Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 07:57 AM EDT

PDB ID	:	3HK2
Title	:	Crystal structure of T. thermophilus Argonaute N478 mutant protein complexed with DNA guide strand and 19-nt RNA target strand
Authors	:	Wang, Y.; Li, H.; Sheng, G.; Patel, D.J.
Deposited on	:	2009-05-22
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:

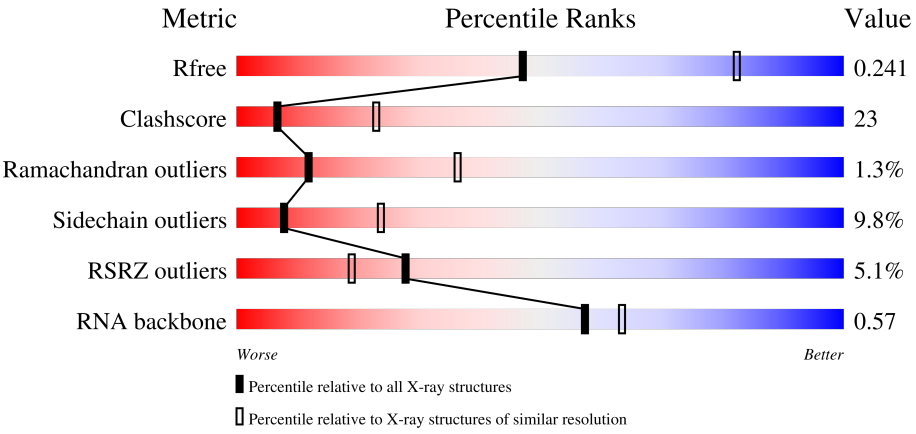
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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 <=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	5% 63% 29% 5% ·
1	B	685	6% 63% 30% 5% ·
2	C	21	10% 52% 19% 19%
2	E	21	24% 43% 14% 19%

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Mol	Chain	Length	Quality of chain
3	D	19	26% 47% 5% 21%
3	F	19	11% 68% 21%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11092 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	664	Total	C	N	O	S	0	0	0
			4869	3105	905	854	5			
1	B	666	Total	C	N	O	S	0	0	0
			4901	3126	912	858	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	478	ASN	ASP	engineered mutation	UNP Q746M7
B	478	ASN	ASP	engineered mutation	UNP Q746M7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	17	Total	C	N	O	P	0	0	0
			342	160	62	103	17			
2	E	17	Total	C	N	O	P	0	0	0
			342	160	62	103	17			

- Molecule 3 is a RNA chain called 5'-R(*UP*AP*UP*AP*CP*AP*AP*CP*CP*UP*AP*CP*UP*AP*CP*CP*UP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	15	Total	C	N	O	P	0	0	0
			310	140	52	103	15			
3	D	15	Total	C	N	O	P	0	0	0
			310	140	52	103	15			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is water.

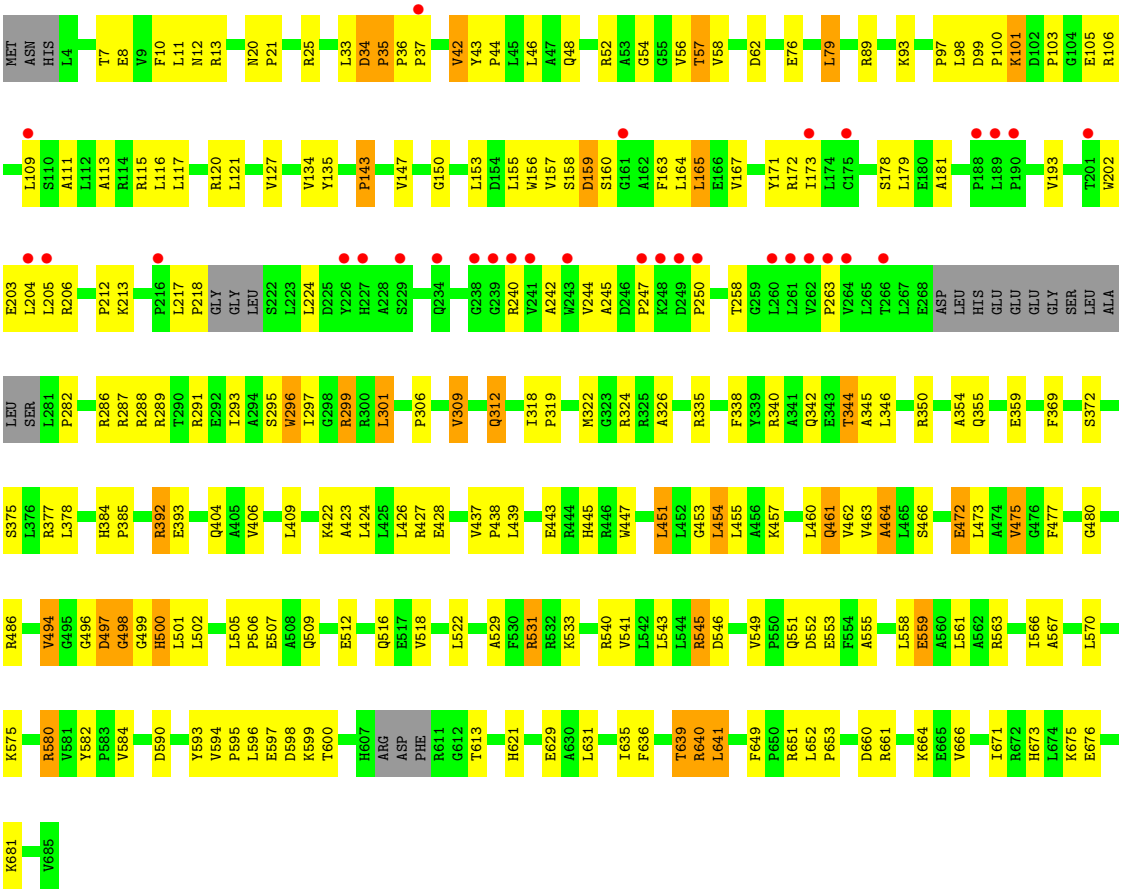
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	6	Total O 6 6	0	0
5	B	5	Total O 5 5	0	0
5	E	3	Total O 3 3	0	0

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.

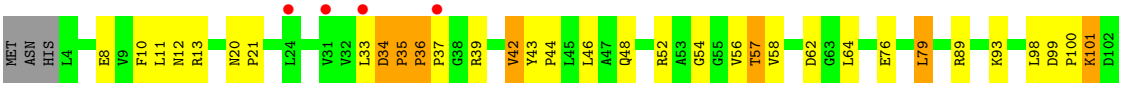
• Molecule 1: Argonaute

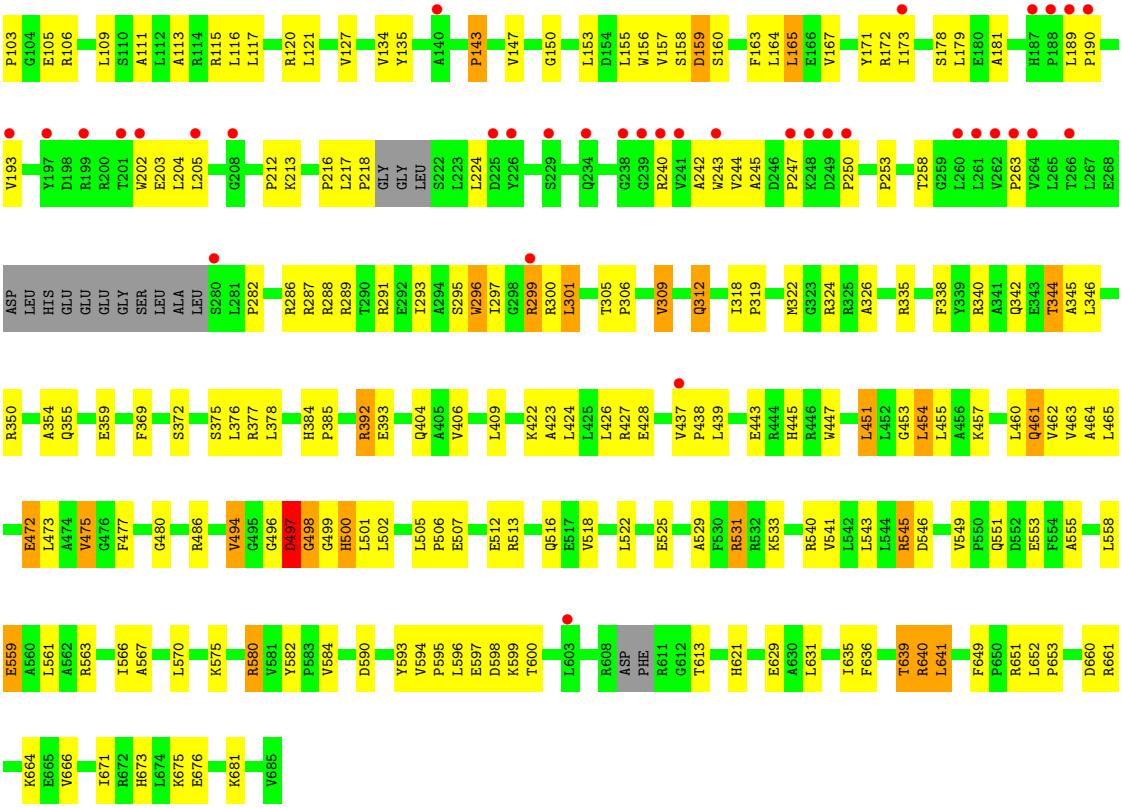
Chain A:



• Molecule 1: Argonaute

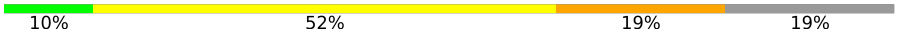
Chain B:

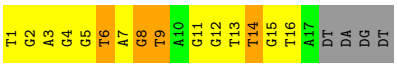




• Molecule 2: 5'-D(P*TP*GP*AP*GP*GP*TP*AP*GP*TP*AP*GP*GP*TP*TP*GP*TP*AP*TP*AP*GP*T)-3'

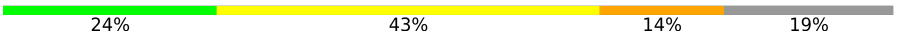
Chain C:

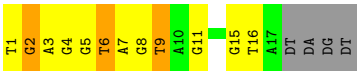




• Molecule 2: 5'-D(P*TP*GP*AP*GP*GP*TP*AP*GP*TP*AP*GP*GP*TP*TP*GP*TP*AP*TP*AP*GP*T)-3'

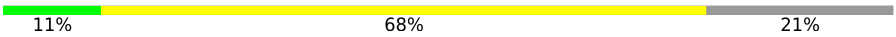
Chain E:

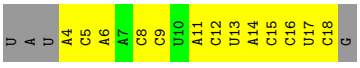




• Molecule 3: 5'-R(*UP*AP*UP*AP*CP*AP*AP*CP*CP*UP*AP*CP*UP*AP*CP*CP*UP*CP*G)-3'

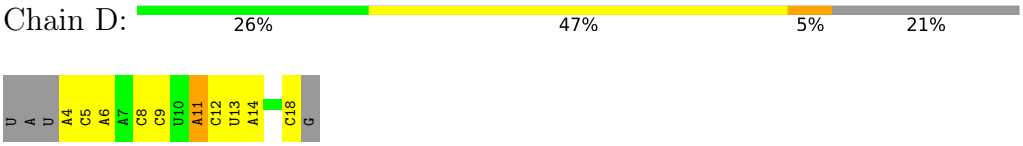
Chain F:





• Molecule 3: 5'-R(*UP*AP*UP*AP*CP*AP*AP*CP*CP*UP*AP*CP*UP*AP*CP*CP*UP*CP*G)-3'

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	111.19Å 110.88Å 174.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.78 – 2.80 46.78 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.3 (46.78-2.80) 99.0 (46.78-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.205 , 0.241 0.208 , 0.241	Depositor DCC
R_{free} test set	2730 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	76.1	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 54.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.477 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11092	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.42	2/4975 (0.0%)	0.62	7/6779 (0.1%)
1	B	0.37	0/5008	0.61	7/6823 (0.1%)
2	C	0.88	1/383 (0.3%)	1.46	9/591 (1.5%)
2	E	0.90	1/383 (0.3%)	1.48	8/591 (1.4%)
3	D	0.51	0/344	1.10	1/531 (0.2%)
3	F	0.51	0/344	1.06	0/531
All	All	0.45	4/11437 (0.0%)	0.75	32/15846 (0.2%)

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	1
1	B	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	DT	OP3-P	-10.80	1.48	1.61
2	C	1	DT	OP3-P	-10.71	1.48	1.61
1	A	464	ALA	C-N	-8.54	1.14	1.34
1	A	466	SER	C-N	7.94	1.47	1.33

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	11	DG	O4'-C1'-N9	9.01	114.31	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	11	DG	O4'-C1'-N9	8.23	113.76	108.00
2	E	2	DG	O4'-C4'-C3'	-7.82	101.31	106.00
2	E	6	DT	O4'-C4'-C3'	-6.96	101.71	104.50
2	C	9	DT	N3-C4-O4	6.35	123.71	119.90
2	E	6	DT	C4'-C3'-C2'	-6.30	97.43	103.10
2	E	9	DT	N3-C4-O4	6.25	123.65	119.90
1	B	218	PRO	N-CA-CB	6.24	110.79	103.30
1	B	247	PRO	N-CA-CB	6.24	110.79	103.30
1	A	247	PRO	N-CA-CB	6.23	110.78	103.30
2	E	16	DT	P-O3'-C3'	6.20	127.14	119.70
1	A	464	ALA	O-C-N	-6.16	112.84	122.70
2	C	6	DT	C4'-C3'-C2'	-6.16	97.56	103.10
1	B	216	PRO	N-CA-CB	6.11	110.63	103.30
1	A	143	PRO	N-CA-CB	6.08	110.60	103.30
1	B	143	PRO	N-CA-CB	6.06	110.58	103.30
2	C	16	DT	O4'-C1'-N1	6.01	112.21	108.00
1	B	282	PRO	N-CA-CB	5.95	110.43	103.30
1	A	282	PRO	N-CA-CB	5.94	110.43	103.30
1	A	218	PRO	N-CA-CB	5.86	110.33	103.30
1	B	250	PRO	N-CA-CB	5.80	110.27	103.30
1	A	250	PRO	N-CA-CB	5.80	110.26	103.30
1	B	212	PRO	N-CA-CB	5.78	110.23	103.30
1	A	212	PRO	N-CA-CB	5.69	110.13	103.30
2	C	6	DT	O4'-C4'-C3'	-5.55	102.28	104.50
2	C	8	DG	O4'-C1'-N9	5.50	111.85	108.00
2	C	14	DT	O4'-C1'-N1	-5.39	104.22	108.00
2	C	6	DT	N3-C4-O4	5.36	123.12	119.90
3	D	11	A	P-O3'-C3'	5.31	126.07	119.70
2	C	9	DT	C5-C4-O4	-5.19	121.26	124.90
2	E	9	DT	C5-C4-O4	-5.14	121.30	124.90
2	E	6	DT	O4'-C1'-N1	5.13	111.59	108.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	498	GLY	Peptide
1	B	498	GLY	Peptide

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	4869	0	4674	230	0
1	B	4901	0	4706	216	0
2	C	342	0	182	24	0
2	E	342	0	182	21	0
3	D	310	0	163	10	0
3	F	310	0	163	14	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
5	A	6	0	0	0	0
5	B	5	0	0	0	0
5	E	3	0	0	0	0
All	All	11092	0	10070	495	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 23.

All (495) 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:296:TRP:HD1	1:A:297:ILE:N	1.30	1.26
1:A:296:TRP:CD1	1:A:297:ILE:N	2.09	1.20
1:A:203:GLU:O	1:A:205:LEU:HD12	1.48	1.10
1:A:117:LEU:HD22	1:A:155:LEU:HB2	1.38	1.05
1:B:593:TYR:CE2	1:B:629:GLU:HG3	1.98	0.99
1:A:296:TRP:CD1	1:A:296:TRP:C	2.37	0.97
1:A:480:GLY:HA2	1:A:486:ARG:HB3	1.46	0.97
1:A:593:TYR:CE2	1:A:629:GLU:HG3	1.98	0.97
1:A:296:TRP:HD1	1:A:297:ILE:CA	1.78	0.96
1:B:480:GLY:HA2	1:B:486:ARG:HB3	1.46	0.94
1:B:34:ASP:O	1:B:36:PRO:HD3	1.66	0.94
1:A:33:LEU:HD12	1:A:37:PRO:HG3	1.50	0.93
1:A:34:ASP:O	1:A:36:PRO:HD3	1.69	0.93
1:B:33:LEU:HD12	1:B:37:PRO:HG3	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:TRP:CD1	1:B:296:TRP:C	2.39	0.92
1:A:286:ARG:HD2	1:A:613:THR:HG21	1.50	0.92
1:B:12:ASN:ND2	1:B:580:ARG:H	1.66	0.92
2:C:5:DG:H2"	2:C:6:DT:H5"	1.52	0.92
1:B:289:ARG:O	1:B:293:ILE:HG12	1.69	0.92
1:A:289:ARG:O	1:A:293:ILE:HG12	1.69	0.91
1:A:12:ASN:ND2	1:A:580:ARG:H	1.67	0.91
2:E:5:DG:H2"	2:E:6:DT:H5"	1.51	0.90
1:B:286:ARG:HD2	1:B:613:THR:HG21	1.52	0.89
1:A:202:TRP:HB3	1:A:244:VAL:HG11	1.55	0.89
1:B:202:TRP:HB3	1:B:244:VAL:HG11	1.55	0.89
1:A:593:TYR:HE2	1:A:629:GLU:HG3	1.39	0.88
1:B:540:ARG:HB2	1:B:567:ALA:HB3	1.54	0.88
1:A:540:ARG:HB2	1:A:567:ALA:HB3	1.54	0.87
1:B:202:TRP:HB3	1:B:244:VAL:CG1	2.05	0.87
1:A:202:TRP:HB3	1:A:244:VAL:CG1	2.05	0.85
1:B:593:TYR:HE2	1:B:629:GLU:HG3	1.40	0.85
1:B:296:TRP:C	1:B:296:TRP:HD1	1.77	0.84
2:C:6:DT:H2"	2:C:7:DA:H5'	1.60	0.83
2:E:15:DG:H1	3:F:5:C:H42	1.27	0.83
1:A:636:PHE:O	1:A:639:THR:HB	1.79	0.82
1:B:636:PHE:O	1:B:639:THR:HB	1.78	0.82
1:A:157:VAL:HG12	1:A:158:SER:H	1.45	0.82
1:A:116:LEU:HD21	1:A:120:ARG:NE	1.95	0.81
1:A:203:GLU:O	1:A:205:LEU:CD1	2.27	0.80
2:C:5:DG:C2'	2:C:6:DT:H5"	2.11	0.80
1:B:157:VAL:HG12	1:B:158:SER:H	1.44	0.80
1:A:422:LYS:O	1:A:426:LEU:HD13	1.81	0.80
1:B:350:ARG:NH2	1:B:354:ALA:HB3	1.97	0.80
1:B:422:LYS:O	1:B:426:LEU:HD13	1.83	0.79
1:A:350:ARG:NH2	1:A:354:ALA:HB3	1.96	0.79
1:A:296:TRP:HD1	1:A:296:TRP:C	1.77	0.79
1:B:34:ASP:O	1:B:36:PRO:CD	2.31	0.78
1:A:202:TRP:CB	1:A:244:VAL:HG11	2.13	0.77
2:C:3:DA:C2'	2:C:4:DG:H5"	2.14	0.77
1:B:202:TRP:CB	1:B:244:VAL:HG11	2.13	0.77
2:E:3:DA:C2'	2:E:4:DG:H5"	2.14	0.77
1:A:116:LEU:HD13	1:A:116:LEU:O	1.84	0.77
1:A:242:ALA:HB2	1:A:258:THR:HG22	1.67	0.77
1:A:34:ASP:O	1:A:36:PRO:CD	2.33	0.76
2:E:5:DG:C2'	2:E:6:DT:H5"	2.14	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LEU:HD13	1:A:116:LEU:C	2.06	0.75
1:B:116:LEU:C	1:B:116:LEU:HD13	2.08	0.75
1:B:242:ALA:HB2	1:B:258:THR:HG22	1.66	0.75
2:C:15:DG:H1	3:D:5:C:H42	1.34	0.75
1:B:296:TRP:NE1	1:B:300:ARG:HD3	2.02	0.74
2:C:4:DG:H8	2:C:4:DG:C5'	2.00	0.74
2:C:3:DA:H2"	2:C:4:DG:H5"	1.70	0.73
1:A:621:HIS:CE1	1:A:631:LEU:HD11	2.25	0.72
1:A:296:TRP:CD1	1:A:297:ILE:CA	2.65	0.72
1:A:42:VAL:O	1:A:46:LEU:HB2	1.90	0.71
1:B:42:VAL:O	1:B:46:LEU:HB2	1.90	0.71
1:B:12:ASN:HD21	1:B:580:ARG:H	1.38	0.71
1:B:473:LEU:HB3	1:B:541:VAL:HG12	1.73	0.70
3:D:11:A:H2'	3:D:12:C:H6	1.56	0.70
1:B:344:THR:HB	1:B:404:GLN:HE22	1.57	0.70
1:A:297:ILE:O	1:A:301:LEU:HB2	1.90	0.70
2:E:4:DG:C5'	2:E:4:DG:H8	2.03	0.70
1:A:117:LEU:HD22	1:A:155:LEU:CB	2.20	0.70
1:B:117:LEU:HD22	1:B:155:LEU:HB2	1.72	0.70
1:B:621:HIS:CE1	1:B:631:LEU:HD11	2.27	0.70
1:A:12:ASN:HD21	1:A:580:ARG:H	1.39	0.69
1:A:205:LEU:HD21	1:A:245:ALA:HB2	1.72	0.69
1:A:344:THR:HB	1:A:404:GLN:HE22	1.56	0.69
3:D:4:A:O2'	3:D:5:C:H5'	1.93	0.69
1:A:205:LEU:HD11	1:A:245:ALA:HB3	1.76	0.68
1:B:639:THR:HG22	1:B:640:ARG:HE	1.57	0.68
1:B:297:ILE:O	1:B:301:LEU:HB2	1.93	0.68
3:D:11:A:H2'	3:D:12:C:C6	2.27	0.68
1:B:109:LEU:HB3	1:B:157:VAL:HG21	1.75	0.68
1:A:296:TRP:HD1	1:A:297:ILE:HA	1.59	0.67
1:A:437:VAL:O	1:A:439:LEU:N	2.27	0.67
3:F:4:A:O2'	3:F:5:C:H5'	1.94	0.67
1:A:473:LEU:HB3	1:A:541:VAL:HG12	1.76	0.67
1:A:486:ARG:HH22	1:A:512:GLU:HB2	1.59	0.67
1:A:639:THR:HG22	1:A:640:ARG:HE	1.58	0.67
1:B:295:SER:HA	1:B:306:PRO:HG2	1.76	0.67
1:B:639:THR:HG22	1:B:640:ARG:HD2	1.77	0.67
1:A:109:LEU:HB3	1:A:157:VAL:HG21	1.75	0.66
1:A:156:TRP:HD1	1:A:157:VAL:O	1.78	0.66
1:B:437:VAL:O	1:B:439:LEU:N	2.28	0.66
1:A:296:TRP:CD1	1:A:297:ILE:HA	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:THR:HG22	1:A:640:ARG:HD2	1.77	0.66
1:B:156:TRP:HD1	1:B:157:VAL:O	1.79	0.66
1:B:486:ARG:HH22	1:B:512:GLU:HB2	1.60	0.66
1:A:244:VAL:HG12	1:A:245:ALA:N	2.11	0.65
1:A:56:VAL:HG13	1:A:115:ARG:HB2	1.78	0.65
1:B:531:ARG:C	1:B:531:ARG:HD3	2.17	0.65
1:B:496:GLY:O	1:B:498:GLY:N	2.30	0.65
1:A:35:PRO:O	1:A:36:PRO:C	2.35	0.65
1:B:244:VAL:HG12	1:B:245:ALA:N	2.12	0.65
1:A:205:LEU:HD12	1:A:205:LEU:N	2.11	0.64
1:B:392:ARG:NH2	1:B:428:GLU:OE2	2.30	0.64
1:B:639:THR:HG22	1:B:640:ARG:NE	2.11	0.64
1:A:506:PRO:HG2	1:A:666:VAL:HG21	1.79	0.64
1:A:639:THR:HG22	1:A:640:ARG:NE	2.12	0.64
2:E:6:DT:H2"	2:E:7:DA:H5'	1.78	0.64
1:B:296:TRP:CD1	1:B:300:ARG:HD3	2.31	0.64
1:A:392:ARG:NH2	1:A:428:GLU:OE2	2.31	0.64
1:A:496:GLY:O	1:A:498:GLY:N	2.30	0.64
1:B:296:TRP:HD1	1:B:297:ILE:N	1.95	0.64
1:A:531:ARG:HD3	1:A:531:ARG:C	2.17	0.63
1:B:113:ALA:HB1	1:B:155:LEU:HD13	1.81	0.63
1:B:506:PRO:HG2	1:B:666:VAL:HG21	1.80	0.63
2:E:15:DG:H1	3:F:5:C:N4	1.94	0.63
1:A:384:HIS:ND1	1:A:385:PRO:HD2	2.14	0.63
1:A:462:VAL:HG23	1:A:463:VAL:HG13	1.81	0.63
1:A:598:ASP:O	1:A:599:LYS:HB2	1.98	0.63
1:B:598:ASP:O	1:B:599:LYS:HB2	1.97	0.63
2:E:3:DA:H2"	2:E:4:DG:H5"	1.81	0.63
1:A:113:ALA:HB1	1:A:155:LEU:HD13	1.80	0.62
1:B:116:LEU:HD21	1:B:120:ARG:NE	2.13	0.62
1:A:472:GLU:HA	1:A:496:GLY:CA	2.30	0.62
1:B:384:HIS:ND1	1:B:385:PRO:HD2	2.14	0.62
1:A:205:LEU:CD1	1:A:245:ALA:N	2.63	0.62
1:B:472:GLU:HA	1:B:496:GLY:CA	2.30	0.62
1:B:20:ASN:HB2	1:B:21:PRO:HD2	1.81	0.62
1:A:639:THR:HG22	1:A:640:ARG:CD	2.30	0.62
2:C:4:DG:C5'	2:C:4:DG:C8	2.82	0.61
1:B:639:THR:HG22	1:B:640:ARG:CD	2.29	0.61
1:B:639:THR:CG2	1:B:640:ARG:HE	2.13	0.61
1:A:205:LEU:HD13	1:A:245:ALA:N	2.16	0.61
1:B:287:ARG:HD3	1:B:291:ARG:HH12	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:15:DG:H1	3:D:5:C:N4	1.99	0.61
1:A:20:ASN:HB2	1:A:21:PRO:HD2	1.81	0.61
1:B:12:ASN:ND2	1:B:580:ARG:N	2.46	0.61
2:C:2:DG:H2'	2:C:3:DA:C8	2.36	0.61
1:A:340:ARG:HH22	1:A:500:HIS:CB	2.14	0.60
1:B:340:ARG:HH22	1:B:500:HIS:CB	2.14	0.60
1:B:445:HIS:NE2	3:F:18:C:H2'	2.16	0.60
1:A:486:ARG:NH2	1:A:512:GLU:HB2	2.16	0.60
2:E:4:DG:C5'	2:E:4:DG:C8	2.84	0.60
1:A:287:ARG:HD3	1:A:291:ARG:HH12	1.66	0.60
1:A:639:THR:CG2	1:A:640:ARG:HE	2.15	0.60
1:B:157:VAL:HG12	1:B:158:SER:N	2.15	0.60
1:A:34:ASP:O	1:A:36:PRO:N	2.35	0.60
1:A:546:ASP:CG	1:A:546:ASP:O	2.40	0.60
1:B:58:VAL:HG11	1:B:111:ALA:C	2.22	0.60
1:B:462:VAL:HG23	1:B:463:VAL:HG13	1.84	0.60
1:A:48:GLN:HE21	1:A:79:LEU:HD11	1.67	0.60
1:B:486:ARG:NH2	1:B:512:GLU:HB2	2.17	0.59
1:A:116:LEU:HD21	1:A:120:ARG:HE	1.67	0.59
2:E:4:DG:H5"	2:E:4:DG:H8	1.65	0.59
1:A:445:HIS:NE2	3:D:18:C:H2'	2.17	0.59
1:B:121:LEU:HD22	1:B:134:VAL:HG21	1.83	0.59
1:A:58:VAL:HG11	1:A:111:ALA:C	2.23	0.59
1:A:157:VAL:HG12	1:A:158:SER:N	2.15	0.59
1:B:465:LEU:O	1:B:497:ASP:O	2.20	0.59
1:B:559:GLU:OE2	1:B:559:GLU:HA	2.02	0.59
2:E:3:DA:H2'	2:E:4:DG:H5"	1.82	0.59
1:B:52:ARG:NH1	1:B:79:LEU:HD13	2.16	0.59
3:F:11:A:H2'	3:F:12:C:H6	1.68	0.59
1:A:52:ARG:NH1	1:A:79:LEU:HD13	2.17	0.59
1:B:48:GLN:HE21	1:B:79:LEU:HD11	1.68	0.59
1:A:559:GLU:HA	1:A:559:GLU:OE2	2.02	0.59
1:B:546:ASP:CG	1:B:546:ASP:O	2.40	0.58
1:B:156:TRP:CD1	1:B:157:VAL:O	2.56	0.58
2:C:6:DT:H6	2:C:6:DT:H5'	1.68	0.58
1:A:501:LEU:HD21	1:A:641:LEU:HD13	1.86	0.58
1:A:156:TRP:CD1	1:A:157:VAL:O	2.55	0.58
1:A:342:GLN:O	1:A:344:THR:HG22	2.03	0.58
1:B:34:ASP:O	1:B:36:PRO:N	2.36	0.58
1:A:116:LEU:HD21	1:A:120:ARG:CZ	2.33	0.57
1:B:593:TYR:CZ	1:B:595:PRO:HG3	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:635:ILE:HG23	1:B:653:PRO:HG3	1.86	0.57
1:A:12:ASN:ND2	1:A:580:ARG:N	2.47	0.57
1:A:25:ARG:HD2	1:A:97:PRO:HG3	1.85	0.57
1:A:121:LEU:HD22	1:A:134:VAL:HG21	1.85	0.57
1:B:342:GLN:O	1:B:344:THR:HG22	2.04	0.57
2:C:4:DG:H5"	2:C:4:DG:H8	1.66	0.57
3:F:13:U:H2'	3:F:14:A:C8	2.38	0.57
1:A:344:THR:HG23	1:A:369:PHE:CE2	2.40	0.57
1:A:593:TYR:CZ	1:A:595:PRO:HG3	2.40	0.57
1:B:501:LEU:HD21	1:B:641:LEU:HD13	1.87	0.57
1:B:494:VAL:HG13	1:B:500:HIS:O	2.04	0.56
1:A:350:ARG:CZ	1:A:354:ALA:HB3	2.35	0.56
1:B:13:ARG:HB2	1:B:309:VAL:HG11	1.87	0.56
1:B:344:THR:HG23	1:B:369:PHE:CE2	2.40	0.56
1:B:480:GLY:CA	1:B:486:ARG:HB3	2.30	0.56
1:B:296:TRP:CD1	1:B:297:ILE:N	2.72	0.56
1:B:350:ARG:CZ	1:B:354:ALA:HB3	2.36	0.56
1:A:48:GLN:HG2	1:A:79:LEU:HD11	1.88	0.56
1:A:213:LYS:HA	1:A:224:LEU:CB	2.37	0.55
1:A:494:VAL:HG13	1:A:500:HIS:O	2.04	0.55
1:B:324:ARG:HA	1:B:324:ARG:NE	2.20	0.55
2:C:4:DG:H8	2:C:4:DG:H5'	1.68	0.55
1:A:155:LEU:HD22	1:A:164:LEU:O	2.06	0.55
1:B:35:PRO:O	1:B:36:PRO:C	2.41	0.55
1:A:13:ARG:HB2	1:A:309:VAL:HG11	1.88	0.55
1:A:33:LEU:CD1	1:A:37:PRO:HG3	2.32	0.55
1:B:296:TRP:CD1	1:B:296:TRP:O	2.58	0.55
1:A:171:TYR:HB2	2:C:8:DG:H5"	1.88	0.55
1:A:205:LEU:HD21	1:A:245:ALA:CB	2.36	0.55
1:A:377:ARG:O	1:A:378:LEU:HD23	2.06	0.55
1:B:33:LEU:CD1	1:B:37:PRO:HG3	2.31	0.55
1:A:453:GLY:O	1:A:457:LYS:HG3	2.07	0.55
1:A:324:ARG:HA	1:A:324:ARG:NE	2.20	0.55
1:A:635:ILE:HG23	1:A:653:PRO:HG3	1.89	0.55
1:A:312:GLN:H	1:A:312:GLN:NE2	2.05	0.54
1:B:377:ARG:O	1:B:378:LEU:HD23	2.06	0.54
1:A:205:LEU:HD11	1:A:245:ALA:CB	2.36	0.54
1:A:217:LEU:HD11	1:B:39:ARG:HD3	1.87	0.54
2:C:2:DG:H2'	2:C:3:DA:H8	1.72	0.54
3:F:11:A:H2'	3:F:12:C:C6	2.40	0.54
1:B:165:LEU:HD13	1:B:167:VAL:CG2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:LYS:HA	1:B:224:LEU:CB	2.37	0.54
1:B:48:GLN:HG2	1:B:79:LEU:HD11	1.88	0.54
1:B:155:LEU:HD22	1:B:164:LEU:O	2.08	0.54
1:B:312:GLN:H	1:B:312:GLN:NE2	2.05	0.54
1:B:531:ARG:HD3	1:B:531:ARG:O	2.07	0.54
2:E:6:DT:H1'	2:E:7:DA:H5"	1.89	0.54
1:A:116:LEU:C	1:A:116:LEU:CD1	2.75	0.54
1:A:531:ARG:HD3	1:A:531:ARG:O	2.07	0.54
1:B:116:LEU:C	1:B:116:LEU:CD1	2.76	0.53
1:B:660:ASP:OD2	1:B:664:LYS:HE3	2.08	0.53
1:A:99:ASP:OD1	1:A:101:LYS:HB2	2.08	0.53
1:A:165:LEU:HD13	1:A:167:VAL:CG2	2.39	0.53
1:B:475:VAL:HG22	1:B:477:PHE:CE1	2.44	0.53
1:A:475:VAL:HG22	1:A:477:PHE:CE1	2.44	0.53
1:B:101:LYS:O	1:B:103:PRO:HD3	2.08	0.53
1:A:121:LEU:HD13	1:A:134:VAL:HG23	1.90	0.53
1:A:660:ASP:OD2	1:A:664:LYS:HE3	2.09	0.53
1:B:99:ASP:OD1	1:B:101:LYS:HB2	2.08	0.53
1:B:172:ARG:HD3	2:E:9:DT:OP1	2.09	0.53
1:B:165:LEU:HD13	1:B:167:VAL:HG23	1.91	0.53
1:A:295:SER:HA	1:A:306:PRO:HG2	1.90	0.52
2:E:2:DG:H2'	2:E:3:DA:C8	2.44	0.52
2:E:6:DT:H5'	2:E:6:DT:H6	1.73	0.52
1:A:242:ALA:HB2	1:A:258:THR:CG2	2.37	0.52
1:A:43:TYR:HB2	1:A:44:PRO:HD3	1.91	0.52
1:A:101:LYS:O	1:A:103:PRO:HD3	2.08	0.52
1:A:472:GLU:HA	1:A:496:GLY:HA2	1.91	0.52
1:B:338:PHE:CZ	1:B:455:LEU:HD13	2.45	0.52
3:D:4:A:C2	3:D:5:C:C2	2.97	0.52
1:B:116:LEU:HD21	1:B:120:ARG:CZ	2.40	0.52
1:B:453:GLY:O	1:B:457:LYS:HG3	2.09	0.52
1:B:155:LEU:HD23	1:B:165:LEU:HD23	1.92	0.51
1:B:242:ALA:HB2	1:B:258:THR:CG2	2.36	0.51
1:A:155:LEU:HD11	1:A:163:PHE:CD2	2.46	0.51
1:B:472:GLU:HA	1:B:496:GLY:HA2	1.92	0.51
1:B:575:LYS:HB3	1:B:651:ARG:NH2	2.24	0.51
1:A:575:LYS:HB3	1:A:651:ARG:NH2	2.26	0.51
1:B:121:LEU:HD13	1:B:134:VAL:HG23	1.92	0.51
1:B:43:TYR:HB2	1:B:44:PRO:HD3	1.92	0.51
1:A:338:PHE:CZ	1:A:455:LEU:HD13	2.46	0.51
1:A:447:TRP:HE3	1:A:451:LEU:HD22	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:GLU:O	1:B:204:LEU:C	2.49	0.51
1:A:13:ARG:HB2	1:A:309:VAL:CG1	2.41	0.50
1:A:165:LEU:HD13	1:A:167:VAL:HG23	1.93	0.50
1:B:447:TRP:HE3	1:B:451:LEU:HD22	1.76	0.50
1:B:155:LEU:HD11	1:B:163:PHE:CD2	2.46	0.50
1:A:205:LEU:HD13	1:A:244:VAL:C	2.31	0.50
1:A:242:ALA:O	1:A:244:VAL:HG23	2.12	0.50
1:B:13:ARG:HB2	1:B:309:VAL:CG1	2.41	0.50
1:B:171:TYR:HB2	2:E:8:DG:H5"	1.94	0.50
2:E:4:DG:H5"	2:E:4:DG:C8	2.47	0.50
3:D:13:U:H2'	3:D:14:A:C8	2.47	0.50
1:A:155:LEU:HD23	1:A:165:LEU:HD23	1.93	0.50
1:A:205:LEU:CD2	1:A:245:ALA:HB2	2.42	0.49
1:B:56:VAL:HG13	1:B:115:ARG:CB	2.42	0.49
2:C:3:DA:H2'	2:C:4:DG:H5"	1.90	0.49
1:A:512:GLU:OE2	1:A:545:ARG:NH2	2.45	0.49
1:A:116:LEU:CD2	1:A:120:ARG:NE	2.72	0.49
1:B:242:ALA:O	1:B:244:VAL:HG23	2.13	0.49
1:A:244:VAL:CG1	1:A:245:ALA:N	2.75	0.49
1:B:512:GLU:OE2	1:B:545:ARG:NH2	2.46	0.49
1:B:100:PRO:HB3	1:B:158:SER:O	2.12	0.49
1:B:115:ARG:O	1:B:116:LEU:C	2.51	0.49
1:A:240:ARG:O	1:A:258:THR:HG23	2.13	0.49
1:A:100:PRO:HB3	1:A:158:SER:O	2.13	0.49
1:A:205:LEU:CD1	1:A:205:LEU:N	2.76	0.49
1:A:480:GLY:CA	1:A:486:ARG:HB3	2.30	0.48
1:B:155:LEU:HA	1:B:164:LEU:O	2.13	0.48
1:B:240:ARG:O	1:B:258:THR:HG23	2.13	0.48
2:C:4:DG:H5"	2:C:4:DG:C8	2.47	0.48
1:B:286:ARG:HD2	1:B:613:THR:CG2	2.35	0.48
1:A:461:GLN:NE2	1:A:500:HIS:HA	2.28	0.48
1:B:243:TRP:CE3	1:B:253:PRO:HB2	2.49	0.48
1:B:461:GLN:NE2	1:B:500:HIS:HA	2.28	0.48
1:B:516:GLN:OE1	1:B:555:ALA:HB3	2.13	0.48
1:B:445:HIS:CE1	3:F:18:C:H2'	2.48	0.48
2:E:4:DG:H8	2:E:4:DG:H5'	1.74	0.48
1:A:640:ARG:HD2	1:A:640:ARG:N	2.28	0.48
1:B:244:VAL:CG1	1:B:245:ALA:N	2.75	0.48
1:A:155:LEU:HA	1:A:164:LEU:O	2.13	0.48
3:F:16:C:H2'	3:F:17:U:H6	1.79	0.48
1:A:494:VAL:O	1:A:499:GLY:HA3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:ALA:HB1	1:A:498:GLY:O	2.13	0.48
1:A:640:ARG:HG3	1:A:649:PHE:CD2	2.49	0.48
1:A:113:ALA:HB1	1:A:155:LEU:CD1	2.42	0.47
1:B:464:ALA:HB1	1:B:498:GLY:O	2.13	0.47
1:A:103:PRO:HG3	1:A:106:ARG:NH2	2.29	0.47
1:B:443:GLU:O	1:B:447:TRP:CD1	2.68	0.47
1:B:640:ARG:HD2	1:B:640:ARG:N	2.29	0.47
1:B:494:VAL:O	1:B:499:GLY:HA3	2.14	0.47
1:B:500:HIS:CE1	1:B:533:LYS:HG2	2.49	0.47
1:A:205:LEU:HD11	1:A:245:ALA:N	2.30	0.47
1:B:135:TYR:HA	1:B:150:GLY:HA3	1.96	0.47
1:A:120:ARG:NH1	1:A:301:LEU:O	2.47	0.47
1:A:443:GLU:O	1:A:447:TRP:CD1	2.67	0.47
1:A:500:HIS:CE1	1:A:533:LYS:HG2	2.50	0.47
1:A:516:GLN:OE1	1:A:555:ALA:HB3	2.13	0.47
1:A:652:LEU:HB3	1:A:653:PRO:HD2	1.97	0.47
1:B:384:HIS:CE1	1:B:385:PRO:HD2	2.48	0.47
1:B:455:LEU:HD22	1:B:460:LEU:HD22	1.96	0.47
1:B:546:ASP:OD1	1:B:575:LYS:NZ	2.46	0.47
1:A:384:HIS:CE1	1:A:385:PRO:HD2	2.49	0.47
1:B:652:LEU:HB3	1:B:653:PRO:HD2	1.97	0.47
1:B:661:ARG:HA	1:B:661:ARG:HD3	1.68	0.47
1:A:116:LEU:CD2	1:A:120:ARG:HE	2.27	0.46
1:A:546:ASP:OD1	1:A:575:LYS:NZ	2.47	0.46
1:B:100:PRO:HB2	1:B:159:ASP:O	2.16	0.46
1:A:205:LEU:HD13	1:A:244:VAL:HA	1.97	0.46
1:B:113:ALA:HB1	1:B:155:LEU:CD1	2.44	0.46
1:B:120:ARG:NH1	1:B:301:LEU:O	2.48	0.46
1:A:109:LEU:CB	1:A:157:VAL:HG21	2.43	0.46
1:A:135:TYR:HA	1:A:150:GLY:HA3	1.96	0.46
1:A:286:ARG:HD2	1:A:613:THR:CG2	2.34	0.46
1:B:598:ASP:O	1:B:599:LYS:CB	2.64	0.46
2:C:6:DT:H5'	2:C:6:DT:C6	2.50	0.46
1:A:172:ARG:HD3	2:C:9:DT:OP1	2.15	0.46
1:A:287:ARG:HD3	1:A:291:ARG:NH1	2.29	0.46
1:B:56:VAL:HG13	1:B:115:ARG:HB2	1.98	0.46
1:B:344:THR:CG2	1:B:369:PHE:CE2	2.99	0.46
1:B:384:HIS:CG	1:B:385:PRO:HD2	2.51	0.46
1:A:11:LEU:C	1:A:13:ARG:H	2.18	0.46
1:A:384:HIS:CG	1:A:385:PRO:HD2	2.51	0.46
1:B:11:LEU:C	1:B:13:ARG:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:PRO:HG3	1:B:106:ARG:NH2	2.30	0.46
2:C:4:DG:C8	2:C:4:DG:H5'	2.49	0.46
3:F:4:A:C2	3:F:5:C:C2	3.04	0.46
1:A:36:PRO:HA	1:A:37:PRO:HD3	1.85	0.46
1:A:344:THR:CG2	1:A:369:PHE:CE2	2.99	0.46
1:B:359:GLU:OE1	1:B:359:GLU:HA	2.15	0.46
1:A:193:VAL:HG11	1:A:204:LEU:HB2	1.98	0.46
1:B:109:LEU:CB	1:B:157:VAL:HG21	2.43	0.46
1:A:121:LEU:HD11	1:A:153:LEU:HD12	1.98	0.45
1:A:359:GLU:OE1	1:A:359:GLU:HA	2.15	0.45
1:B:287:ARG:HD3	1:B:291:ARG:NH1	2.29	0.45
1:B:640:ARG:HG3	1:B:649:PHE:CD2	2.51	0.45
1:B:457:LYS:O	1:B:681:LYS:HG2	2.16	0.45
1:B:121:LEU:HD11	1:B:153:LEU:HD12	1.99	0.45
1:B:203:GLU:O	1:B:205:LEU:HD23	2.16	0.45
1:A:661:ARG:HD3	1:A:661:ARG:HA	1.68	0.45
1:B:344:THR:CB	1:B:404:GLN:HE22	2.27	0.45
1:B:596:LEU:O	1:B:597:GLU:C	2.55	0.45
1:A:393:GLU:CD	1:B:531:ARG:HH21	2.19	0.45
1:B:54:GLY:O	1:B:57:THR:CG2	2.65	0.45
1:A:531:ARG:HH21	1:B:393:GLU:CD	2.19	0.45
2:C:14:DT:H1'	2:C:15:DG:H5'	1.99	0.45
1:A:445:HIS:CE1	3:D:18:C:H2'	2.52	0.44
1:A:596:LEU:O	1:A:597:GLU:C	2.54	0.44
1:B:594:VAL:O	1:B:594:VAL:HG12	2.16	0.44
1:B:545:ARG:HG2	1:B:549:VAL:HG22	1.99	0.44
1:B:561:LEU:HA	1:B:561:LEU:HD23	1.77	0.44
1:A:423:ALA:HB1	1:A:673:HIS:CE1	2.52	0.44
1:A:594:VAL:HG12	1:A:594:VAL:O	2.17	0.44
1:B:461:GLN:HG3	1:B:500:HIS:HB2	1.99	0.44
1:A:100:PRO:HB2	1:A:159:ASP:O	2.16	0.44
1:B:299:ARG:C	1:B:301:LEU:H	2.21	0.44
1:A:8:GLU:O	1:A:584:VAL:HG23	2.18	0.44
1:A:545:ARG:HG2	1:A:549:VAL:HG22	1.99	0.44
1:B:286:ARG:HG2	1:B:582:TYR:OH	2.18	0.44
1:B:545:ARG:HD3	1:B:553:GLU:OE2	2.18	0.44
1:A:299:ARG:C	1:A:301:LEU:H	2.21	0.44
1:A:505:LEU:HD12	1:B:675:LYS:HB2	1.99	0.44
1:A:179:LEU:HA	1:A:263:PRO:HG3	2.00	0.44
1:A:54:GLY:O	1:A:57:THR:CG2	2.66	0.44
1:B:340:ARG:HH22	1:B:500:HIS:HB2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ARG:HG2	1:A:582:TYR:OH	2.18	0.43
1:A:507:GLU:OE2	1:B:671:ILE:HG22	2.18	0.43
1:A:455:LEU:HD22	1:A:460:LEU:HD22	1.99	0.43
1:B:561:LEU:HD22	1:B:566:ILE:HB	1.99	0.43
1:B:147:VAL:HG22	1:B:173:ILE:HA	1.99	0.43
2:E:3:DA:H2'	2:E:4:DG:C8	2.52	0.43
1:A:147:VAL:HG22	1:A:173:ILE:HA	1.99	0.43
1:A:461:GLN:HG3	1:A:500:HIS:HB2	2.00	0.43
3:F:15:C:H2'	3:F:16:C:C6	2.53	0.43
1:A:98:LEU:HG	1:A:105:GLU:HB3	1.99	0.43
1:B:423:ALA:HB1	1:B:673:HIS:CE1	2.53	0.43
1:B:461:GLN:HG3	1:B:500:HIS:CB	2.48	0.43
1:A:159:ASP:N	1:A:159:ASP:OD1	2.50	0.43
1:A:178:SER:H	1:A:181:ALA:HB3	1.83	0.43
1:A:461:GLN:HG3	1:A:500:HIS:CB	2.48	0.43
1:A:518:VAL:O	1:A:522:LEU:HG	2.18	0.43
1:B:98:LEU:HG	1:B:105:GLU:HB3	2.01	0.43
1:B:159:ASP:OD1	1:B:159:ASP:N	2.51	0.43
1:A:345:ALA:HB2	1:A:377:ARG:CZ	2.48	0.43
1:B:345:ALA:HB2	1:B:377:ARG:CZ	2.48	0.43
1:A:340:ARG:HH22	1:A:500:HIS:HB2	1.82	0.43
1:A:344:THR:CB	1:A:404:GLN:HE22	2.27	0.43
1:A:346:LEU:CD2	1:A:454:LEU:HD13	2.48	0.43
1:B:178:SER:H	1:B:181:ALA:HB3	1.83	0.43
1:B:451:LEU:HD12	1:B:451:LEU:HA	1.87	0.43
1:A:350:ARG:HG2	1:A:409:LEU:HB2	2.01	0.43
1:A:509:GLN:HE21	1:A:509:GLN:HB3	1.69	0.43
1:A:545:ARG:HD3	1:A:553:GLU:OE2	2.19	0.43
1:B:496:GLY:C	1:B:498:GLY:H	2.22	0.43
1:A:8:GLU:HB3	1:A:584:VAL:HG21	2.01	0.43
1:A:496:GLY:C	1:A:498:GLY:H	2.22	0.43
3:F:15:C:H2'	3:F:16:C:H6	1.84	0.43
1:A:322:MET:SD	1:A:326:ALA:HA	2.59	0.42
1:B:496:GLY:C	1:B:498:GLY:N	2.72	0.42
3:F:8:C:H2'	3:F:9:C:O4'	2.19	0.42
1:A:346:LEU:HD23	1:A:454:LEU:HD13	2.02	0.42
1:A:551:GLN:O	1:A:552:ASP:HB2	2.19	0.42
1:B:455:LEU:HD22	1:B:460:LEU:CD2	2.48	0.42
2:E:6:DT:H5'	2:E:6:DT:C6	2.54	0.42
1:A:205:LEU:CD1	1:A:245:ALA:H	2.31	0.42
1:A:427:ARG:HH11	1:A:673:HIS:CE1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:LEU:HD23	1:A:641:LEU:HA	1.87	0.42
1:B:8:GLU:O	1:B:584:VAL:HG23	2.19	0.42
1:B:115:ARG:HD2	1:B:115:ARG:HA	1.61	0.42
1:B:179:LEU:HA	1:B:263:PRO:HG3	2.00	0.42
1:B:193:VAL:HG13	1:B:193:VAL:O	2.19	0.42
1:A:496:GLY:C	1:A:498:GLY:N	2.73	0.42
1:B:116:LEU:HD13	1:B:116:LEU:O	2.19	0.42
1:B:318:ILE:HA	1:B:319:PRO:HD3	1.88	0.42
1:B:350:ARG:HG2	1:B:409:LEU:HB2	2.02	0.42
2:C:6:DT:H1'	2:C:7:DA:H5"	2.02	0.42
1:A:48:GLN:NE2	1:A:79:LEU:HD11	2.32	0.42
1:B:217:LEU:HD12	1:B:217:LEU:HA	1.85	0.42
2:C:3:DA:H2'	2:C:4:DG:C8	2.54	0.42
1:A:324:ARG:NE	1:A:324:ARG:CA	2.83	0.42
1:A:451:LEU:HD12	1:A:451:LEU:HA	1.88	0.42
1:B:10:PHE:CE2	1:B:584:VAL:HA	2.55	0.42
1:A:461:GLN:CG	1:A:500:HIS:HB2	2.49	0.42
1:B:305:THR:HA	1:B:306:PRO:HD3	1.71	0.42
1:B:461:GLN:CG	1:B:500:HIS:HB2	2.49	0.42
1:A:344:THR:HG21	1:A:460:LEU:HD11	2.01	0.42
1:A:561:LEU:HD22	1:A:566:ILE:HB	2.00	0.42
1:B:502:LEU:C	1:B:502:LEU:HD12	2.39	0.42
1:A:598:ASP:O	1:A:599:LYS:CB	2.64	0.42
1:B:500:HIS:C	1:B:500:HIS:CD2	2.93	0.42
2:C:12:DG:H2'	2:C:13:DT:H71	2.02	0.42
3:F:16:C:O2'	3:F:17:U:H5'	2.20	0.42
1:A:193:VAL:CG1	1:A:204:LEU:HB2	2.50	0.41
1:B:8:GLU:HB3	1:B:584:VAL:HG21	2.01	0.41
1:B:344:THR:HG21	1:B:460:LEU:HD11	2.02	0.41
1:B:346:LEU:CD2	1:B:454:LEU:HD13	2.49	0.41
1:B:502:LEU:HD21	1:B:529:ALA:HB1	2.01	0.41
1:A:193:VAL:HG13	1:A:193:VAL:O	2.19	0.41
1:A:502:LEU:HD21	1:A:529:ALA:HB1	2.01	0.41
1:A:561:LEU:HA	1:A:561:LEU:HD23	1.80	0.41
1:A:76:GLU:HG2	1:A:89:ARG:HD2	2.02	0.41
1:A:502:LEU:HD12	1:A:502:LEU:C	2.40	0.41
1:B:324:ARG:NE	1:B:324:ARG:CA	2.83	0.41
1:A:7:THR:HG22	1:A:8:GLU:N	2.36	0.41
1:B:427:ARG:HH11	1:B:673:HIS:CE1	2.38	0.41
2:E:6:DT:H5'	2:E:6:DT:H2'	1.75	0.41
1:A:640:ARG:HG3	1:A:649:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:GLU:HG2	1:B:89:ARG:HD2	2.03	0.41
1:A:10:PHE:CE2	1:A:584:VAL:HA	2.55	0.41
1:B:20:ASN:HB2	1:B:21:PRO:CD	2.48	0.41
1:B:48:GLN:NE2	1:B:79:LEU:HD11	2.33	0.41
1:B:322:MET:SD	1:B:326:ALA:HA	2.60	0.41
1:B:376:LEU:HD11	1:B:378:LEU:HD21	2.02	0.41
1:A:93:LYS:HA	1:A:93:LYS:HD3	1.80	0.41
1:A:455:LEU:HD22	1:A:460:LEU:CD2	2.50	0.41
1:A:500:HIS:C	1:A:500:HIS:CD2	2.94	0.41
1:A:671:ILE:HG22	1:B:507:GLU:OE2	2.21	0.41
1:B:189:LEU:HA	1:B:190:PRO:HD3	1.82	0.41
1:B:193:VAL:HG11	1:B:204:LEU:HB2	2.03	0.41
1:B:465:LEU:O	1:B:498:GLY:HA3	2.21	0.41
1:B:465:LEU:HB2	1:B:498:GLY:HA3	2.02	0.41
1:B:500:HIS:O	1:B:500:HIS:HD2	2.03	0.41
1:B:518:VAL:O	1:B:522:LEU:HG	2.20	0.41
1:B:640:ARG:HG3	1:B:649:PHE:CE2	2.56	0.41
1:A:205:LEU:HD13	1:A:244:VAL:CA	2.51	0.41
1:B:93:LYS:HA	1:B:93:LYS:HD3	1.81	0.41
1:A:318:ILE:HA	1:A:319:PRO:HD3	1.88	0.40
1:A:427:ARG:HD2	1:B:525:GLU:OE1	2.21	0.40
1:B:299:ARG:HD2	1:B:300:ARG:HG3	2.03	0.40
1:A:500:HIS:O	1:A:500:HIS:HD2	2.05	0.40
1:A:158:SER:HB3	1:A:164:LEU:HD12	2.04	0.40
1:A:675:LYS:HB2	1:B:505:LEU:HD12	2.03	0.40
1:B:513:ARG:NH2	1:B:551:GLN:O	2.52	0.40
1:B:621:HIS:ND1	1:B:631:LEU:HD11	2.36	0.40
3:D:8:C:H2'	3:D:9:C:O4'	2.22	0.40
1:A:457:LYS:O	1:A:681:LYS:HG2	2.20	0.40
1:A:621:HIS:ND1	1:A:631:LEU:HD11	2.35	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	656/685 (96%)	581 (89%)	67 (10%)	8 (1%)	13	39
1	B	658/685 (96%)	581 (88%)	68 (10%)	9 (1%)	11	34
All	All	1314/1370 (96%)	1162 (88%)	135 (10%)	17 (1%)	12	36

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	PRO
1	A	497	ASP
1	B	143	PRO
1	B	497	ASP
1	A	127	VAL
1	B	127	VAL
1	A	563	ARG
1	A	34	ASP
1	A	35	PRO
1	B	34	ASP
1	B	35	PRO
1	B	288	ARG
1	A	288	ARG
1	B	563	ARG
1	B	36	PRO
1	A	438	PRO
1	B	438	PRO

5.3.2 Protein sidechains (i)

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	437/549 (80%)	394 (90%)	43 (10%)	8	24
1	B	440/549 (80%)	397 (90%)	43 (10%)	8	24
All	All	877/1098 (80%)	791 (90%)	86 (10%)	8	24

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	VAL
1	A	57	THR
1	A	62	ASP
1	A	79	LEU
1	A	101	LYS
1	A	159	ASP
1	A	160	SER
1	A	165	LEU
1	A	206	ARG
1	A	296	TRP
1	A	299	ARG
1	A	301	LEU
1	A	309	VAL
1	A	312	GLN
1	A	335	ARG
1	A	344	THR
1	A	355	GLN
1	A	372	SER
1	A	375	SER
1	A	392	ARG
1	A	406	VAL
1	A	424	LEU
1	A	451	LEU
1	A	454	LEU
1	A	461	GLN
1	A	472	GLU
1	A	475	VAL
1	A	494	VAL
1	A	497	ASP
1	A	500	HIS
1	A	531	ARG
1	A	543	LEU
1	A	545	ARG
1	A	558	LEU
1	A	559	GLU
1	A	570	LEU
1	A	580	ARG
1	A	590	ASP
1	A	600	THR
1	A	639	THR
1	A	640	ARG
1	A	641	LEU

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Mol	Chain	Res	Type
1	A	676	GLU
1	B	42	VAL
1	B	57	THR
1	B	62	ASP
1	B	64	LEU
1	B	79	LEU
1	B	101	LYS
1	B	159	ASP
1	B	160	SER
1	B	165	LEU
1	B	296	TRP
1	B	299	ARG
1	B	301	LEU
1	B	309	VAL
1	B	312	GLN
1	B	335	ARG
1	B	344	THR
1	B	355	GLN
1	B	372	SER
1	B	375	SER
1	B	392	ARG
1	B	406	VAL
1	B	424	LEU
1	B	451	LEU
1	B	454	LEU
1	B	461	GLN
1	B	472	GLU
1	B	475	VAL
1	B	494	VAL
1	B	497	ASP
1	B	500	HIS
1	B	531	ARG
1	B	543	LEU
1	B	545	ARG
1	B	558	LEU
1	B	559	GLU
1	B	570	LEU
1	B	580	ARG
1	B	590	ASP
1	B	600	THR
1	B	639	THR
1	B	640	ARG

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Mol	Chain	Res	Type
1	B	641	LEU
1	B	676	GLU

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	12	ASN
1	A	48	GLN
1	A	256	HIS
1	A	312	GLN
1	A	355	GLN
1	A	382	HIS
1	A	404	GLN
1	A	445	HIS
1	A	461	GLN
1	A	509	GLN
1	B	12	ASN
1	B	48	GLN
1	B	256	HIS
1	B	312	GLN
1	B	355	GLN
1	B	382	HIS
1	B	404	GLN
1	B	445	HIS
1	B	461	GLN
1	B	509	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	D	14/19 (73%)	1 (7%)	0
3	F	14/19 (73%)	1 (7%)	0
All	All	28/38 (73%)	2 (7%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	F	6	A
3	D	6	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 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	464:ALA	C	465:LEU	N	1.14

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, 95^{th} 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	664/685 (96%)	0.28	31 (4%) 31 22	37, 71, 146, 179	0
1	B	666/685 (97%)	0.30	40 (6%) 21 14	37, 71, 146, 179	0
2	C	17/21 (80%)	-0.28	0 100 100	61, 79, 114, 127	0
2	E	17/21 (80%)	-0.30	0 100 100	61, 81, 113, 132	0
3	D	15/19 (78%)	-0.17	0 100 100	66, 102, 127, 138	0
3	F	15/19 (78%)	-0.19	0 100 100	66, 101, 127, 137	0
All	All	1394/1450 (96%)	0.27	71 (5%) 28 19	37, 72, 146, 179	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	250	PRO	5.4
1	B	247	PRO	5.2
1	A	248	LYS	5.0
1	B	243	TRP	4.7
1	A	247	PRO	4.3
1	B	248	LYS	4.2
1	A	264	VAL	4.1
1	A	239	GLY	4.1
1	A	234	GLN	4.1
1	B	229	SER	4.1
1	A	188	PRO	4.0
1	A	250	PRO	3.9
1	B	249	ASP	3.8
1	B	263	PRO	3.8
1	A	201	THR	3.6
1	B	238	GLY	3.6
1	B	239	GLY	3.6
1	A	238	GLY	3.6
1	B	208	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	241	VAL	3.6
1	A	37	PRO	3.6
1	B	266	THR	3.5
1	B	205	LEU	3.4
1	B	37	PRO	3.4
1	A	205	LEU	3.4
1	B	225	ASP	3.4
1	B	193	VAL	3.4
1	A	161	GLY	3.3
1	A	249	ASP	3.3
1	B	260	LEU	3.3
1	A	260	LEU	3.3
1	A	261	LEU	3.3
1	B	201	THR	3.2
1	B	234	GLN	3.1
1	B	188	PRO	3.1
1	A	266	THR	3.1
1	B	240	ARG	2.9
1	B	261	LEU	2.9
1	B	264	VAL	2.9
1	B	280	SER	2.8
1	B	262	VAL	2.8
1	A	227	HIS	2.8
1	B	190	PRO	2.7
1	A	173	ILE	2.7
1	B	31	VAL	2.7
1	A	216	PRO	2.7
1	B	199	ARG	2.6
1	B	173	ILE	2.6
1	A	226	TYR	2.6
1	A	240	ARG	2.5
1	A	189	LEU	2.5
1	A	204	LEU	2.5
1	B	197	TYR	2.4
1	A	190	PRO	2.4
1	B	24	LEU	2.4
1	A	263	PRO	2.4
1	A	109	LEU	2.3
1	B	189	LEU	2.3
1	B	603	LEU	2.3
1	B	187	HIS	2.3
1	A	175	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	33	LEU	2.2
1	A	262	VAL	2.2
1	B	241	VAL	2.2
1	A	229	SER	2.1
1	A	243	TRP	2.1
1	B	437	VAL	2.1
1	B	226	TYR	2.0
1	B	140	ALA	2.0
1	B	299	ARG	2.0
1	B	202	TRP	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 monosaccharides 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, 95^{th} 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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	C	22	1/1	0.89	0.20	46,46,46,46	0
4	MG	B	686	1/1	0.90	0.12	75,75,75,75	0
4	MG	A	686	1/1	0.90	0.13	71,71,71,71	0
4	MG	E	22	1/1	0.95	0.20	52,52,52,52	0

6.5 Other polymers (i)

There are no such residues in this entry.