



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:43 PM UTC

PDB ID : 4N41 / pdb_00004n41
Title : Structure of Thermus thermophilus Argonaute bound to guide DNA and 15-mer target DNA
Authors : Sheng, G.; Zhao, H.; Wang, J.; Rao, Y.; Wang, Y.
Deposited on : 2013-10-08
Resolution : 2.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

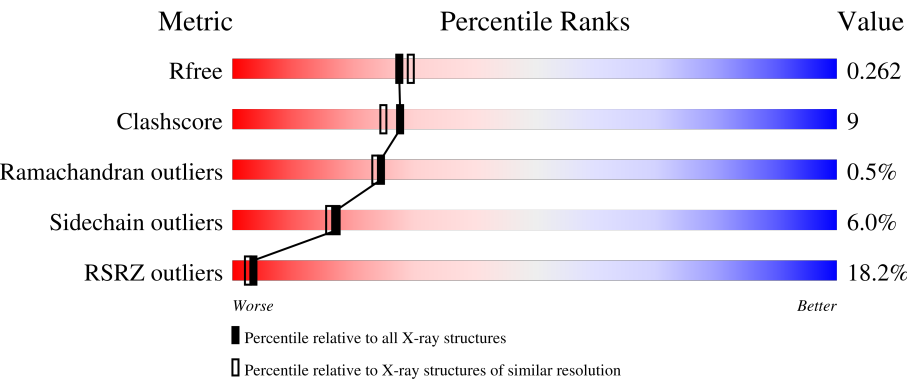
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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	685	15% 76% 18% • •
1	B	685	21% 75% 20% • •
2	C	21	33% 24% 14% 29%
2	E	21	5% 29% 29% 19% 24%
3	D	13	38% 62%

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Mol	Chain	Length	Quality of chain
4	F	14	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: green (36%), yellow (57%), and orange (7%).

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11432 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 Argonaute.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	658	Total	C	N	O	S	0	1	0
			4977	3177	937	857	6			
1	B	667	Total	C	N	O	S	0	0	0
			5093	3261	949	877	6			

- Molecule 2 is a DNA chain called 5'-D(P*TP*GP*AP*GP*GP*TP*AP*GP*TP*AP*GP*GP*TP*T*GP*TP*AP*TP*AP*GP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	15	Total	C	N	O	P	0	0	0
			315	150	60	91	14			
2	E	16	Total	C	N	O	P	0	0	0
			338	160	62	100	16			

- Molecule 3 is a DNA chain called 5'-D(P*AP*CP*CP*TP*AP*CP*TP*AP*CP*CP*TP*C P*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	13	Total	C	N	O	P	0	0	0
			259	124	44	78	13			

- Molecule 4 is a DNA chain called 5'-D(*AP*AP*CP*CP*TP*AP*CP*TP*GP*CP*CP*TP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	14	Total	C	N	O	P	0	0	0
			277	134	49	81	13			

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Mg 1	0	0
5	C	1	Total 1	Mg 1	0	0
5	E	1	Total 1	Mg 1	0	0

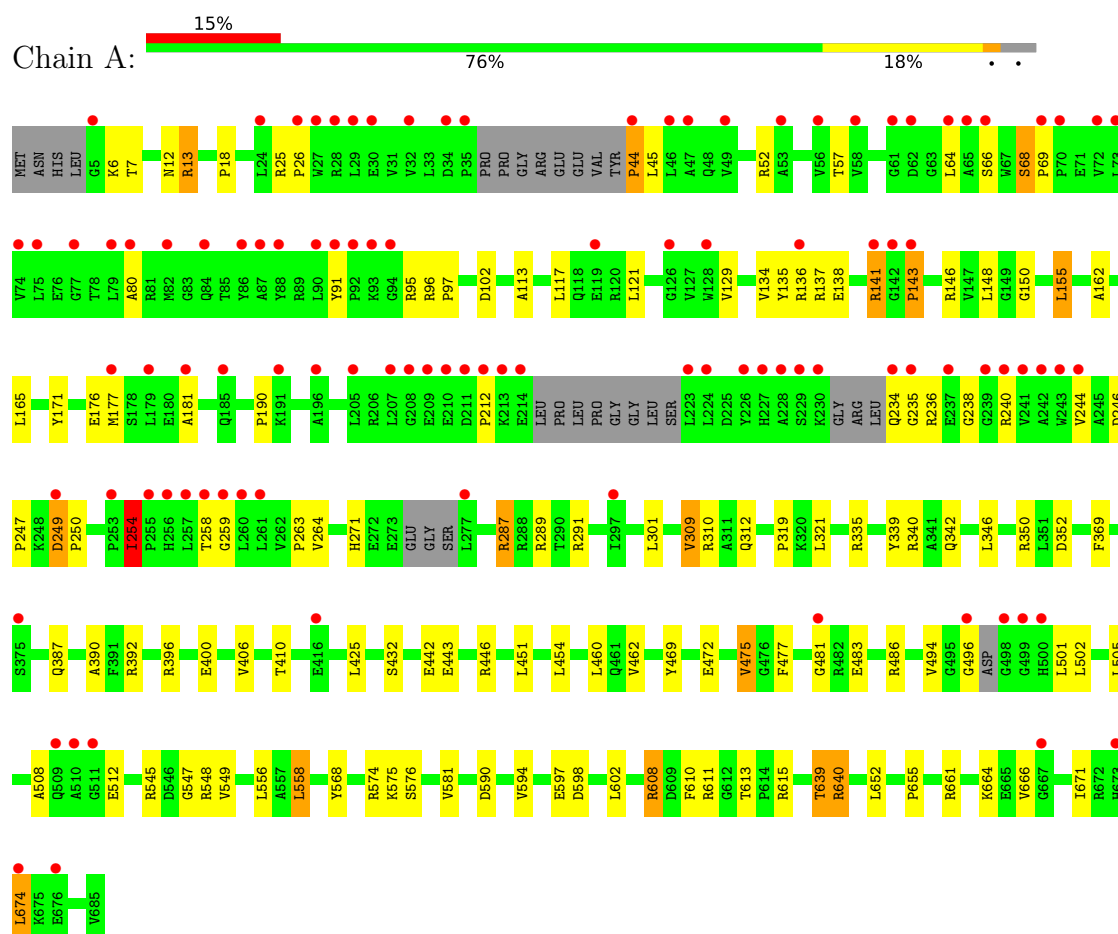
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	126	Total 126	O 126	0	0
6	B	14	Total 14	O 14	0	0
6	C	15	Total 15	O 15	0	0
6	E	6	Total 6	O 6	0	0
6	D	8	Total 8	O 8	0	0
6	F	1	Total 1	O 1	0	0

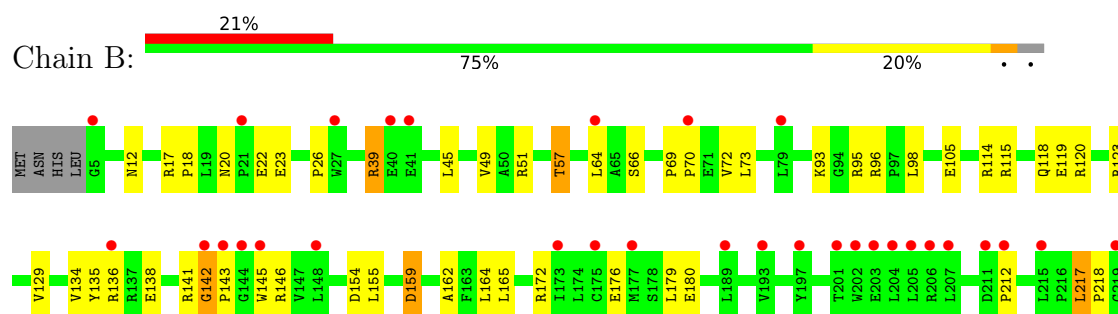
3 Residue-property plots [i](#)

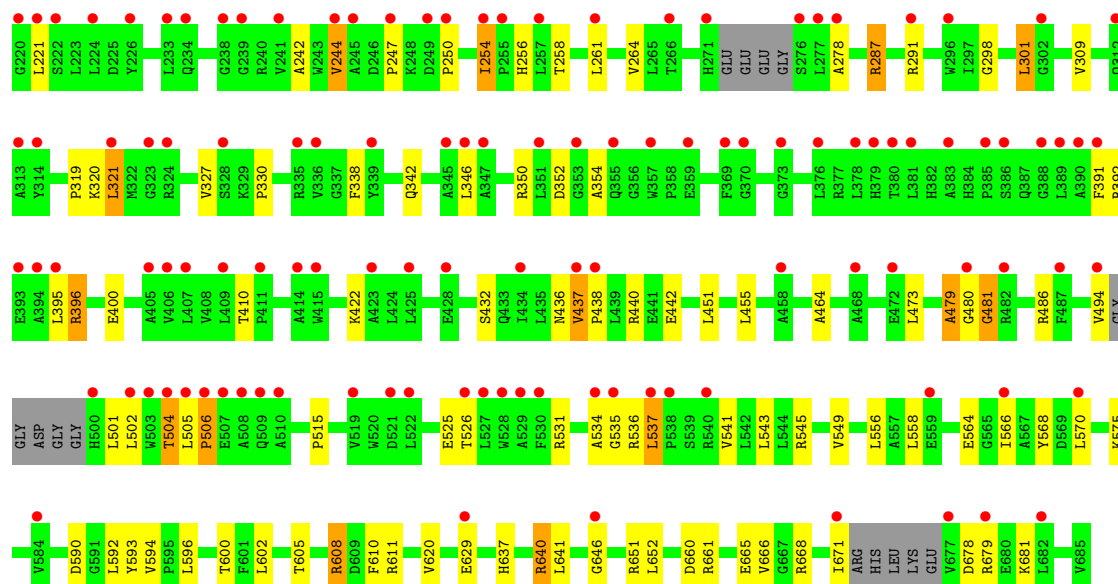
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Argonaute



• Molecule 1: Argonaute





• Molecule 2: 5'-D(P*TP*GP*AP*GP*GP*TP*AP*GP*TP*AP*GP*GP*TP*T*GP*TP*AP*T
P*AP*GP*T)-3'

Chain C: 33% 24% 14% 29%



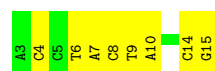
• Molecule 2: 5'-D(P*TP*GP*AP*GP*GP*TP*AP*GP*TP*AP*GP*GP*TP*T*GP*TP*AP*T
P*AP*GP*T)-3'

Chain E: 5% 29% 29% 19% 24%



• Molecule 3: 5'-D(P*AP*CP*CP*TP*AP*CP*TP*AP*CP*CP*TP*CP*G)-3'

Chain D: 38% 62%



• Molecule 4: 5'-D(*AP*AP*CP*CP*TP*AP*CP*TP*GP*CP*CP*TP*CP*G)-3'

Chain F: 36% 57% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.51Å 101.70Å 153.02Å 90.00° 93.52° 90.00°	Depositor
Resolution (Å)	45.52 – 2.25 45.52 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.52-2.25) 99.7 (45.52-2.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.223 , 0.259 0.228 , 0.262	Depositor DCC
R_{free} test set	4330 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.437	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11432	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 4.26% 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

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.67	2/5092 (0.0%)	0.92	20/6922 (0.3%)
1	B	0.41	1/5212 (0.0%)	0.84	8/7090 (0.1%)
2	C	0.35	0/353	1.39	6/542 (1.1%)
2	E	0.24	0/378	1.19	5/580 (0.9%)
3	D	0.35	0/288	1.31	2/440 (0.5%)
4	F	0.24	0/309	1.06	1/473 (0.2%)
All	All	0.53	3/11632 (0.0%)	0.93	42/16047 (0.3%)

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	A	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	44	PRO	C-N	24.15	1.67	1.33
1	A	12	ASN	C-N	-5.38	1.26	1.33
1	B	278	ALA	CA-C	-5.33	1.46	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	PRO	N-CA-CB	8.26	111.69	102.60
1	A	598	ASP	N-CA-C	8.17	120.19	111.28
1	B	250	PRO	N-CA-CB	7.49	110.31	103.20
1	B	481	GLY	N-CA-C	-7.42	105.49	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	218	PRO	N-CA-CB	7.20	110.81	103.25
1	A	249	ASP	N-CA-C	-6.96	94.43	109.81
1	B	143	PRO	N-CA-CB	6.93	110.22	102.60
1	B	212	PRO	N-CA-CB	6.67	110.25	103.25
1	A	44	PRO	O-C-N	-6.63	112.39	123.00
1	B	247	PRO	N-CA-CB	6.56	110.55	103.33
1	A	102	ASP	CA-C-N	6.50	126.00	119.24
1	A	102	ASP	C-N-CA	6.50	126.00	119.24
2	C	8	DG	N9-C1'-C2'	-6.33	104.01	113.50
1	A	410	THR	CA-C-N	-6.27	113.92	120.38
1	A	410	THR	C-N-CA	-6.27	113.92	120.38
1	A	212	PRO	N-CA-CB	6.22	109.79	103.25
3	D	4	DC	N1-C1'-C2'	-6.20	104.20	113.50
2	C	2	DG	O5'-C5'-C4'	-6.06	101.72	110.80
2	C	12	DG	N9-C1'-C2'	-6.04	104.44	113.50
1	B	479	ALA	N-CA-C	-6.04	101.53	110.46
1	A	247	PRO	N-CA-CB	5.87	109.95	103.26
1	A	250	PRO	N-CA-CB	5.86	109.41	103.25
2	E	14	DT	C5'-C4'-O4'	-5.78	100.73	109.40
2	E	8	DG	N9-C1'-C2'	-5.75	104.87	113.50
2	C	6	DT	C4'-C3'-O3'	-5.54	101.69	110.00
2	E	11	DG	N9-C1'-C2'	-5.39	105.41	113.50
3	D	7	DA	C5'-C4'-C3'	-5.36	106.86	114.90
1	A	469	TYR	CA-C-N	5.32	124.78	119.24
1	A	469	TYR	C-N-CA	5.32	124.78	119.24
1	A	254	ILE	CA-C-N	5.30	125.20	119.85
1	A	254	ILE	C-N-CA	5.30	125.20	119.85
4	F	7	DA	C5'-C4'-C3'	-5.30	106.95	114.90
1	A	13	ARG	N-CA-C	5.24	118.26	110.14
2	E	7	DA	O5'-C5'-C4'	5.24	118.66	110.80
1	A	91	TYR	CA-C-N	5.21	126.35	119.84
1	A	91	TYR	C-N-CA	5.21	126.35	119.84
2	C	10	DA	C2'-C3'-O3'	-5.19	103.71	111.50
2	C	10	DA	N9-C1'-C2'	-5.10	105.85	113.50
2	E	5	DG	O5'-C5'-C4'	-5.07	103.20	110.80
1	A	68	SER	CA-C-N	5.07	123.36	119.66
1	A	68	SER	C-N-CA	5.07	123.36	119.66
1	B	12	ASN	N-CA-C	-5.02	107.65	112.97

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	508	ALA	Peptide
1	A	597	GLU	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	4977	0	4894	83	0
1	B	5093	0	5046	95	0
2	C	315	0	173	10	0
2	E	338	0	184	7	0
3	D	259	0	147	6	0
4	F	277	0	159	9	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
6	A	126	0	0	9	0
6	B	14	0	0	1	0
6	C	15	0	0	1	0
6	D	8	0	0	1	0
6	E	6	0	0	0	0
6	F	1	0	0	0	0
All	All	11432	0	10603	195	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 9.

All (195) 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:44:PRO:C	1:A:45:LEU:N	1.67	1.46
1:A:545:ARG:NH2	1:A:549:VAL:O	2.11	0.84
1:B:545:ARG:NH2	1:B:549:VAL:O	2.11	0.82
1:A:113:ALA:HB1	1:A:155:LEU:HD13	1.62	0.80
1:A:350:ARG:NH2	1:A:352:ASP:OD1	2.16	0.79
1:A:246:ASP:O	1:A:249:ASP:O	2.01	0.78
1:B:575:LYS:HE2	1:B:652:LEU:HD11	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:GLU:O	1:A:496:GLY:N	2.24	0.69
1:B:440:ARG:NE	1:B:442:GLU:OE2	2.25	0.68
1:A:141:ARG:NH2	1:A:176:GLU:OE1	2.26	0.68
1:A:335:ARG:NH1	6:A:785:HOH:O	2.22	0.66
1:B:350:ARG:NH2	1:B:352:ASP:OD1	2.29	0.66
1:B:22:GLU:OE1	1:B:95:ARG:NH2	2.27	0.66
1:B:575:LYS:O	1:B:651:ARG:NH2	2.26	0.66
1:A:52:ARG:HH12	1:A:80:ALA:H	1.42	0.65
1:A:129:VAL:HG22	1:A:134:VAL:HG12	1.77	0.65
2:E:13:DT:H2''	2:E:14:DT:H5'	1.79	0.65
2:E:4:DG:H2'	2:E:5:DG:C8	2.32	0.65
1:B:473:LEU:HB3	1:B:541:VAL:HG12	1.78	0.64
1:A:319:PRO:HG2	1:A:640:ARG:HG3	1.79	0.64
1:B:605:THR:O	1:B:640:ARG:NH2	2.28	0.63
1:B:120:ARG:NH1	1:B:301:LEU:O	2.31	0.63
1:B:504:THR:HG22	1:B:679:ARG:HH21	1.62	0.62
1:B:525:GLU:HG3	1:B:679:ARG:HH22	1.64	0.62
3:D:8:DC:H2'	3:D:9:DT:C6	2.35	0.62
1:A:44:PRO:C	1:A:45:LEU:CA	2.71	0.61
1:A:590:ASP:OD2	3:D:15:DG:N1	2.18	0.61
1:A:350:ARG:HH22	1:A:352:ASP:CG	2.07	0.61
1:B:531:ARG:HE	1:B:537:LEU:HD13	1.65	0.61
1:A:146:ARG:NH1	1:A:176:GLU:OE2	2.34	0.61
1:A:350:ARG:NH1	6:A:797:HOH:O	2.30	0.60
1:A:25:ARG:HH22	1:A:95:ARG:NH2	2.00	0.60
1:A:271:HIS:HD2	3:D:10:DA:H5''	1.66	0.59
4:F:9:DT:H2'	4:F:10:DA:C8	2.38	0.59
1:A:639:THR:HG21	1:A:640:ARG:HH21	1.68	0.59
1:B:17:ARG:NH1	1:B:18:PRO:O	2.33	0.58
1:A:639:THR:CG2	1:A:640:ARG:HH21	2.16	0.58
4:F:8:DC:H2'	4:F:9:DT:C6	2.38	0.58
1:A:575:LYS:HE2	1:A:652:LEU:HD11	1.84	0.58
1:A:350:ARG:HH21	1:A:350:ARG:HB3	1.68	0.58
1:A:481:GLY:HA3	3:D:6:DT:H5'	1.86	0.58
1:B:242:ALA:HB2	1:B:258:THR:HG22	1.85	0.57
1:B:330:PRO:HB2	1:B:646:GLY:HA2	1.85	0.57
1:B:593:TYR:CE2	1:B:629:GLU:HG3	2.39	0.57
1:A:171:TYR:OH	1:A:289:ARG:NH2	2.37	0.57
1:B:437:VAL:HG23	1:B:438:PRO:HD3	1.87	0.56
1:B:138:GLU:OE2	1:B:141:ARG:HB3	2.06	0.55
1:A:392:ARG:HB3	1:A:396:ARG:HH21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:LEU:O	1:B:49:VAL:HG23	2.07	0.55
1:B:534:ALA:O	1:B:536:ARG:N	2.39	0.55
1:B:537:LEU:HD23	1:B:566:ILE:HD11	1.88	0.54
1:A:138:GLU:OE2	1:A:141:ARG:HG3	2.08	0.54
1:B:464:ALA:HA	1:B:641:LEU:HD21	1.90	0.54
1:B:558:LEU:HG	1:B:568:TYR:CE1	2.43	0.54
1:B:608:ARG:HG2	1:B:610:PHE:CE2	2.43	0.54
1:A:611:ARG:HD3	2:C:5:DG:H1'	1.90	0.53
1:B:665:GLU:OE1	1:B:668:ARG:NH2	2.41	0.53
1:A:608:ARG:HG2	1:A:610:PHE:CE2	2.44	0.53
1:B:590:ASP:OD2	4:F:15:DG:N1	2.29	0.53
1:B:129:VAL:HG22	1:B:134:VAL:HG12	1.92	0.52
1:B:217:LEU:HD11	2:E:21:DT:H2'	1.91	0.52
1:B:481:GLY:HA3	4:F:6:DT:H5'	1.90	0.52
1:A:234:GLN:O	1:A:236:ARG:N	2.36	0.52
1:B:115:ARG:NH1	1:B:118:GLN:OE1	2.43	0.52
1:A:287:ARG:HD3	1:A:291:ARG:CZ	2.41	0.51
6:A:737:HOH:O	2:C:7:DA:H5''	2.09	0.51
1:B:180:GLU:OE1	1:B:258:THR:OG1	2.21	0.51
1:A:18:PRO:HA	1:A:162:ALA:HA	1.91	0.51
3:D:9:DT:H2'	3:D:10:DA:C8	2.46	0.51
2:C:7:DA:OP1	6:C:202:HOH:O	2.19	0.51
4:F:4:DC:H2'	4:F:5:DC:C6	2.46	0.51
1:B:57:THR:HG22	1:B:66:SER:OG	2.11	0.51
1:B:594:VAL:HB	1:B:602:LEU:HB2	1.93	0.51
1:B:319:PRO:HG2	1:B:640:ARG:HG3	1.93	0.50
4:F:4:DC:H2'	4:F:5:DC:H6	1.77	0.50
1:A:594:VAL:HB	1:A:602:LEU:HB2	1.94	0.50
1:B:531:ARG:NE	1:B:537:LEU:HD13	2.26	0.50
2:C:6:DT:H2'	2:C:7:DA:H8	1.77	0.50
1:B:422:LYS:NZ	2:E:1:DT:OP1	2.36	0.50
1:A:240:ARG:O	1:A:258:THR:HG23	2.12	0.49
1:B:159:ASP:OD2	1:B:159:ASP:N	2.45	0.49
1:B:70:PRO:HA	1:B:73:LEU:HD12	1.94	0.49
1:B:479:ALA:C	1:B:481:GLY:H	2.19	0.49
1:A:291:ARG:NH1	6:A:711:HOH:O	2.46	0.49
1:B:525:GLU:HG3	1:B:679:ARG:NH2	2.27	0.49
1:A:350:ARG:NE	6:A:797:HOH:O	2.42	0.49
1:A:13:ARG:HG3	1:A:309:VAL:HG13	1.95	0.49
1:A:608:ARG:NH2	6:A:723:HOH:O	2.45	0.48
1:A:135:TYR:HA	1:A:150:GLY:HA3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:THR:O	1:B:436:ASN:HA	2.14	0.48
2:E:7:DA:H2'	2:E:8:DG:C8	2.48	0.48
1:A:494:VAL:HG22	1:A:501:LEU:CD2	2.44	0.48
1:A:264:VAL:HG11	2:C:10:DA:H5'	1.96	0.48
1:B:264:VAL:HG11	2:E:10:DA:H5'	1.96	0.48
1:A:442:GLU:H	1:A:442:GLU:CD	2.20	0.48
1:B:114:ARG:NH2	1:B:154:ASP:OD2	2.43	0.48
1:B:319:PRO:HG3	1:B:637:HIS:CD2	2.49	0.48
1:A:611:ARG:HD3	2:C:5:DG:C1'	2.44	0.47
1:B:350:ARG:HH21	1:B:350:ARG:HB3	1.79	0.47
1:B:392:ARG:NH1	1:B:396:ARG:HH22	2.12	0.47
1:A:547:GLY:HA3	1:A:574:ARG:HG3	1.95	0.47
1:A:190:PRO:HG3	1:A:263:PRO:HB3	1.96	0.47
1:B:217:LEU:HB2	1:B:221:LEU:O	2.15	0.47
1:B:506:PRO:O	1:B:671:ILE:HD11	2.14	0.47
1:A:483:GLU:HA	1:A:548:ARG:HG3	1.95	0.47
1:B:600:THR:HG22	1:B:620:VAL:HG22	1.96	0.47
1:A:319:PRO:HG2	1:A:640:ARG:CG	2.45	0.47
1:A:666:VAL:HA	1:A:671:ILE:HG22	1.97	0.47
4:F:9:DT:H2'	4:F:10:DA:H8	1.79	0.47
1:B:142:GLY:N	1:B:145:TRP:O	2.48	0.47
1:B:494:VAL:HG22	1:B:501:LEU:HD22	1.96	0.46
1:A:26:PRO:HD2	1:A:96:ARG:O	2.15	0.46
1:A:310:ARG:HD3	6:A:776:HOH:O	2.15	0.46
1:A:238:GLY:HA2	1:A:259:GLY:HA3	1.96	0.46
1:B:396:ARG:O	1:B:400:GLU:HG3	2.16	0.46
1:B:146:ARG:HD3	1:B:176:GLU:OE2	2.16	0.46
1:A:396:ARG:O	1:A:400:GLU:HG3	2.16	0.46
1:B:17:ARG:HH22	1:B:23:GLU:CD	2.22	0.46
3:D:14:DC:OP1	6:D:102:HOH:O	2.21	0.46
1:A:671:ILE:HD11	1:A:674:LEU:HB2	1.97	0.46
1:B:666:VAL:HG13	1:B:671:ILE:HB	1.98	0.46
1:B:17:ARG:NH2	1:B:23:GLU:OE1	2.44	0.46
1:B:422:LYS:HD2	1:B:432:SER:OG	2.16	0.46
1:B:531:ARG:NH1	1:B:536:ARG:HA	2.31	0.45
1:B:298:GLY:O	6:B:801:HOH:O	2.21	0.45
1:A:177:MET:HB2	1:A:181:ALA:HB3	1.98	0.45
1:A:136:ARG:HG3	1:A:137:ARG:N	2.31	0.45
1:A:339:TYR:CD2	1:A:340:ARG:HG3	2.52	0.45
1:B:486:ARG:HG2	1:B:515:PRO:HD3	1.99	0.45
1:A:576:SER:HA	1:A:615:ARG:HH21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:ASP:HB3	1:B:437:VAL:HG21	1.99	0.44
1:A:57:THR:HG22	1:A:66:SER:OG	2.18	0.44
1:B:504:THR:HG21	1:B:526:THR:OG1	2.16	0.44
1:B:479:ALA:O	1:B:481:GLY:N	2.45	0.44
1:A:254:ILE:HG13	2:C:21:DT:H1'	1.99	0.44
1:B:287:ARG:HD3	1:B:291:ARG:CZ	2.47	0.44
1:B:610:PHE:CG	4:F:13:DT:H4'	2.53	0.44
1:B:244:VAL:HG12	1:B:254:ILE:HG23	2.00	0.44
1:B:564:GLU:HB3	1:B:566:ILE:HG13	1.99	0.44
1:A:6:LYS:HD3	1:A:312:GLN:HE21	1.83	0.44
1:A:494:VAL:HG23	1:A:655:PRO:HG3	1.99	0.44
1:B:442:GLU:H	1:B:442:GLU:CD	2.25	0.44
1:B:338:PHE:CZ	1:B:455:LEU:HD13	2.53	0.44
1:B:39:ARG:H	1:B:39:ARG:NE	2.15	0.44
1:A:319:PRO:CG	1:A:640:ARG:HG3	2.47	0.43
1:B:155:LEU:HD12	1:B:164:LEU:O	2.18	0.43
1:A:574:ARG:NH2	6:A:751:HOH:O	2.52	0.43
1:B:69:PRO:O	1:B:72:VAL:HG22	2.17	0.43
1:B:494:VAL:HG11	1:B:641:LEU:HD13	1.99	0.43
1:A:68:SER:HA	1:A:69:PRO:HD3	1.90	0.43
1:B:18:PRO:HA	1:B:162:ALA:HA	2.00	0.43
2:C:6:DT:H2'	2:C:7:DA:C8	2.54	0.43
1:A:425:LEU:HD12	1:A:432:SER:HB3	2.01	0.43
1:B:678:ASP:HB2	1:B:681:LYS:HG3	2.00	0.43
1:A:96:ARG:HA	1:A:97:PRO:HD3	1.82	0.43
1:A:350:ARG:CZ	6:A:797:HOH:O	2.67	0.43
1:A:369:PHE:CZ	1:A:460:LEU:HD21	2.53	0.43
1:A:613:THR:O	2:C:6:DT:H5''	2.18	0.43
1:B:611:ARG:HD3	2:E:5:DG:H1'	2.00	0.43
1:A:121:LEU:HD22	1:A:134:VAL:HG11	2.01	0.42
1:B:98:LEU:HD22	1:B:105:GLU:HG2	2.00	0.42
1:B:321:LEU:HB3	1:B:327:VAL:HG23	2.00	0.42
1:B:115:ARG:O	1:B:119:GLU:HG2	2.19	0.42
1:A:13:ARG:HG3	1:A:309:VAL:CG1	2.49	0.42
1:A:475:VAL:HG22	1:A:477:PHE:CE1	2.55	0.42
1:A:486:ARG:HD3	1:A:512:GLU:OE2	2.19	0.42
1:B:20:ASN:OD1	1:B:23:GLU:N	2.48	0.42
1:A:558:LEU:HG	1:A:568:TYR:CE1	2.55	0.42
1:B:505:LEU:HD21	1:B:666:VAL:HG21	2.01	0.42
1:A:146:ARG:HE	1:A:148:LEU:HD21	1.85	0.42
1:A:505:LEU:HD21	1:A:666:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:LEU:HD23	1:A:505:LEU:HA	1.79	0.42
1:A:674:LEU:HD23	1:A:674:LEU:HA	1.73	0.42
1:A:664:LYS:HE3	1:A:664:LYS:HB2	1.85	0.41
1:A:117:LEU:O	1:A:121:LEU:HG	2.20	0.41
1:B:26:PRO:HD2	1:B:96:ARG:O	2.19	0.41
1:B:51:ARG:NH2	1:B:115:ARG:HH12	2.18	0.41
1:B:135:TYR:CE2	1:B:172:ARG:HB2	2.55	0.41
1:A:387:GLN:HB3	1:A:390:ALA:HB3	2.03	0.41
1:B:179:LEU:N	1:B:261:LEU:O	2.48	0.41
1:A:287:ARG:HD3	1:A:291:ARG:NH1	2.35	0.41
1:B:531:ARG:HG3	1:B:536:ARG:C	2.46	0.41
1:B:256:HIS:HB3	1:B:261:LEU:HD11	2.03	0.41
4:F:6:DT:H2'	4:F:7:DA:C8	2.55	0.41
1:A:443:GLU:CD	1:A:446:ARG:HH21	2.28	0.41
1:B:93:LYS:HA	1:B:93:LYS:HD3	1.92	0.41
1:B:321:LEU:HD23	1:B:321:LEU:HA	1.85	0.41
1:B:534:ALA:C	1:B:536:ARG:H	2.29	0.41
1:B:596:LEU:HD11	1:B:602:LEU:HG	2.03	0.40
1:A:117:LEU:HD22	1:A:155:LEU:HB2	2.02	0.40
1:B:51:ARG:NH2	1:B:115:ARG:HH22	2.20	0.40
1:B:536:ARG:NH1	1:B:537:LEU:O	2.55	0.40
2:C:7:DA:H2'	2:C:8:DG:C8	2.56	0.40
1:B:350:ARG:NH2	1:B:354:ALA:HB3	2.37	0.40
1:B:391:PHE:CE2	1:B:395:LEU:HD11	2.57	0.40

There are no symmetry-related clashes.

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	647/685 (94%)	623 (96%)	22 (3%)	2 (0%)	36 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	659/685 (96%)	638 (97%)	16 (2%)	5 (1%)	16	13
All	All	1306/1370 (95%)	1261 (97%)	38 (3%)	7 (0%)	24	23

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	PRO
1	B	142	GLY
1	A	235	GLY
1	B	535	GLY
1	B	506	PRO
1	B	480	GLY
1	B	437	VAL

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	466/549 (85%)	439 (94%)	27 (6%)	18	17
1	B	484/549 (88%)	454 (94%)	30 (6%)	16	15
All	All	950/1098 (86%)	893 (94%)	57 (6%)	17	16

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	64	LEU
1	A	141	ARG
1	A	155	LEU
1	A	165	LEU
1	A	244	VAL
1	A	254	ILE
1	A	287	ARG
1	A	301	LEU

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Mol	Chain	Res	Type
1	A	309	VAL
1	A	321	LEU
1	A	342	GLN
1	A	346	LEU
1	A	406	VAL
1	A	451	LEU
1	A	454	LEU
1	A	462	VAL
1	A	475	VAL
1	A	502	LEU
1	A	556	LEU
1	A	558	LEU
1	A	581	VAL
1	A	608	ARG
1	A	639	THR
1	A	640	ARG
1	A	661	ARG
1	A	674	LEU
1	B	39	ARG
1	B	57	THR
1	B	64	LEU
1	B	123	ARG
1	B	136	ARG
1	B	159	ASP
1	B	165	LEU
1	B	217	LEU
1	B	244	VAL
1	B	254	ILE
1	B	287	ARG
1	B	301	LEU
1	B	309	VAL
1	B	320	LYS
1	B	321	LEU
1	B	342	GLN
1	B	346	LEU
1	B	396	ARG
1	B	451	LEU
1	B	502	LEU
1	B	504	THR
1	B	537	LEU
1	B	543	LEU
1	B	556	LEU

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Mol	Chain	Res	Type
1	B	570	LEU
1	B	592	LEU
1	B	608	ARG
1	B	640	ARG
1	B	660	ASP
1	B	661	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	HIS
1	A	312	GLN
1	A	673	HIS
1	B	382	HIS

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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	44:PRO	C	45:LEU	N	1.67

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	658/685 (96%)	0.81	104 (15%) 5 4	28, 50, 120, 138	1 (0%)
1	B	667/685 (97%)	1.37	147 (22%) 2 1	49, 78, 106, 126	0
2	C	15/21 (71%)	0.22	0 100 100	38, 45, 110, 114	0
2	E	16/21 (76%)	0.57	1 (6%) 26 24	58, 66, 95, 105	0
3	D	13/13 (100%)	0.19	0 100 100	38, 53, 73, 86	0
4	F	14/14 (100%)	0.68	0 100 100	51, 74, 92, 95	0
All	All	1383/1439 (96%)	1.06	252 (18%) 3 2	28, 69, 114, 138	1 (0%)

All (252) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	241	VAL	6.2
1	A	90	LEU	5.5
1	A	243	TRP	5.3
1	A	44	PRO	5.3
1	A	87	ALA	5.1
1	A	230	LYS	4.9
1	B	500	HIS	4.8
1	B	407	LEU	4.8
1	A	46	LEU	4.7
1	A	227	HIS	4.6
1	B	277	LEU	4.6
1	A	223	LEU	4.6
1	A	91	TYR	4.6
1	A	226	TYR	4.6
1	B	487	PHE	4.4
1	A	92	PRO	4.4
1	A	29	LEU	4.3
1	A	47	ALA	4.2
1	A	510	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	229	SER	4.1
1	B	271	HIS	4.1
1	A	234	GLN	4.0
1	B	276	SER	4.0
1	B	530	PHE	4.0
1	B	266	THR	4.0
1	B	508	ALA	3.9
1	A	88	TYR	3.8
1	B	254	ILE	3.8
1	A	673	HIS	3.8
1	B	504	THR	3.7
1	A	260	LEU	3.7
1	A	34	ASP	3.7
1	A	53	ALA	3.7
1	A	498	GLY	3.6
1	A	499	GLY	3.6
1	A	72	VAL	3.5
1	B	390	ALA	3.5
1	B	386	SER	3.5
1	B	389	LEU	3.5
1	A	49	VAL	3.5
1	A	509	GLN	3.5
1	A	242	ALA	3.5
1	B	355	GLN	3.4
1	A	253	PRO	3.4
1	A	244	VAL	3.4
1	B	136	ARG	3.3
1	B	313	ALA	3.3
1	A	70	PRO	3.3
1	B	391	PHE	3.3
1	A	249	ASP	3.3
1	B	646	GLY	3.2
1	B	278	ALA	3.2
1	B	415	TRP	3.2
1	A	93	LYS	3.2
1	A	64	LEU	3.2
1	A	142	GLY	3.2
1	A	26	PRO	3.2
1	B	221	LEU	3.2
1	A	212	PRO	3.1
1	A	667	GLY	3.1
1	A	228	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	56	VAL	3.1
1	B	438	PRO	3.1
1	B	204	LEU	3.1
1	A	82	MET	3.1
1	B	211	ASP	3.0
1	B	241	VAL	3.0
1	B	205	LEU	3.0
1	B	505	LEU	3.0
1	A	27	TRP	3.0
1	A	94	GLY	3.0
1	B	482	ARG	3.0
1	B	528	TRP	3.0
1	A	224	LEU	2.9
1	B	226	TYR	2.9
1	A	30	GLU	2.9
1	B	671	ILE	2.9
1	A	35	PRO	2.9
1	A	136	ARG	2.9
1	A	179	LEU	2.9
1	B	193	VAL	2.9
1	A	239	GLY	2.9
1	B	224	LEU	2.9
1	A	209	GLU	2.9
1	B	201	THR	2.9
1	A	481	GLY	2.8
1	A	75	LEU	2.8
1	B	677	VAL	2.8
1	B	526	THR	2.8
1	B	220	GLY	2.8
1	B	346	LEU	2.8
1	B	425	LEU	2.8
1	A	196	ALA	2.8
1	B	27	TRP	2.8
1	A	208	GLY	2.8
1	B	409	LEU	2.8
1	B	245	ALA	2.8
1	B	510	ALA	2.8
1	B	323	GLY	2.7
1	A	255	PRO	2.7
1	B	79	LEU	2.7
1	A	32	VAL	2.7
1	B	388	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	383	ALA	2.7
1	B	468	ALA	2.7
1	B	335	ARG	2.7
1	A	205	LEU	2.7
1	A	207	LEU	2.7
1	B	381	LEU	2.7
1	B	395	LEU	2.7
1	B	394	ALA	2.7
1	B	353	GLY	2.7
1	A	80	ALA	2.6
1	A	84	GLN	2.6
1	A	74	VAL	2.6
1	B	238	GLY	2.6
1	A	143	PRO	2.6
1	A	256	HIS	2.6
1	A	86	TYR	2.6
1	B	406	VAL	2.6
1	A	511	GLY	2.6
1	B	142	GLY	2.6
1	B	247	PRO	2.6
1	B	250	PRO	2.6
1	A	73	LEU	2.6
1	B	244	VAL	2.6
1	B	379	HIS	2.6
1	B	537	LEU	2.6
1	A	240	ARG	2.6
1	B	351	LEU	2.5
1	B	522	LEU	2.5
1	B	405	ALA	2.5
1	A	5	GLY	2.5
1	A	61	GLY	2.5
1	B	378	LEU	2.5
1	B	239	GLY	2.5
1	B	480	GLY	2.5
1	B	509	GLN	2.5
1	B	679	ARG	2.5
1	A	674	LEU	2.5
1	A	211	ASP	2.5
1	A	416	GLU	2.5
1	A	676	GLU	2.5
1	B	584	VAL	2.5
1	A	500	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	324	ARG	2.4
1	B	173	ILE	2.4
1	B	336	VAL	2.4
1	B	494	VAL	2.4
1	B	145	TRP	2.4
1	B	296	TRP	2.4
1	B	215	LEU	2.4
1	A	69	PRO	2.4
1	B	21	PRO	2.4
1	B	40	GLU	2.4
1	A	258	THR	2.4
1	A	66	SER	2.4
1	A	79	LEU	2.4
1	B	41	GLU	2.4
1	A	259	GLY	2.4
1	A	213	LYS	2.4
1	B	175	CYS	2.4
1	B	519	VAL	2.4
1	A	24	LEU	2.4
1	B	682	LEU	2.4
1	B	503	TRP	2.4
1	B	339	TYR	2.4
1	B	411	PRO	2.4
1	B	144	GLY	2.4
1	B	222	SER	2.4
1	B	434	ILE	2.4
1	B	540	ARG	2.4
1	A	496	GLY	2.3
1	A	181	ALA	2.3
1	A	58	VAL	2.3
1	A	261	LEU	2.3
1	A	119	GLU	2.3
1	B	5	GLY	2.3
1	B	373	GLY	2.3
1	A	210	GLU	2.3
1	A	257	LEU	2.3
1	B	64	LEU	2.3
1	A	235	GLY	2.3
1	B	347	ALA	2.3
1	B	423	ALA	2.3
1	A	28	ARG	2.3
1	B	207	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	70	PRO	2.3
1	B	538	PRO	2.3
1	B	206	ARG	2.3
1	B	257	LEU	2.2
1	B	529	ALA	2.2
1	B	380	THR	2.2
1	B	629	GLU	2.2
1	B	202	TRP	2.2
1	B	189	LEU	2.2
1	A	62	ASP	2.2
2	E	14	DT	2.2
1	B	370	GLY	2.2
1	A	65	ALA	2.2
1	B	534	ALA	2.2
1	B	233	LEU	2.2
1	B	143	PRO	2.2
1	B	177	MET	2.2
1	B	302	GLY	2.2
1	B	535	GLY	2.2
1	B	203	GLU	2.2
1	B	507	GLU	2.2
1	B	566	ILE	2.2
1	A	141	ARG	2.2
1	B	393	GLU	2.2
1	B	458	ALA	2.2
1	B	197	TYR	2.1
1	A	297	ILE	2.1
1	B	376	LEU	2.1
1	B	521	ASP	2.1
1	B	312	GLN	2.1
1	B	328	SER	2.1
1	A	277	LEU	2.1
1	B	212	PRO	2.1
1	B	369	PHE	2.1
1	B	219	GLY	2.1
1	A	177	MET	2.1
1	A	214	GLU	2.1
1	B	261	LEU	2.1
1	B	428	GLU	2.1
1	B	314	TYR	2.1
1	B	255	PRO	2.1
1	A	128	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	357	TRP	2.1
1	B	414	ALA	2.1
1	B	359	GLU	2.1
1	B	472	GLU	2.1
1	B	559	GLU	2.1
1	B	502	LEU	2.1
1	B	249	ASP	2.1
1	B	291	ARG	2.1
1	A	191	LYS	2.0
1	A	375	SER	2.0
1	A	237	GLU	2.0
1	B	345	ALA	2.0
1	A	185	GLN	2.0
1	B	570	LEU	2.0
1	B	385	PRO	2.0
1	B	506	PRO	2.0
1	B	437	VAL	2.0
1	A	77	GLY	2.0
1	A	126	GLY	2.0
1	B	234	GLN	2.0
1	B	148	LEU	2.0
1	B	321	LEU	2.0
1	B	527	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	B	701	1/1	0.92	0.11	68,68,68,68	0
5	MG	E	101	1/1	0.92	0.11	71,71,71,71	0
5	MG	C	101	1/1	0.99	0.04	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.