Full wwPDB X-ray Structure Validation Report ⓘ

Jul 1, 2024 – 02:12 PM JST

PDB ID	:	8K0K
Title	:	Crystal structure of Csy complex
Authors	:	Feng, Y.; Wang, H.
Deposited on	:	2023-07-09
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:

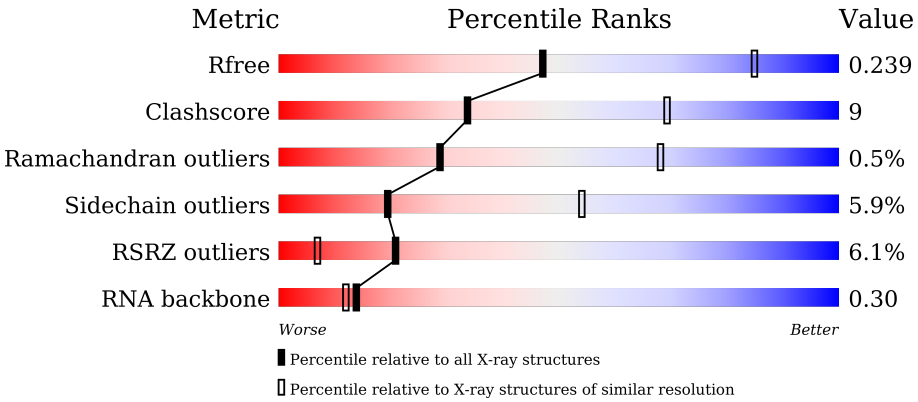
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 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 <=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	179	80% 17%
2	B	248	4% 76% 22%
3	C	306	5% 83% 14%
3	D	306	4% 82% 16%

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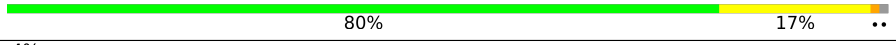
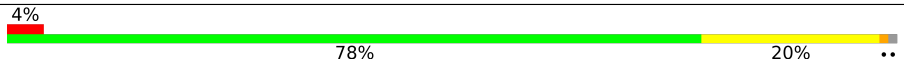
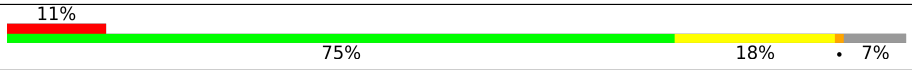
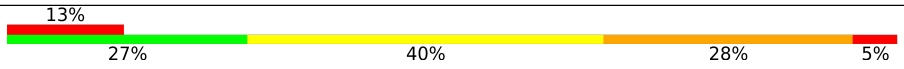
Mol	Chain	Length	Quality of chain
3	E	306	
3	F	306	
3	G	306	
3	H	306	
4	I	168	
5	J	60	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19734 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 Csy1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	177	Total	C	N	O	S	0	0	0
			1418	898	235	274	11			

- Molecule 2 is a protein called Csy2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	248	Total	C	N	O	S	0	0	0
			1919	1223	322	360	14			

- Molecule 3 is a protein called Csy3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	304	Total	C	N	O	S	0	0	0
			2333	1468	396	462	7			
3	D	302	Total	C	N	O	S	0	0	0
			2320	1460	393	460	7			
3	E	304	Total	C	N	O	S	0	0	0
			2332	1467	395	462	8			
3	F	303	Total	C	N	O	S	0	0	0
			2328	1465	394	461	8			
3	G	303	Total	C	N	O	S	0	0	0
			2328	1465	394	461	8			
3	H	285	Total	C	N	O	S	0	0	0
			2198	1391	367	432	8			

- Molecule 4 is a protein called Csy4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	166	Total	C	N	O	S	0	0	0
			1298	823	222	246	7			

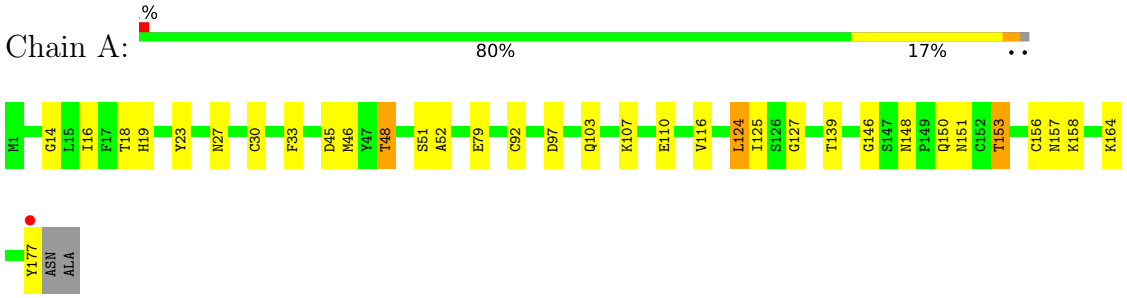
- Molecule 5 is a RNA chain called RNA (60-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
5	J	60	1260	565	210	425	60	0	0	0

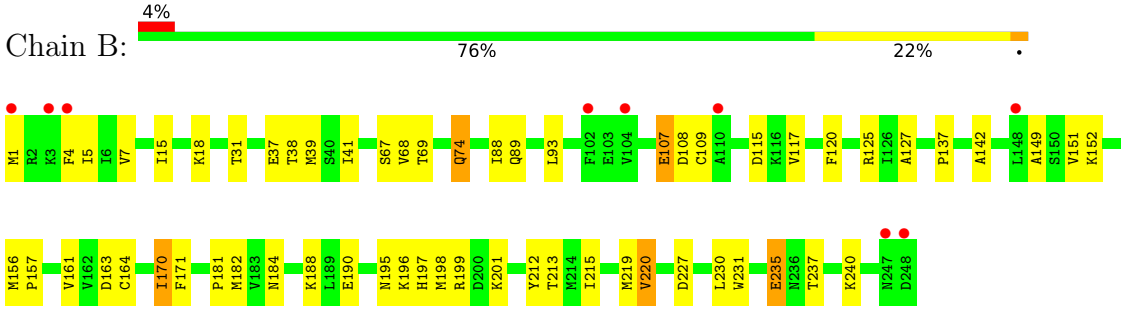
3 Residue-property plots (i)

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.

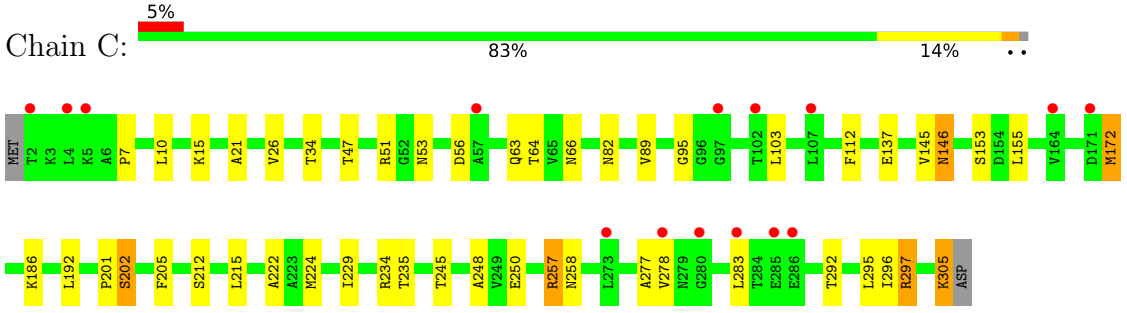
• Molecule 1: Csy1



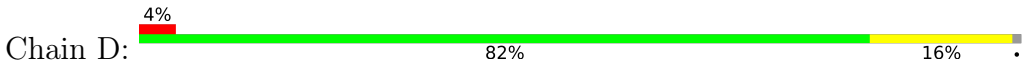
• Molecule 2: Csy2

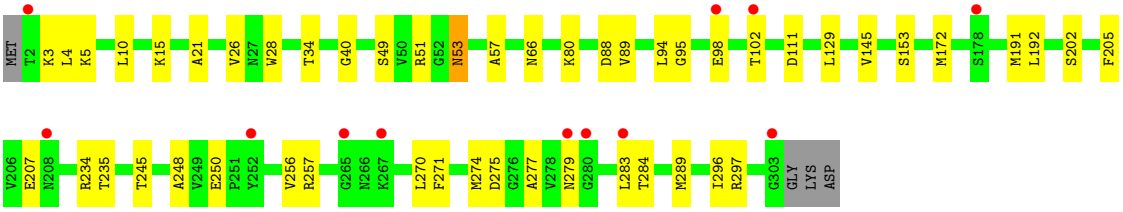


• Molecule 3: Csy3

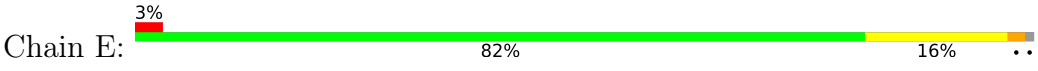


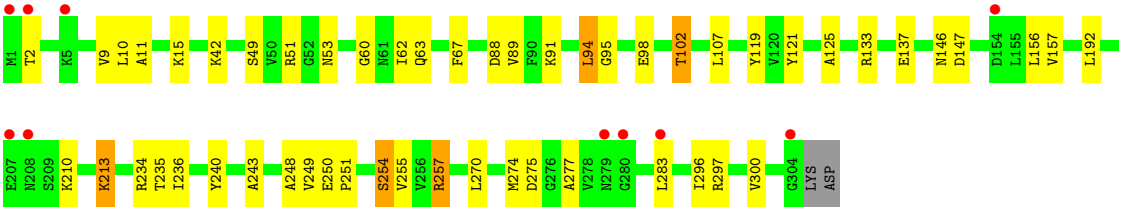
• Molecule 3: Csy3



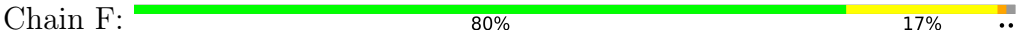


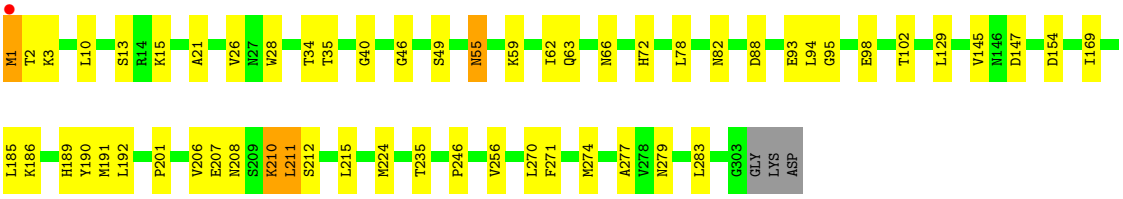
• Molecule 3: Csy3



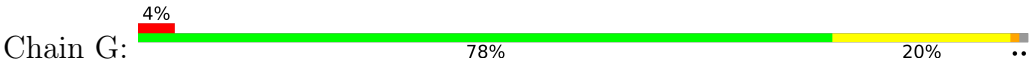


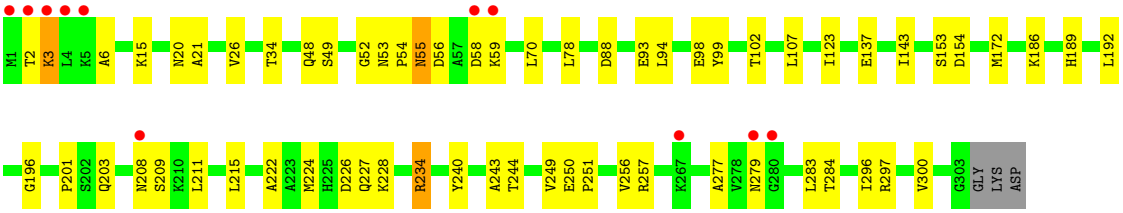
• Molecule 3: Csy3



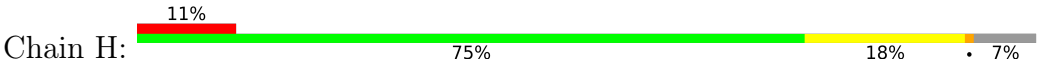


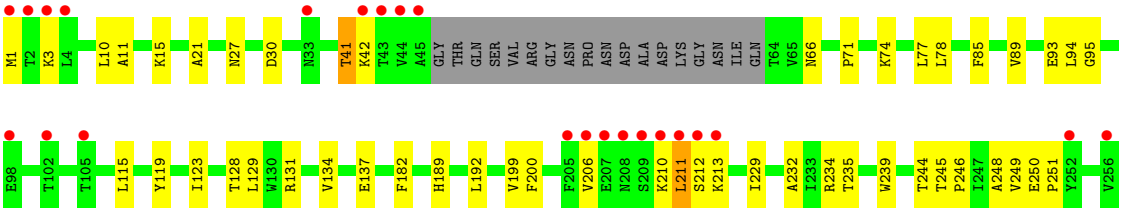
• Molecule 3: Csy3

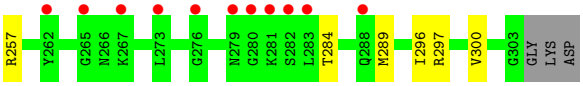




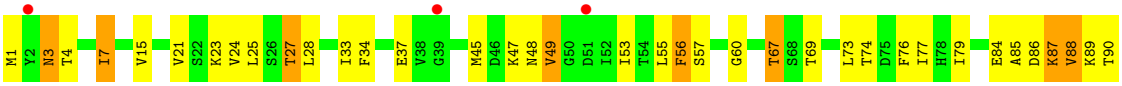
• Molecule 3: Csy3

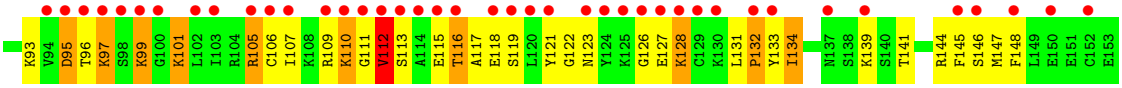


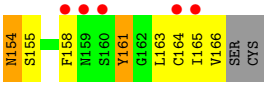




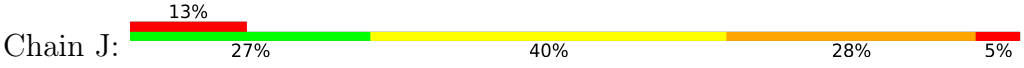
• Molecule 4: Csy4

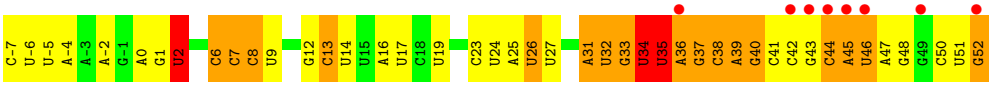






• Molecule 5: RNA (60-MER)





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	238.85Å 95.08Å 204.03Å 90.00° 93.16° 90.00°	Depositor
Resolution (Å)	46.30 – 3.00 47.80 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.4 (46.30-3.00) 92.4 (47.80-3.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.198 , 0.238 0.200 , 0.239	Depositor DCC
R_{free} test set	4261 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	57.2	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 41.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	19734	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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

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	0.30	0/1451	0.45	0/1959
2	B	0.29	0/1956	0.47	0/2645
3	C	0.28	0/2373	0.48	0/3221
3	D	0.29	0/2360	0.47	0/3205
3	E	0.28	0/2372	0.47	0/3220
3	F	0.30	0/2368	0.50	0/3215
3	G	0.30	0/2368	0.48	0/3215
3	H	0.27	0/2236	0.46	0/3035
4	I	0.36	0/1316	0.56	0/1767
5	J	0.33	0/1404	1.09	11/2181 (0.5%)
All	All	0.30	0/20204	0.55	11/27663 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	13	C	C2-N1-C1'	8.73	128.40	118.80
5	J	13	C	N1-C2-O2	7.60	123.46	118.90
5	J	34	U	P-O3'-C3'	7.11	128.23	119.70
5	J	2	U	O4'-C1'-N1	6.45	113.36	108.20
5	J	13	C	C6-N1-C1'	-6.41	113.11	120.80
5	J	13	C	N3-C2-O2	-6.35	117.45	121.90
5	J	34	U	O4'-C1'-N1	6.20	113.16	108.20
5	J	34	U	C2-N1-C1'	5.81	124.68	117.70
5	J	34	U	C6-N1-C1'	-5.11	114.05	121.20
5	J	35	U	C2-N1-C1'	5.09	123.81	117.70
5	J	35	U	N3-C2-O2	-5.04	118.67	122.20

There are no chirality outliers.

There are no planarity outliers.

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	1418	0	1360	17	1
2	B	1919	0	1935	42	0
3	C	2333	0	2281	27	0
3	D	2320	0	2265	31	0
3	E	2332	0	2280	33	1
3	F	2328	0	2277	36	0
3	G	2328	0	2277	36	0
3	H	2198	0	2155	34	0
4	I	1298	0	1345	82	0
5	J	1260	0	641	53	0
All	All	19734	0	18816	329	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (329) 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)
2:B:182:MET:CE	2:B:215:ILE:HG21	1.83	1.07
4:I:1:MET:HG2	4:I:86:ASP:HB2	1.58	0.86
2:B:182:MET:HE1	2:B:215:ILE:HG21	1.57	0.84
1:A:153:THR:HG22	1:A:156:CYS:H	1.44	0.81
3:C:112:PHE:HE1	3:C:292:THR:HG21	1.47	0.79
4:I:105:ARG:HH12	5:J:41:C:H5	1.31	0.79
3:D:49:SER:HB3	3:E:251:PRO:HG2	1.65	0.78
3:H:206:VAL:H	5:J:31:A:H2	1.33	0.77
2:B:182:MET:CE	2:B:215:ILE:CG2	2.62	0.77
4:I:145:PHE:CE2	4:I:147:MET:HA	2.20	0.76
1:A:16:ILE:HG12	1:A:46:MET:HG2	1.69	0.75
4:I:144:ARG:HD2	5:J:36:A:N6	2.03	0.74
3:H:131:ARG:NH1	4:I:15:VAL:O	2.20	0.73
3:E:250:GLU:OE1	3:E:297:ARG:NH1	2.21	0.73
4:I:90:THR:HG21	4:I:154:ASN:HA	1.69	0.73
4:I:97:LYS:NZ	5:J:40:G:O6	2.22	0.73
4:I:101:LYS:HG2	5:J:39:A:H5"	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:101:LYS:HD3	4:I:105:ARG:HE	1.55	0.72
3:C:7:PRO:HA	3:C:305:LYS:HE3	1.72	0.71
2:B:182:MET:HE2	2:B:215:ILE:HG21	1.70	0.69
3:F:210:LYS:HD3	3:F:211:LEU:HD22	1.76	0.68
3:C:250:GLU:OE1	3:C:297:ARG:NH1	2.27	0.68
3:H:15:LYS:HB2	3:H:296:ILE:HG23	1.76	0.68
3:G:257:ARG:NH2	5:J:26:U:OP1	2.26	0.67
2:B:182:MET:HE2	2:B:215:ILE:CG2	2.25	0.67
3:D:15:LYS:HB2	3:D:296:ILE:HG23	1.77	0.66
3:C:51:ARG:NH2	3:D:275:ASP:OD1	2.29	0.66
1:A:107:LYS:HE3	1:A:110:GLU:HA	1.77	0.66
1:A:139:THR:HG21	1:A:164:LYS:HE3	1.78	0.66
4:I:112:VAL:HG22	4:I:117:ALA:HB1	1.77	0.66
4:I:131:LEU:HD22	4:I:148:PHE:CD2	2.31	0.66
4:I:155:SER:HB3	4:I:163:LEU:HD22	1.76	0.66
3:G:49:SER:HB2	3:H:251:PRO:HG2	1.78	0.65
5:J:31:A:H4'	5:J:32:U:OP1	1.95	0.65
3:F:145:VAL:HG22	3:F:185:LEU:HD22	1.77	0.65
3:H:211:LEU:HD13	3:H:212:SER:H	1.60	0.65
4:I:7:ILE:HG23	4:I:79:ILE:HG12	1.78	0.65
4:I:56:PHE:HD1	4:I:88:VAL:HG11	1.62	0.65
3:G:53:ASN:ND2	3:G:56:ASP:OD2	2.30	0.65
3:C:10:LEU:HD12	3:C:95:GLY:HA3	1.80	0.64
4:I:144:ARG:HD2	5:J:36:A:H61	1.61	0.64
2:B:5:ILE:HD13	2:B:117:VAL:HG21	1.80	0.63
4:I:109:ARG:NH1	5:J:42:C:OP1	2.32	0.63
4:I:90:THR:HG23	4:I:163:LEU:HD11	1.80	0.63
3:D:257:ARG:HG3	3:E:94:LEU:HD11	1.78	0.63
4:I:21:VAL:HG13	4:I:53:ILE:HD11	1.79	0.63
3:H:234:ARG:HG2	3:H:249:VAL:H	1.64	0.61
3:F:13:SER:HB3	3:F:93:GLU:HG3	1.82	0.61
4:I:141:THR:CG2	5:J:52:G:H21	2.13	0.61
3:F:145:VAL:CG2	3:F:185:LEU:HD22	2.31	0.61
4:I:134:ILE:HD12	5:J:35:U:OP1	2.00	0.60
3:E:98:GLU:O	3:E:102:THR:HG23	2.00	0.60
2:B:170:ILE:HD11	2:B:212:TYR:CG	2.36	0.60
2:B:199:ARG:NH1	5:J:-6:U:OP2	2.34	0.60
4:I:96:THR:CG2	4:I:131:LEU:HD21	2.31	0.60
1:A:30:CYS:HB2	1:A:97:ASP:HB3	1.82	0.60
1:A:124:LEU:HD12	1:A:125:ILE:HG13	1.84	0.60
4:I:112:VAL:CG2	4:I:117:ALA:HB1	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:3:ASN:HA	4:I:84:GLU:OE1	2.01	0.59
4:I:93:LYS:HA	4:I:148:PHE:O	2.03	0.59
3:F:10:LEU:HD12	3:F:95:GLY:HA3	1.85	0.59
4:I:28:LEU:HD22	4:I:33:ILE:HD12	1.84	0.59
3:C:146:ASN:ND2	3:C:172:MET:SD	2.76	0.58
3:E:11:ALA:HB3	3:E:94:LEU:HB2	1.84	0.58
4:I:106:CYS:HA	4:I:110:LYS:HB2	1.83	0.58
3:E:234:ARG:HG3	3:E:249:VAL:H	1.66	0.58
5:J:35:U:H3'	5:J:36:A:H8	1.68	0.58
4:I:133:TYR:O	4:I:148:PHE:HA	2.03	0.58
3:C:235:THR:HA	3:C:248:ALA:HA	1.86	0.58
2:B:68:VAL:HG13	2:B:88:ILE:HD11	1.85	0.58
3:H:41:THR:HG23	3:H:66:ASN:HD21	1.69	0.57
5:J:33:G:H4'	5:J:34:U:OP2	2.03	0.57
4:I:99:LYS:NZ	4:I:126:GLY:HA3	2.18	0.57
3:C:15:LYS:HB2	3:C:296:ILE:HG23	1.87	0.56
4:I:145:PHE:CD1	5:J:38:C:C4	2.93	0.56
3:E:10:LEU:HD12	3:E:95:GLY:HA3	1.88	0.56
4:I:87:LYS:HZ1	4:I:89:LYS:HG3	1.70	0.56
2:B:182:MET:HE1	2:B:215:ILE:CG2	2.28	0.56
3:F:59:LYS:HD2	3:F:62:ILE:HD11	1.88	0.55
4:I:45:MET:HG3	4:I:49:VAL:HA	1.88	0.55
3:C:202:SER:HB2	3:C:224:MET:HA	1.88	0.55
3:H:250:GLU:OE2	3:H:297:ARG:NH1	2.39	0.55
3:D:257:ARG:NH2	5:J:8:C:O2	2.38	0.55
4:I:7:ILE:HD11	4:I:55:LEU:HD11	1.88	0.55
4:I:139:LYS:NZ	4:I:161:TYR:OH	2.38	0.55
3:G:52:GLY:O	3:G:54:PRO:HD3	2.07	0.55
4:I:48:ASN:HD21	5:J:35:U:P	2.30	0.55
1:A:103:GLN:HG2	1:A:116:VAL:HG22	1.89	0.54
3:F:1:MET:SD	3:F:1:MET:N	2.77	0.54
4:I:23:LYS:O	4:I:27:THR:OG1	2.25	0.54
4:I:134:ILE:HA	4:I:147:MET:O	2.07	0.54
5:J:37:G:H4'	5:J:38:C:OP1	2.06	0.54
3:C:26:VAL:HG12	3:C:34:THR:HA	1.89	0.54
5:J:8:C:H2'	5:J:9:U:H6	1.72	0.54
5:J:47:A:H2'	5:J:48:G:O4'	2.08	0.54
4:I:67:THR:HG23	4:I:79:ILE:HD12	1.90	0.54
4:I:99:LYS:HD2	4:I:126:GLY:H	1.72	0.54
3:C:257:ARG:NH2	5:J:2:U:H5'	2.22	0.54
3:F:98:GLU:O	3:F:102:THR:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:15:LYS:HB2	3:E:296:ILE:HG23	1.89	0.54
3:C:112:PHE:CE1	3:C:292:THR:HG21	2.36	0.54
3:F:201:PRO:HG2	3:F:215:LEU:HD13	1.90	0.53
5:J:8:C:H2'	5:J:9:U:C6	2.44	0.53
3:D:53:ASN:OD1	3:D:53:ASN:N	2.41	0.53
3:F:72:HIS:NE2	3:G:20:ASN:O	2.38	0.53
4:I:134:ILE:CG2	4:I:146:SER:HB3	2.39	0.53
2:B:170:ILE:HD11	2:B:212:TYR:CB	2.39	0.53
3:H:257:ARG:CZ	5:J:32:U:H4'	2.39	0.53
3:H:15:LYS:HE3	3:H:89:VAL:HA	1.91	0.53
3:H:131:ARG:HG2	4:I:15:VAL:HG13	1.91	0.53
3:E:133:ARG:CZ	3:E:157:VAL:HG21	2.39	0.53
3:F:55:ASN:N	3:F:55:ASN:OD1	2.41	0.52
4:I:145:PHE:CD1	4:I:146:SER:N	2.77	0.52
3:C:15:LYS:HG3	3:C:89:VAL:HG12	1.92	0.52
2:B:184:ASN:HD22	2:B:213:THR:HB	1.75	0.52
2:B:152:LYS:HG3	2:B:220:VAL:HG12	1.92	0.52
2:B:161:VAL:HG13	2:B:215:ILE:HD13	1.91	0.51
4:I:3:ASN:N	4:I:57:SER:O	2.43	0.51
4:I:95:ASP:OD1	4:I:95:ASP:N	2.41	0.51
1:A:23:TYR:OH	1:A:45:ASP:OD2	2.20	0.51
3:E:257:ARG:HG3	5:J:12:G:C6	2.45	0.51
3:E:51:ARG:HA	3:F:271:PHE:CE2	2.45	0.51
3:E:15:LYS:HG3	3:E:89:VAL:HG12	1.93	0.50
3:F:206:VAL:HG12	3:F:208:ASN:H	1.77	0.50
3:C:257:ARG:HH22	5:J:2:U:H5'	1.76	0.50
3:D:28:TRP:HB2	3:D:192:LEU:HD13	1.93	0.50
3:F:21:ALA:HB3	3:F:224:MET:HB2	1.94	0.50
4:I:107:ILE:HA	4:I:112:VAL:HG12	1.93	0.50
2:B:125:ARG:NH2	5:J:-2:A:OP1	2.43	0.50
2:B:182:MET:SD	2:B:215:ILE:HG21	2.50	0.50
3:G:93:GLU:HG3	3:G:94:LEU:HD13	1.94	0.50
1:A:150:GLN:HA	1:A:157:ASN:HB2	1.93	0.50
3:F:26:VAL:HG12	3:F:34:THR:HA	1.94	0.50
3:D:15:LYS:HE3	3:D:89:VAL:HA	1.93	0.50
3:D:205:PHE:HB2	5:J:7:C:C5	2.46	0.50
3:F:270:LEU:O	3:F:274:MET:HB2	2.12	0.49
1:A:48:THR:HG21	1:A:52:ALA:O	2.11	0.49
3:E:235:THR:HA	3:E:248:ALA:HA	1.94	0.49
3:H:10:LEU:HD12	3:H:95:GLY:HA3	1.93	0.49
2:B:199:ARG:HD3	5:J:-4:A:C2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:121:TYR:OH	3:E:156:LEU:O	2.26	0.49
4:I:33:ILE:HG22	4:I:34:PHE:H	1.76	0.49
3:H:27:ASN:HB2	3:H:30:ASP:HB3	1.94	0.49
2:B:37:GLU:O	2:B:41:ILE:HG12	2.12	0.49
4:I:121:TYR:OH	5:J:46:U:OP2	2.31	0.48
2:B:188:LYS:NZ	2:B:237:THR:HG21	2.28	0.48
3:E:137:GLU:HB3	3:E:192:LEU:HB3	1.95	0.48
3:D:235:THR:HA	3:D:248:ALA:HA	1.95	0.48
3:F:3:LYS:HE3	3:F:279:ASN:HB3	1.96	0.48
4:I:96:THR:HG23	4:I:131:LEU:HD21	1.95	0.48
2:B:15:ILE:HG23	2:B:127:ALA:HB3	1.94	0.48
2:B:163:ASP:HB2	2:B:231:TRP:CH2	2.47	0.48
2:B:7:VAL:HG22	2:B:137:PRO:HB3	1.95	0.48
3:F:3:LYS:HB3	3:F:279:ASN:ND2	2.29	0.48
3:H:131:ARG:HH11	4:I:15:VAL:HG12	1.79	0.48
4:I:112:VAL:HG22	4:I:117:ALA:CB	2.44	0.48
3:C:137:GLU:HB3	3:C:192:LEU:HB3	1.96	0.48
3:H:11:ALA:HB2	3:H:300:VAL:HG22	1.96	0.48
1:A:18:THR:HG23	1:A:19:HIS:ND1	2.29	0.48
4:I:86:ASP:O	4:I:87:LYS:CB	2.62	0.48
3:F:49:SER:HB3	3:G:251:PRO:HG2	1.96	0.47
2:B:235:GLU:H	2:B:235:GLU:HG3	1.39	0.47
3:D:26:VAL:HG12	3:D:34:THR:HA	1.96	0.47
4:I:87:LYS:O	4:I:87:LYS:HD3	2.14	0.47
3:G:228:LYS:NZ	5:J:24:U:O2	2.47	0.47
3:E:94:LEU:HD13	3:E:94:LEU:HA	1.71	0.47
1:A:124:LEU:HD12	1:A:125:ILE:H	1.79	0.47
1:A:124:LEU:HD12	1:A:125:ILE:N	2.29	0.47
5:J:36:A:H1'	5:J:37:G:H5"	1.96	0.47
2:B:31:THR:HG21	2:B:127:ALA:HB2	1.95	0.47
2:B:38:THR:OG1	5:J:-7:C:H4'	2.14	0.47
2:B:195:ASN:HA	2:B:198:MET:HG2	1.96	0.47
2:B:37:GLU:HB3	5:J:-7:C:H5'	1.97	0.47
3:D:3:LYS:HB3	3:D:279:ASN:HD21	1.80	0.47
3:C:277:ALA:HB2	3:C:283:LEU:HD11	1.97	0.47
3:D:51:ARG:NH2	3:E:275:ASP:OD1	2.48	0.47
3:D:57:ALA:O	3:E:254:SER:HB3	2.14	0.47
3:G:201:PRO:HG3	3:G:222:ALA:HB1	1.97	0.47
3:H:137:GLU:HB3	3:H:192:LEU:HB3	1.97	0.47
3:D:10:LEU:HD12	3:D:95:GLY:HA3	1.97	0.46
3:E:240:TYR:CE2	3:E:243:ALA:HA	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:66:ASN:HD22	3:C:215:LEU:H	1.63	0.46
3:D:257:ARG:CZ	5:J:8:C:H1'	2.46	0.46
3:E:277:ALA:HB2	3:E:283:LEU:HD11	1.97	0.46
3:G:3:LYS:HD2	3:G:3:LYS:HA	1.61	0.46
3:G:250:GLU:OE2	3:G:297:ARG:NH1	2.48	0.46
4:I:115:GLU:O	4:I:118:GLU:N	2.49	0.46
3:G:15:LYS:HB2	3:G:296:ILE:HG23	1.98	0.46
1:A:48:THR:HG22	1:A:51:SER:HA	1.97	0.46
3:C:201:PRO:HG3	3:C:222:ALA:HB1	1.98	0.46
4:I:87:LYS:HD3	4:I:87:LYS:C	2.35	0.46
4:I:141:THR:HG21	5:J:52:G:H21	1.80	0.46
3:D:129:LEU:HD13	3:D:191:MET:SD	2.55	0.46
3:E:62:ILE:H	3:E:62:ILE:HG13	1.59	0.46
3:E:213:LYS:HE3	5:J:16:A:H62	1.80	0.46
4:I:126:GLY:C	4:I:128:LYS:H	2.19	0.46
4:I:21:VAL:HG11	4:I:49:VAL:HG21	1.96	0.46
4:I:110:LYS:HG3	5:J:45:A:C6	2.50	0.46
3:C:21:ALA:HB2	3:C:229:ILE:HD11	1.97	0.46
4:I:126:GLY:O	4:I:128:LYS:N	2.45	0.46
3:G:203:GLN:NE2	5:J:27:U:OP2	2.49	0.46
3:H:245:THR:HB	3:H:246:PRO:HD2	1.98	0.46
2:B:74:GLN:OE1	5:J:-2:A:H1'	2.16	0.45
3:D:270:LEU:O	3:D:274:MET:HB2	2.16	0.45
3:G:153:SER:O	3:G:154:ASP:C	2.54	0.45
3:G:55:ASN:OD1	3:G:55:ASN:N	2.47	0.45
4:I:84:GLU:OE1	4:I:84:GLU:HA	2.16	0.45
3:F:235:THR:HG22	3:F:246:PRO:HB2	1.98	0.45
3:C:258:ASN:ND2	3:D:94:LEU:O	2.48	0.45
4:I:90:THR:OG1	4:I:163:LEU:HD21	2.16	0.45
3:E:255:VAL:HG23	3:E:255:VAL:O	2.17	0.45
3:G:209:SER:C	3:G:211:LEU:H	2.20	0.45
3:F:277:ALA:HB2	3:F:283:LEU:HD11	1.99	0.45
4:I:96:THR:HG21	4:I:131:LEU:HD21	1.99	0.45
3:H:78:LEU:HA	3:H:189:HIS:O	2.15	0.45
3:C:47:THR:HG22	3:D:256:VAL:HG13	1.98	0.45
3:F:28:TRP:HB2	3:F:192:LEU:HD13	1.99	0.45
4:I:110:LYS:HG3	5:J:45:A:C5	2.52	0.45
5:J:35:U:H3'	5:J:36:A:C8	2.50	0.44
5:J:44:C:H4'	5:J:45:A:OP1	2.17	0.44
3:G:58:ASP:CG	3:G:59:LYS:HZ2	2.21	0.44
3:H:235:THR:HA	3:H:248:ALA:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196:LYS:HD2	2:B:197:HIS:CE1	2.52	0.44
3:D:94:LEU:HA	3:D:94:LEU:HD12	1.84	0.44
3:H:134:VAL:HG22	4:I:76:PHE:CE2	2.52	0.44
4:I:127:GLU:O	4:I:128:LYS:HB2	2.18	0.44
3:C:145:VAL:HG22	3:C:146:ASN:ND2	2.32	0.44
3:E:60:GLY:HA2	3:F:256:VAL:HG11	1.99	0.44
3:G:98:GLU:O	3:G:102:THR:HG22	2.18	0.44
1:A:146:GLY:O	1:A:148:ASN:N	2.49	0.44
2:B:219:MET:O	2:B:220:VAL:C	2.55	0.44
3:E:125:ALA:HB1	3:E:157:VAL:HG22	2.00	0.44
3:H:134:VAL:HG21	4:I:15:VAL:HG11	1.99	0.44
4:I:95:ASP:OD2	5:J:50:C:N4	2.50	0.44
4:I:145:PHE:CG	4:I:146:SER:N	2.86	0.44
5:J:36:A:C4'	5:J:37:G:OP1	2.66	0.44
3:F:129:LEU:HD21	3:F:189:HIS:CG	2.53	0.43
3:F:10:LEU:HA	3:F:95:GLY:CA	2.48	0.43
3:D:98:GLU:O	3:D:102:THR:HG23	2.17	0.43
2:B:108:ASP:OD1	2:B:109:CYS:N	2.45	0.43
2:B:170:ILE:HD13	2:B:181:PRO:HB3	2.00	0.43
3:D:250:GLU:OE1	3:D:297:ARG:NH1	2.51	0.43
3:H:131:ARG:HD2	3:H:200:PHE:CE2	2.53	0.43
3:F:59:LYS:HA	3:G:256:VAL:HG11	2.00	0.43
3:F:145:VAL:HG21	3:F:169:ILE:HG23	2.00	0.43
3:G:49:SER:CB	3:H:251:PRO:HG2	2.46	0.43
3:F:82:ASN:ND2	3:F:186:LYS:HE3	2.34	0.43
3:G:137:GLU:HB3	3:G:192:LEU:HB3	2.01	0.43
4:I:112:VAL:HG13	4:I:113:SER:N	2.33	0.43
3:F:94:LEU:HD12	3:F:94:LEU:HA	1.84	0.43
3:F:129:LEU:HD13	3:F:191:MET:SD	2.59	0.43
4:I:115:GLU:O	4:I:116:THR:C	2.55	0.43
4:I:118:GLU:O	4:I:122:GLY:N	2.42	0.43
4:I:126:GLY:O	4:I:127:GLU:HB2	2.18	0.43
3:C:82:ASN:HD21	3:C:186:LYS:HE3	1.84	0.43
4:I:164:CYS:HB3	4:I:165:ILE:H	1.63	0.43
3:E:9:VAL:O	3:E:94:LEU:HB3	2.19	0.43
3:H:71:PRO:HG2	3:H:74:LYS:HB2	1.99	0.43
3:H:77:LEU:HD13	3:H:199:VAL:HG11	1.99	0.43
3:E:270:LEU:O	3:E:274:MET:HB2	2.19	0.42
1:A:33:PHE:CG	1:A:92:CYS:HB3	2.53	0.42
2:B:184:ASN:HB3	2:B:213:THR:HG22	2.01	0.42
3:G:240:TYR:CE2	3:G:243:ALA:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:85:PHE:O	3:H:182:PHE:HA	2.19	0.42
3:G:201:PRO:HG2	3:G:215:LEU:HD13	2.00	0.42
3:E:300:VAL:HG23	5:J:9:U:O2	2.19	0.42
3:F:129:LEU:HD21	3:F:189:HIS:CD2	2.55	0.42
3:H:42:LYS:HA	3:H:42:LYS:HD3	1.63	0.42
5:J:37:G:H1'	5:J:38:C:O5'	2.20	0.42
3:C:63:GLN:HG3	3:C:212:SER:HB2	2.01	0.42
3:G:3:LYS:HE2	3:G:279:ASN:HD22	1.84	0.42
3:C:145:VAL:HG22	3:C:146:ASN:CG	2.40	0.42
3:D:234:ARG:NH2	3:D:250:GLU:OE2	2.33	0.42
3:D:257:ARG:HA	3:D:257:ARG:HD2	1.63	0.42
3:E:119:TYR:CE1	3:E:236:ILE:HD13	2.55	0.42
3:G:21:ALA:HB3	3:G:224:MET:HB2	2.01	0.42
3:G:78:LEU:HA	3:G:189:HIS:O	2.19	0.42
4:I:141:THR:OG1	5:J:52:G:N2	2.51	0.42
3:D:21:ALA:HA	3:D:80:LYS:O	2.20	0.42
4:I:155:SER:H	4:I:163:LEU:HD22	1.83	0.42
2:B:1:MET:HG3	2:B:142:ALA:O	2.20	0.42
3:D:234:ARG:NH1	5:J:6:C:OP2	2.53	0.42
3:F:78:LEU:HD13	3:F:190:TYR:CE1	2.55	0.42
3:H:119:TYR:O	3:H:123:ILE:HG13	2.19	0.41
2:B:156:MET:HA	2:B:157:PRO:HA	1.82	0.41
3:F:49:SER:CB	3:G:251:PRO:HG2	2.50	0.41
3:G:277:ALA:HB2	3:G:283:LEU:HD11	2.00	0.41
4:I:48:ASN:ND2	5:J:34:U:O3'	2.53	0.41
2:B:15:ILE:O	2:B:93:LEU:HA	2.20	0.41
2:B:39:MET:HB2	2:B:120:PHE:CE2	2.56	0.41
3:G:26:VAL:HG12	3:G:34:THR:HA	2.02	0.41
3:D:277:ALA:HB2	3:D:283:LEU:HD11	2.02	0.41
3:G:6:ALA:HB2	3:G:99:TYR:CZ	2.56	0.41
4:I:4:THR:HA	4:I:55:LEU:O	2.21	0.41
3:F:46:GLY:HA3	5:J:23:C:H1'	2.03	0.41
3:G:234:ARG:HG3	3:G:249:VAL:HB	2.03	0.41
3:H:21:ALA:HB2	3:H:229:ILE:HD11	2.02	0.41
3:E:42:LYS:HB3	3:E:67:PHE:CE1	2.56	0.41
3:G:70:LEU:O	3:G:196:GLY:HA2	2.21	0.41
3:H:257:ARG:NH2	5:J:32:U:OP1	2.54	0.41
1:A:127:GLY:HA3	2:B:171:PHE:CE2	2.55	0.41
2:B:4:PHE:CD2	2:B:151:VAL:HG11	2.56	0.41
2:B:149:ALA:HA	2:B:152:LYS:HE3	2.03	0.41
3:G:123:ILE:HG22	3:G:143:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:234:ARG:NH2	3:G:297:ARG:HD2	2.36	0.41
4:I:45:MET:HA	4:I:49:VAL:O	2.20	0.41
4:I:90:THR:CG2	4:I:163:LEU:HD11	2.50	0.41
3:D:111:ASP:HB3	3:D:289:MET:SD	2.61	0.41
3:G:186:LYS:HE2	3:G:186:LYS:HB3	1.96	0.41
3:G:226:ASP:OD1	3:G:227:GLN:N	2.54	0.41
3:H:129:LEU:HD21	3:H:189:HIS:CG	2.56	0.41
4:I:24:VAL:HG22	4:I:77:ILE:HD11	2.02	0.41
4:I:99:LYS:HZ3	4:I:126:GLY:HA3	1.84	0.41
4:I:84:GLU:CD	4:I:85:ALA:H	2.25	0.40
4:I:101:LYS:HE2	4:I:101:LYS:HA	2.03	0.40
3:C:51:ARG:HA	3:D:271:PHE:CE2	2.56	0.40
3:E:15:LYS:HE3	3:E:89:VAL:HA	2.03	0.40
3:E:213:LYS:NZ	5:J:17:U:O4	2.51	0.40
5:J:38:C:H2'	5:J:39:A:H8	1.86	0.40
2:B:227:ASP:HA	2:B:230:LEU:HD12	2.03	0.40
3:F:207:GLU:O	3:F:208:ASN:C	2.60	0.40
3:H:93:GLU:HG3	3:H:94:LEU:HD12	2.03	0.40
3:F:40:GLY:O	3:F:66:ASN:HA	2.21	0.40
3:H:115:LEU:HD21	3:H:289:MET:HB3	2.03	0.40
3:H:128:THR:HG22	3:H:232:ALA:HB3	2.03	0.40
2:B:107:GLU:H	2:B:107:GLU:CD	2.25	0.40
3:C:103:LEU:HD13	3:C:278:VAL:HG23	2.03	0.40
3:D:40:GLY:O	3:D:66:ASN:HA	2.22	0.40
3:E:91:LYS:HA	3:E:91:LYS:HD2	1.91	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLU:OE1	3:E:146:ASN:OD1[1_565]	2.11	0.09

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	175/179 (98%)	163 (93%)	11 (6%)	1 (1%)	25 64
2	B	246/248 (99%)	227 (92%)	19 (8%)	0	100 100
3	C	302/306 (99%)	282 (93%)	20 (7%)	0	100 100
3	D	300/306 (98%)	280 (93%)	19 (6%)	1 (0%)	41 76
3	E	302/306 (99%)	283 (94%)	19 (6%)	0	100 100
3	F	301/306 (98%)	275 (91%)	25 (8%)	1 (0%)	41 76
3	G	301/306 (98%)	281 (93%)	20 (7%)	0	100 100
3	H	281/306 (92%)	264 (94%)	16 (6%)	1 (0%)	34 72
4	I	164/168 (98%)	135 (82%)	21 (13%)	8 (5%)	2 13
All	All	2372/2431 (98%)	2190 (92%)	170 (7%)	12 (0%)	29 68

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	207	GLU
4	I	87	LYS
4	I	60	GLY
4	I	111	GLY
4	I	123	ASN
4	I	128	LYS
4	I	132	PRO
1	A	14	GLY
3	F	154	ASP
3	H	244	THR
4	I	49	VAL
4	I	112	VAL

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	156/157 (99%)	149 (96%)	7 (4%)	27 64
2	B	211/211 (100%)	197 (93%)	14 (7%)	16 49
3	C	249/251 (99%)	234 (94%)	15 (6%)	19 53
3	D	248/251 (99%)	238 (96%)	10 (4%)	31 68
3	E	249/251 (99%)	236 (95%)	13 (5%)	23 59
3	F	249/251 (99%)	238 (96%)	11 (4%)	28 65
3	G	249/251 (99%)	237 (95%)	12 (5%)	25 62
3	H	235/251 (94%)	227 (97%)	8 (3%)	37 72
4	I	149/151 (99%)	122 (82%)	27 (18%)	1 9
All	All	1995/2025 (98%)	1878 (94%)	117 (6%)	19 54

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	48	THR
1	A	124	LEU
1	A	151	ASN
1	A	153	THR
1	A	158	LYS
1	A	177	TYR
2	B	18	LYS
2	B	67	SER
2	B	69	THR
2	B	74	GLN
2	B	89	GLN
2	B	107	GLU
2	B	115	ASP
2	B	164	CYS
2	B	170	ILE
2	B	190	GLU
2	B	201	LYS
2	B	220	VAL
2	B	235	GLU
2	B	240	LYS
3	C	53	ASN
3	C	56	ASP
3	C	64	THR
3	C	146	ASN
3	C	153	SER

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Mol	Chain	Res	Type
3	C	155	LEU
3	C	172	MET
3	C	202	SER
3	C	205	PHE
3	C	234	ARG
3	C	245	THR
3	C	257	ARG
3	C	295	LEU
3	C	297	ARG
3	C	305	LYS
3	D	4	LEU
3	D	5	LYS
3	D	53	ASN
3	D	88	ASP
3	D	145	VAL
3	D	153	SER
3	D	172	MET
3	D	202	SER
3	D	245	THR
3	D	284	THR
3	E	2	THR
3	E	49	SER
3	E	53	ASN
3	E	63	GLN
3	E	88	ASP
3	E	94	LEU
3	E	102	THR
3	E	107	LEU
3	E	147	ASP
3	E	210	LYS
3	E	213	LYS
3	E	254	SER
3	E	257	ARG
3	F	1	MET
3	F	2	THR
3	F	15	LYS
3	F	35	THR
3	F	55	ASN
3	F	63	GLN
3	F	88	ASP
3	F	147	ASP
3	F	210	LYS

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Mol	Chain	Res	Type
3	F	211	LEU
3	F	212	SER
3	G	2	THR
3	G	3	LYS
3	G	48	GLN
3	G	55	ASN
3	G	88	ASP
3	G	107	LEU
3	G	172	MET
3	G	208	ASN
3	G	234	ARG
3	G	244	THR
3	G	284	THR
3	G	300	VAL
3	H	1	MET
3	H	3	LYS
3	H	41	THR
3	H	210	LYS
3	H	211	LEU
3	H	213	LYS
3	H	239	TRP
3	H	284	THR
4	I	3	ASN
4	I	7	ILE
4	I	25	LEU
4	I	27	THR
4	I	37	GLU
4	I	47	LYS
4	I	56	PHE
4	I	67	THR
4	I	69	THR
4	I	73	LEU
4	I	74	THR
4	I	88	VAL
4	I	95	ASP
4	I	97	LYS
4	I	99	LYS
4	I	101	LYS
4	I	105	ARG
4	I	110	LYS
4	I	112	VAL
4	I	116	THR

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Mol	Chain	Res	Type
4	I	119	SER
4	I	132	PRO
4	I	134	ILE
4	I	154	ASN
4	I	158	PHE
4	I	161	TYR
4	I	166	VAL

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

Mol	Chain	Res	Type
1	A	148	ASN
3	C	63	GLN
3	F	208	ASN
4	I	48	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	J	59/60 (98%)	27 (45%)	5 (8%)

All (27) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	J	-5	U
5	J	0	A
5	J	1	G
5	J	2	U
5	J	6	C
5	J	7	C
5	J	8	C
5	J	13	C
5	J	14	U
5	J	19	U
5	J	25	A
5	J	26	U
5	J	31	A
5	J	32	U
5	J	34	U
5	J	35	U

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Mol	Chain	Res	Type
5	J	36	A
5	J	37	G
5	J	38	C
5	J	39	A
5	J	40	G
5	J	43	G
5	J	44	C
5	J	45	A
5	J	46	U
5	J	51	U
5	J	52	G

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	J	33	G
5	J	34	U
5	J	36	A
5	J	37	G
5	J	44	C

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

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	177/179 (98%)	-0.01	1 (0%) 89 72	25, 44, 74, 100	0
2	B	248/248 (100%)	0.32	9 (3%) 42 17	24, 56, 91, 107	0
3	C	304/306 (99%)	0.30	15 (4%) 29 11	22, 55, 80, 110	0
3	D	302/306 (98%)	0.22	12 (3%) 38 15	23, 48, 82, 107	0
3	E	304/306 (99%)	0.03	10 (3%) 46 20	21, 38, 67, 119	0
3	F	303/306 (99%)	-0.12	1 (0%) 94 84	21, 35, 70, 95	0
3	G	303/306 (99%)	0.15	11 (3%) 42 17	36, 58, 89, 114	0
3	H	285/306 (93%)	0.74	34 (11%) 4 1	51, 79, 102, 123	0
4	I	166/168 (98%)	1.44	49 (29%) 0 0	70, 94, 139, 141	0
5	J	60/60 (100%)	0.83	8 (13%) 3 1	26, 54, 145, 153	0
All	All	2452/2491 (98%)	0.31	150 (6%) 21 7	21, 54, 100, 153	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	I	127	GLU	7.5
4	I	120	LEU	6.3
4	I	112	VAL	6.1
4	I	126	GLY	6.0
3	H	45	ALA	5.9
3	H	212	SER	5.5
4	I	111	GLY	5.5
4	I	159	ASN	5.3
4	I	95	ASP	5.2
3	H	2	THR	5.1
3	H	210	LYS	5.1
3	G	1	MET	5.1
3	H	1	MET	5.1

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Mol	Chain	Res	Type	RSRZ
4	I	105	ARG	4.6
3	G	2	THR	4.6
3	H	209	SER	4.5
4	I	97	LYS	4.5
4	I	129	CYS	4.5
4	I	125	LYS	4.5
4	I	107	ILE	4.5
4	I	103	ILE	4.2
4	I	119	SER	4.1
3	E	1	MET	4.1
4	I	121	TYR	4.1
4	I	130	LYS	4.0
4	I	128	LYS	4.0
4	I	116	THR	3.9
3	H	273	LEU	3.9
4	I	124	TYR	3.9
3	H	262	TYR	3.9
3	H	280	GLY	3.7
2	B	4	PHE	3.7
4	I	118	GLU	3.7
4	I	139	LYS	3.6
3	E	2	THR	3.6
3	H	283	LEU	3.6
3	H	211	LEU	3.6
4	I	94	VAL	3.6
3	D	2	THR	3.5
4	I	106	CYS	3.5
4	I	113	SER	3.3
3	H	265	GLY	3.3
5	J	44	C	3.3
4	I	158	PHE	3.3
3	E	304	GLY	3.3
2	B	3	LYS	3.3
3	C	4	LEU	3.3
4	I	164	CYS	3.2
3	H	281	LYS	3.2
3	C	278	VAL	3.2
4	I	137	ASN	3.2
3	D	303	GLY	3.1
3	H	207	GLU	3.1
4	I	115	GLU	3.1
3	H	43	THR	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	248	ASP	3.1
4	I	96	THR	3.1
3	C	285	GLU	3.1
3	G	4	LEU	3.1
4	I	145	PHE	3.0
4	I	102	LEU	3.0
4	I	160	SER	3.0
3	C	171	ASP	2.9
3	G	5	LYS	2.9
4	I	132	PRO	2.9
2	B	1	MET	2.8
3	H	279	ASN	2.8
3	D	252	TYR	2.8
4	I	98	SER	2.8
3	G	267	LYS	2.7
3	G	58	ASP	2.7
3	E	279	ASN	2.7
4	I	51	ASP	2.7
3	D	267	LYS	2.7
3	C	2	THR	2.7
2	B	247	ASN	2.6
3	D	265	GLY	2.6
3	C	283	LEU	2.6
5	J	45	A	2.6
1	A	177	TYR	2.6
3	H	252	TYR	2.6
4	I	109	ARG	2.6
3	G	3	LYS	2.6
3	H	208	ASN	2.6
5	J	43	G	2.5
3	G	208	ASN	2.5
3	D	280	GLY	2.5
3	D	102	THR	2.5
3	G	279	ASN	2.5
4	I	133	TYR	2.4
5	J	52	G	2.4
3	H	102	THR	2.4
3	H	44	VAL	2.4
3	H	205	PHE	2.4
3	H	256	VAL	2.4
3	C	273	LEU	2.4
3	H	282	SER	2.4

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Mol	Chain	Res	Type	RSRZ
3	E	208	ASN	2.4
4	I	123	ASN	2.4
4	I	110	LYS	2.4
3	G	59	LYS	2.4
5	J	42	C	2.4
4	I	146	SER	2.4
2	B	148	LEU	2.4
3	C	164	VAL	2.4
3	D	208	ASN	2.4
3	H	98	GLU	2.3
3	H	206	VAL	2.3
3	C	97	GLY	2.3
3	E	280	GLY	2.3
3	H	3	LYS	2.3
4	I	2	TYR	2.3
2	B	104	VAL	2.3
3	H	288	GLN	2.3
3	H	105	THR	2.2
3	E	154	ASP	2.2
3	H	42	LYS	2.2
3	D	283	LEU	2.2
4	I	150	GLU	2.2
3	E	207	GLU	2.2
3	E	283	LEU	2.2
3	E	5	LYS	2.2
4	I	100	GLY	2.2
3	G	280	GLY	2.2
4	I	114	ALA	2.2
3	C	57	ALA	2.2
4	I	148	PHE	2.2
5	J	36	A	2.1
2	B	110	ALA	2.1
3	C	286	GLU	2.1
3	C	5	LYS	2.1
3	C	107	LEU	2.1
3	H	267	LYS	2.1
3	C	102	THR	2.1
3	H	4	LEU	2.1
4	I	99	LYS	2.1
4	I	39	GLY	2.1
2	B	102	PHE	2.1
3	H	213	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
3	H	276	GLY	2.1
3	C	280	GLY	2.1
3	D	98	GLU	2.1
3	D	279	ASN	2.0
3	D	178	SER	2.0
5	J	46	U	2.0
3	H	33	ASN	2.0
3	F	1	MET	2.0
4	I	152	CYS	2.0
4	I	165	ILE	2.0
5	J	49	G	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.