



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:04 PM UTC

PDB ID : 5Y58 / pdb_00005y58
Title : Crystal structure of Ku70/80 and TLC1
Authors : Chen, H.; Xue, J.; Wu, J.; Lei, M.
Deposited on : 2017-08-08
Resolution : 2.80 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

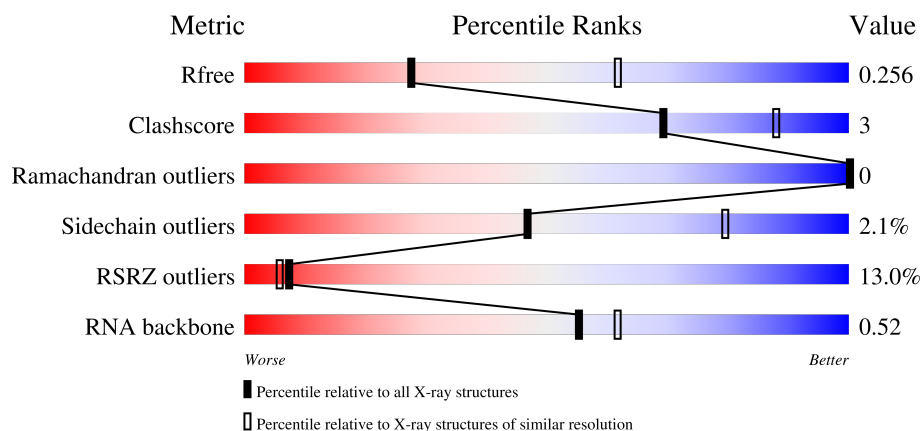
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)
RNA backbone	3983	1114 (3.00-2.60)

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	575	4% 83% 12% • 5%
1	C	575	2% 83% 11% • 5%
1	E	575	20% 84% 11% • 5%
2	B	628	12% 81% 8% • 10%

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Mol	Chain	Length	Quality of chain
2	D	628	9% 79% 10% 11%
2	F	628	25% 80% 9% 10%
3	X	30	7% 90% 7%
3	Y	30	3% 83% 13%
3	Z	30	13% 83% 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29320 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 ATP-dependent DNA helicase II subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	0	0	0
			4549	2926	743	863	17			
1	C	548	Total	C	N	O	S	0	0	0
			4549	2926	743	863	17			
1	E	548	Total	C	N	O	S	0	0	0
			4549	2926	743	863	17			

- Molecule 2 is a protein called ATP-dependent DNA helicase II subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	568	Total	C	N	O	S	0	0	0
			4509	2849	750	887	23			
2	D	560	Total	C	N	O	S	0	0	0
			4442	2812	737	870	23			
2	F	565	Total	C	N	O	S	0	0	0
			4493	2841	747	882	23			

- Molecule 3 is a RNA chain called TLC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	30	Total	C	N	O	P	0	0	0
			641	287	116	208	30			
3	Y	30	Total	C	N	O	P	0	0	0
			641	287	116	208	30			
3	Z	30	Total	C	N	O	P	0	0	0
			641	287	116	208	30			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	60	Total	O	0	0
			60	60		

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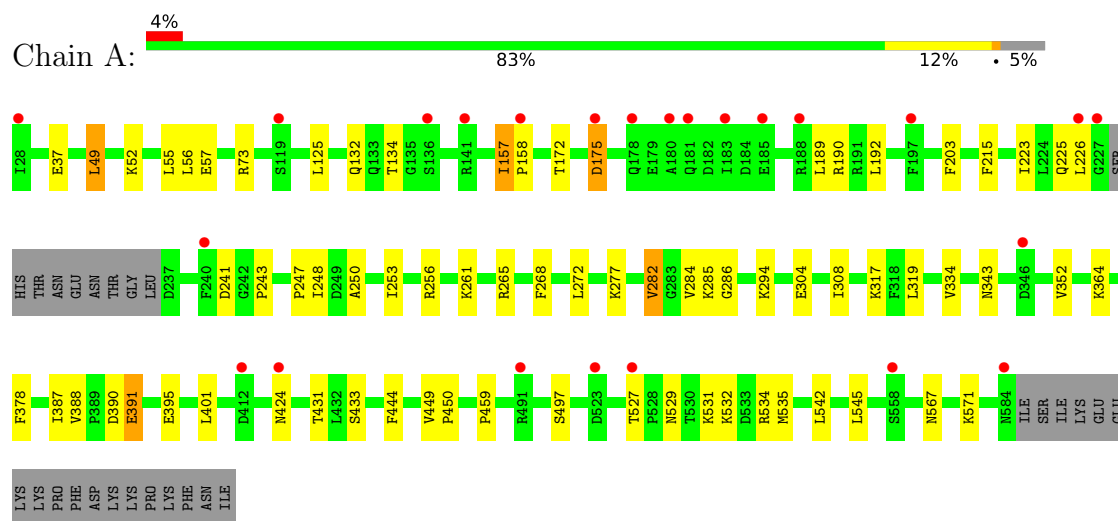
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	66	Total 66	O 66	0	0
4	X	14	Total 14	O 14	0	0
4	C	19	Total 19	O 19	0	0
4	D	48	Total 48	O 48	0	0
4	Y	13	Total 13	O 13	0	0
4	E	34	Total 34	O 34	0	0
4	F	45	Total 45	O 45	0	0
4	Z	7	Total 7	O 7	0	0

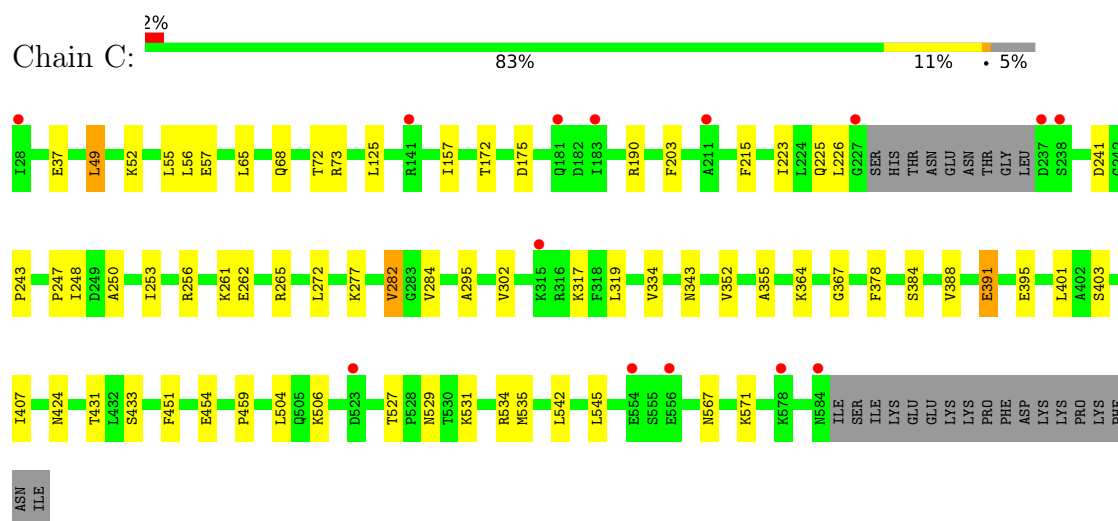
3 Residue-property plots

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.

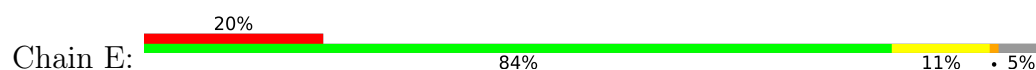
- Molecule 1: ATP-dependent DNA helicase II subunit 1

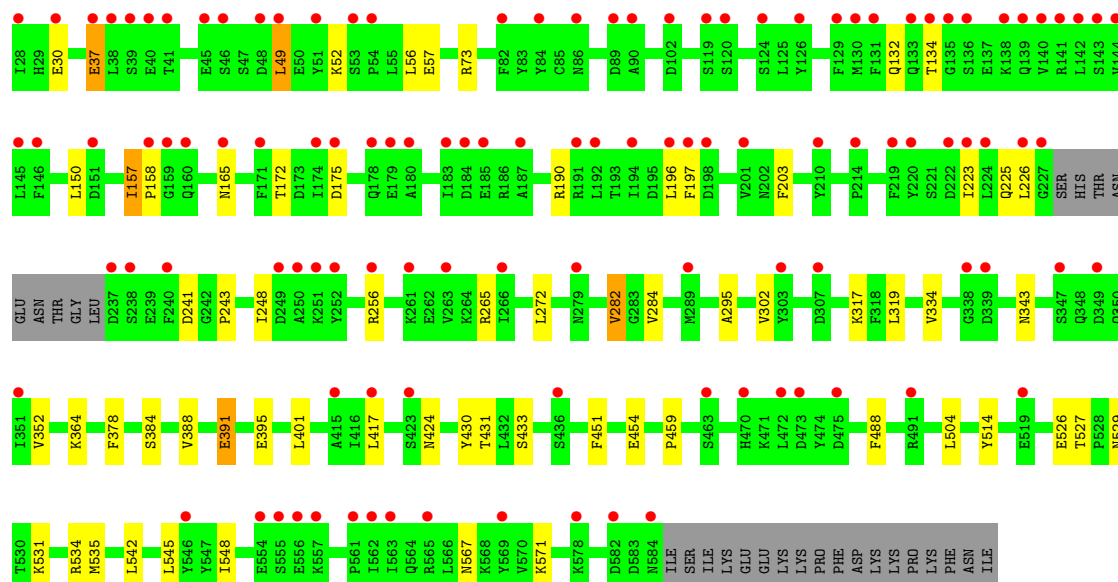


- Molecule 1: ATP-dependent DNA helicase II subunit 1

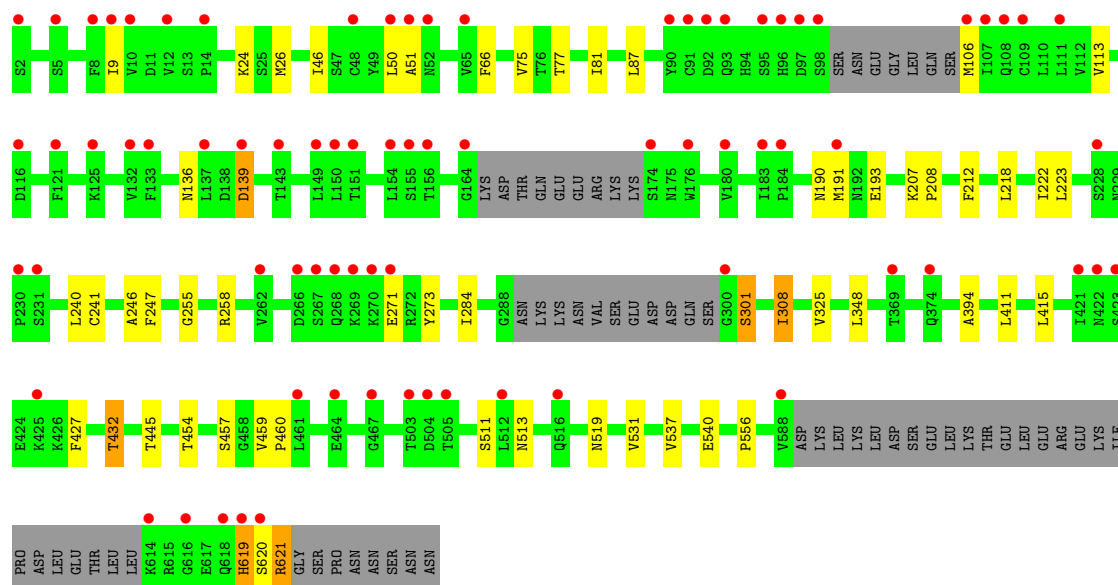
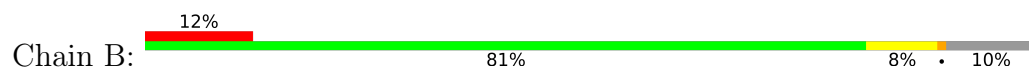


- Molecule 1: ATP-dependent DNA helicase II subunit 1

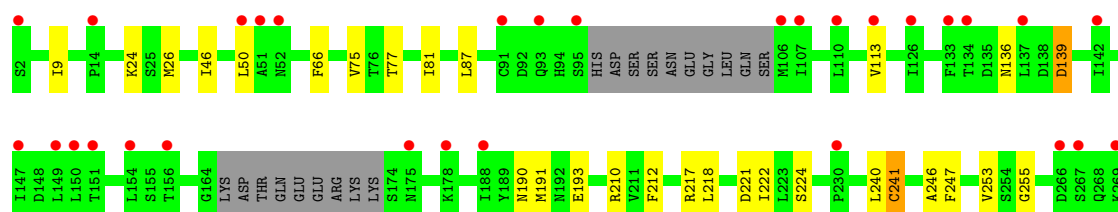
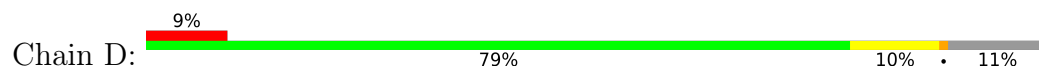


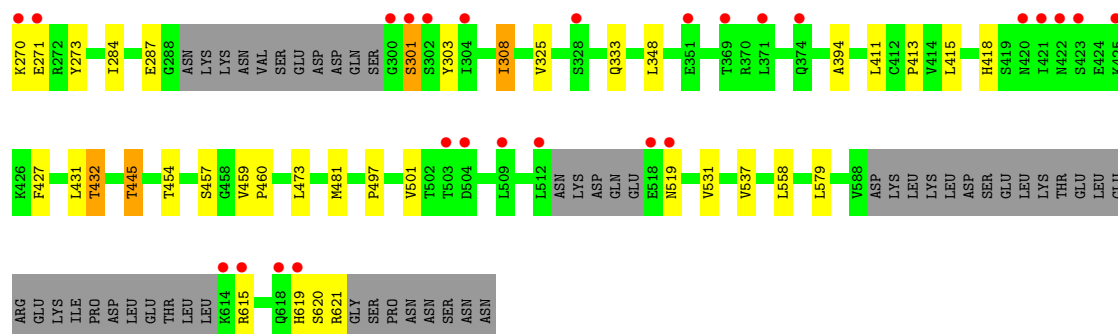


• Molecule 2: ATP-dependent DNA helicase II subunit 2

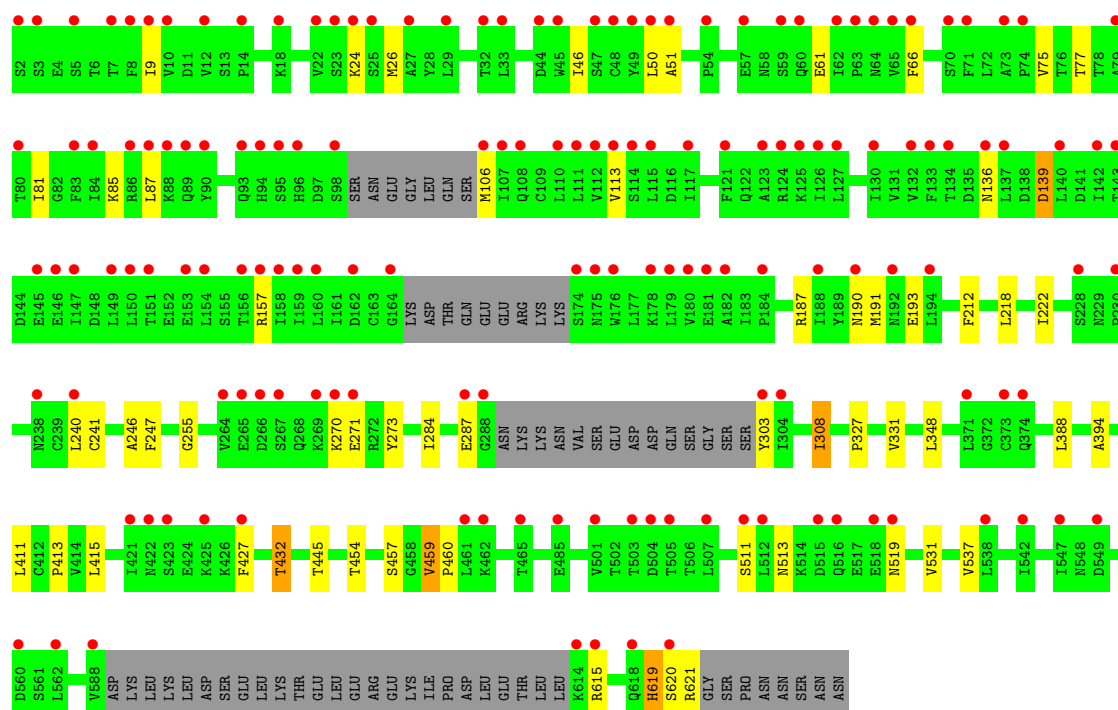
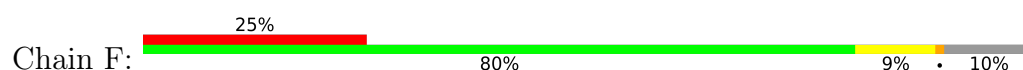


• Molecule 2: ATP-dependent DNA helicase II subunit 2

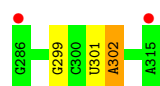
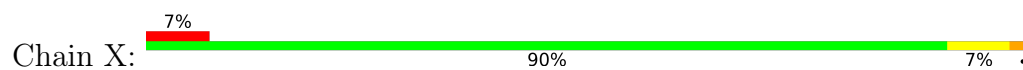




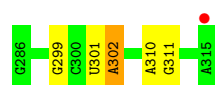
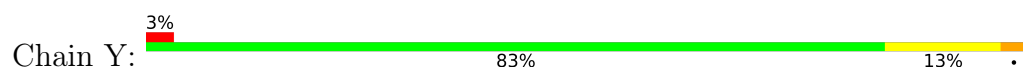
• Molecule 2: ATP-dependent DNA helicase II subunit 2



• Molecule 3: TLC1

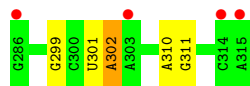


• Molecule 3: TLC1



● Molecule 3: TLC1

Chain Z: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	116.30Å 115.16Å 115.85Å 77.43° 78.48° 63.73°	Depositor
Resolution (Å)	44.11 – 2.80 44.11 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.8 (44.11-2.80) 91.8 (44.11-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.215 , 0.258 0.219 , 0.256	Depositor DCC
R_{free} test set	5915 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 60.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	29320	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 4.29% 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	0.28	0/4647	0.68	2/6253 (0.0%)
1	C	0.31	0/4647	0.68	2/6253 (0.0%)
1	E	0.29	0/4647	0.68	2/6253 (0.0%)
2	B	0.29	0/4583	0.71	2/6203 (0.0%)
2	D	0.30	0/4514	0.70	3/6109 (0.0%)
2	F	0.30	0/4567	0.71	3/6182 (0.0%)
3	X	0.12	0/717	0.22	0/1115
3	Y	0.11	0/717	0.23	0/1115
3	Z	0.17	0/717	0.24	0/1115
All	All	0.29	0/29756	0.67	14/40598 (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
2	B	0	1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	157	ILE	CA-C-N	6.30	127.72	119.84
1	C	157	ILE	C-N-CA	6.30	127.72	119.84
1	A	157	ILE	CA-C-N	6.12	127.49	119.84
1	A	157	ILE	C-N-CA	6.12	127.49	119.84
1	E	157	ILE	CA-C-N	5.97	127.30	119.84
1	E	157	ILE	C-N-CA	5.97	127.30	119.84
2	B	519	ASN	N-CA-C	-5.62	106.19	113.16
2	F	620	SER	N-CA-C	5.45	117.68	109.23
2	F	270	LYS	N-CA-C	-5.44	103.51	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	270	LYS	N-CA-C	-5.40	103.57	110.53
2	D	519	ASN	N-CA-C	-5.27	106.62	113.16
2	D	301	SER	CB-CA-C	-5.16	109.66	115.79
2	F	519	ASN	N-CA-C	-5.13	106.80	113.16
2	B	301	SER	CB-CA-C	-5.10	109.72	115.79

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	258	ARG	Sidechain

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	4549	0	4523	39	0
1	C	4549	0	4523	38	0
1	E	4549	0	4523	37	0
2	B	4509	0	4542	28	0
2	D	4442	0	4488	39	0
2	F	4493	0	4529	34	0
3	X	641	0	323	3	0
3	Y	641	0	323	3	0
3	Z	641	0	323	3	0
4	A	60	0	0	0	0
4	B	66	0	0	0	0
4	C	19	0	0	0	0
4	D	48	0	0	0	0
4	E	34	0	0	0	0
4	F	45	0	0	0	0
4	X	14	0	0	0	0
4	Y	13	0	0	0	0
4	Z	7	0	0	0	0
All	All	29320	0	28097	198	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 3.

All (198) 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:30:GLU:HG3	1:E:165:ASN:HB3	1.67	0.74
2:B:212:PHE:HB3	2:B:246:ALA:HB3	1.73	0.70
1:C:506:LYS:HE3	2:D:333:GLN:O	1.91	0.70
1:E:526:GLU:OE2	1:E:534:ARG:HD3	1.91	0.69
2:F:615:ARG:HH21	2:F:619:HIS:HB2	1.57	0.69
2:F:212:PHE:HB3	2:F:246:ALA:HB3	1.75	0.68
1:C:531:LYS:HE2	1:C:535:MET:HE3	1.76	0.66
2:D:212:PHE:HB3	2:D:246:ALA:HB3	1.76	0.66
2:B:190:ASN:HB2	2:B:193:GLU:HB2	1.78	0.65
1:C:49:LEU:HG	1:C:57:GLU:HG3	1.78	0.65
2:B:255:GLY:HA2	2:B:531:VAL:HG22	1.79	0.65
2:D:394:ALA:HB3	2:D:411:LEU:HB2	1.79	0.64
1:E:531:LYS:HE2	1:E:535:MET:HE3	1.80	0.64
2:D:190:ASN:HB2	2:D:193:GLU:HB2	1.80	0.64
1:C:52:LYS:HG3	1:C:56:LEU:HD23	1.82	0.61
1:A:391:GLU:HG2	1:A:395:GLU:HA	1.83	0.61
1:A:531:LYS:HE2	1:A:535:MET:HE3	1.83	0.60
1:E:49:LEU:HG	1:E:57:GLU:HG3	1.84	0.60
1:A:272:LEU:HB3	1:A:282:VAL:HG12	1.82	0.60
1:A:378:PHE:HA	2:B:432:THR:HG21	1.84	0.59
1:C:378:PHE:HA	2:D:432:THR:HG21	1.85	0.59
2:F:190:ASN:HB2	2:F:193:GLU:HB2	1.83	0.59
1:E:203:PHE:HB2	1:E:243:PRO:HG3	1.83	0.58
1:A:203:PHE:HB2	1:A:243:PRO:HG3	1.85	0.58
1:E:378:PHE:HA	2:F:432:THR:HG21	1.85	0.58
1:C:190:ARG:HG3	1:C:223:ILE:HA	1.86	0.57
1:C:203:PHE:HB2	1:C:243:PRO:HG3	1.86	0.57
2:F:255:GLY:HA2	2:F:531:VAL:HG22	1.85	0.57
2:B:394:ALA:HB3	2:B:411:LEU:HB2	1.86	0.57
1:C:272:LEU:HB3	1:C:282:VAL:HG12	1.86	0.57
2:D:255:GLY:HA2	2:D:531:VAL:HG22	1.86	0.56
1:A:190:ARG:HG3	1:A:223:ILE:HA	1.87	0.56
1:E:284:VAL:HG12	1:E:401:LEU:HD11	1.87	0.56
1:E:52:LYS:HG3	1:E:56:LEU:HD23	1.86	0.56
1:A:49:LEU:HG	1:A:57:GLU:HG3	1.88	0.56
1:A:52:LYS:HG3	1:A:56:LEU:HD23	1.88	0.56
1:E:352:VAL:HG22	2:F:537:VAL:HG21	1.88	0.55
2:F:394:ALA:HB3	2:F:411:LEU:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:317:LYS:HE2	1:E:319:LEU:HD21	1.89	0.54
2:D:9:ILE:HD11	2:D:113:VAL:HG21	1.88	0.54
1:C:284:VAL:HG12	1:C:401:LEU:HD11	1.90	0.54
2:F:218:LEU:HB3	2:F:240:LEU:HB2	1.90	0.54
1:C:352:VAL:HG22	2:D:537:VAL:HG21	1.90	0.54
1:E:190:ARG:HG3	1:E:223:ILE:HA	1.90	0.53
2:D:218:LEU:HB3	2:D:240:LEU:HB2	1.89	0.53
1:E:248:ILE:HD13	1:E:256:ARG:HD3	1.90	0.53
1:E:527:THR:HG22	1:E:529:ASN:H	1.74	0.52
1:E:30:GLU:CG	1:E:165:ASN:HB3	2.36	0.52
1:C:317:LYS:HE2	1:C:319:LEU:HD21	1.93	0.51
2:D:325:VAL:HG23	2:D:619:HIS:HE1	1.74	0.51
2:F:51:ALA:HB1	2:F:106:MET:HG2	1.92	0.51
1:E:73:ARG:HD2	1:E:265:ARG:HH21	1.75	0.51
2:F:24:LYS:HB3	2:F:191:MET:HE2	1.92	0.51
2:B:218:LEU:HB3	2:B:240:LEU:HB2	1.92	0.51
2:D:46:ILE:HG12	2:D:75:VAL:HG22	1.93	0.51
2:F:9:ILE:HD11	2:F:113:VAL:HG21	1.93	0.51
2:B:540:GLU:HG3	2:B:556:PRO:HG3	1.92	0.51
2:D:24:LYS:HB3	2:D:191:MET:HE2	1.93	0.51
2:D:271:GLU:HB3	2:D:273:TYR:HE1	1.76	0.51
2:B:620:SER:O	2:B:621:ARG:HB2	2.10	0.51
1:A:317:LYS:HE2	1:A:319:LEU:HD21	1.93	0.50
1:E:272:LEU:HB3	1:E:282:VAL:HG12	1.91	0.50
1:A:226:LEU:HB2	1:A:241:ASP:HA	1.93	0.50
1:A:542:LEU:HD22	2:B:222:ILE:HD12	1.94	0.50
1:E:542:LEU:HD22	2:F:222:ILE:HD12	1.92	0.50
3:X:299:G:O2'	3:X:302:A:N7	2.40	0.50
1:A:175:ASP:OD1	1:A:215:PHE:HA	2.12	0.50
1:C:302:VAL:HB	2:D:615:ARG:NH2	2.26	0.50
1:E:132:GLN:HB3	1:E:134:THR:HG23	1.94	0.50
1:E:391:GLU:HG2	1:E:395:GLU:HA	1.94	0.50
1:E:459:PRO:HG3	2:F:247:PHE:CD1	2.47	0.50
1:C:451:PHE:HB2	1:C:454:GLU:HG3	1.94	0.49
2:F:26:MET:HE2	2:F:87:LEU:HG	1.94	0.49
1:C:567:ASN:O	1:C:571:LYS:HG2	2.12	0.49
2:D:50:LEU:HD12	2:D:66:PHE:HD2	1.77	0.49
2:F:50:LEU:HD12	2:F:66:PHE:HD2	1.77	0.49
1:C:542:LEU:HD22	2:D:222:ILE:HD12	1.93	0.49
1:A:37:GLU:HB3	1:A:172:THR:HA	1.94	0.49
2:B:9:ILE:HD11	2:B:113:VAL:HG21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:454:THR:HG22	2:D:460:PRO:HA	1.94	0.49
2:B:51:ALA:HB1	2:B:106:MET:HG2	1.94	0.48
2:B:511:SER:C	2:B:513:ASN:H	2.21	0.48
1:C:55:LEU:HD23	1:C:125:LEU:HD13	1.95	0.48
1:C:545:LEU:HB2	2:D:222:ILE:HD11	1.95	0.48
1:A:334:VAL:HG12	1:A:343:ASN:HB2	1.95	0.48
1:A:352:VAL:HG22	2:B:537:VAL:HG21	1.95	0.48
1:C:73:ARG:HD2	1:C:265:ARG:HH21	1.79	0.48
2:D:26:MET:HE2	2:D:87:LEU:HG	1.95	0.48
1:E:514:TYR:CE2	2:F:621:ARG:HG3	2.49	0.48
1:E:150:LEU:HD13	1:E:196:LEU:HD23	1.96	0.48
1:A:248:ILE:HD13	1:A:256:ARG:HD3	1.95	0.48
1:C:226:LEU:HB2	1:C:241:ASP:HA	1.96	0.48
1:A:73:ARG:HD2	1:A:265:ARG:HH21	1.79	0.47
2:B:50:LEU:HD12	2:B:66:PHE:HD2	1.78	0.47
1:E:30:GLU:HG3	1:E:165:ASN:CB	2.42	0.47
2:F:415:LEU:HD22	2:F:427:PHE:HB3	1.97	0.47
2:B:46:ILE:HG12	2:B:75:VAL:HG22	1.95	0.47
2:D:620:SER:O	2:D:621:ARG:HB2	2.15	0.47
1:C:334:VAL:HG12	1:C:343:ASN:HB2	1.97	0.47
2:F:284:ILE:HG23	2:F:308:ILE:HG12	1.97	0.47
2:F:46:ILE:HG12	2:F:75:VAL:HG22	1.96	0.47
3:Z:299:G:O2'	3:Z:302:A:N7	2.48	0.47
2:B:77:THR:O	2:B:81:ILE:HG12	2.16	0.46
2:D:415:LEU:HD22	2:D:427:PHE:HB3	1.97	0.46
1:A:532:LYS:HE2	2:B:223:LEU:HD11	1.97	0.46
2:F:287:GLU:HA	2:F:303:TYR:HA	1.98	0.46
2:F:136:ASN:HB3	2:F:139:ASP:HB2	1.98	0.46
1:A:284:VAL:HG12	1:A:401:LEU:HD11	1.96	0.46
1:E:295:ALA:HB2	1:E:504:LEU:HD23	1.98	0.46
1:E:545:LEU:HB2	2:F:222:ILE:HD11	1.98	0.46
1:A:459:PRO:HG3	2:B:247:PHE:CD1	2.51	0.45
2:D:284:ILE:HG23	2:D:308:ILE:HG12	1.98	0.45
1:E:157:ILE:HA	1:E:158:PRO:HD2	1.73	0.45
2:F:77:THR:O	2:F:81:ILE:HG12	2.17	0.45
2:F:388:LEU:HG	2:F:413:PRO:HB2	1.97	0.45
2:F:81:ILE:HG22	2:F:85:LYS:HE2	1.98	0.45
2:F:511:SER:C	2:F:513:ASN:H	2.25	0.45
3:Z:310:A:H2'	3:Z:311:G:C8	2.52	0.45
1:C:459:PRO:HG3	2:D:247:PHE:CD1	2.52	0.45
1:E:226:LEU:HB2	1:E:241:ASP:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LEU:HD23	1:A:192:LEU:HD12	1.99	0.45
2:D:77:THR:O	2:D:81:ILE:HG12	2.17	0.45
3:Y:302:A:H2'	3:Y:302:A:N3	2.32	0.45
1:C:65:LEU:HG	1:C:261:LYS:HD3	1.99	0.45
2:D:221:ASP:HB3	2:D:224:SER:HB2	1.99	0.45
3:Z:302:A:H2'	3:Z:302:A:N3	2.32	0.45
3:Y:299:G:O2'	3:Y:302:A:N7	2.44	0.44
1:E:37:GLU:HB3	1:E:172:THR:HA	1.98	0.44
1:C:37:GLU:HB3	1:C:172:THR:HA	1.99	0.44
1:E:526:GLU:OE2	1:E:531:LYS:HA	2.18	0.44
3:X:302:A:N3	3:X:302:A:H2'	2.32	0.44
1:C:367:GLY:HA2	2:D:481:MET:HB3	2.00	0.44
2:F:454:THR:HG22	2:F:460:PRO:HA	2.00	0.44
2:F:271:GLU:HB3	2:F:273:TYR:HE1	1.83	0.43
1:A:294:LYS:NZ	3:X:299:G:N7	2.62	0.43
1:E:334:VAL:HG12	1:E:343:ASN:HB2	1.99	0.43
2:B:24:LYS:HB3	2:B:191:MET:HE2	2.00	0.43
2:B:26:MET:HE2	2:B:87:LEU:HG	1.99	0.43
1:C:248:ILE:HD13	1:C:256:ARG:HD3	2.00	0.43
3:Y:310:A:H2'	3:Y:311:G:C8	2.53	0.43
1:C:364:LYS:HB3	1:C:364:LYS:HE2	1.85	0.43
1:C:527:THR:HG22	1:C:529:ASN:H	1.82	0.43
2:D:473:LEU:HB2	2:D:579:LEU:HD13	2.00	0.43
1:A:55:LEU:HD23	1:A:125:LEU:HD13	1.99	0.43
2:B:284:ILE:HG23	2:B:308:ILE:HG12	2.00	0.43
1:E:567:ASN:O	1:E:571:LYS:HG2	2.18	0.43
1:A:364:LYS:HB3	1:A:364:LYS:HE2	1.83	0.43
2:D:136:ASN:HB3	2:D:139:ASP:HB2	2.00	0.42
1:C:403:SER:O	1:C:407:ILE:HG12	2.19	0.42
1:A:567:ASN:O	1:A:571:LYS:HG2	2.19	0.42
1:C:277:LYS:HE2	1:C:277:LYS:HB3	1.87	0.42
2:B:207:LYS:HA	2:B:208:PRO:HD3	1.91	0.42
1:C:355:ALA:HB1	2:D:558:LEU:HB2	2.01	0.42
1:A:157:ILE:HA	1:A:158:PRO:HD2	1.73	0.42
1:A:49:LEU:HD12	1:A:49:LEU:HA	1.90	0.42
1:C:295:ALA:HB2	1:C:504:LEU:HD23	2.02	0.42
1:A:387:ILE:HB	1:A:444:PHE:HB2	2.02	0.42
1:A:527:THR:HG22	1:A:529:ASN:H	1.84	0.42
2:B:415:LEU:HD22	2:B:427:PHE:HB3	2.02	0.42
1:E:197:PHE:HD2	1:E:226:LEU:HD21	1.84	0.42
1:A:277:LYS:HE2	1:A:277:LYS:HB3	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:GLU:HA	1:A:308:ILE:O	2.20	0.42
2:B:271:GLU:HB3	2:B:273:TYR:HE1	1.84	0.42
1:C:391:GLU:HG2	1:C:395:GLU:HA	2.00	0.42
1:A:250:ALA:HA	1:A:253:ILE:HG13	2.02	0.41
2:B:454:THR:HG22	2:B:460:PRO:HA	2.00	0.41
2:D:413:PRO:HA	2:D:431:LEU:HD23	2.02	0.41
2:D:620:SER:O	2:D:621:ARG:CB	2.68	0.41
2:F:287:GLU:HG3	2:F:303:TYR:HB3	2.01	0.41
2:F:157:ARG:HH22	2:F:187:ARG:HH12	1.68	0.41
1:A:215:PHE:HB3	1:A:247:PRO:HB3	2.02	0.41
1:A:545:LEU:HB2	2:B:222:ILE:HD11	2.02	0.41
1:E:302:VAL:HB	2:F:615:ARG:NH2	2.35	0.41
1:C:302:VAL:HB	2:D:615:ARG:HH22	1.85	0.41
2:D:271:GLU:HB3	2:D:273:TYR:CE1	2.56	0.41
1:C:262:GLU:HB2	2:D:445:THR:HG23	2.02	0.41
1:A:285:LYS:HG3	1:A:390:ASP:HB2	2.02	0.41
1:C:454:GLU:HG2	2:D:253:VAL:HG22	2.02	0.41
2:D:418:HIS:CE1	2:D:497:PRO:HG3	2.55	0.41
1:E:488:PHE:CE1	1:E:548:ILE:HG23	2.56	0.41
2:F:459:VAL:HA	2:F:460:PRO:HD3	1.91	0.41
1:A:261:LYS:HE3	1:A:261:LYS:HB3	1.94	0.41
2:B:325:VAL:HG23	2:B:619:HIS:CE1	2.55	0.41
1:E:364:LYS:HB3	1:E:364:LYS:HE2	1.90	0.41
1:A:268:PHE:CE1	1:A:286:GLY:HA3	2.55	0.41
2:B:136:ASN:HB3	2:B:139:ASP:HB2	2.03	0.41
1:C:250:ALA:HA	1:C:253:ILE:HG13	2.02	0.41
2:D:325:VAL:HB	2:D:619:HIS:HE2	1.86	0.41
2:F:327:PRO:O	2:F:331:VAL:HG23	2.21	0.41
2:D:287:GLU:HA	2:D:303:TYR:HA	2.03	0.41
2:F:271:GLU:HB3	2:F:273:TYR:CE1	2.56	0.41
1:A:449:VAL:HA	1:A:450:PRO:HD3	1.97	0.40
1:C:215:PHE:HB3	1:C:247:PRO:HB3	2.02	0.40
1:E:417:LEU:HB2	1:E:430:TYR:HB2	2.01	0.40
1:E:451:PHE:HB2	1:E:454:GLU:HG3	2.03	0.40
1:A:132:GLN:HB3	1:A:134:THR:HG23	2.04	0.40
2:D:217:ARG:HG2	2:D:241:CYS:SG	2.61	0.40
1:C:68:GLN:OE1	1:C:261:LYS:HE2	2.22	0.40

There are no symmetry-related clashes.

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	544/575 (95%)	529 (97%)	15 (3%)	0	100	100
1	C	544/575 (95%)	526 (97%)	18 (3%)	0	100	100
1	E	544/575 (95%)	527 (97%)	17 (3%)	0	100	100
2	B	558/628 (89%)	539 (97%)	19 (3%)	0	100	100
2	D	548/628 (87%)	531 (97%)	17 (3%)	0	100	100
2	F	555/628 (88%)	536 (97%)	19 (3%)	0	100	100
All	All	3293/3609 (91%)	3188 (97%)	105 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	510/536 (95%)	499 (98%)	11 (2%)	45	78
1	C	510/536 (95%)	498 (98%)	12 (2%)	43	77
1	E	510/536 (95%)	499 (98%)	11 (2%)	45	78
2	B	527/585 (90%)	516 (98%)	11 (2%)	47	79
2	D	519/585 (89%)	508 (98%)	11 (2%)	47	79
2	F	525/585 (90%)	515 (98%)	10 (2%)	50	81
All	All	3101/3363 (92%)	3035 (98%)	66 (2%)	47	79

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	LEU
1	A	175	ASP
1	A	225	GLN
1	A	282	VAL
1	A	388	VAL
1	A	391	GLU
1	A	424	ASN
1	A	431	THR
1	A	433	SER
1	A	497	SER
1	A	534	ARG
2	B	139	ASP
2	B	241	CYS
2	B	301	SER
2	B	308	ILE
2	B	348	LEU
2	B	432	THR
2	B	445	THR
2	B	457	SER
2	B	459	VAL
2	B	619	HIS
2	B	621	ARG
1	C	49	LEU
1	C	72	THR
1	C	175	ASP
1	C	225	GLN
1	C	282	VAL
1	C	384	SER
1	C	388	VAL
1	C	391	GLU
1	C	424	ASN
1	C	431	THR
1	C	433	SER
1	C	534	ARG
2	D	139	ASP
2	D	210	ARG
2	D	241	CYS
2	D	301	SER
2	D	308	ILE
2	D	348	LEU
2	D	432	THR
2	D	445	THR

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Mol	Chain	Res	Type
2	D	457	SER
2	D	459	VAL
2	D	501	VAL
1	E	37	GLU
1	E	49	LEU
1	E	175	ASP
1	E	225	GLN
1	E	282	VAL
1	E	384	SER
1	E	388	VAL
1	E	391	GLU
1	E	424	ASN
1	E	431	THR
1	E	433	SER
2	F	61	GLU
2	F	139	ASP
2	F	241	CYS
2	F	308	ILE
2	F	348	LEU
2	F	432	THR
2	F	445	THR
2	F	457	SER
2	F	459	VAL
2	F	619	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	21	ASN
2	B	175	ASN
2	B	390	ASN
1	C	426	HIS
2	D	21	ASN
2	D	229	ASN
2	D	285	HIS
2	D	390	ASN
1	E	426	HIS
1	E	525	ASN
2	F	21	ASN
2	F	60	GLN
2	F	229	ASN
2	F	390	ASN

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Mol	Chain	Res	Type
2	F	407	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	X	29/30 (96%)	2 (6%)	0
3	Y	29/30 (96%)	2 (6%)	0
3	Z	29/30 (96%)	2 (6%)	0
All	All	87/90 (96%)	6 (6%)	0

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	X	301	U
3	X	302	A
3	Y	301	U
3	Y	302	A
3	Z	301	U
3	Z	302	A

There are no RNA pucker outliers to report.

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

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	548/575 (95%)	0.24	24 (4%) 39 31	16, 51, 99, 142	0
1	C	548/575 (95%)	0.03	14 (2%) 57 47	17, 46, 94, 150	0
1	E	548/575 (95%)	1.11	115 (20%) 2 2	29, 71, 130, 181	0
2	B	568/628 (90%)	0.66	77 (13%) 7 5	16, 64, 143, 204	0
2	D	560/628 (89%)	0.52	56 (10%) 12 9	18, 64, 149, 189	0
2	F	565/628 (89%)	1.28	154 (27%) 1 1	22, 82, 163, 200	0
3	X	30/30 (100%)	0.10	2 (6%) 24 17	32, 55, 109, 130	0
3	Y	30/30 (100%)	-0.04	1 (3%) 49 39	34, 57, 100, 122	0
3	Z	30/30 (100%)	0.34	4 (13%) 7 5	35, 55, 116, 126	0
All	All	3427/3699 (92%)	0.63	447 (13%) 7 6	16, 60, 140, 204	0

All (447) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	267	SER	6.4
2	B	270	LYS	6.0
1	A	178	GLN	5.7
2	D	106	MET	5.7
2	F	270	LYS	5.5
2	F	107	ILE	5.5
1	E	131	PHE	5.5
2	B	150	LEU	5.1
2	D	269	LYS	5.0
2	F	60	GLN	5.0
1	E	240	PHE	4.9
2	F	108	GLN	4.9
2	F	59	SER	4.7
2	B	516	GLN	4.7
2	F	10	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
2	D	512	LEU	4.6
2	F	507	LEU	4.6
2	D	271	GLU	4.6
2	D	421	ILE	4.5
1	A	227	GLY	4.5
2	F	271	GLU	4.5
2	F	620	SER	4.5
2	D	270	LYS	4.5
3	Z	315	A	4.3
2	B	230	PRO	4.3
2	B	149	LEU	4.2
2	B	133	PHE	4.2
2	D	107	ILE	4.2
1	E	28	ILE	4.2
2	D	425	LYS	4.1
2	F	134	THR	4.1
2	B	98	SER	4.1
2	F	71	PHE	4.1
1	E	183	ILE	4.1
2	F	461	LEU	4.0
2	F	269	LYS	4.0
2	F	3	SER	4.0
2	F	160	LEU	4.0
2	F	427	PHE	4.0
2	B	369	THR	4.0
2	F	14	PRO	3.9
2	F	106	MET	3.9
2	D	267	SER	3.9
1	E	227	GLY	3.8
2	F	158	ILE	3.8
2	D	151	THR	3.8
1	E	38	LEU	3.8
2	F	137	LEU	3.8
2	B	97	ASP	3.8
2	F	51	ALA	3.8
1	E	569	TYR	3.7
2	F	9	ILE	3.7
2	F	133	PHE	3.7
2	B	151	THR	3.7
1	C	28	ILE	3.7
2	D	2	SER	3.7
2	F	516	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
2	F	371	LEU	3.7
1	C	227	GLY	3.7
2	F	8	PHE	3.7
2	F	62	ILE	3.7
2	D	423	SER	3.6
2	F	114	SER	3.6
2	F	115	LEU	3.6
2	B	619	HIS	3.5
2	F	421	ILE	3.5
2	F	180	VAL	3.5
2	F	70	SER	3.5
1	A	28	ILE	3.4
1	A	183	ILE	3.4
2	B	106	MET	3.4
2	D	178	LYS	3.4
1	E	226	LEU	3.4
2	F	73	ALA	3.4
1	E	84	TYR	3.4
2	F	80	THR	3.4
1	E	140	VAL	3.4
2	F	164	GLY	3.4
1	E	54	PRO	3.4
2	F	94	HIS	3.4
2	F	188	ILE	3.3
2	F	151	THR	3.3
2	F	87	LEU	3.3
2	F	110	LEU	3.3
1	E	45	GLU	3.3
1	E	192	LEU	3.3
1	E	197	PHE	3.3
1	A	141	ARG	3.3
1	E	49	LEU	3.3
2	F	2	SER	3.3
2	F	504	ASP	3.3
1	E	146	PHE	3.3
1	C	554	GLU	3.2
2	F	66	PHE	3.2
2	B	176	TRP	3.2
1	E	133	GLN	3.2
1	E	251	LYS	3.2
3	X	315	A	3.2
1	E	180	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	201	VAL	3.2
1	E	160	GLN	3.2
2	F	63	PRO	3.2
1	E	347	SER	3.1
2	F	615	ARG	3.1
1	E	561	PRO	3.1
2	B	614	LYS	3.1
2	F	425	LYS	3.1
1	E	120	SER	3.1
1	C	141	ARG	3.1
1	E	196	LEU	3.1
2	B	137	LEU	3.1
2	D	137	LEU	3.1
2	F	111	LEU	3.1
2	F	143	THR	3.1
1	E	90	ALA	3.1
2	D	328	SER	3.1
1	E	584	ASN	3.1
2	D	618	GLN	3.1
1	E	126	TYR	3.0
1	E	339	ASP	3.0
2	B	5	SER	3.0
2	F	48	CYS	3.0
2	B	421	ILE	3.0
2	B	51	ALA	3.0
2	F	23	SER	3.0
2	F	44	ASP	3.0
2	F	64	ASN	3.0
2	B	300	GLY	3.0
1	E	557	LYS	3.0
2	F	125	LYS	3.0
2	F	65	VAL	3.0
1	E	252	TYR	3.0
1	E	562	ILE	3.0
1	E	222	ASP	3.0
2	B	512	LEU	3.0
2	B	620	SER	3.0
2	F	33	LEU	3.0
2	F	47	SER	3.0
1	E	41	THR	3.0
2	D	503	THR	3.0
2	F	7	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	436	SER	3.0
2	F	266	ASP	3.0
2	B	271	GLU	3.0
1	E	129	PHE	3.0
2	F	124	ARG	2.9
1	A	180	ALA	2.9
1	A	527	THR	2.9
2	B	10	VAL	2.9
1	E	138	LYS	2.9
1	C	237	ASP	2.9
1	E	184	ASP	2.9
2	D	615	ARG	2.9
2	F	562	LEU	2.9
1	E	220	TYR	2.9
2	B	108	GLN	2.9
2	F	49	TYR	2.9
2	F	518	GLU	2.9
1	E	249	ASP	2.9
2	B	132	VAL	2.9
2	F	84	ILE	2.9
2	D	154	LEU	2.9
2	F	154	LEU	2.9
2	F	288	GLY	2.9
1	E	175	ASP	2.9
2	B	2	SER	2.9
2	F	140	LEU	2.9
1	E	40	GLU	2.8
2	F	25	SER	2.8
2	D	149	LEU	2.8
1	E	30	GLU	2.8
2	F	176	TRP	2.8
2	F	123	ALA	2.8
1	E	46	SER	2.8
2	B	143	THR	2.8
2	F	373	CYS	2.8
2	F	265	GLU	2.8
2	F	93	GLN	2.8
2	B	180	VAL	2.8
2	B	107	ILE	2.8
2	F	159	ILE	2.8
2	D	14	PRO	2.8
1	A	181	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
2	F	121	PHE	2.7
1	E	145	LEU	2.7
2	D	519	ASN	2.7
2	B	266	ASP	2.7
2	F	505	THR	2.7
2	D	95	SER	2.7
2	B	14	PRO	2.7
1	A	188	ARG	2.7
2	F	89	GLN	2.7
1	A	185	GLU	2.7
1	E	563	ILE	2.7
2	D	420	ASN	2.7
2	B	504	ASP	2.7
1	E	143	SER	2.7
2	F	98	SER	2.7
1	A	240	PHE	2.7
2	B	154	LEU	2.7
2	F	614	LYS	2.7
2	F	96	HIS	2.7
1	A	424	ASN	2.7
1	C	584	ASN	2.7
1	E	565	ARG	2.7
1	E	554	GLU	2.7
2	F	174	SER	2.7
1	E	134	THR	2.7
2	F	54	PRO	2.7
1	E	48	ASP	2.7
1	E	519	GLU	2.7
2	B	155	SER	2.7
2	B	423	SER	2.7
2	B	96	HIS	2.6
2	D	150	LEU	2.6
2	F	149	LEU	2.6
2	F	179	LEU	2.6
1	A	558	SER	2.6
1	C	211	ALA	2.6
1	E	289	MET	2.6
2	F	95	SER	2.6
3	X	286	G	2.6
2	B	8	PHE	2.6
1	E	555	SER	2.6
2	F	5	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	158	PRO	2.6
2	B	111	LEU	2.6
2	B	156	THR	2.6
1	A	412	ASP	2.6
2	F	228	SER	2.6
1	C	315	LYS	2.6
2	B	90	TYR	2.6
2	F	150	LEU	2.6
2	B	9	ILE	2.6
2	F	192	ASN	2.6
2	F	462	LYS	2.5
2	F	50	LEU	2.5
2	F	588	VAL	2.5
1	E	307	ASP	2.5
2	B	95	SER	2.5
2	B	588	VAL	2.5
2	F	113	VAL	2.5
1	E	556	GLU	2.5
1	E	250	ALA	2.5
1	E	491	ARG	2.5
1	A	136	SER	2.5
2	F	127	LEU	2.5
2	F	157	ARG	2.5
1	E	237	ASP	2.5
2	F	515	ASP	2.5
2	B	616	GLY	2.5
2	F	45	TRP	2.5
2	F	88	LYS	2.5
3	Z	314	C	2.5
2	B	91	CYS	2.5
2	B	422	ASN	2.5
1	E	142	LEU	2.4
2	F	512	LEU	2.4
2	F	74	PRO	2.4
2	D	300	GLY	2.4
2	F	145	GLU	2.4
1	A	584	ASN	2.4
1	A	226	LEU	2.4
1	C	183	ILE	2.4
1	E	194	ILE	2.4
2	F	147	ILE	2.4
2	B	12	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	39	SER	2.4
1	E	136	SER	2.4
2	B	174	SER	2.4
1	C	578	LYS	2.4
1	E	261	LYS	2.4
2	D	133	PHE	2.4
2	F	18	LYS	2.4
2	F	181	GLU	2.4
2	F	156	THR	2.4
2	F	465	THR	2.4
1	E	223	ILE	2.4
2	B	48	CYS	2.4
2	B	184	PRO	2.4
2	D	126	ILE	2.4
2	F	547	ILE	2.4
1	A	346	ASP	2.4
2	F	112	VAL	2.4
2	D	371	LEU	2.4
1	E	279	ASN	2.4
2	D	52	ASN	2.4
2	F	175	ASN	2.4
1	A	197	PHE	2.4
3	Z	303	A	2.4
1	E	53	SER	2.4
2	D	230	PRO	2.4
2	F	178	LYS	2.3
2	B	164	GLY	2.3
2	B	92	ASP	2.3
2	D	518	GLU	2.3
1	E	124	SER	2.3
2	F	423	SER	2.3
2	F	130	ILE	2.3
2	F	24	LYS	2.3
2	F	264	VAL	2.3
1	E	86	ASN	2.3
1	E	338	GLY	2.3
1	E	187	ALA	2.3
2	B	109	CYS	2.3
2	D	509	LEU	2.3
1	E	470	HIS	2.3
2	D	619	HIS	2.3
1	E	174	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	147	ILE	2.3
2	D	113	VAL	2.3
2	F	132	VAL	2.3
1	E	159	GLY	2.3
2	B	121	PHE	2.3
2	F	287	GLU	2.3
2	B	50	LEU	2.3
2	D	50	LEU	2.3
1	C	238	SER	2.3
2	B	228	SER	2.3
2	F	503	THR	2.3
1	E	210	TYR	2.3
1	E	256	ARG	2.3
2	F	230	PRO	2.3
3	Y	315	A	2.3
1	E	135	GLY	2.3
2	D	175	ASN	2.3
2	F	190	ASN	2.3
2	F	238	ASN	2.3
1	E	185	GLU	2.3
2	D	93	GLN	2.3
2	B	269	LYS	2.3
1	E	463	SER	2.3
2	B	65	VAL	2.3
2	F	501	VAL	2.3
2	D	51	ALA	2.2
2	B	374	GLN	2.2
2	B	139	ASP	2.2
2	D	504	ASP	2.2
2	F	142	ILE	2.2
2	B	503	THR	2.2
1	E	144	VAL	2.2
1	E	303	TYR	2.2
1	E	546	TYR	2.2
2	B	231	SER	2.2
2	B	267	SER	2.2
2	F	12	VAL	2.2
2	F	511	SER	2.2
1	E	130	MET	2.2
1	E	415	ALA	2.2
1	E	417	LEU	2.2
2	B	425	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	461	LEU	2.2
2	F	153	GLU	2.2
2	B	93	GLN	2.2
1	A	523	ASP	2.2
1	E	191	ARG	2.2
2	B	505	THR	2.2
2	D	369	THR	2.2
1	E	51	TYR	2.2
2	F	90	TYR	2.2
1	E	171	PHE	2.2
1	E	224	LEU	2.2
2	D	351	GLU	2.2
2	B	183	ILE	2.2
2	F	304	ILE	2.2
2	D	91	CYS	2.2
1	E	119	SER	2.2
2	D	302	SER	2.2
2	F	538	LEU	2.2
2	F	57	GLU	2.2
2	F	485	GLU	2.2
1	E	139	GLN	2.2
1	E	178	GLN	2.2
1	E	263	VAL	2.2
1	E	582	ASP	2.2
2	D	156	THR	2.2
2	B	618	GLN	2.1
2	F	374	GLN	2.1
2	B	52	ASN	2.1
1	C	523	ASP	2.1
2	F	560	ASP	2.1
1	E	578	LYS	2.1
2	B	125	LYS	2.1
2	D	110	LEU	2.1
2	F	27	ALA	2.1
1	E	351	ILE	2.1
2	F	422	ASN	2.1
1	E	214	PRO	2.1
1	E	102	ASP	2.1
2	F	549	ASP	2.1
2	F	29	LEU	2.1
1	C	556	GLU	2.1
2	F	146	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
3	Z	286	G	2.1
2	B	191	MET	2.1
2	B	262	VAL	2.1
2	F	136	ASN	2.1
2	F	184	PRO	2.1
1	A	175	ASP	2.1
1	E	349	ASP	2.1
1	E	472	LEU	2.1
2	B	116	ASP	2.1
2	F	162	ASP	2.1
2	F	194	LEU	2.1
2	F	240	LEU	2.1
2	D	134	THR	2.1
2	F	86	ARG	2.1
2	D	304	ILE	2.1
2	F	126	ILE	2.1
2	F	618	GLN	2.1
1	E	165	ASN	2.1
2	D	422	ASN	2.1
2	F	519	ASN	2.1
1	E	219	PHE	2.1
2	B	467	GLY	2.1
2	F	83	PHE	2.1
1	E	151	ASP	2.1
1	E	473	ASP	2.1
2	F	32	THR	2.1
2	D	142	ILE	2.1
2	F	79	ALA	2.1
1	E	238	SER	2.0
1	E	423	SER	2.0
2	D	301	SER	2.0
2	B	268	GLN	2.0
2	D	374	GLN	2.0
1	A	491	ARG	2.0
1	E	82	PHE	2.0
1	E	141	ARG	2.0
1	E	198	ASP	2.0
2	D	266	ASP	2.0
2	F	542	ILE	2.0
1	E	37	GLU	2.0
2	B	464	GLU	2.0
2	F	303	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	119	SER	2.0
1	C	181	GLN	2.0
1	A	158	PRO	2.0
1	E	266	ILE	2.0
2	D	188	ILE	2.0
2	F	117	ILE	2.0
2	F	182	ALA	2.0
1	E	89	ASP	2.0
1	E	179	GLU	2.0
1	E	475	ASP	2.0
2	D	614	LYS	2.0
2	F	22	VAL	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.