426:ALA:HA	2.01	0.41
1:C:788:GLU:OE1	1:C:788:GLU:N	2.53	0.41
1:C:175:ILE:HG22	1:C:717:PHE:CD1	2.56	0.41
1:C:752:ALA:HB1	1:C:764:GLU:OE1	2.20	0.41
1:D:406:ASN:O	1:D:406:ASN:ND2	2.45	0.41
1:A:180:ASN:ND2	1:A:184:ASN:O	2.54	0.41
1:B:104:VAL:HG21	1:B:779:ALA:HB3	2.02	0.41
1:B:140:ASN:HB3	1:B:158:PHE:CD2	2.56	0.41
1:A:380:VAL:HB	1:A:389:THR:HG23	2.03	0.41
1:A:757:ASP:N	1:A:757:ASP:OD1	2.51	0.41
1:C:97:ASN:HB2	1:C:103:MET:HE3	2.03	0.41
1:C:220:TYR:CZ	1:C:222:THR:HG22	2.55	0.41
1:A:396:GLY:HA2	1:A:427:THR:O	2.20	0.41
1:A:687:ASN:O	1:B:586:GLN:HG3	2.20	0.41
1:C:106:ASP:OD1	1:C:107:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:PHE:CZ	1:D:779:ALA:O	2.74	0.41
1:D:339:LYS:HG2	2:D:1137:HOH:O	2.21	0.41
1:D:787:LEU:HD11	1:D:796:LYS:N	2.35	0.41
1:D:811:THR:O	1:D:814:ARG:NE	2.54	0.41
1:D:104:VAL:HA	1:D:113:TYR:O	2.21	0.41
1:D:152:ARG:HA	1:D:152:ARG:HH11	1.86	0.41
1:C:714:LYS:NZ	2:C:922:HOH:O	2.35	0.40
1:C:520:TYR:CG	1:C:573:LYS:HD2	2.56	0.40
1:B:171:THR:OG1	1:B:741:ASP:OD2	2.24	0.40
1:C:691:LEU:HD21	1:C:694:TYR:HD1	1.86	0.40
1:D:361:LYS:O	2:D:907:HOH:O	2.22	0.40
1:D:383:ASN:O	1:D:386:GLN:NE2	2.48	0.40
1:A:160:ASP:HA	1:A:161:PRO:HD3	1.84	0.40
1:B:158:PHE:CG	1:B:159:ILE:N	2.90	0.40
1:D:181:SER:HB3	1:D:728:SER:OG	2.21	0.40
1:D:757:ASP:HB2	1:D:815:GLY:HA2	2.04	0.40

All (1) 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:C:785:SER:N	1:D:783:ASN:O[2_454]	2.08	0.12

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	724/741 (98%)	701 (97%)	19 (3%)	4 (1%)	21	27
1	B	724/741 (98%)	681 (94%)	34 (5%)	9 (1%)	10	11
1	C	724/741 (98%)	699 (96%)	21 (3%)	4 (1%)	21	27
1	D	724/741 (98%)	699 (96%)	20 (3%)	5 (1%)	18	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2896/2964 (98%)	2780 (96%)	94 (3%)	22 (1%)	16 20

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	159	ILE
1	C	102	PHE
1	C	785	SER
1	D	784	ASN
1	A	111	THR
1	B	196	ASP
1	A	813	GLY
1	B	158	PHE
1	B	783	ASN
1	B	813	GLY
1	C	111	THR
1	A	102	PHE
1	A	119	ASP
1	B	790	ILE
1	D	111	THR
1	B	102	PHE
1	B	104	VAL
1	D	781	VAL
1	D	786	GLY
1	B	791	GLY
1	C	813	GLY
1	D	813	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	581/595 (98%)	572 (98%)	9 (2%)	57 70
1	B	581/595 (98%)	559 (96%)	22 (4%)	29 43
1	C	581/595 (98%)	566 (97%)	15 (3%)	40 55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	581/595 (98%)	571 (98%)	10 (2%)	53 67
All	All	2324/2380 (98%)	2268 (98%)	56 (2%)	43 58

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	VAL
1	A	110	LEU
1	A	135	VAL
1	A	329	THR
1	A	421	GLN
1	A	424	GLN
1	A	719	THR
1	A	808	GLU
1	A	814	ARG
1	B	94	VAL
1	B	103	MET
1	B	153	THR
1	B	159	ILE
1	B	251	ASP
1	B	294	VAL
1	B	328	ASP
1	B	338	VAL
1	B	389	THR
1	B	419	THR
1	B	429	VAL
1	B	566	ASN
1	B	651	ASP
1	B	719	THR
1	B	726	LEU
1	B	762	LEU
1	B	790	ILE
1	B	794	LEU
1	B	797	VAL
1	B	803	ASN
1	B	804	ILE
1	B	814	ARG
1	C	110	LEU
1	C	113	TYR
1	C	135	VAL
1	C	141	ILE
1	C	207	ARG

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Mol	Chain	Res	Type
1	C	329	THR
1	C	383	ASN
1	C	421	GLN
1	C	424	GLN
1	C	648	THR
1	C	754	ARG
1	C	755	VAL
1	C	761	ILE
1	C	789	GLU
1	C	803	ASN
1	D	103	MET
1	D	110	LEU
1	D	135	VAL
1	D	153	THR
1	D	251	ASP
1	D	349	VAL
1	D	402	THR
1	D	406	ASN
1	D	421	GLN
1	D	806	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	295	ASN
1	A	467	GLN
1	A	700	ASN
1	A	723	ASN
1	B	225	ASN
1	B	467	GLN
1	B	617	GLN
1	B	637	HIS
1	B	723	ASN
1	C	140	ASN
1	C	199	HIS
1	C	295	ASN
1	C	306	GLN
1	C	533	GLN
1	C	562	ASN
1	C	712	GLN
1	C	723	ASN
1	D	295	ASN

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Mol	Chain	Res	Type
1	D	562	ASN
1	D	712	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	726/741 (97%)	0.16	20 (2%) 55 56	29, 51, 98, 126	0
1	B	726/741 (97%)	0.16	50 (6%) 23 20	23, 47, 118, 150	0
1	C	726/741 (97%)	0.44	88 (12%) 8 7	25, 48, 249, 302	0
1	D	726/741 (97%)	0.57	81 (11%) 10 8	27, 63, 190, 248	0
All	All	2904/2964 (97%)	0.33	239 (8%) 17 15	23, 52, 192, 302	0

All (239) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	776	ILE	13.3
1	C	777	ALA	9.5
1	C	779	ALA	7.0
1	C	804	ILE	6.6
1	A	100	GLY	6.4
1	C	773	VAL	6.1
1	C	139	TRP	5.9
1	C	781	VAL	5.6
1	C	102	PHE	5.5
1	C	778	MET	5.5
1	A	815	GLY	5.5
1	C	806	VAL	5.4
1	D	806	VAL	5.3
1	C	805	VAL	5.3
1	C	138	GLY	5.3
1	D	159	ILE	5.3
1	B	819	THR	5.3
1	C	122	LEU	5.1
1	D	790	ILE	4.8
1	C	110	LEU	4.8
1	C	101	PHE	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	782	ALA	4.6
1	C	124	ALA	4.6
1	C	158	PHE	4.5
1	C	114	LEU	4.5
1	C	148	ILE	4.5
1	C	771	PHE	4.5
1	B	159	ILE	4.4
1	D	649	THR	4.3
1	D	98	GLY	4.3
1	B	157	ILE	4.2
1	C	784	ASN	4.2
1	C	790	ILE	4.1
1	D	804	ILE	4.0
1	D	795	PHE	4.0
1	C	780	SER	4.0
1	D	115	THR	4.0
1	C	807	GLY	4.0
1	C	748	LEU	3.9
1	C	753	ILE	3.9
1	D	811	THR	3.9
1	C	797	VAL	3.9
1	D	128	PHE	3.8
1	D	807	GLY	3.8
1	A	96	ILE	3.8
1	C	128	PHE	3.7
1	D	102	PHE	3.7
1	C	762	LEU	3.7
1	C	803	ASN	3.7
1	C	109	GLY	3.7
1	D	652	GLY	3.6
1	C	794	LEU	3.6
1	C	159	ILE	3.6
1	D	650	GLN	3.6
1	C	750	PRO	3.5
1	B	104	VAL	3.5
1	D	779	ALA	3.5
1	C	150	SER	3.5
1	C	143	TRP	3.4
1	B	813	GLY	3.4
1	C	775	LYS	3.4
1	B	379	ALA	3.3
1	B	158	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	129	VAL	3.3
1	D	776	ILE	3.3
1	B	110	LEU	3.3
1	C	813	GLY	3.3
1	B	779	ALA	3.3
1	D	114	LEU	3.3
1	C	792	GLY	3.3
1	A	101	PHE	3.2
1	C	98	GLY	3.2
1	D	629	ILE	3.2
1	C	149	ASP	3.2
1	B	425	ALA	3.2
1	D	784	ASN	3.1
1	B	148	ILE	3.1
1	D	794	LEU	3.1
1	D	812	GLY	3.1
1	B	776	ILE	3.1
1	A	102	PHE	3.1
1	C	134	PHE	3.1
1	D	134	PHE	3.1
1	B	113	TYR	3.0
1	D	94	VAL	3.0
1	B	125	TYR	3.0
1	B	781	VAL	3.0
1	D	805	VAL	3.0
1	A	819	THR	3.0
1	C	799	ALA	3.0
1	D	633	LEU	3.0
1	C	146	GLN	3.0
1	D	819	THR	2.9
1	D	809	ALA	2.9
1	D	96	ILE	2.9
1	D	778	MET	2.9
1	D	126	GLY	2.9
1	C	761	ILE	2.9
1	B	797	VAL	2.9
1	C	104	VAL	2.9
1	C	758	LYS	2.9
1	C	96	ILE	2.8
1	A	804	ILE	2.8
1	D	753	ILE	2.8
1	B	101	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	120	PHE	2.8
1	B	100	GLY	2.8
1	D	129	VAL	2.8
1	D	423	PRO	2.8
1	B	803	ASN	2.8
1	C	161	PRO	2.8
1	D	781	VAL	2.8
1	C	772	ALA	2.8
1	C	103	MET	2.8
1	B	815	GLY	2.7
1	D	101	PHE	2.8
1	C	94	VAL	2.7
1	C	147	THR	2.7
1	D	122	LEU	2.7
1	B	196	ASP	2.7
1	C	133	GLY	2.7
1	D	143	TRP	2.7
1	D	104	VAL	2.7
1	C	809	ALA	2.7
1	C	814	ARG	2.7
1	B	795	PHE	2.7
1	D	168	ALA	2.7
1	D	746	GLY	2.7
1	D	810	GLY	2.7
1	C	132	ALA	2.7
1	B	791	GLY	2.6
1	A	110	LEU	2.6
1	B	790	ILE	2.6
1	D	793	ASN	2.6
1	A	379	ALA	2.6
1	D	95	ALA	2.6
1	A	109	GLY	2.6
1	D	103	MET	2.6
1	B	804	ILE	2.6
1	D	157	ILE	2.5
1	B	424	GLN	2.5
1	D	136	VAL	2.5
1	A	398	ALA	2.5
1	B	126	GLY	2.5
1	D	100	GLY	2.5
1	A	94	VAL	2.5
1	B	156	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	783	ASN	2.5
1	B	777	ALA	2.5
1	B	792	GLY	2.5
1	C	802	GLY	2.5
1	D	815	GLY	2.5
1	C	130	ASN	2.5
1	D	777	ALA	2.5
1	C	105	SER	2.5
1	D	105	SER	2.5
1	B	154	PRO	2.5
1	C	759	GLY	2.5
1	D	97	ASN	2.5
1	A	423	PRO	2.4
1	D	773	VAL	2.4
1	C	774	ALA	2.4
1	B	105	SER	2.4
1	D	158	PHE	2.4
1	A	104	VAL	2.4
1	C	151	SER	2.4
1	B	786	GLY	2.4
1	D	813	GLY	2.4
1	D	787	LEU	2.4
1	C	152	ARG	2.4
1	C	113	TYR	2.4
1	B	782	ALA	2.4
1	C	165	ILE	2.4
1	D	331	ASP	2.4
1	B	102	PHE	2.4
1	A	97	ASN	2.4
1	D	169	LYS	2.4
1	D	782	ALA	2.4
1	A	422	PRO	2.3
1	B	96	ILE	2.3
1	C	153	THR	2.3
1	C	787	LEU	2.3
1	D	651	ASP	2.3
1	B	274	PHE	2.3
1	D	166	PRO	2.3
1	C	115	THR	2.3
1	B	805	VAL	2.3
1	D	797	VAL	2.3
1	C	111	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	114	LEU	2.3
1	C	157	ILE	2.3
1	D	148	ILE	2.3
1	D	135	VAL	2.3
1	B	423	PRO	2.3
1	C	154	PRO	2.3
1	B	95	ALA	2.2
1	D	112	ASN	2.2
1	D	113	TYR	2.3
1	B	122	LEU	2.2
1	D	771	PHE	2.2
1	D	220	TYR	2.2
1	A	807	GLY	2.2
1	B	802	GLY	2.2
1	D	780	SER	2.2
1	B	778	MET	2.2
1	D	110	LEU	2.2
1	C	765	PHE	2.2
1	D	721	GLY	2.2
1	C	196	ASP	2.2
1	D	750	PRO	2.2
1	C	769	LYS	2.2
1	C	136	VAL	2.1
1	C	140	ASN	2.1
1	D	290	ALA	2.1
1	D	425	ALA	2.1
1	A	792	GLY	2.1
1	C	791	GLY	2.1
1	D	109	GLY	2.1
1	D	648	THR	2.1
1	C	121	LYS	2.1
1	B	97	ASN	2.1
1	A	790	ILE	2.1
1	D	196	ASP	2.1
1	D	709	PRO	2.1
1	C	763	GLY	2.1
1	B	799	ALA	2.1
1	D	124	ALA	2.1
1	B	794	LEU	2.1
1	D	139	TRP	2.1
1	D	207	ARG	2.1
1	A	329	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	121	LYS	2.1
1	B	103	MET	2.1
1	B	136	VAL	2.0
1	B	139	TRP	2.0
1	C	108	GLY	2.0
1	C	795	PHE	2.0
1	C	216	THR	2.0
1	C	785	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.