



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 10:00 PM JST

PDB ID : 6AEB
Title : Crystal structure of xCas9 in complex with sgRNA and target DNA (AAG PAM)
Authors : Guo, M.; Ren, K.; Zhu, Y.; Huang, Z.
Deposited on : 2018-08-04
Resolution : 3.00 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 : 2.36
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) : 2.36

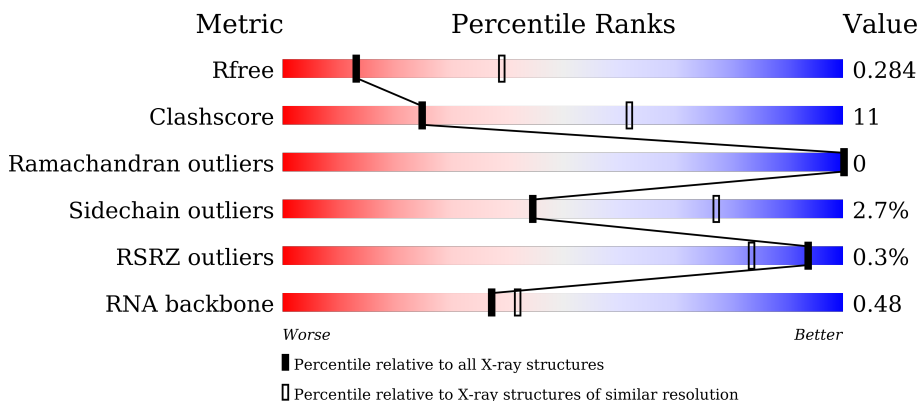
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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	100	 45% 35% 15% 5%
1	E	100	 44% 39% 11% 5%
2	C	28	 43% 46% 11%
2	G	28	 64% 25% 11%

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Mol	Chain	Length	Quality of chain
3	D	11	 55% 45%
3	H	11	 45% 55%
4	B	1368	 72% 23% ..
4	F	1368	 72% 24% ..

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 26351 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 RNA chain called RNA (95-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	95	2032	911	372	654	95	0	0	0
1	E	95	2032	911	372	654	95	0	0	0

- Molecule 2 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	25	506	247	83	152	24	0	0	0
2	G	25	506	247	83	152	24	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	D	11	227	110	46	61	10	0	0	0
3	H	11	227	110	46	61	10	0	0	0

- Molecule 4 is a protein called DNA Nuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	1322	10411	6656	1811	1923	21	0	0	0
4	F	1322	10409	6655	1811	1922	21	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	10	ALA	ASP	engineered mutation	UNP Q99ZW2
B	262	THR	ALA	engineered mutation	UNP Q99ZW2
B	324	LEU	ARG	engineered mutation	UNP Q99ZW2
B	409	ILE	SER	engineered mutation	UNP Q99ZW2
B	480	LYS	GLU	engineered mutation	UNP Q99ZW2
B	543	ASP	GLU	engineered mutation	UNP Q99ZW2
B	694	ILE	MET	engineered mutation	UNP Q99ZW2
B	840	ALA	HIS	engineered mutation	UNP Q99ZW2
B	1219	VAL	GLU	engineered mutation	UNP Q99ZW2
F	10	ALA	ASP	engineered mutation	UNP Q99ZW2
F	262	THR	ALA	engineered mutation	UNP Q99ZW2
F	324	LEU	ARG	engineered mutation	UNP Q99ZW2
F	409	ILE	SER	engineered mutation	UNP Q99ZW2
F	480	LYS	GLU	engineered mutation	UNP Q99ZW2
F	543	ASP	GLU	engineered mutation	UNP Q99ZW2
F	694	ILE	MET	engineered mutation	UNP Q99ZW2
F	840	ALA	HIS	engineered mutation	UNP Q99ZW2
F	1219	VAL	GLU	engineered mutation	UNP Q99ZW2

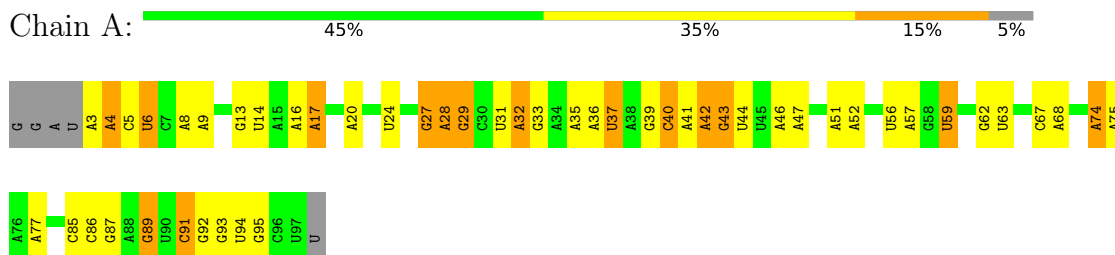
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O 1 1	0	0

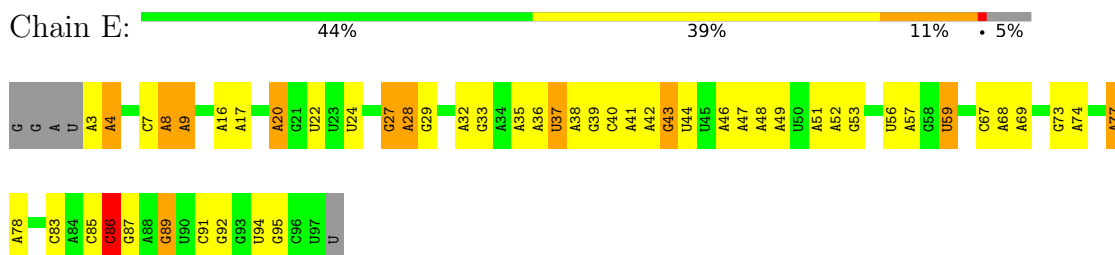
3 Residue-property plots [i](#)

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.

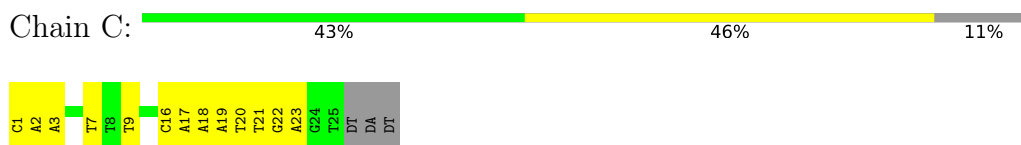
- Molecule 1: RNA (95-MER)



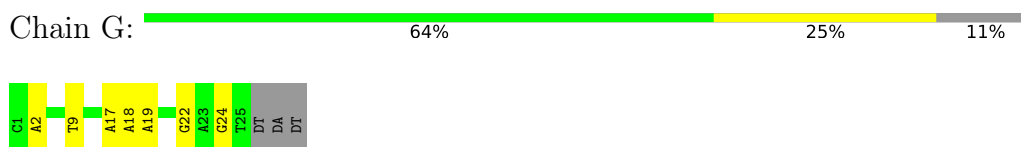
- Molecule 1: RNA (95-MER)



- Molecule 2: DNA (25-MER)



- Molecule 2: DNA (25-MER)

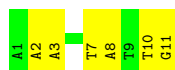


- Molecule 3: DNA (5'-D(*AP*AP*AP*AP*AP*GP*TP*AP*TP*TP*G)-3')

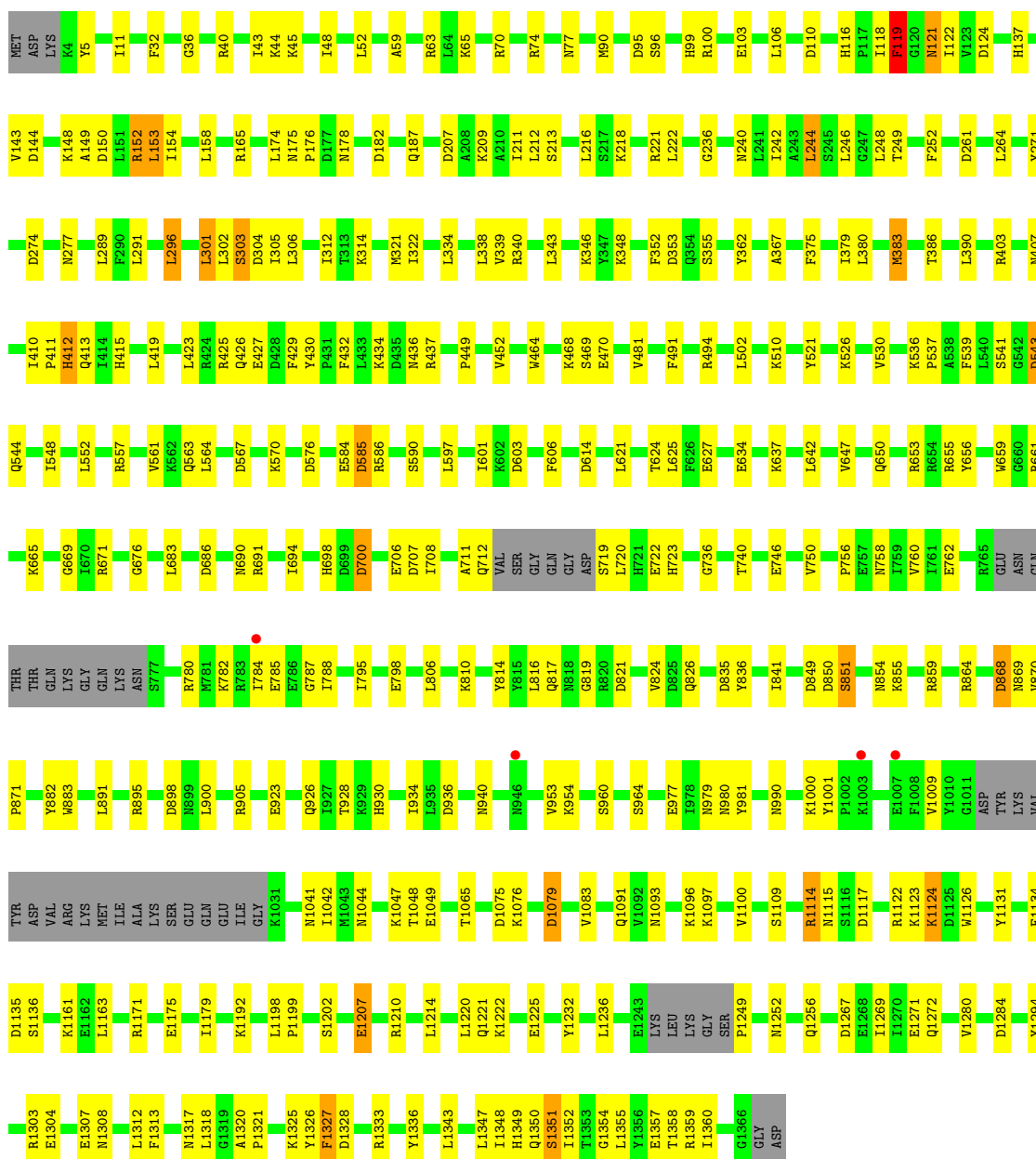




● Molecule 3: DNA (5'-D(*AP*AP*AP*AP*AP*GP*TP*AP*TP*TP*G)-3')



● Molecule 4: DNA Nuclease



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	361.85Å 71.13Å 198.32Å 90.00° 101.75° 90.00°	Depositor
Resolution (Å)	49.45 – 3.00 49.45 – 3.01	Depositor EDS
% Data completeness (in resolution range)	97.7 (49.45-3.00) 86.1 (49.45-3.01)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.74 (at 3.01Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.231 , 0.283 0.232 , 0.284	Depositor DCC
R_{free} test set	1981 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	62.2	Xtrriage
Anisotropy	0.704	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	26351	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.30 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4091e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 i

5.1 Standard geometry i

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	0.35	0/2277	1.00	0/3546
1	E	0.36	0/2277	0.99	1/3546 (0.0%)
2	C	0.77	0/565	1.19	0/870
2	G	0.77	0/565	1.17	0/870
3	D	0.73	0/256	0.98	0/394
3	H	0.74	0/256	0.99	0/394
4	B	0.36	1/10600 (0.0%)	0.52	11/14316 (0.1%)
4	F	0.34	0/10598	0.50	4/14313 (0.0%)
All	All	0.39	1/27394 (0.0%)	0.68	16/38249 (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
4	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	119	PHE	C-N	-6.62	1.21	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	175	ASN	C-N-CD	-10.49	97.52	120.60
4	B	119	PHE	N-CA-C	-8.90	86.98	111.00
4	B	119	PHE	O-C-N	-8.07	109.48	123.20
4	B	118	ILE	CB-CA-C	-6.44	98.71	111.60
4	B	586	ARG	N-CA-CB	-6.35	99.17	110.60
4	F	1075	ASP	N-CA-C	-6.17	94.34	111.00
4	F	586	ARG	N-CA-CB	-5.92	99.93	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	851	SER	N-CA-CB	5.84	119.26	110.50
4	B	153	LEU	CB-CA-C	5.82	121.25	110.20
4	B	585	ASP	N-CA-C	-5.68	95.67	111.00
4	B	1083	VAL	CB-CA-C	-5.56	100.84	111.40
4	B	121	ASN	N-CA-C	-5.45	96.29	111.00
4	B	119	PHE	CA-C-N	5.42	127.05	116.20
1	E	86	C	C2-N1-C1'	5.38	124.72	118.80
4	B	850	ASP	N-CA-C	-5.24	96.86	111.00
4	F	585	ASP	N-CA-C	-5.11	97.20	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	B	119	PHE	Mainchain

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	2032	0	1021	42	0
1	E	2032	0	1021	27	0
2	C	506	0	289	18	0
2	G	506	0	289	9	0
3	D	227	0	126	7	0
3	H	227	0	126	5	0
4	B	10411	0	10286	238	0
4	F	10409	0	10281	224	0
5	B	1	0	0	0	0
All	All	26351	0	23439	517	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 11.

All (517) 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:63:U:N3	4:B:65:LYS:NZ	1.95	1.13
4:F:1047:LYS:O	4:F:1076:LYS:NZ	1.89	1.05
4:B:150:ASP:OD1	4:B:152:ARG:HG2	1.69	0.93
4:F:1062:LEU:O	4:F:1076:LYS:HG3	1.69	0.92
4:B:561:VAL:HG23	4:B:585:ASP:O	1.70	0.91
1:A:63:U:H3	4:B:65:LYS:HZ1	1.20	0.89
1:A:63:U:C2	4:B:65:LYS:NZ	2.42	0.87
4:F:514:LEU:HG	4:F:667:ILE:HD11	1.56	0.86
4:B:870:VAL:HG22	4:B:871:PRO:HD2	1.57	0.85
4:B:1124:LYS:HE3	4:B:1124:LYS:HA	1.58	0.85
1:A:29:G:H1	1:A:40:C:H42	1.21	0.85
1:A:3:A:H2'	1:A:4:A:H8	1.43	0.84
1:A:63:U:H3	4:B:65:LYS:NZ	1.70	0.82
4:F:1205:GLU:OE1	4:F:1359:ARG:NH2	2.13	0.81
4:F:832:ARG:NH1	4:F:835:ASP:OD2	2.13	0.81
1:E:3:A:H2'	1:E:4:A:H8	1.46	0.81
4:B:700:ASP:OD1	4:B:700:ASP:N	2.15	0.80
4:B:898:ASP:O	4:B:905:ARG:NH2	2.15	0.79
1:E:86:C:N4	1:E:92:G:O6	2.16	0.78
4:B:627:GLU:O	4:B:655:ARG:NH2	2.17	0.78
1:E:33:G:N2	1:E:36:A:OP2	2.16	0.78
3:D:8:DA:OP1	4:B:1114:ARG:NH1	2.17	0.77
4:B:152:ARG:O	4:B:153:LEU:C	2.20	0.77
4:B:1308:ASN:OD1	4:B:1326:TYR:O	2.03	0.77
4:B:209:LYS:O	4:B:213:SER:OG	2.04	0.76
4:B:621:LEU:HD11	4:B:625:LEU:HD22	1.67	0.75
1:A:32:A:N6	1:A:37:U:O4	2.15	0.75
4:B:780:ARG:NH1	4:B:806:LEU:O	2.19	0.75
3:H:8:DA:OP1	4:F:1114:ARG:NH1	2.20	0.75
4:F:557:ARG:NH2	4:F:596:ASP:OD1	2.20	0.75
4:F:870:VAL:HG22	4:F:871:PRO:HD2	1.69	0.74
4:F:986:ASP:O	4:F:990:ASN:ND2	2.20	0.74
2:C:7:DT:O4	3:D:5:DA:N6	2.19	0.73
4:B:1124:LYS:HA	4:B:1124:LYS:CE	2.16	0.73
2:C:22:DG:O3'	4:B:895:ARG:NH1	2.20	0.73
4:F:175:ASN:CG	4:F:176:PRO:HD2	2.09	0.73
4:B:158:LEU:HD22	4:B:419:LEU:HD12	1.69	0.72
4:B:1308:ASN:HB3	4:B:1326:TYR:O	1.89	0.72
1:A:67:C:OP2	4:B:1097:LYS:NZ	2.19	0.72
4:B:1303:ARG:NH2	4:B:1307:GLU:OE2	2.23	0.72
4:B:548:ILE:HG23	4:B:552:LEU:HD12	1.72	0.72
4:F:826:GLN:OE1	4:F:859:ARG:NH2	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1267:ASP:OD1	4:B:1294:TYR:OH	2.09	0.71
4:F:1207:GLU:OE1	4:F:1210:ARG:NH1	2.21	0.71
2:G:22:DG:O3'	4:F:895:ARG:NH1	2.23	0.71
4:F:971:GLN:O	4:F:1234:ASN:ND2	2.24	0.71
4:B:1357:GLU:OE1	4:B:1359:ARG:NH1	2.24	0.70
1:A:91:C:H5''	4:B:1091:GLN:HG3	1.73	0.70
4:F:274:ASP:OD1	4:F:653:ARG:NH1	2.24	0.70
4:B:427:GLU:HB2	4:B:434:LYS:HB2	1.72	0.69
4:B:817:GLN:O	4:B:882:TYR:OH	2.11	0.68
2:G:19:DA:OP1	4:F:497:ASN:ND2	2.25	0.68
4:F:719:SER:OG	4:F:720:LEU:N	2.27	0.68
4:B:362:TYR:HA	4:B:367:ALA:HB3	1.76	0.68
4:B:96:SER:OG	4:B:100:ARG:NH1	2.27	0.68
4:F:209:LYS:O	4:F:213:SER:OG	2.11	0.67
4:F:170:ILE:O	4:F:413:GLN:NE2	2.27	0.67
4:F:82:LEU:HD22	4:F:162:ILE:HD12	1.76	0.67
1:A:41:A:OP2	4:B:340:ARG:NH1	2.28	0.67
1:A:29:G:H1	1:A:40:C:N4	1.93	0.66
4:F:780:ARG:NH1	4:F:806:LEU:O	2.27	0.66
1:A:33:G:N2	1:A:36:A:OP2	2.26	0.66
4:F:841:ILE:HD13	4:F:900:LEU:CD1	2.25	0.66
1:E:92:G:O6	4:F:44:LYS:NZ	2.29	0.66
4:F:469:SER:OG	4:F:470:GLU:N	2.29	0.66
4:F:817:GLN:O	4:F:882:TYR:OH	2.13	0.65
4:B:148:LYS:HE3	4:B:429:PHE:HB3	1.77	0.65
4:F:625:LEU:HD13	4:F:659:TRP:CH2	2.31	0.65
1:E:3:A:H2'	1:E:4:A:C8	2.31	0.64
4:F:1194:LEU:HD13	4:F:1365:LEU:HB3	1.78	0.64
1:A:89:G:O6	4:B:1272:GLN:NE2	2.26	0.64
4:B:137:HIS:HA	4:B:322:ILE:HD11	1.80	0.63
4:F:1161:LYS:NZ	4:F:1365:LEU:O	2.22	0.63
4:B:432:PHE:O	4:B:436:ASN:ND2	2.27	0.63
4:B:936:ASP:OD1	4:B:940:ASN:ND2	2.31	0.63
4:B:1124:LYS:HE3	4:B:1124:LYS:CA	2.28	0.63
4:F:277:ASN:OD1	4:F:650:GLN:NE2	2.31	0.63
4:F:1000:LYS:NZ	4:F:1065:THR:O	2.30	0.63
4:B:826:GLN:OE1	4:B:859:ARG:NH2	2.31	0.63
4:F:1267:ASP:OD1	4:F:1294:TYR:OH	2.09	0.63
4:F:218:LYS:NZ	4:F:246:LEU:O	2.30	0.63
4:F:1061:PRO:O	4:F:1076:LYS:HE3	1.99	0.62
4:B:570:LYS:NZ	4:B:576:ASP:OD1	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:694:ILE:O	4:B:698:HIS:CD2	2.52	0.62
4:B:561:VAL:CG2	4:B:585:ASP:O	2.46	0.62
4:B:625:LEU:HD13	4:B:659:TRP:HH2	1.65	0.62
4:B:1135:ASP:OD1	4:B:1136:SER:N	2.33	0.62
1:A:92:G:O6	4:B:44:LYS:NZ	2.33	0.62
4:B:526:LYS:NZ	4:B:690:ASN:O	2.33	0.62
4:B:1207:GLU:OE2	4:B:1210:ARG:NH1	2.32	0.61
1:A:27:G:N2	1:A:44:U:OP2	2.33	0.61
1:A:3:A:OP1	4:B:661:ARG:NH1	2.33	0.61
4:B:980:ASN:ND2	4:B:1225:GLU:OE2	2.31	0.61
4:F:601:ILE:HD11	4:F:607:LEU:HD21	1.81	0.61
2:C:19:DA:H5 ^{''}	2:C:19:DA:H8	1.65	0.61
1:A:16:A:OP2	4:B:70:ARG:NH2	2.34	0.60
4:B:48:ILE:O	4:B:1093:ASN:ND2	2.26	0.60
4:F:427:GLU:HB2	4:F:434:LYS:HB2	1.82	0.60
4:B:274:ASP:OD1	4:B:653:ARG:NH1	2.34	0.60
4:B:277:ASN:OD1	4:B:650:GLN:NE2	2.35	0.60
4:F:1194:LEU:HD22	4:F:1365:LEU:HD13	1.84	0.60
4:F:1060:ARG:NE	4:F:1064:GLU:OE2	2.27	0.60
4:B:1123:LYS:HB2	4:B:1126:TRP:CD2	2.37	0.60
4:B:1047:LYS:O	4:B:1076:LYS:NZ	2.28	0.59
1:A:5:C:OP1	4:B:510:LYS:NZ	2.35	0.59
4:B:756:PRO:O	4:B:953:VAL:HG22	2.02	0.59
4:F:179:SER:OG	4:F:312:ILE:HD12	2.02	0.59
2:C:19:DA:H5 ^{''}	2:C:19:DA:C8	2.37	0.59
4:B:787:GLY:HA3	4:B:891:LEU:HD21	1.85	0.58
2:G:19:DA:H8	2:G:19:DA:H5 ^{''}	1.69	0.58
4:F:809:GLU:OE1	4:F:855:LYS:NZ	2.29	0.58
4:F:1295:ASN:HA	4:F:1298:ARG:HD2	1.86	0.58
1:E:67:C:OP2	4:F:1097:LYS:NZ	2.28	0.57
4:F:175:ASN:OD1	4:F:176:PRO:HD2	2.03	0.57
4:F:432:PHE:O	4:F:436:ASN:ND2	2.32	0.57
4:F:1357:GLU:OE1	4:F:1359:ARG:NH1	2.35	0.57
2:C:1:DC:N3	3:D:11:DG:N2	2.47	0.57
4:B:45:LYS:NZ	4:B:1357:GLU:OE2	2.26	0.57
4:B:1163:LEU:HD11	4:B:1198:LEU:HD12	1.87	0.57
4:F:353:ASP:OD1	4:F:355:SER:OG	2.20	0.57
4:F:548:ILE:HG23	4:F:552:LEU:HD12	1.85	0.57
4:F:1207:GLU:CD	4:F:1210:ARG:HH11	2.07	0.57
4:B:841:ILE:O	4:B:864:ARG:NH2	2.38	0.57
1:A:17:A:OP2	4:B:74:ARG:NH1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:A:OP2	1:A:62:G:N2	2.33	0.56
4:F:625:LEU:HD13	4:F:659:TRP:HH2	1.68	0.56
4:B:1252:ASN:O	4:B:1256:GLN:N	2.31	0.56
4:F:11:ILE:HD11	4:F:740:THR:HG21	1.87	0.56
4:F:854:ASN:O	4:F:854:ASN:ND2	2.38	0.56
4:B:11:ILE:HD11	4:B:740:THR:HG21	1.88	0.56
4:F:121:ASN:OD1	4:F:124:ASP:N	2.34	0.56
4:F:404:THR:OG1	4:F:405:PHE:N	2.37	0.56
4:F:535:ARG:HG2	4:F:536:LYS:HG2	1.88	0.56
4:F:967:ARG:NH2	4:F:972:PHE:O	2.38	0.56
4:B:762:GLU:OE2	4:B:960:SER:OG	2.23	0.56
4:F:144:ASP:O	4:F:425:ARG:NH2	2.39	0.56
4:F:594:TYR:OH	4:F:608:ASP:OD1	2.14	0.56
4:B:719:SER:OG	4:B:720:LEU:N	2.39	0.55
4:B:212:LEU:HD22	4:B:246:LEU:HD21	1.88	0.55
4:B:977:GLU:N	4:B:977:GLU:OE2	2.40	0.55
4:B:782:LYS:HA	4:B:785:GLU:HB2	1.87	0.55
4:F:869:ASN:OD1	4:F:870:VAL:N	2.38	0.55
2:C:2:DA:H61	3:D:10:DT:H3	1.55	0.54
4:F:1207:GLU:CD	4:F:1207:GLU:H	2.09	0.54
1:E:8:A:H2'	1:E:9:A:C8	2.42	0.54
4:F:978:ILE:HD12	4:F:1233:VAL:HG13	1.89	0.54
1:A:14:U:OP2	4:B:63:ARG:NH1	2.37	0.54
4:B:302:LEU:HD22	4:B:306:LEU:HD21	1.89	0.54
4:B:1222:LYS:HD2	4:B:1317:ASN:O	2.07	0.54
4:F:469:SER:OG	4:F:471:GLU:HG2	2.07	0.54
4:B:469:SER:OG	4:B:470:GLU:N	2.33	0.54
4:F:474:THR:N	4:F:477:ASN:OD1	2.35	0.54
4:F:1000:LYS:HG3	4:F:1001:TYR:CE1	2.43	0.54
2:C:23:DA:P	4:B:895:ARG:HH12	2.30	0.54
4:F:1328:ASP:N	4:F:1328:ASP:OD1	2.41	0.54
1:A:94:U:H2'	1:A:95:G:C8	2.43	0.54
4:B:207:ASP:O	4:B:211:ILE:HG13	2.08	0.54
4:F:148:LYS:HE3	4:F:429:PHE:HB3	1.88	0.54
4:F:492:ILE:O	4:F:496:THR:HG23	2.08	0.54
4:B:1179:ILE:HD11	4:B:1192:LYS:HG3	1.90	0.54
1:A:13:G:OP1	4:B:59:ALA:N	2.37	0.53
4:F:368:SER:N	4:F:371:GLU:OE1	2.28	0.53
4:F:100:ARG:NH2	4:F:119:PHE:O	2.42	0.53
1:A:93:G:O6	4:B:44:LYS:NZ	2.36	0.53
2:G:2:DA:H61	3:H:10:DT:H3	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:9:DT:OP2	4:F:1107:LYS:HB3	2.09	0.53
4:F:246:LEU:HD23	4:F:300:ILE:HD13	1.91	0.53
4:F:492:ILE:HD13	4:F:625:LEU:O	2.09	0.53
4:F:1312:LEU:HA	4:F:1324:PHE:CE2	2.44	0.53
4:B:1284:ASP:OD1	4:B:1284:ASP:N	2.41	0.52
4:F:103:GLU:O	4:F:111:LYS:NZ	2.41	0.52
4:F:677:LYS:HB2	4:F:682:PHE:CE1	2.44	0.52
4:B:469:SER:HB3	4:B:481:VAL:HG13	1.89	0.52
4:F:340:ARG:O	4:F:344:PRO:HG3	2.09	0.52
1:E:20:A:OP2	4:F:403:ARG:NH1	2.42	0.52
4:F:86:PHE:O	4:F:90:MET:HB3	2.10	0.52
4:F:305:ILE:HG22	4:F:306:LEU:HD13	1.92	0.52
4:F:339:VAL:O	4:F:343:LEU:N	2.32	0.52
4:B:625:LEU:HD13	4:B:659:TRP:CH2	2.45	0.52
4:B:1308:ASN:CB	4:B:1326:TYR:O	2.56	0.52
4:F:561:VAL:HG23	4:F:585:ASP:O	2.08	0.52
4:F:628:ASP:O	4:F:629:ARG:C	2.46	0.52
4:B:252:PHE:CD2	4:B:264:LEU:HD13	2.45	0.52
4:B:1000:LYS:HG3	4:B:1001:TYR:CE1	2.44	0.52
4:F:46:ASN:O	4:F:48:ILE:N	2.41	0.52
4:F:249:THR:O	4:F:249:THR:OG1	2.26	0.52
4:B:212:LEU:O	4:B:221:ARG:NH2	2.43	0.51
4:F:1062:LEU:O	4:F:1076:LYS:CG	2.52	0.51
4:B:706:GLU:HG3	4:B:707:ASP:N	2.25	0.51
4:B:1199:PRO:O	4:B:1202:SER:OG	2.21	0.51
4:F:212:LEU:HD22	4:F:246:LEU:HD21	1.93	0.51
1:A:41:A:OP1	4:B:340:ARG:NH2	2.44	0.51
4:B:883:TRP:CD2	4:B:900:LEU:HD23	2.45	0.51
4:F:628:ASP:O	4:F:631:MET:N	2.44	0.51
4:B:870:VAL:HG22	4:B:871:PRO:CD	2.35	0.51
4:F:841:ILE:HG21	4:F:900:LEU:HD12	1.93	0.51
4:B:869:ASN:OD1	4:B:870:VAL:N	2.44	0.51
4:B:144:ASP:O	4:B:425:ARG:NH2	2.44	0.51
4:F:784:ILE:O	4:F:788:ILE:HG12	2.11	0.51
4:B:1232:TYR:HB3	4:B:1269:ILE:HD11	1.93	0.50
4:B:821:ASP:HB3	4:B:824:VAL:O	2.11	0.50
4:B:1214:LEU:HD23	4:B:1220:LEU:HD23	1.93	0.50
4:B:1349:HIS:HB2	4:B:1358:THR:HB	1.92	0.50
4:B:143:VAL:O	4:B:425:ARG:NE	2.42	0.50
4:F:165:ARG:O	4:F:412:HIS:HA	2.11	0.50
4:F:48:ILE:O	4:F:1093:ASN:ND2	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:C:H42	2:G:22:DG:H1	1.60	0.50
4:F:1135:ASP:OD1	4:F:1136:SER:N	2.45	0.50
4:F:1207:GLU:OE1	4:F:1210:ARG:NE	2.43	0.49
4:B:411:PRO:HB2	4:B:413:GLN:OE1	2.11	0.49
4:B:1161:LYS:O	4:B:1343:LEU:HD13	2.12	0.49
4:F:441:GLU:O	4:F:445:THR:HG23	2.12	0.49
4:F:601:ILE:HG22	4:F:647:VAL:HG11	1.94	0.49
1:A:46:A:OP1	4:B:403:ARG:NH2	2.43	0.49
4:B:221:ARG:NH2	4:B:304:ASP:OD1	2.42	0.49
4:B:686:ASP:OD2	4:B:691:ARG:HG3	2.13	0.49
4:B:1321:PRO:O	4:B:1333:ARG:HD2	2.12	0.49
4:F:95:ASP:OD1	4:F:95:ASP:N	2.45	0.49
1:A:67:C:N4	4:B:1100:VAL:O	2.44	0.49
1:E:16:A:OP1	4:F:74:ARG:NH2	2.22	0.49
2:G:17:DA:H2'	2:G:18:DA:C8	2.48	0.49
4:F:518:PHE:HB2	4:F:667:ILE:HD12	1.94	0.49
1:A:3:A:H2'	1:A:4:A:C8	2.34	0.49
4:B:339:VAL:O	4:B:343:LEU:N	2.39	0.49
4:B:671:ARG:NH1	4:B:676:GLY:O	2.36	0.49
4:F:733:ILE:O	4:F:737:ILE:HG13	2.13	0.49
4:B:851:SER:N	4:B:855:LYS:HE2	2.28	0.49
1:E:59:U:OP1	4:F:473:ILE:HG13	2.12	0.49
4:F:526:LYS:NZ	4:F:690:ASN:O	2.32	0.49
4:F:1206:LEU:HB3	4:F:1207:GLU:OE2	2.12	0.49
4:F:137:HIS:HA	4:F:322:ILE:HD11	1.94	0.49
4:F:777:SER:OG	4:F:778:ARG:N	2.45	0.49
4:F:1312:LEU:HD23	4:F:1324:PHE:HE2	1.78	0.49
4:B:723:HIS:O	4:B:723:HIS:ND1	2.46	0.48
4:B:1312:LEU:HD21	4:B:1326:TYR:HD1	1.77	0.48
4:B:379:ILE:O	4:B:383:MET:HG3	2.12	0.48
4:B:464:TRP:CZ2	4:B:491:PHE:HD1	2.31	0.48
4:B:222:LEU:HD13	4:B:242:ILE:HG22	1.96	0.48
4:F:302:LEU:O	4:F:305:ILE:N	2.45	0.48
4:F:841:ILE:O	4:F:864:ARG:NH2	2.46	0.48
4:F:1214:LEU:HD23	4:F:1220:LEU:HD23	1.96	0.48
4:B:343:LEU:HD13	4:B:346:LYS:HD2	1.96	0.48
4:B:423:LEU:HD13	4:B:437:ARG:HA	1.95	0.48
4:B:603:ASP:OD1	4:B:606:PHE:N	2.40	0.48
4:F:96:SER:OG	4:F:100:ARG:NH1	2.47	0.48
4:B:100:ARG:NH2	4:B:119:PHE:O	2.47	0.47
4:B:810:LYS:NZ	4:B:836:TYR:O	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:100:ARG:NH2	4:F:118:ILE:O	2.43	0.47
4:F:526:LYS:HE2	4:F:695:GLN:HE22	1.79	0.47
4:F:1042:ILE:HG23	4:F:1043:MET:HG2	1.96	0.47
4:F:1286:ASN:ND2	4:F:1332:ASP:O	2.47	0.47
4:B:548:ILE:HD13	4:B:564:LEU:HD11	1.95	0.47
4:F:45:LYS:NZ	4:F:1354:GLY:O	2.47	0.47
4:F:236:GLY:O	4:F:240:ASN:ND2	2.34	0.47
4:F:832:ARG:NH1	4:F:832:ARG:HB3	2.29	0.47
4:F:1321:PRO:O	4:F:1333:ARG:HD2	2.14	0.47
2:C:16:DC:H2'	2:C:17:DA:C8	2.50	0.47
4:B:1312:LEU:HD21	4:B:1326:TYR:CD1	2.50	0.47
4:F:1117:ASP:OD1	4:F:1117:ASP:N	2.46	0.47
4:F:396:GLU:O	4:F:400:ARG:HD3	2.13	0.47
4:F:584:GLU:O	4:F:585:ASP:C	2.51	0.47
4:B:979:ASN:OD1	4:B:981:TYR:N	2.47	0.47
1:E:37:U:H2'	1:E:38:A:O4'	2.15	0.47
4:F:1161:LYS:O	4:F:1343:LEU:HD13	2.15	0.47
4:F:1236:LEU:O	4:F:1240:SER:OG	2.22	0.47
4:B:719:SER:HB3	4:B:722:GLU:HB3	1.96	0.47
4:B:1079:ASP:OD1	4:B:1079:ASP:N	2.48	0.47
4:F:278:LEU:O	4:F:282:ILE:HG12	2.14	0.47
4:F:993:VAL:O	4:F:997:LEU:HB2	2.15	0.47
4:B:746:GLU:OE1	4:B:1351:SER:OG	2.33	0.47
4:B:1117:ASP:OD1	4:B:1117:ASP:N	2.45	0.47
4:B:149:ALA:O	4:B:430:TYR:OH	2.22	0.47
4:B:187:GLN:HG2	4:B:187:GLN:O	2.15	0.47
4:B:530:VAL:HB	4:B:537:PRO:HA	1.96	0.47
4:B:563:GLN:O	4:B:567:ASP:HB2	2.14	0.47
4:B:746:GLU:O	4:B:750:VAL:HG23	2.13	0.47
4:B:1232:TYR:CD1	4:B:1269:ILE:HG13	2.50	0.47
4:B:36:GLY:HA3	4:B:1359:ARG:O	2.15	0.46
4:F:1312:LEU:HA	4:F:1324:PHE:HE2	1.80	0.46
1:A:46:A:H2'	1:A:47:A:C8	2.50	0.46
1:A:74:A:H2'	1:A:75:A:O4'	2.14	0.46
4:B:218:LYS:NZ	4:B:246:LEU:O	2.28	0.46
4:B:380:LEU:O	4:B:386:THR:OG1	2.23	0.46
4:B:841:ILE:HD12	4:B:854:ASN:HA	1.95	0.46
4:F:627:GLU:O	4:F:655:ARG:NH2	2.48	0.46
4:F:711:ALA:HA	4:F:712:GLN:HA	1.59	0.46
2:C:23:DA:H5'	4:B:895:ARG:NH1	2.30	0.46
4:B:165:ARG:O	4:B:412:HIS:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1313:PHE:O	4:B:1317:ASN:N	2.46	0.46
4:F:672:ASP:OD2	4:F:675:SER:OG	2.30	0.46
4:B:468:LYS:N	4:B:481:VAL:O	2.46	0.46
4:B:1214:LEU:HD23	4:B:1214:LEU:HA	1.78	0.46
1:E:94:U:H2'	1:E:95:G:C8	2.51	0.46
4:F:777:SER:HB2	4:F:803:ASN:O	2.15	0.46
4:F:217:SER:O	4:F:221:ARG:HD3	2.16	0.46
4:F:1200:LYS:HE2	4:F:1201:TYR:CZ	2.50	0.46
4:B:252:PHE:HD2	4:B:264:LEU:HD13	1.80	0.46
4:B:634:GLU:O	4:B:637:LYS:HG2	2.15	0.46
4:B:52:LEU:HB2	4:B:1096:LYS:HD2	1.97	0.46
4:B:584:GLU:O	4:B:585:ASP:C	2.53	0.46
1:E:16:A:OP2	4:F:70:ARG:NH2	2.49	0.46
4:F:433:LEU:O	4:F:437:ARG:N	2.49	0.46
4:F:832:ARG:HB3	4:F:832:ARG:HH11	1.81	0.46
1:A:27:G:H5'	1:A:28:A:C5'	2.45	0.46
4:B:353:ASP:OD1	4:B:355:SER:OG	2.20	0.46
4:B:1304:GLU:O	4:B:1308:ASN:ND2	2.45	0.46
4:F:892:ILE:HB	4:F:896:LYS:HD3	1.98	0.46
1:A:5:C:H2'	1:A:6:U:H6	1.81	0.45
1:E:27:G:H5'	1:E:28:A:C5'	2.45	0.45
1:E:43:G:O6	4:F:351:PHE:HB3	2.15	0.45
4:F:8:GLY:HA3	4:F:991:ALA:HB2	1.97	0.45
4:F:544:GLN:NE2	4:F:573:GLU:OE2	2.49	0.45
4:F:1006:SER:OG	4:F:1007:GLU:N	2.48	0.45
4:F:1351:SER:HB2	4:F:1356:TYR:HB2	1.99	0.45
4:B:621:LEU:CD1	4:B:625:LEU:HD22	2.43	0.45
4:F:31:LYS:HG2	4:F:44:LYS:HD2	1.98	0.45
4:F:869:ASN:HD21	4:F:908:LEU:H	1.64	0.45
4:F:1210:ARG:HD2	4:F:1212:ARG:NH2	2.30	0.45
4:F:1214:LEU:HD22	4:F:1216:SER:O	2.16	0.45
4:B:264:LEU:HD23	4:B:271:TYR:CE2	2.52	0.45
4:B:1222:LYS:O	4:B:1318:LEU:HD12	2.16	0.45
4:F:314:LYS:HE2	4:F:314:LYS:HB3	1.76	0.45
4:F:666:LEU:HD12	4:F:670:ILE:HD11	1.97	0.45
4:B:1048:THR:OG1	4:B:1049:GLU:N	2.49	0.45
4:F:563:GLN:O	4:F:567:ASP:HB2	2.16	0.45
4:B:1210:ARG:HD3	4:B:1280:VAL:HA	1.98	0.45
4:F:624:THR:HA	4:F:656:TYR:O	2.16	0.45
4:F:846:PHE:O	4:F:920:GLN:NE2	2.50	0.45
4:F:799:HIS:O	4:F:815:TYR:OH	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:1120:ILE:HB	4:F:1134:PHE:HB2	1.99	0.45
4:F:1206:LEU:HD21	4:F:1341:GLU:HG3	1.97	0.45
4:B:339:VAL:HA	4:B:383:MET:CE	2.47	0.45
1:E:27:G:H4'	1:E:28:A:OP2	2.16	0.45
4:B:930:HIS:O	4:B:934:ILE:HG13	2.17	0.45
2:G:24:DG:OP1	4:F:902:LYS:NZ	2.34	0.45
4:F:699:ASP:C	4:F:701:SER:N	2.67	0.45
4:F:940:ASN:OD1	4:F:953:VAL:N	2.46	0.45
2:C:2:DA:H2'	2:C:3:DA:C8	2.52	0.44
2:C:18:DA:H2'	2:C:19:DA:C8	2.52	0.44
4:B:784:ILE:O	4:B:788:ILE:HG12	2.18	0.44
4:F:490:SER:O	4:F:494:ARG:HG3	2.17	0.44
4:B:1001:TYR:HE2	4:B:1042:ILE:HG13	1.82	0.44
1:E:41:A:P	4:F:340:ARG:HH22	2.41	0.44
4:F:1264:HIS:H	4:F:1264:HIS:CD2	2.36	0.44
4:B:32:PHE:HE2	4:B:1355:LEU:HD22	1.82	0.44
4:B:106:LEU:HA	4:B:1131:TYR:HE1	1.82	0.44
4:B:175:ASN:HB3	4:B:178:ASN:ND2	2.32	0.44
4:F:380:LEU:HB3	4:F:390:LEU:HD21	2.00	0.44
4:B:601:ILE:HG22	4:B:647:VAL:HG11	1.99	0.44
4:B:760:VAL:HG11	4:B:990:ASN:O	2.17	0.44
4:F:361:GLY:HA2	4:F:365:GLY:HA3	1.99	0.44
1:A:5:C:H2'	1:A:6:U:C6	2.53	0.44
4:B:302:LEU:O	4:B:306:LEU:HD22	2.18	0.44
4:B:407:ASN:O	4:B:410:ILE:HG12	2.17	0.44
4:B:541:SER:OG	4:B:544:GLN:HG3	2.17	0.44
4:B:1001:TYR:CE2	4:B:1042:ILE:HG13	2.52	0.44
1:E:48:A:H2'	1:E:49:A:C8	2.51	0.44
4:F:918:LYS:O	4:F:922:VAL:HG23	2.18	0.44
4:F:923:GLU:HG2	4:F:928:THR:HG21	1.99	0.44
4:F:1083:VAL:O	4:F:1086:VAL:N	2.51	0.44
3:D:10:DT:H2''	3:D:11:DG:H5''	2.00	0.44
4:B:95:ASP:OD1	4:B:95:ASP:N	2.45	0.44
4:B:526:LYS:HD2	4:B:526:LYS:HA	1.72	0.44
4:B:1308:ASN:CG	4:B:1326:TYR:O	2.54	0.44
1:E:83:C:H42	1:E:95:G:H1	1.66	0.44
4:F:1284:ASP:N	4:F:1284:ASP:OD1	2.51	0.44
2:C:20:DT:OP1	4:B:930:HIS:HE1	1.99	0.44
4:B:348:LYS:O	4:B:352:PHE:HB2	2.18	0.44
4:B:557:ARG:O	4:B:590:SER:OG	2.22	0.44
4:B:923:GLU:HG2	4:B:928:THR:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:524:LEU:HD23	4:F:524:LEU:HA	1.81	0.44
4:F:1270:ILE:HG13	4:F:1294:TYR:CZ	2.52	0.44
4:B:165:ARG:O	4:B:415:HIS:HD2	2.01	0.44
4:B:614:ASP:OD1	4:B:614:ASP:N	2.48	0.44
4:B:1163:LEU:HD21	4:B:1214:LEU:HD11	2.00	0.44
4:B:1163:LEU:HB2	4:B:1343:LEU:HD21	2.00	0.44
4:F:37:ASN:HD21	4:F:1361:ASP:H	1.66	0.44
4:F:841:ILE:HD11	4:F:896:LYS:HE3	2.00	0.44
4:B:1171:ARG:NE	4:B:1175:GLU:OE1	2.43	0.43
4:F:755:LYS:HE2	4:F:939:MET:O	2.18	0.43
4:F:760:VAL:HG11	4:F:990:ASN:O	2.17	0.43
4:F:883:TRP:CD2	4:F:900:LEU:HD23	2.53	0.43
4:B:1041:ASN:HB3	4:B:1044:ASN:ND2	2.33	0.43
4:F:729:GLY:O	4:F:734:LYS:HE2	2.19	0.43
4:B:116:HIS:CE1	4:B:122:ILE:HB	2.53	0.43
1:E:22:U:O2'	4:F:1110:ILE:O	2.36	0.43
4:F:961:LYS:HE2	4:F:961:LYS:HB2	1.83	0.43
4:F:967:ARG:HA	4:F:972:PHE:HB2	2.01	0.43
4:F:1249:PRO:O	4:F:1252:ASN:ND2	2.51	0.43
4:F:1300:LYS:HA	4:F:1300:LYS:HD3	1.81	0.43
1:A:59:U:H1'	4:B:77:ASN:ND2	2.33	0.43
4:B:99:HIS:O	4:B:103:GLU:HG2	2.18	0.43
4:B:665:LYS:HA	4:B:669:GLY:HA3	2.00	0.43
4:F:593:THR:HA	4:F:596:ASP:HB2	2.00	0.43
4:B:296:LEU:HD23	4:B:296:LEU:HA	1.83	0.43
4:B:642:LEU:HD12	4:B:642:LEU:HA	1.78	0.43
4:B:1351:SER:OG	4:B:1352:ILE:N	2.52	0.43
3:H:2:DA:H2''	3:H:3:DA:C8	2.53	0.43
4:F:103:GLU:CD	4:F:112:LYS:H	2.21	0.43
4:F:1066:ASN:OD1	4:F:1069:THR:N	2.50	0.43
2:C:9:DT:OP2	4:B:1109:SER:N	2.52	0.43
2:C:21:DT:OP1	4:B:926:GLN:N	2.47	0.43
4:B:65:LYS:HZ2	4:B:65:LYS:HG3	1.75	0.43
4:B:464:TRP:HB3	4:B:494:ARG:HD3	2.00	0.43
4:F:1084:ARG:O	4:F:1088:SER:OG	2.18	0.43
1:A:27:G:H5'	1:A:28:A:O5'	2.19	0.43
1:A:29:G:N2	1:A:40:C:N3	2.50	0.43
4:B:216:LEU:O	4:B:221:ARG:HD2	2.19	0.43
4:F:301:LEU:O	4:F:305:ILE:HG12	2.19	0.43
4:F:784:ILE:HD11	4:F:812:TYR:CD1	2.53	0.43
1:A:27:G:H4'	1:A:28:A:OP2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:264:LEU:HD23	4:F:271:TYR:CE1	2.54	0.42
4:F:1045:PHE:O	4:F:1064:GLU:HG3	2.19	0.42
4:B:5:TYR:CE2	4:B:756:PRO:HB3	2.54	0.42
4:B:175:ASN:HA	4:B:176:PRO:HD3	1.69	0.42
4:B:521:TYR:HB3	4:B:683:LEU:HB3	2.01	0.42
4:B:1347:LEU:HB3	4:B:1360:ILE:HB	2.01	0.42
1:E:36:A:N6	1:E:37:U:O2	2.52	0.42
4:F:665:LYS:O	4:F:670:ILE:HG12	2.18	0.42
4:F:828:LEU:HD23	4:F:828:LEU:HA	1.84	0.42
4:F:1297:HIS:O	4:F:1300:LYS:HB2	2.20	0.42
2:C:2:DA:N6	3:D:10:DT:H3	2.17	0.42
4:F:1206:LEU:HB3	4:F:1207:GLU:H	1.67	0.42
4:B:289:LEU:HA	4:B:289:LEU:HD12	1.80	0.42
4:B:1249:PRO:O	4:B:1252:ASN:ND2	2.53	0.42
4:F:449:PRO:HD2	4:F:452:VAL:HG11	1.99	0.42
4:F:625:LEU:HD12	4:F:625:LEU:HA	1.71	0.42
1:A:27:G:H22	1:A:44:U:P	2.43	0.42
4:B:244:LEU:HA	4:B:244:LEU:HD23	1.75	0.42
4:B:597:LEU:O	4:B:601:ILE:HG12	2.19	0.42
4:B:849:ASP:O	4:B:851:SER:N	2.52	0.42
1:E:89:G:O6	4:F:1272:GLN:NE2	2.46	0.42
4:F:625:LEU:HD13	4:F:659:TRP:CZ2	2.54	0.42
4:F:1212:ARG:NH2	4:F:1336:TYR:HE2	2.17	0.42
4:B:543:ASP:N	4:B:543:ASP:OD1	2.53	0.42
4:B:954:LYS:HB3	4:B:1009:VAL:HG11	2.02	0.42
2:G:19:DA:H5''	2:G:19:DA:C8	2.51	0.42
3:H:10:DT:H2''	3:H:11:DG:H5''	2.02	0.42
3:D:7:DT:H5''	4:B:1135:ASP:OD1	2.20	0.42
4:B:305:ILE:HG22	4:B:306:LEU:HD13	2.01	0.42
4:B:334:LEU:O	4:B:338:LEU:HB2	2.20	0.42
4:B:390:LEU:HD13	4:B:390:LEU:HA	1.85	0.42
4:F:1000:LYS:HA	4:F:1000:LYS:HD2	1.76	0.42
4:B:45:LYS:NZ	4:B:1354:GLY:O	2.52	0.42
4:B:1236:LEU:HD23	4:B:1236:LEU:HA	1.82	0.42
1:E:46:A:H2'	1:E:47:A:C8	2.55	0.42
4:F:615:ILE:HG23	4:F:639:TYR:CE1	2.54	0.42
4:F:652:LYS:HB2	4:F:652:LYS:HE3	1.81	0.42
1:A:59:U:H1'	4:B:77:ASN:HD22	1.85	0.42
4:F:853:ASP:OD1	4:F:893:THR:OG1	2.26	0.42
4:F:1169:MET:HE2	4:F:1169:MET:HB2	1.90	0.42
4:B:154:ILE:HD11	4:B:426:GLN:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:1222:LYS:H	4:F:1222:LYS:HG2	1.57	0.41
4:F:97:PHE:CE1	4:F:152:ARG:HB3	2.55	0.41
4:B:758:ASN:HA	4:B:954:LYS:O	2.20	0.41
4:B:795:ILE:HA	4:B:798:GLU:HB2	2.01	0.41
1:E:52:A:N7	1:E:53:G:H1'	2.36	0.41
4:F:628:ASP:O	4:F:630:GLU:N	2.54	0.41
4:B:213:SER:HB2	4:B:303:SER:OG	2.20	0.41
4:F:22:THR:O	4:F:25:TYR:N	2.48	0.41
4:F:249:THR:HG22	4:F:265:GLN:CD	2.41	0.41
4:F:824:VAL:HG12	4:F:826:GLN:HG2	2.01	0.41
4:F:977:GLU:OE2	4:F:977:GLU:N	2.36	0.41
4:F:1149:VAL:O	4:F:1157:LEU:HA	2.20	0.41
4:B:816:LEU:HD23	4:B:816:LEU:HA	1.92	0.41
1:A:94:U:H2'	1:A:95:G:H8	1.83	0.41
4:B:43:ILE:HG21	4:B:45:LYS:HE3	2.02	0.41
4:B:301:LEU:HA	4:B:301:LEU:HD23	1.82	0.41
4:F:651:LEU:HD12	4:F:651:LEU:HA	1.86	0.41
1:A:42:A:O2'	1:A:43:G:OP1	2.32	0.41
4:B:218:LYS:HB3	4:B:248:LEU:HD21	2.02	0.41
4:B:249:THR:HA	4:B:264:LEU:O	2.21	0.41
4:B:868:ASP:OD1	4:B:868:ASP:N	2.54	0.41
4:B:1348:ILE:HG22	4:B:1350:GLN:HG3	2.02	0.41
4:F:185:PHE:O	4:F:188:LEU:N	2.50	0.41
4:B:736:GLY:O	4:B:740:THR:OG1	2.27	0.41
4:B:814:TYR:CE2	4:B:819:GLY:HA2	2.55	0.41
4:B:1267:ASP:O	4:B:1271:GLU:HG2	2.20	0.41
2:C:23:DA:H5'	4:B:895:ARG:HH12	1.86	0.41
4:B:1075:ASP:HB3	4:B:1079:ASP:OD1	2.21	0.41
4:F:287:ALA:O	4:F:291:LEU:N	2.50	0.41
4:F:334:LEU:HD22	4:F:389:LEU:HD11	2.03	0.41
4:F:1207:GLU:OE1	4:F:1210:ARG:CZ	2.68	0.41
2:C:19:DA:H2''	2:C:20:DT:C5'	2.51	0.41
2:C:23:DA:OP1	4:B:895:ARG:NH2	2.41	0.41
4:B:236:GLY:O	4:B:240:ASN:ND2	2.48	0.41
4:B:502:LEU:HD23	4:B:502:LEU:HA	1.94	0.41
4:B:1000:LYS:NZ	4:B:1065:THR:O	2.48	0.41
4:F:696:LEU:C	4:F:698:HIS:H	2.25	0.41
4:F:784:ILE:HG21	4:F:815:TYR:HB3	2.03	0.41
1:E:27:G:N2	1:E:44:U:OP2	2.54	0.40
1:A:3:A:O2'	1:A:4:A:H5'	2.21	0.40
4:B:624:THR:HA	4:B:656:TYR:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:711:ALA:HA	4:B:712:GLN:HA	1.52	0.40
4:F:90:MET:HB2	4:F:90:MET:HE2	1.89	0.40
4:F:1163:LEU:HD13	4:F:1343:LEU:HD21	2.03	0.40
4:B:152:ARG:HG2	4:B:152:ARG:H	1.55	0.40
4:B:1122:ARG:HG3	4:B:1134:PHE:CE2	2.56	0.40
4:B:1220:LEU:HB2	4:B:1336:TYR:HB2	2.03	0.40
1:E:77:A:H2'	1:E:78:A:H8	1.86	0.40
4:F:350:ILE:HD11	4:F:379:ILE:HD13	2.04	0.40
4:F:830:ILE:O	4:F:833:LEU:HG	2.20	0.40
4:F:1044:ASN:O	4:F:1047:LYS:N	2.51	0.40
4:B:708:ILE:O	4:B:711:ALA:N	2.54	0.40
4:B:849:ASP:OD1	4:B:851:SER:OG	2.30	0.40
4:B:1221:GLN:HE21	4:B:1320:ALA:HB2	1.87	0.40
4:F:25:TYR:O	4:F:988:TYR:OH	2.27	0.40
4:F:561:VAL:CG2	4:F:585:ASP:O	2.70	0.40
4:F:1148:LYS:HG2	4:F:1159:SER:HA	2.03	0.40
4:B:121:ASN:HD21	4:B:124:ASP:HB2	1.87	0.40
4:B:449:PRO:HB2	4:B:452:VAL:HG12	2.03	0.40
4:B:869:ASN:OD1	4:B:870:VAL:HG12	2.21	0.40
4:B:1304:GLU:HB3	4:B:1327:PHE:HZ	1.87	0.40
3:H:7:DT:H5''	4:F:1135:ASP:OD1	2.22	0.40
4:F:107:VAL:O	4:F:111:LYS:HG3	2.22	0.40
4:F:135:ILE:HG21	4:F:160:HIS:CE1	2.56	0.40
4:F:189:VAL:HG21	4:F:203:ALA:HB2	2.03	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
4	B	1312/1368 (96%)	1188 (90%)	124 (10%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	F	1312/1368 (96%)	1181 (90%)	131 (10%)	0	100	100
All	All	2624/2736 (96%)	2369 (90%)	255 (10%)	0	100	100

There are no Ramachandran outliers to report.

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	
4	B	1086/1226 (89%)	1052 (97%)	34 (3%)	40	75
4	F	1085/1226 (88%)	1061 (98%)	24 (2%)	52	81
All	All	2171/2452 (88%)	2113 (97%)	58 (3%)	44	77

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	40	ARG
4	B	90	MET
4	B	110	ASP
4	B	152	ARG
4	B	174	LEU
4	B	182	ASP
4	B	244	LEU
4	B	261	ASP
4	B	291	LEU
4	B	296	LEU
4	B	301	LEU
4	B	303	SER
4	B	312	ILE
4	B	314	LYS
4	B	321	MET
4	B	375	PHE
4	B	383	MET
4	B	412	HIS

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Mol	Chain	Res	Type
4	B	536	LYS
4	B	539	PHE
4	B	543	ASP
4	B	700	ASP
4	B	835	ASP
4	B	868	ASP
4	B	964	SER
4	B	1079	ASP
4	B	1114	ARG
4	B	1115	ASN
4	B	1124	LYS
4	B	1207	GLU
4	B	1325	LYS
4	B	1327	PHE
4	B	1328	ASP
4	B	1351	SER
4	F	40	ARG
4	F	65	LYS
4	F	174	LEU
4	F	179	SER
4	F	187	GLN
4	F	244	LEU
4	F	314	LYS
4	F	383	MET
4	F	476	TRP
4	F	543	ASP
4	F	605	ASP
4	F	612	ASN
4	F	644	ASP
4	F	645	ASP
4	F	785	GLU
4	F	847	LEU
4	F	976	ARG
4	F	1060	ARG
4	F	1115	ASN
4	F	1159	SER
4	F	1222	LYS
4	F	1234	ASN
4	F	1264	HIS
4	F	1325	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
4	B	265	GLN
4	B	459	ASN
4	B	698	HIS
4	B	930	HIS
4	B	1308	ASN
4	F	265	GLN
4	F	277	ASN
4	F	394	ASN
4	F	497	ASN
4	F	650	GLN
4	F	695	GLN
4	F	881	ASN
4	F	930	HIS
4	F	1101	GLN
4	F	1264	HIS
4	F	1305	GLN
4	F	1308	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	94/100 (94%)	28 (29%)	4 (4%)
1	E	94/100 (94%)	28 (29%)	5 (5%)
All	All	188/200 (94%)	56 (29%)	9 (4%)

All (56) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	A
1	A	6	U
1	A	9	A
1	A	17	A
1	A	20	A
1	A	24	U
1	A	28	A
1	A	29	G
1	A	31	U
1	A	32	A
1	A	35	A
1	A	37	U
1	A	39	G
1	A	40	C

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Mol	Chain	Res	Type
1	A	42	A
1	A	43	G
1	A	51	A
1	A	56	U
1	A	57	A
1	A	59	U
1	A	68	A
1	A	74	A
1	A	77	A
1	A	85	C
1	A	86	C
1	A	87	G
1	A	89	G
1	A	91	C
1	E	4	A
1	E	9	A
1	E	17	A
1	E	20	A
1	E	24	U
1	E	28	A
1	E	29	G
1	E	32	A
1	E	35	A
1	E	37	U
1	E	39	G
1	E	40	C
1	E	42	A
1	E	43	G
1	E	51	A
1	E	56	U
1	E	57	A
1	E	59	U
1	E	68	A
1	E	69	A
1	E	73	G
1	E	74	A
1	E	77	A
1	E	85	C
1	E	86	C
1	E	87	G
1	E	89	G
1	E	91	C

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	27	G
1	A	28	A
1	A	42	A
1	E	8	A
1	E	27	G
1	E	28	A
1	E	42	A
1	E	68	A

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	95/100 (95%)	-0.11	0	100 100	51, 79, 116, 149	0
1	E	95/100 (95%)	-0.12	0	100 100	49, 79, 118, 148	0
2	C	25/28 (89%)	-0.23	0	100 100	58, 67, 105, 120	0
2	G	25/28 (89%)	-0.14	0	100 100	56, 68, 112, 126	0
3	D	11/11 (100%)	0.10	0	100 100	53, 72, 117, 118	0
3	H	11/11 (100%)	0.05	0	100 100	55, 69, 115, 121	0
4	B	1322/1368 (96%)	-0.07	4 (0%)	94 84	51, 79, 103, 138	0
4	F	1322/1368 (96%)	-0.05	6 (0%)	91 75	46, 79, 104, 134	0
All	All	2906/3014 (96%)	-0.07	10 (0%)	94 84	46, 79, 105, 149	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	1053	ALA	3.3
4	B	1003	LYS	3.0
4	F	1312	LEU	2.8
4	F	1054	ASN	2.6
4	B	946	ASN	2.4
4	F	338	LEU	2.4
4	F	1039	TYR	2.2
4	B	1007	GLU	2.1
4	F	1194	LEU	2.1
4	B	784	ILE	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.