



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:25 PM UTC

PDB ID : 6LTP / pdb_00006ltp
Title : Crystal structure of Cas12i2 binary complex
Authors : Huang, X.; Sun, W.; Cheng, Z.; Chen, M.; Li, X.; Wang, J.; Sheng, G.; Gong, W.; Wang, Y.
Deposited on : 2020-01-23
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

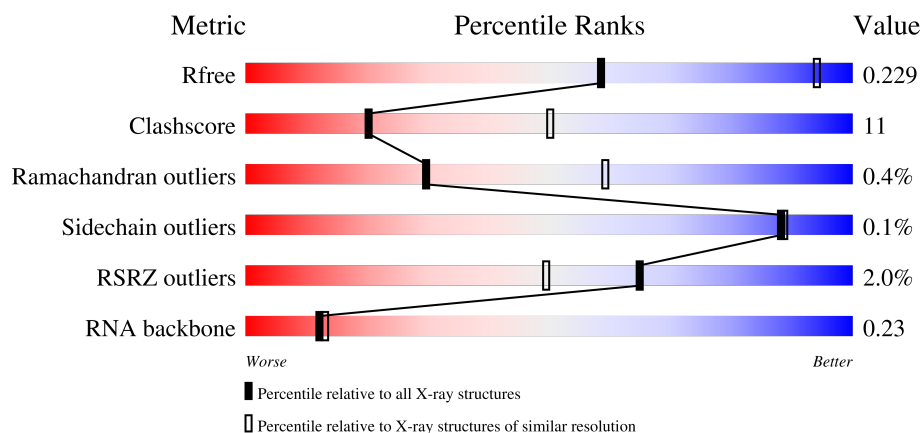
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)
RNA backbone	3983	1157 (3.80-3.00)

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	1055	2% 66% 21% 13%
1	G	1055	% 65% 22% 13%
2	B	56	4% 23% 32% 20% 25%
2	H	56	4% 27% 30% 18% 25%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16382 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 Cas12i2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	920	Total	C	N	O	S	0	0	0
			7244	4606	1267	1345	26			
1	G	923	Total	C	N	O	S	0	0	0
			7348	4681	1292	1349	26			

- Molecule 2 is a RNA chain called crRNA (56-mer RNA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	42	Total	C	N	O	P	0	0	0
			889	400	157	291	41			
2	H	42	Total	C	N	O	P	0	0	0
			889	400	157	291	41			

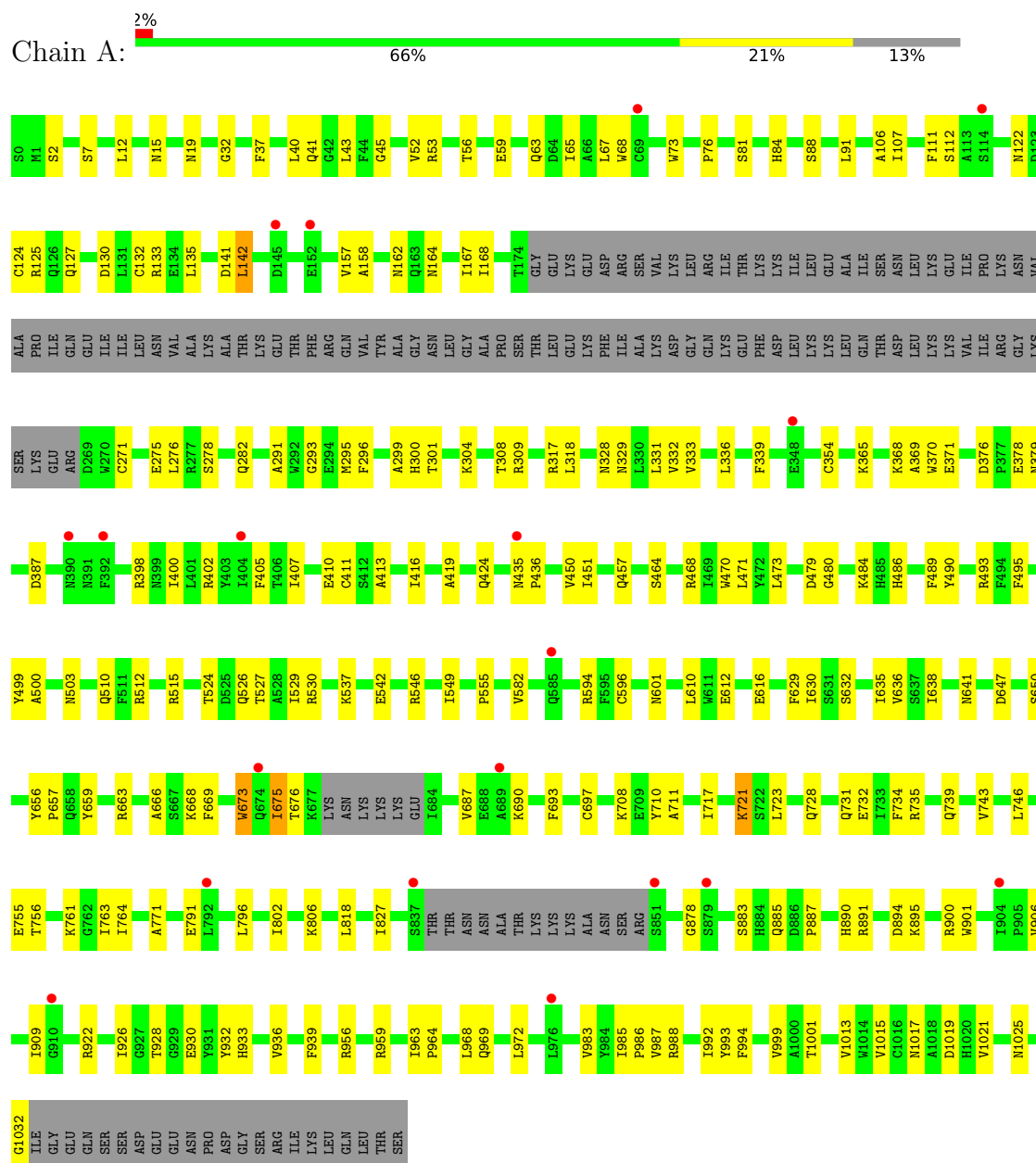
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		
3	B	1	Total	O	0	0
			1	1		
3	G	7	Total	O	0	0
			7	7		

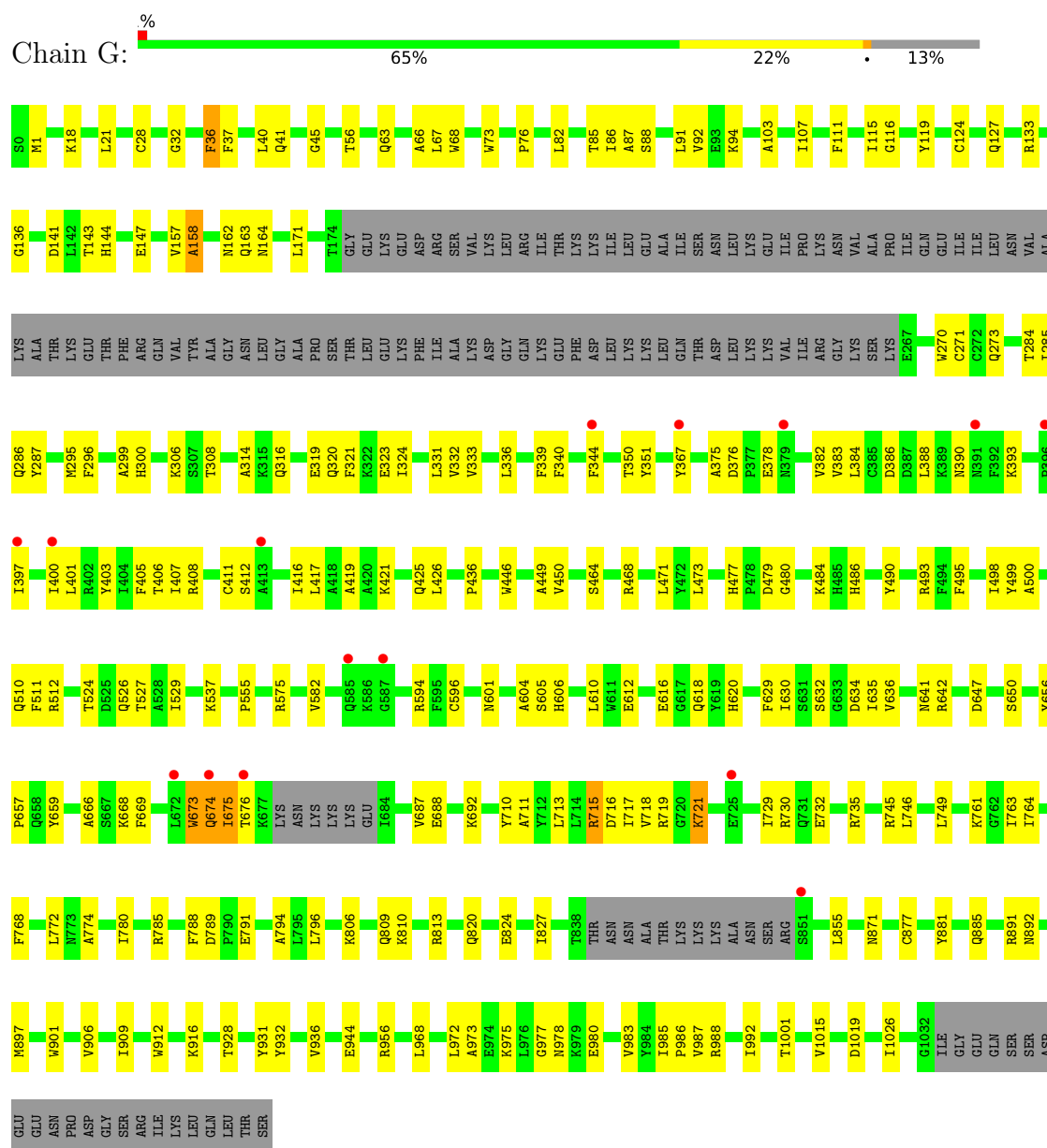
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Cas12i2



• Molecule 1: Cas12i2



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	146.31Å 146.31Å 144.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.71 – 3.40 48.71 – 3.40	Depositor EDS
% Data completeness (in resolution range)	94.8 (48.71-3.40) 94.8 (48.71-3.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.207 , 0.230 0.207 , 0.229	Depositor DCC
R_{free} test set	2152 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	48.4	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.032 for -h,-l,-k 0.026 for -h,l,k 0.026 for l,-k,h 0.034 for -l,-k,-h 0.047 for h,-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	16382	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [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	0.32	0/7399	0.70	7/10025 (0.1%)
1	G	0.37	3/7505 (0.0%)	0.72	12/10154 (0.1%)
2	B	0.26	0/992	0.68	0/1538
2	H	0.26	0/992	0.69	0/1538
All	All	0.34	3/16888 (0.0%)	0.70	19/23255 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	634	ASP	CG-OD2	6.05	1.36	1.25
1	G	891	ARG	CZ-NH2	5.65	1.40	1.33
1	G	891	ARG	N-CA	-5.19	1.39	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	ASN	N-CA-C	7.64	119.24	111.07
1	A	142	LEU	CB-CG-CD2	-6.41	91.47	110.70
1	G	634	ASP	N-CA-CB	6.33	120.94	110.63
1	A	739	GLN	CA-C-N	5.98	132.96	121.54
1	A	739	GLN	C-N-CA	5.98	132.96	121.54
1	A	673	TRP	N-CA-C	-5.88	101.76	110.46
1	G	367	TYR	N-CA-CB	5.67	118.46	110.12
1	G	721	LYS	N-CA-C	5.62	117.55	110.24
1	G	891	ARG	CD-NE-CZ	5.48	132.07	124.40
1	G	36	PHE	N-CA-CB	5.36	118.48	110.22
1	G	673	TRP	N-CA-C	-5.35	102.54	110.46
1	A	410	GLU	N-CA-C	5.33	117.91	111.40
1	G	891	ARG	CB-CA-C	-5.31	102.71	111.36
1	A	721	LYS	N-CA-C	5.27	117.09	110.24
1	G	393	LYS	N-CA-C	5.14	116.74	110.41
1	G	715	ARG	CG-CD-NE	-5.14	100.70	112.00
1	G	674	GLN	CA-C-N	5.05	131.06	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	674	GLN	C-N-CA	5.05	131.06	121.97
1	G	1	MET	CB-CG-SD	-5.01	97.66	112.70

There are no chirality outliers.

There are no planarity outliers.

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	7244	0	6970	173	0
1	G	7348	0	7182	175	0
2	B	889	0	453	20	0
2	H	889	0	453	20	0
3	A	4	0	0	0	0
3	B	1	0	0	0	0
3	G	7	0	0	0	0
All	All	16382	0	15058	354	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 (354) 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:G:928:THR:HG23	1:G:988:ARG:HH22	1.06	1.13
1:G:715:ARG:HH21	1:G:719:ARG:HH21	1.07	0.95
1:A:376:ASP:HB2	1:A:379:ASN:HD21	1.34	0.91
1:G:692:LYS:HD3	1:G:713:LEU:HD13	1.51	0.90
1:G:928:THR:HG23	1:G:988:ARG:NH2	1.90	0.86
1:G:909:ILE:HG21	1:G:968:LEU:HD23	1.58	0.84
1:A:636:VAL:HG12	1:A:638:ILE:HG13	1.60	0.83
1:A:387:ASP:OD1	1:A:928:THR:HG23	1.79	0.82
1:G:378:GLU:O	1:G:382:VAL:HG23	1.80	0.81
1:A:336:LEU:O	1:A:339:PHE:HB3	1.82	0.80
1:G:715:ARG:HH21	1:G:719:ARG:NH2	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ASN:ND2	1:A:300:HIS:CE1	2.50	0.79
1:G:674:GLN:HG3	1:G:688:GLU:CB	2.14	0.78
1:G:171:LEU:O	1:G:273:GLN:NE2	2.16	0.76
1:G:715:ARG:NH2	1:G:719:ARG:HH21	1.84	0.76
2:B:44:U:O4	2:H:51:A:N6	2.18	0.75
1:G:331:LEU:HD12	1:G:332:VAL:HG13	1.65	0.75
2:B:51:A:N6	2:H:44:U:O4	2.19	0.75
1:A:601:ASN:ND2	1:A:1019:ASP:OD2	2.19	0.75
1:G:339:PHE:CZ	1:G:400:ILE:HG22	2.20	0.75
1:A:612:GLU:HB2	1:A:630:ILE:HD11	1.69	0.75
2:H:11:C:OP1	1:G:806:LYS:NZ	2.20	0.74
1:G:632:SER:HB3	1:G:1001:THR:H	1.53	0.73
1:G:972:LEU:HD13	1:G:983:VAL:HG11	1.68	0.73
1:G:375:ALA:HB1	1:G:956:ARG:HH12	1.53	0.72
1:A:673:TRP:HE1	1:A:721:LYS:HE2	1.54	0.72
2:H:2:G:N7	1:G:18:LYS:NZ	2.38	0.71
1:A:88:SER:HA	1:A:91:LEU:HD11	1.74	0.69
1:G:676:THR:CG2	1:G:717:ILE:HA	2.22	0.69
1:A:275:GLU:OE2	1:A:275:GLU:N	2.25	0.69
1:G:384:LEU:HD23	1:G:384:LEU:C	2.17	0.69
1:G:676:THR:HG21	1:G:717:ILE:HA	1.74	0.69
1:G:163:GLN:HA	1:G:163:GLN:OE1	1.94	0.68
1:G:612:GLU:HB2	1:G:630:ILE:HD11	1.74	0.68
1:G:512:ARG:NH1	1:G:555:PRO:O	2.27	0.67
1:A:708:LYS:NZ	1:A:755:GLU:OE1	2.24	0.67
1:A:328:ASN:OD1	1:A:329:ASN:N	2.27	0.67
2:H:12:U:O2	1:G:641:ASN:ND2	2.27	0.67
2:B:38:G:H2'	2:B:39:U:H4'	1.77	0.67
1:A:278:SER:O	1:A:282:GLN:HG3	1.96	0.66
1:A:407:ILE:HD12	1:A:411:CYS:SG	2.37	0.65
1:A:806:LYS:NZ	2:B:11:C:OP1	2.29	0.65
1:G:479:ASP:OD1	1:G:480:GLY:N	2.29	0.65
1:A:632:SER:HB3	1:A:1001:THR:H	1.62	0.65
1:A:512:ARG:NH1	1:A:555:PRO:O	2.29	0.65
1:G:162:ASN:ND2	1:G:300:HIS:CE1	2.66	0.63
1:G:41:GLN:NE2	1:G:127:GLN:OE1	2.24	0.63
1:A:510:GLN:HG3	1:G:616:GLU:OE1	1.98	0.63
1:A:676:THR:CG2	1:A:717:ILE:HA	2.28	0.63
1:A:616:GLU:OE1	1:G:510:GLN:HG3	1.98	0.63
1:G:473:LEU:O	1:G:484:LYS:HA	1.99	0.63
1:G:56:THR:HG21	1:G:63:GLN:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:TRP:CE2	1:A:158:ALA:HB1	2.33	0.62
1:G:384:LEU:HD23	1:G:384:LEU:O	1.99	0.62
1:A:387:ASP:OD1	1:A:928:THR:CG2	2.47	0.62
1:G:715:ARG:NH1	1:G:716:ASP:OD1	2.31	0.62
1:G:321:PHE:O	1:G:324:ILE:HG22	1.99	0.62
1:G:711:ALA:HA	1:G:763:ILE:HD11	1.82	0.62
1:A:76:PRO:HG2	1:A:436:PRO:HA	1.82	0.62
1:A:909:ILE:O	1:A:969:GLN:NE2	2.33	0.62
1:G:68:TRP:CE2	1:G:158:ALA:HB1	2.35	0.61
1:G:901:TRP:CZ3	1:G:986:PRO:HD3	2.36	0.61
1:A:503:ASN:ND2	1:A:549:ILE:O	2.32	0.61
1:A:141:ASP:HB3	1:A:271:CYS:SG	2.41	0.60
1:A:669:PHE:CD2	1:A:732:GLU:HG3	2.36	0.60
1:A:376:ASP:HB2	1:A:379:ASN:ND2	2.13	0.60
1:A:656:TYR:HB3	1:A:657:PRO:HD3	1.83	0.60
1:G:76:PRO:HG2	1:G:436:PRO:HA	1.84	0.60
1:G:340:PHE:CE2	1:G:350:THR:HA	2.36	0.60
1:A:972:LEU:HD13	1:A:983:VAL:HG11	1.84	0.59
1:G:375:ALA:HB1	1:G:956:ARG:NH1	2.16	0.59
1:G:87:ALA:O	1:G:91:LEU:HG	2.02	0.59
1:A:45:GLY:O	1:A:125:ARG:HD2	2.03	0.59
1:G:732:GLU:OE2	1:G:735:ARG:NH1	2.36	0.59
1:A:636:VAL:CG1	1:A:638:ILE:HG13	2.32	0.59
1:A:901:TRP:CZ3	1:A:986:PRO:HD3	2.39	0.58
1:A:500:ALA:O	1:A:512:ARG:NH2	2.34	0.58
1:A:59:GLU:HG2	1:A:63:GLN:HG2	1.84	0.58
1:A:673:TRP:NE1	1:A:721:LYS:HE2	2.18	0.58
1:G:730:ARG:NH1	1:G:789:ASP:OD2	2.36	0.58
1:G:116:GLY:HA3	1:G:119:TYR:HD2	1.68	0.58
1:G:143:THR:O	1:G:147:GLU:HG3	2.03	0.58
1:G:764:ILE:HG21	1:G:796:LEU:HG	1.84	0.57
1:A:331:LEU:HD12	1:A:332:VAL:HG13	1.85	0.57
1:A:666:ALA:HB1	1:A:710:TYR:CE1	2.40	0.57
1:A:301:THR:HA	1:A:304:LYS:HE2	1.86	0.57
1:A:732:GLU:OE2	1:A:735:ARG:NH1	2.37	0.57
1:A:368:LYS:O	1:A:371:GLU:HG2	2.04	0.57
1:A:370:TRP:CZ2	1:A:405:PHE:HB2	2.40	0.57
1:A:635:ILE:HD11	1:A:818:LEU:HD13	1.86	0.57
1:G:675:ILE:O	1:G:721:LYS:NZ	2.27	0.57
1:G:673:TRP:HE1	1:G:721:LYS:HE2	1.68	0.56
1:A:473:LEU:O	1:A:484:LYS:HA	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:332:VAL:HG23	1:G:419:ALA:HB2	1.86	0.56
1:G:397:ILE:HG23	1:G:400:ILE:HG12	1.88	0.56
1:A:91:LEU:H	1:A:91:LEU:HD12	1.71	0.56
1:G:32:GLY:HA3	1:G:295:MET:SD	2.46	0.56
1:A:52:VAL:HB	1:A:65:ILE:HG23	1.88	0.55
1:G:144:HIS:HD1	1:G:271:CYS:HG	1.53	0.55
2:H:37:G:OP2	1:G:692:LYS:CE	2.54	0.55
1:A:376:ASP:O	1:A:379:ASN:ND2	2.40	0.55
1:A:130:ASP:HA	1:A:133:ARG:HG3	1.89	0.54
1:G:63:GLN:HE21	1:G:68:TRP:HE1	1.54	0.54
1:G:669:PHE:CD2	1:G:732:GLU:HG3	2.42	0.54
1:G:63:GLN:NE2	1:G:68:TRP:HE1	2.05	0.54
1:G:76:PRO:CB	1:G:115:ILE:HD11	2.37	0.54
1:G:629:PHE:HZ	1:G:632:SER:HB2	1.72	0.54
1:G:944:GLU:OE1	1:G:975:LYS:NZ	2.39	0.54
1:A:479:ASP:OD1	1:A:480:GLY:N	2.40	0.54
1:A:641:ASN:ND2	2:B:12:U:O2	2.41	0.54
1:G:407:ILE:HD12	1:G:411:CYS:SG	2.48	0.54
1:G:647:ASP:OD2	1:G:650:SER:OG	2.23	0.54
1:A:336:LEU:HD21	1:A:416:ILE:HD12	1.90	0.54
1:A:468:ARG:HG3	2:B:4:A:H2	1.73	0.54
1:G:76:PRO:HB3	1:G:115:ILE:HD11	1.90	0.54
1:G:718:VAL:HG22	1:G:729:ILE:HG21	1.90	0.54
1:G:772:LEU:HD21	1:G:788:PHE:CD2	2.43	0.54
1:A:527:THR:HG22	1:A:529:ILE:HG13	1.89	0.53
1:A:956:ARG:HB2	1:A:959:ARG:HD2	1.89	0.53
1:G:916:LYS:HZ3	1:G:988:ARG:HG3	1.73	0.53
1:G:768:PHE:CG	1:G:785:ARG:HG2	2.43	0.53
1:G:774:ALA:HB2	1:G:780:ILE:HG23	1.89	0.53
1:A:32:GLY:HA3	1:A:295:MET:SD	2.47	0.53
1:A:132:CYS:SG	1:A:142:LEU:HD23	2.49	0.53
2:H:14:U:O2	1:G:642:ARG:HD2	2.09	0.53
1:A:668:LYS:HD2	1:A:668:LYS:C	2.34	0.53
1:A:676:THR:HG21	1:A:717:ILE:HA	1.90	0.53
1:G:133:ARG:O	1:G:136:GLY:N	2.38	0.53
1:A:354:CYS:HB3	1:A:424:GLN:NE2	2.24	0.52
1:G:86:ILE:HG23	1:G:91:LEU:HD21	1.91	0.52
1:A:107:ILE:HG22	1:A:111:PHE:CE2	2.44	0.52
1:A:647:ASP:OD2	1:A:650:SER:OG	2.25	0.52
1:G:82:LEU:HD21	1:G:85:THR:CG2	2.39	0.52
1:A:610:LEU:HD22	1:A:827:ILE:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:ALA:HA	1:A:763:ILE:HD11	1.92	0.52
1:G:582:VAL:HG12	1:G:871:ASN:HB2	1.92	0.52
1:A:162:ASN:ND2	1:A:300:HIS:HE1	2.04	0.52
1:G:336:LEU:O	1:G:339:PHE:HB3	2.09	0.52
1:G:666:ALA:HB1	1:G:710:TYR:CE1	2.45	0.52
1:A:336:LEU:HD11	1:A:416:ILE:HD11	1.91	0.52
2:H:25:A:O2'	1:G:575:ARG:HD2	2.09	0.52
1:A:932:TYR:CZ	1:A:988:ARG:HD3	2.45	0.52
1:A:12:LEU:HD23	1:A:489:PHE:HB3	1.92	0.52
1:A:464:SER:OG	2:B:3:A:N1	2.42	0.52
1:G:344:PHE:CE2	1:G:403:TYR:HD1	2.27	0.51
1:A:764:ILE:HG21	1:A:796:LEU:HG	1.92	0.51
1:G:405:PHE:CD1	1:G:408:ARG:HD3	2.45	0.51
1:G:973:ALA:O	1:G:977:GLY:N	2.43	0.51
1:A:167:ILE:HG21	1:A:296:PHE:CE2	2.45	0.51
2:H:7:C:C4	1:G:493:ARG:HB2	2.45	0.51
2:H:37:G:OP2	1:G:692:LYS:HE3	2.10	0.51
1:G:673:TRP:NE1	1:G:721:LYS:HE2	2.26	0.51
1:A:40:LEU:HD23	1:A:43:LEU:HD12	1.91	0.51
1:A:56:THR:HG21	1:A:63:GLN:HB2	1.93	0.51
1:A:378:GLU:OE1	1:A:378:GLU:N	2.40	0.51
1:A:515:ARG:HD3	2:B:23:G:OP1	2.11	0.51
1:G:897:MET:HG3	1:G:931:TYR:CZ	2.46	0.51
1:A:932:TYR:CE1	1:A:988:ARG:HD3	2.46	0.51
1:A:493:ARG:HB2	2:B:7:C:C4	2.46	0.51
1:A:985:ILE:HG22	1:A:987:VAL:HG13	1.92	0.51
1:A:336:LEU:HD21	1:A:416:ILE:CD1	2.41	0.50
2:H:37:G:OP2	1:G:692:LYS:NZ	2.42	0.50
1:A:333:VAL:HG22	1:A:419:ALA:HB1	1.93	0.50
1:G:932:TYR:O	1:G:936:VAL:HG23	2.10	0.50
1:A:641:ASN:ND2	2:B:12:U:H1'	2.27	0.50
1:A:909:ILE:HD11	1:A:983:VAL:HG21	1.93	0.50
1:G:405:PHE:O	1:G:408:ARG:HG2	2.12	0.50
1:G:610:LEU:HD22	1:G:827:ILE:HG13	1.92	0.50
1:G:316:GLN:O	1:G:320:GLN:HG3	2.12	0.50
1:G:985:ILE:HG22	1:G:987:VAL:HG13	1.94	0.49
1:G:88:SER:HA	1:G:91:LEU:CD1	2.42	0.49
1:G:157:VAL:HG12	1:G:158:ALA:H	1.77	0.49
1:G:601:ASN:HB2	1:G:605:SER:O	2.12	0.49
1:A:73:TRP:O	1:A:124:CYS:HB2	2.12	0.49
1:A:471:LEU:O	1:A:486:HIS:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ASP:CB	1:A:379:ASN:HD21	2.17	0.49
1:A:413:ALA:O	1:A:416:ILE:HG22	2.12	0.49
1:G:386:ASP:O	1:G:390:ASN:ND2	2.44	0.49
1:G:978:ASN:ND2	1:G:980:GLU:HB2	2.28	0.49
1:A:112:SER:C	1:A:317:ARG:HH12	2.21	0.49
1:A:40:LEU:HD11	1:A:296:PHE:CD1	2.48	0.48
1:G:68:TRP:HH2	1:G:308:THR:HG23	1.78	0.48
1:A:909:ILE:HG21	1:A:968:LEU:HD23	1.94	0.48
1:A:878:GLY:N	1:A:1032:GLY:HA2	2.28	0.48
1:A:993:TYR:CD2	1:A:1021:VAL:HG11	2.48	0.48
1:A:728:GLN:O	1:A:731:GLN:HG3	2.14	0.48
2:H:4:A:H1'	1:G:490:TYR:OH	2.14	0.48
1:G:339:PHE:CE2	1:G:400:ILE:HG22	2.49	0.48
2:H:39:U:O3'	1:G:912:TRP:CE3	2.66	0.48
1:A:157:VAL:HG12	1:A:158:ALA:H	1.77	0.48
1:G:500:ALA:O	1:G:512:ARG:NH2	2.47	0.48
1:A:524:THR:HG23	1:A:526:GLN:H	1.79	0.47
1:G:601:ASN:ND2	1:G:1019:ASP:OD2	2.47	0.47
1:G:636:VAL:HG23	1:G:647:ASP:CG	2.39	0.47
1:A:7:SER:HG	2:B:24:A:HO2'	1.58	0.47
1:A:906:VAL:HG23	1:A:909:ILE:HD12	1.96	0.47
1:A:656:TYR:CZ	1:A:663:ARG:NH2	2.83	0.47
1:A:675:ILE:O	1:A:721:LYS:NZ	2.42	0.47
1:A:41:GLN:OE1	1:A:122:ASN:ND2	2.47	0.47
1:A:495:PHE:HA	1:A:499:TYR:HB3	1.97	0.47
1:G:906:VAL:HG23	1:G:909:ILE:HD12	1.96	0.47
1:A:398:ARG:O	1:A:402:ARG:HG3	2.13	0.47
1:A:992:ILE:HG23	1:A:1015:VAL:HG13	1.95	0.47
1:A:2:SER:OG	1:A:582:VAL:HG13	2.14	0.47
1:A:723:LEU:HD11	1:A:771:ALA:O	2.15	0.47
1:G:82:LEU:HD21	1:G:85:THR:HG22	1.96	0.47
1:A:451:ILE:HG12	1:A:470:TRP:O	2.15	0.47
2:H:2:G:O2'	1:G:468:ARG:NH1	2.48	0.47
1:A:1017:ASN:O	1:A:1021:VAL:HG23	2.14	0.47
1:G:384:LEU:C	1:G:384:LEU:CD2	2.85	0.47
1:A:656:TYR:HA	1:A:659:TYR:CE1	2.50	0.46
1:G:306:LYS:HD2	1:G:436:PRO:O	2.14	0.46
1:A:629:PHE:HZ	1:A:632:SER:HB2	1.81	0.46
1:G:40:LEU:HD11	1:G:296:PHE:CE1	2.51	0.46
1:A:112:SER:O	1:A:317:ARG:NH1	2.48	0.46
1:G:45:GLY:HA3	1:G:124:CYS:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:TRP:HH2	1:A:308:THR:HG23	1.80	0.46
1:A:530:ARG:NH1	2:B:17:U:O2'	2.49	0.46
1:G:56:THR:HG22	1:G:56:THR:O	2.14	0.46
1:G:340:PHE:HE2	1:G:350:THR:HA	1.79	0.46
1:A:59:GLU:HG2	1:A:63:GLN:CG	2.44	0.46
1:A:468:ARG:HG2	1:A:490:TYR:CZ	2.51	0.46
1:G:36:PHE:HD2	1:G:296:PHE:HA	1.81	0.46
1:G:336:LEU:HD21	1:G:416:ILE:HB	1.98	0.46
1:G:416:ILE:HG13	1:G:417:LEU:N	2.31	0.46
1:A:339:PHE:CZ	1:A:400:ILE:HG12	2.51	0.46
1:A:885:GLN:HB2	1:A:1025:ASN:ND2	2.31	0.45
1:A:676:THR:HG22	1:A:717:ILE:HA	1.98	0.45
1:G:916:LYS:NZ	1:G:988:ARG:HG3	2.32	0.45
1:A:690:LYS:O	1:A:693:PHE:HB3	2.16	0.45
1:A:734:PHE:CZ	1:A:791:GLU:HG2	2.51	0.45
1:A:930:GLU:O	1:A:933:HIS:HB3	2.16	0.45
1:A:135:LEU:HD11	1:A:276:LEU:HD21	1.97	0.45
1:A:162:ASN:HD22	1:A:300:HIS:CE1	2.33	0.45
1:G:498:ILE:HD11	1:G:511:PHE:HE1	1.81	0.45
1:A:503:ASN:ND2	1:A:549:ILE:HG23	2.31	0.45
2:H:14:U:OP1	1:G:745:ARG:NH2	2.50	0.45
1:G:66:ALA:C	1:G:107:ILE:HD11	2.42	0.45
1:G:92:VAL:HG13	1:G:103:ALA:CB	2.47	0.45
1:G:270:TRP:HB2	1:G:273:GLN:HB2	1.97	0.45
1:A:537:LYS:HB2	2:B:6:U:O2	2.16	0.45
1:A:922:ARG:HH12	1:A:956:ARG:NE	2.14	0.45
1:G:324:ILE:HD11	1:G:426:LEU:HD13	1.98	0.45
1:G:524:THR:HG23	1:G:526:GLN:H	1.82	0.45
1:G:606:HIS:HB3	1:G:635:ILE:HD12	1.98	0.45
1:G:656:TYR:HB3	1:G:657:PRO:HD3	1.98	0.45
2:H:26:C:H3'	2:H:27:A:C8	2.52	0.45
1:G:284:THR:OG1	1:G:285:ILE:N	2.49	0.45
1:G:768:PHE:CD1	1:G:785:ARG:HG2	2.52	0.45
1:A:734:PHE:HZ	1:A:791:GLU:HG2	1.82	0.45
1:A:994:PHE:HE1	1:A:1015:VAL:HG22	1.82	0.45
1:G:916:LYS:HB3	1:G:916:LYS:HE3	1.84	0.45
1:A:596:CYS:HB3	1:A:610:LEU:HD23	1.99	0.45
1:G:450:VAL:HG22	1:G:471:LEU:CD2	2.47	0.45
1:G:596:CYS:HB3	1:G:610:LEU:HD23	1.98	0.45
1:G:820:GLN:O	1:G:824:GLU:HG3	2.17	0.45
1:G:28:CYS:SG	1:G:285:ILE:HG21	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:668:LYS:C	1:G:668:LYS:HD3	2.42	0.44
1:A:657:PRO:HG2	2:B:43:A:N1	2.32	0.44
1:A:926:ILE:HG23	1:A:926:ILE:O	2.17	0.44
1:G:978:ASN:HD21	1:G:980:GLU:HB2	1.81	0.44
1:A:594:ARG:HB3	1:A:827:ILE:HD13	2.00	0.44
1:A:894:ASP:O	1:A:895:LYS:HB2	2.16	0.44
1:G:421:LYS:O	1:G:425:GLN:HG2	2.17	0.44
1:A:106:ALA:HB2	1:A:318:LEU:HD22	1.99	0.44
1:A:802:ILE:HG22	1:A:806:LYS:HD2	1.98	0.44
1:G:388:LEU:HD23	1:G:388:LEU:HA	1.79	0.44
1:G:604:ALA:HB1	1:G:855:LEU:HD23	1.99	0.44
1:A:67:LEU:HD13	1:A:107:ILE:HG12	2.00	0.44
1:A:84:HIS:NE2	1:A:130:ASP:OD2	2.43	0.44
1:G:791:GLU:O	1:G:794:ALA:HB3	2.18	0.43
1:A:370:TRP:CH2	1:A:405:PHE:HB2	2.54	0.43
2:H:13:U:H4'	1:G:746:LEU:HD11	1.99	0.43
1:G:809:GLN:O	1:G:813:ARG:HG3	2.18	0.43
1:A:732:GLU:O	1:A:735:ARG:HG2	2.18	0.43
1:A:743:VAL:HG11	1:A:756:THR:HG22	2.00	0.43
1:G:471:LEU:O	1:G:486:HIS:HA	2.18	0.43
1:A:936:VAL:O	1:A:939:PHE:HB3	2.18	0.43
1:G:21:LEU:HD11	1:G:477:HIS:ND1	2.33	0.43
1:G:37:PHE:HA	1:G:299:ALA:HB1	1.99	0.43
1:G:383:VAL:HG13	1:G:988:ARG:NH2	2.33	0.43
1:G:403:TYR:O	1:G:406:THR:HB	2.17	0.43
1:G:527:THR:HG22	1:G:529:ILE:HG13	2.00	0.43
1:G:91:LEU:HB3	1:G:111:PHE:CD1	2.54	0.43
1:A:15:ASN:O	1:A:19:ASN:HB2	2.18	0.43
1:A:365:LYS:O	1:A:369:ALA:N	2.42	0.43
2:H:3:A:N1	1:G:464:SER:OG	2.52	0.43
1:G:286:GLN:HG2	1:G:287:TYR:N	2.34	0.43
1:G:340:PHE:HZ	1:G:351:TYR:CD1	2.37	0.43
1:G:67:LEU:HD21	1:G:314:ALA:HB3	2.00	0.42
1:G:333:VAL:HG22	1:G:419:ALA:HB1	2.01	0.42
1:A:636:VAL:HG11	1:A:638:ILE:HD11	2.01	0.42
1:A:887:PRO:HG2	1:A:999:VAL:HG21	2.01	0.42
2:H:6:U:O2	1:G:537:LYS:HB2	2.18	0.42
1:G:40:LEU:HD11	1:G:296:PHE:CD1	2.54	0.42
1:A:162:ASN:ND2	1:A:300:HIS:ND1	2.66	0.42
1:A:890:HIS:CD2	1:A:891:ARG:HG3	2.54	0.42
1:G:992:ILE:HG23	1:G:1015:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:LEU:HD23	1:A:276:LEU:HA	1.52	0.42
1:A:332:VAL:HG23	1:A:419:ALA:HB2	2.02	0.42
1:A:542:GLU:OE2	1:A:546:ARG:HD3	2.19	0.42
1:A:162:ASN:CG	1:A:300:HIS:HE1	2.28	0.42
1:G:446:TRP:HB3	1:G:449:ALA:HB2	2.02	0.42
1:G:620:HIS:HA	1:G:892:ASN:ND2	2.35	0.42
1:G:711:ALA:CA	1:G:763:ILE:HD11	2.48	0.42
1:G:881:TYR:O	1:G:885:GLN:HG3	2.20	0.42
1:A:309:ARG:CB	1:A:435:ASN:HD22	2.33	0.42
1:A:656:TYR:OH	1:A:697:CYS:HB3	2.20	0.42
1:A:900:ARG:HB2	1:A:932:TYR:OH	2.20	0.42
1:G:162:ASN:ND2	1:G:300:HIS:ND1	2.67	0.42
1:G:774:ALA:HB2	1:G:780:ILE:CG2	2.50	0.42
1:G:877:CYS:SG	1:G:1026:ILE:HG23	2.59	0.42
1:A:339:PHE:CE2	1:A:400:ILE:HG12	2.55	0.42
1:A:743:VAL:HA	1:A:746:LEU:O	2.20	0.42
2:B:35:A:H1'	2:B:36:G:C5	2.55	0.42
1:A:40:LEU:HD23	1:A:40:LEU:HA	1.91	0.41
1:G:88:SER:HA	1:G:91:LEU:HD11	2.01	0.41
1:A:52:VAL:O	1:A:56:THR:OG1	2.35	0.41
1:A:451:ILE:CD1	1:A:470:TRP:HB2	2.50	0.41
1:G:376:ASP:OD1	1:G:378:GLU:HB3	2.20	0.41
1:G:594:ARG:HB3	1:G:827:ILE:HD13	2.02	0.41
1:G:656:TYR:HA	1:G:659:TYR:CE1	2.55	0.41
1:A:37:PHE:HA	1:A:299:ALA:HB1	2.02	0.41
1:A:40:LEU:HD11	1:A:296:PHE:CE1	2.55	0.41
1:A:81:SER:O	1:A:81:SER:OG	2.35	0.41
1:A:457:GLN:HB3	2:B:1:A:N7	2.35	0.41
1:A:641:ASN:HD22	2:B:12:U:H1'	1.84	0.41
1:A:883:SER:HB3	1:A:900:ARG:NH1	2.36	0.41
1:G:141:ASP:O	1:G:144:HIS:HB3	2.21	0.41
1:A:56:THR:O	1:A:56:THR:HG22	2.20	0.41
1:A:450:VAL:HG22	1:A:471:LEU:CD2	2.51	0.41
1:G:674:GLN:HG2	1:G:675:ILE:H	1.85	0.41
1:A:84:HIS:CE1	1:A:127:GLN:HA	2.55	0.41
1:A:291:ALA:O	1:A:295:MET:HG3	2.21	0.41
1:A:711:ALA:CA	1:A:763:ILE:HD11	2.50	0.41
1:G:331:LEU:HD12	1:G:332:VAL:N	2.36	0.41
1:G:495:PHE:HA	1:G:499:TYR:HB3	2.03	0.41
1:G:761:LYS:HB3	1:G:761:LYS:HE2	1.75	0.41
2:B:46:A:N1	2:H:50:A:N6	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:319:GLU:O	1:G:323:GLU:HG3	2.21	0.41
1:G:400:ILE:HG13	1:G:401:LEU:N	2.35	0.41
1:G:636:VAL:HG23	1:G:647:ASP:OD2	2.21	0.41
1:A:761:LYS:HB3	1:A:761:LYS:HE2	1.84	0.40
1:A:994:PHE:HB3	1:A:1013:VAL:HG11	2.03	0.40
1:A:376:ASP:OD1	1:A:376:ASP:N	2.55	0.40
1:A:963:ILE:HA	1:A:964:PRO:HD3	1.90	0.40
1:G:331:LEU:CD1	1:G:332:VAL:HG13	2.45	0.40
1:A:168:ILE:HG13	1:A:293:GLY:HA2	2.02	0.40
2:B:34:C:O2	2:B:34:C:C2'	2.70	0.40
1:G:73:TRP:O	1:G:124:CYS:HB2	2.21	0.40
1:G:909:ILE:HD11	1:G:983:VAL:HG21	2.02	0.40
1:A:53:ARG:HG3	1:A:65:ILE:HD13	2.03	0.40
2:B:35:A:H1'	2:B:36:G:N7	2.37	0.40
1:G:749:LEU:O	1:G:810:LYS:NZ	2.39	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	912/1055 (86%)	873 (96%)	37 (4%)	2 (0%)	43	71
1	G	915/1055 (87%)	867 (95%)	43 (5%)	5 (0%)	24	54
All	All	1827/2110 (87%)	1740 (95%)	80 (4%)	7 (0%)	30	59

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	675	ILE
1	G	412	SER
1	G	675	ILE

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Mol	Chain	Res	Type
1	G	164	ASN
1	G	158	ALA
1	A	687	VAL
1	G	687	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	748/931 (80%)	748 (100%)	0	100	100
1	G	770/931 (83%)	768 (100%)	2 (0%)	86	84
All	All	1518/1862 (82%)	1516 (100%)	2 (0%)	88	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	94	LYS
1	G	618	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	126	GLN
1	A	164	ASN
1	A	273	GLN
1	A	356	HIS
1	A	379	ASN
1	A	409	GLN
1	A	448	ASN
1	A	496	GLN
1	A	606	HIS
1	A	618	GLN
1	A	641	ASN

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Mol	Chain	Res	Type
1	A	658	GLN
1	A	1012	GLN
1	G	58	GLN
1	G	63	GLN
1	G	162	ASN
1	G	496	GLN
1	G	606	HIS
1	G	658	GLN
1	G	861	ASN
1	G	978	ASN
1	G	1012	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	40/56 (71%)	18 (45%)	5 (12%)
2	H	40/56 (71%)	18 (45%)	5 (12%)
All	All	80/112 (71%)	36 (45%)	10 (12%)

All (36) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	G
2	B	3	A
2	B	6	U
2	B	13	U
2	B	18	U
2	B	24	A
2	B	27	A
2	B	35	A
2	B	36	G
2	B	37	G
2	B	38	G
2	B	39	U
2	B	44	U
2	B	45	U
2	B	46	A
2	B	48	U
2	B	49	U
2	B	51	A
2	H	3	A

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Mol	Chain	Res	Type
2	H	4	A
2	H	6	U
2	H	13	U
2	H	18	U
2	H	24	A
2	H	26	C
2	H	27	A
2	H	35	A
2	H	36	G
2	H	37	G
2	H	38	G
2	H	39	U
2	H	44	U
2	H	45	U
2	H	46	A
2	H	48	U
2	H	51	A

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	26	C
2	B	34	C
2	B	35	A
2	B	36	G
2	B	47	U
2	H	3	A
2	H	34	C
2	H	35	A
2	H	37	G
2	H	47	U

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	920/1055 (87%)	0.22	19 (2%) 63 48	7, 52, 96, 122	0
1	G	923/1055 (87%)	0.04	15 (1%) 70 56	8, 41, 89, 123	0
2	B	42/56 (75%)	0.11	2 (4%) 35 26	13, 41, 166, 175	0
2	H	42/56 (75%)	0.09	2 (4%) 35 26	10, 35, 167, 178	0
All	All	1927/2222 (86%)	0.13	38 (1%) 65 49	7, 46, 97, 178	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	879	SER	4.3
1	G	587	GLY	3.6
1	A	674	GLN	3.5
1	G	851	SER	3.5
1	A	404	ILE	3.5
1	A	910	GLY	3.0
1	G	672	LEU	2.9
1	A	851	SER	2.9
1	G	397	ILE	2.9
2	B	34	C	2.8
1	A	114	SER	2.7
1	G	676	THR	2.6
1	A	689	ALA	2.5
1	G	725	GLU	2.5
1	A	145	ASP	2.4
1	G	400	ILE	2.4
1	A	904	ILE	2.4
1	G	413	ALA	2.4
2	B	48	U	2.4
1	A	976	LEU	2.3
1	A	585	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	152	GLU	2.3
1	A	837	SER	2.3
1	A	435	ASN	2.3
1	A	348	GLU	2.3
1	G	396	PRO	2.2
1	A	390	ASN	2.2
1	G	674	GLN	2.1
2	H	50	A	2.1
1	A	792	LEU	2.1
1	G	379	ASN	2.1
1	A	69	CYS	2.1
2	H	48	U	2.1
1	A	392	PHE	2.1
1	G	391	ASN	2.1
1	G	585	GLN	2.1
1	G	367	TYR	2.0
1	G	344	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.