



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:52 AM UTC

PDB ID : 5CD4 / pdb_00005cd4
Title : The Type IE CRISPR Cascade complex from E. coli, with two assemblies in the asymmetric unit arranged back-to-back
Authors : Jackson, R.N.; Golden, S.M.; Carter, J.; Wiedenheft, B.
Deposited on : 2015-07-03
Resolution : 3.20 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
Mogul : 2022.3.0, CSD as543be (2022)
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

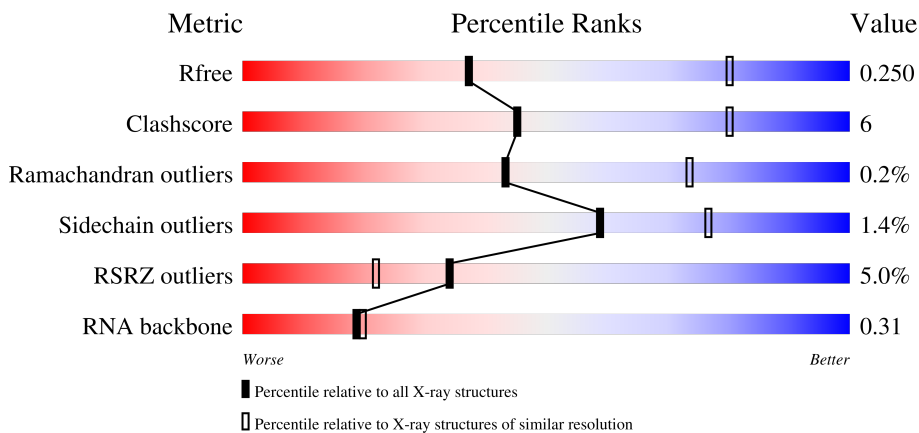
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

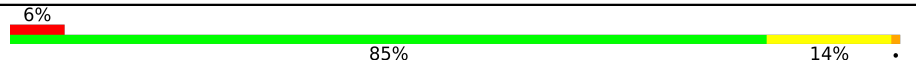

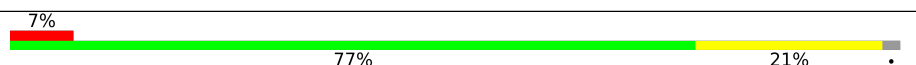
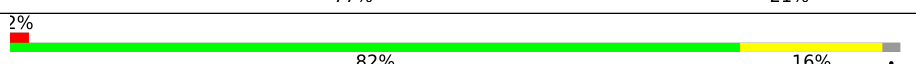
The reported resolution of this entry is 3.20 Å.

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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

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	199	 6% 85% 14%
1	M	199	 12% 83% 13%
2	B	363	 7% 77% 21%
2	C	363	 2% 82% 16%

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Mol	Chain	Length	Quality of chain
2	D	363	
2	E	363	
2	F	363	
2	G	363	
2	N	363	
2	O	363	
2	P	363	
2	Q	363	
2	R	363	
2	S	363	
3	H	224	
3	T	224	
4	I	502	
4	U	502	
5	J	165	
5	K	165	
5	V	165	
5	W	165	
6	L	61	
6	X	61	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 53308 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 CRISPR system Cascade subunit CasE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	199	1523	975	273	269	6	0	0	0
1	M	192	1354	864	245	240	5	0	0	0

- Molecule 2 is a protein called CRISPR system Cascade subunit CasC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	357	2673	1677	474	507	15	0	0	0
2	C	356	2670	1671	477	507	15	0	0	0
2	D	355	2674	1672	478	508	16	0	0	0
2	E	362	2748	1722	490	520	16	0	0	0
2	F	363	2746	1719	490	521	16	0	0	0
2	G	362	2749	1716	490	528	15	0	0	0
2	N	356	2544	1595	464	471	14	0	0	0
2	O	351	2546	1593	464	475	14	0	0	0
2	P	359	2645	1659	478	493	15	0	0	0
2	Q	359	2706	1695	485	510	16	0	0	0
2	R	357	2688	1685	483	504	16	0	0	0
2	S	353	2634	1649	473	497	15	0	0	0

- Molecule 3 is a protein called CRISPR system Cascade subunit CasD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	219	Total	C	N	O	S	0	0	0
			1715	1087	302	317	9			
3	T	219	Total	C	N	O	S	0	0	0
			1716	1087	303	317	9			

- Molecule 4 is a protein called CRISPR system Cascade subunit CasA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	I	494	Total	C	N	O	S	0	0	0
			3792	2424	671	678	19			
4	U	492	Total	C	N	O	S	0	0	0
			3709	2371	655	665	18			

- Molecule 5 is a protein called CRISPR system Cascade subunit CasB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	J	156	Total	C	N	O	S	0	0	0
			1215	767	231	210	7			
5	K	154	Total	C	N	O	S	0	0	0
			1263	791	243	222	7			
5	V	152	Total	C	N	O	S	0	0	0
			1161	741	216	197	7			
5	W	151	Total	C	N	O	S	0	0	0
			1235	775	239	214	7			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	-4	GLY	-	expression tag	UNP P76632
J	-3	PRO	-	expression tag	UNP P76632
J	-2	GLY	-	expression tag	UNP P76632
J	-1	TYR	-	expression tag	UNP P76632
J	0	GLN	-	expression tag	UNP P76632
K	-4	GLY	-	expression tag	UNP P76632
K	-3	PRO	-	expression tag	UNP P76632
K	-2	GLY	-	expression tag	UNP P76632
K	-1	TYR	-	expression tag	UNP P76632
K	0	GLN	-	expression tag	UNP P76632
V	-4	GLY	-	expression tag	UNP P76632
V	-3	PRO	-	expression tag	UNP P76632
V	-2	GLY	-	expression tag	UNP P76632

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Chain	Residue	Modelled	Actual	Comment	Reference
V	-1	TYR	-	expression tag	UNP P76632
V	0	GLN	-	expression tag	UNP P76632
W	-4	GLY	-	expression tag	UNP P76632
W	-3	PRO	-	expression tag	UNP P76632
W	-2	GLY	-	expression tag	UNP P76632
W	-1	TYR	-	expression tag	UNP P76632
W	0	GLN	-	expression tag	UNP P76632

- Molecule 6 is a RNA chain called crRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
6	L	61	1300	580	233	426	61	0	0	0
6	X	61	1300	580	233	426	61	0	0	0

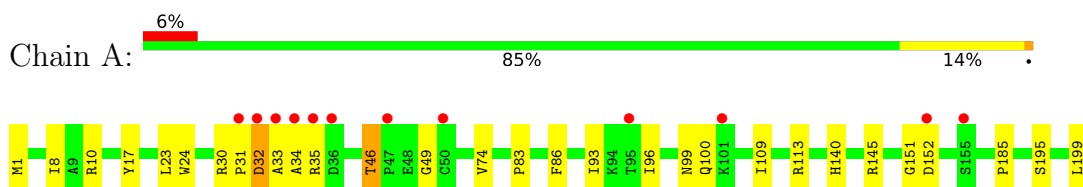
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	1	Total	Zn	0	0
			1	1		
7	U	1	Total	Zn	0	0
			1	1		

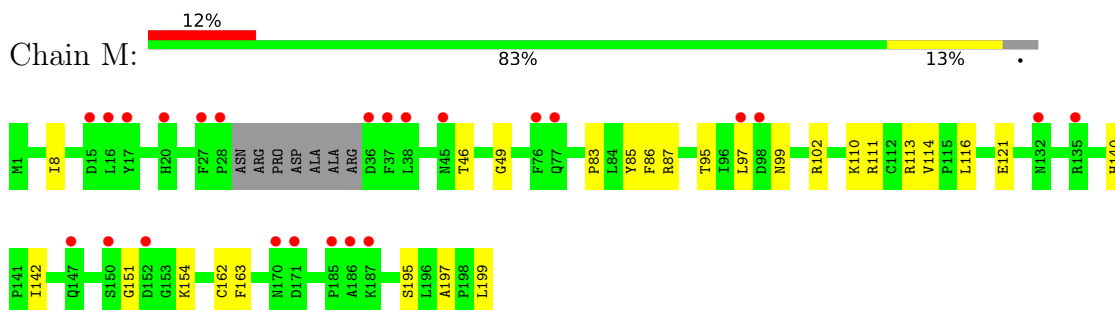
3 Residue-property plots [i](#)

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.

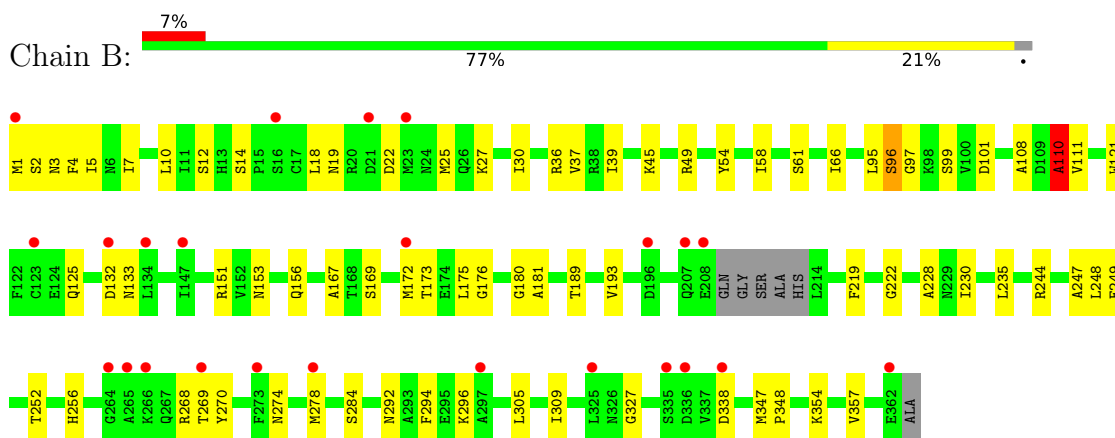
- Molecule 1: CRISPR system Cascade subunit CasE



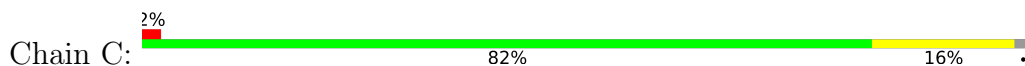
- Molecule 1: CRISPR system Cascade subunit CasE

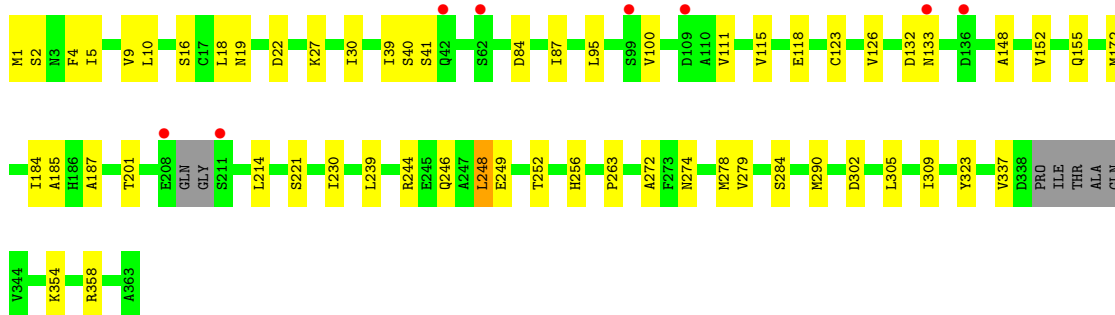


- Molecule 2: CRISPR system Cascade subunit CasC

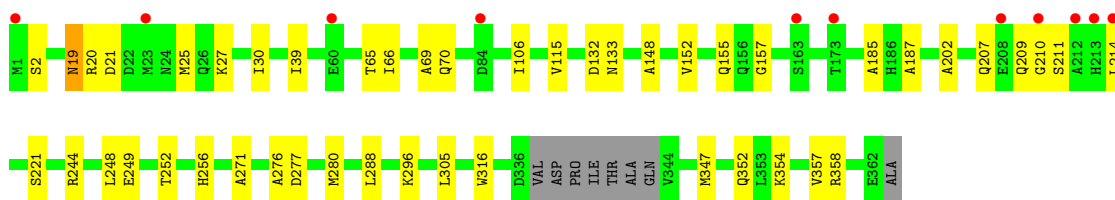
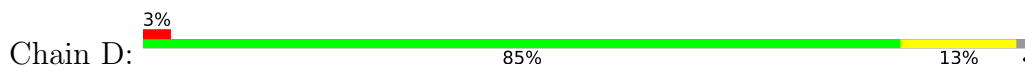


- Molecule 2: CRISPR system Cascade subunit CasC

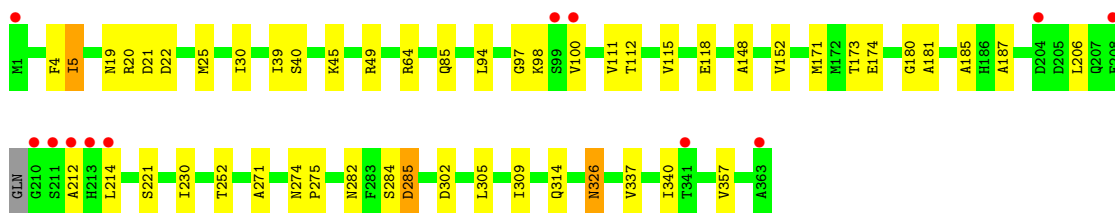
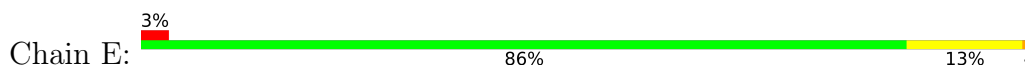




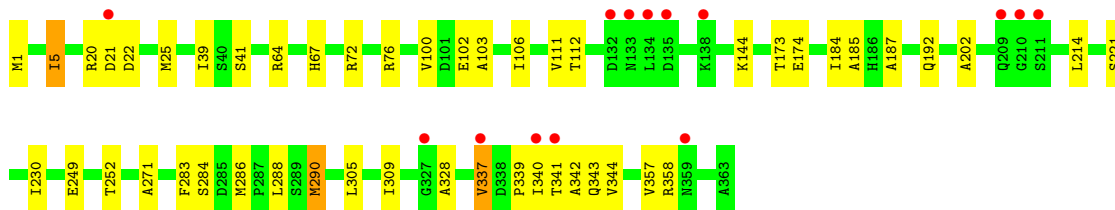
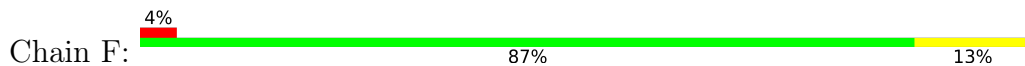
- Molecule 2: CRISPR system Cascade subunit CasC



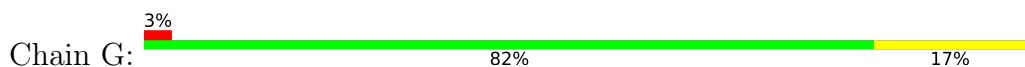
- Molecule 2: CRISPR system Cascade subunit CasC

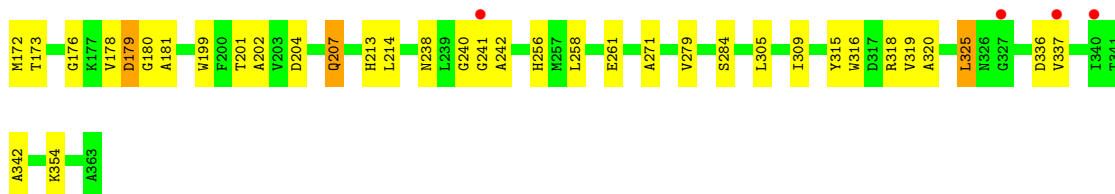


- Molecule 2: CRISPR system Cascade subunit CasC

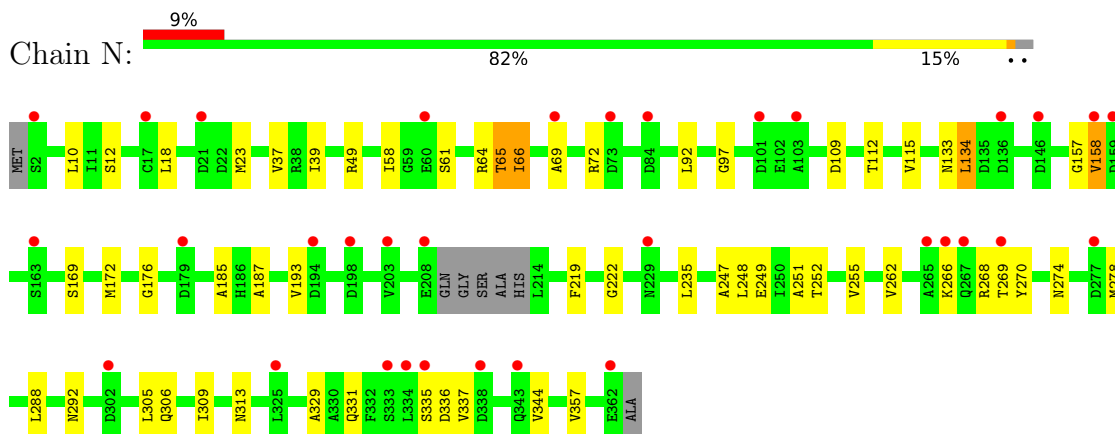


- Molecule 2: CRISPR system Cascade subunit CasC

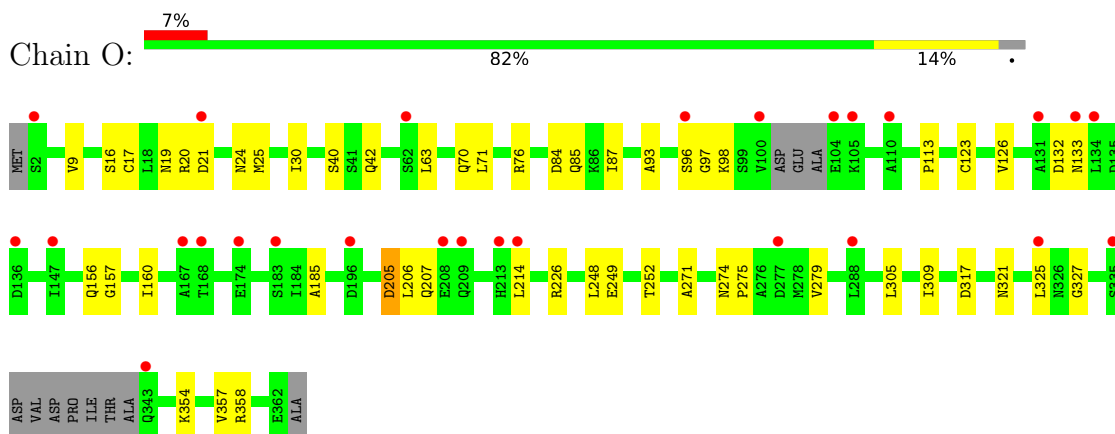




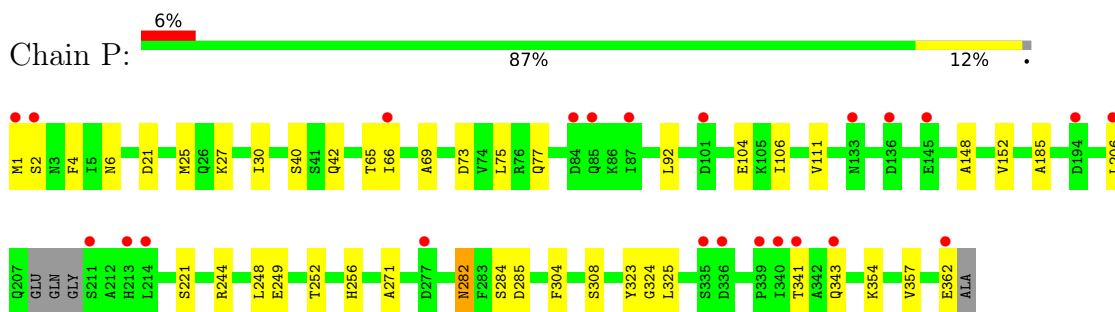
- Molecule 2: CRISPR system Cascade subunit CasC



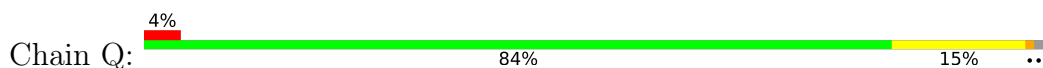
- Molecule 2: CRISPR system Cascade subunit CasC

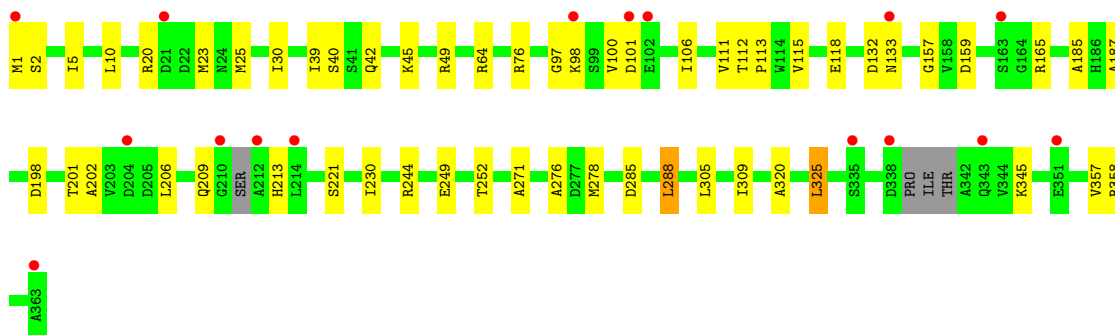


- Molecule 2: CRISPR system Cascade subunit CasC

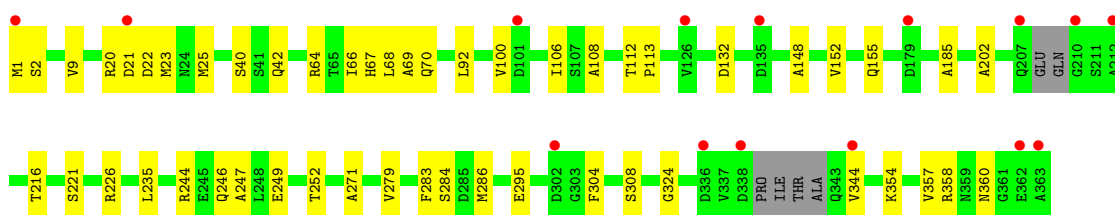
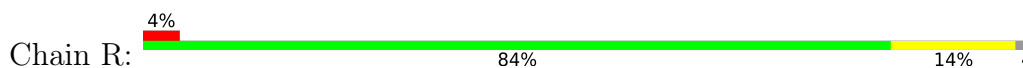


- Molecule 2: CRISPR system Cascade subunit CasC

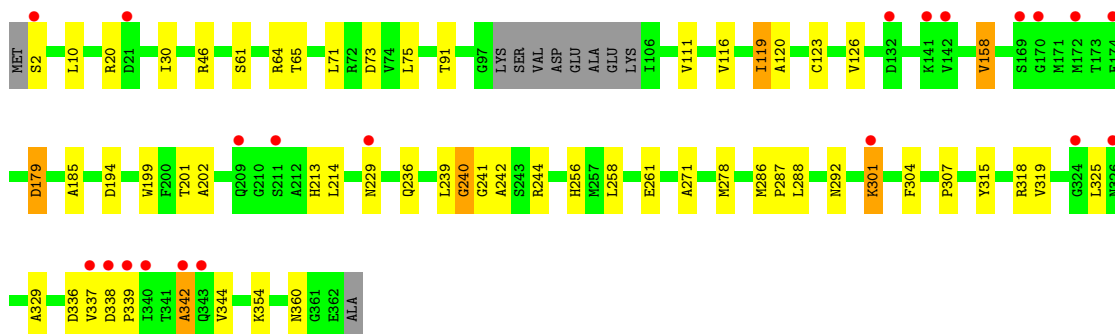
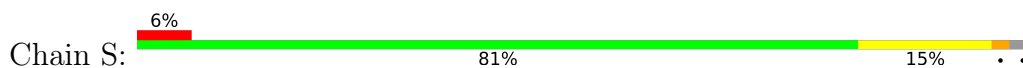




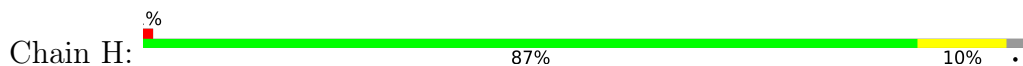
- Molecule 2: CRISPR system Cascade subunit CasC



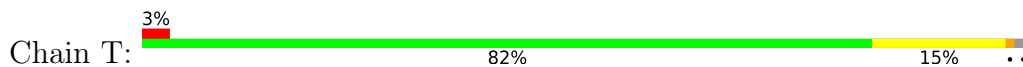
- Molecule 2: CRISPR system Cascade subunit CasC



- Molecule 3: CRISPR system Cascade subunit CasD

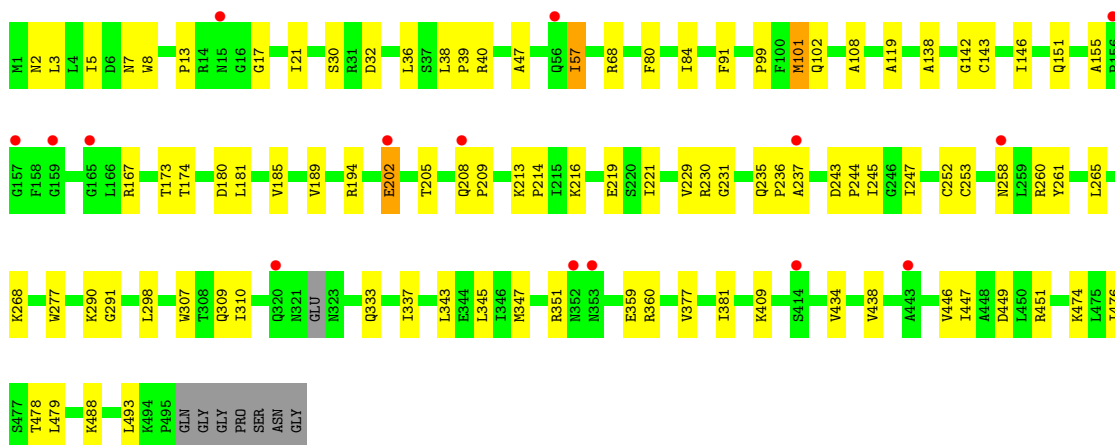
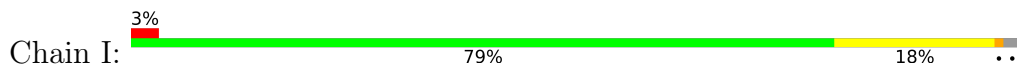


- Molecule 3: CRISPR system Cascade subunit CasD

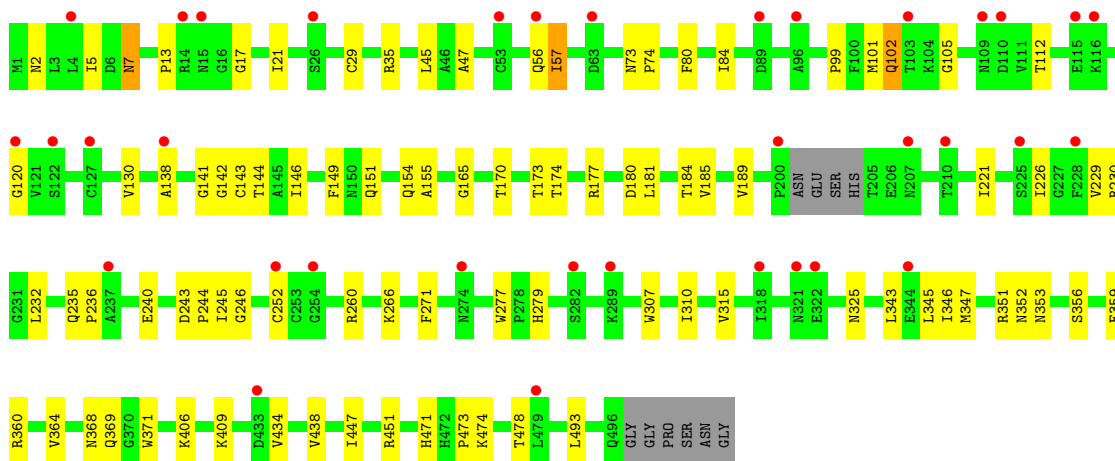
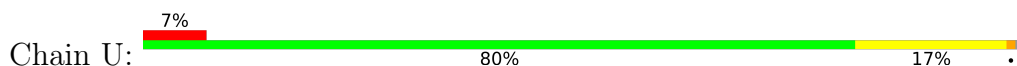




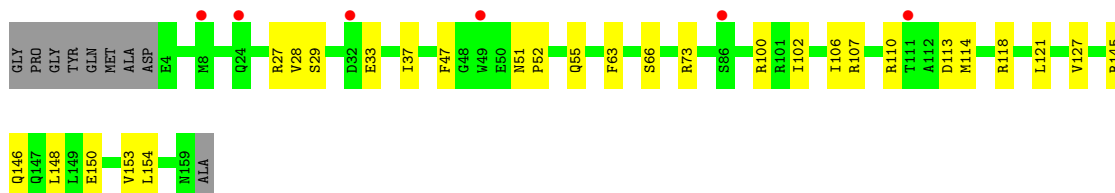
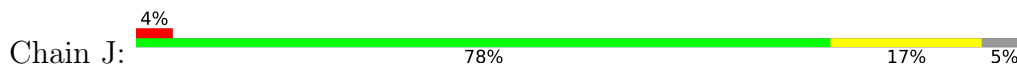
- Molecule 4: CRISPR system Cascade subunit CasA



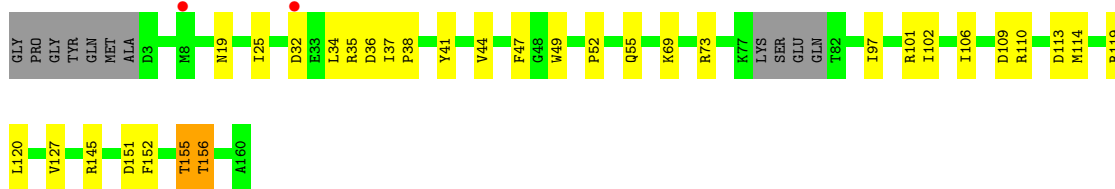
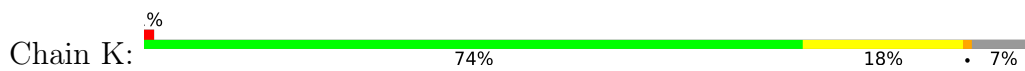
- Molecule 4: CRISPR system Cascade subunit CasA



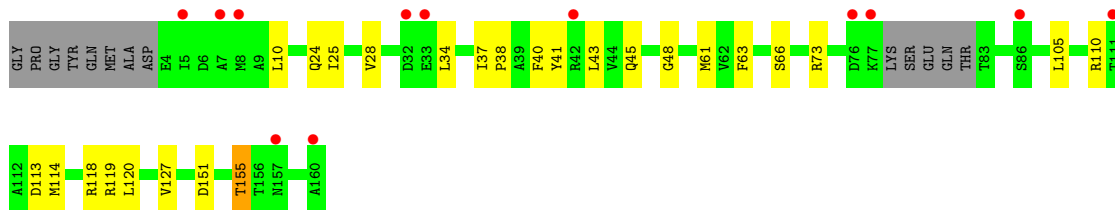
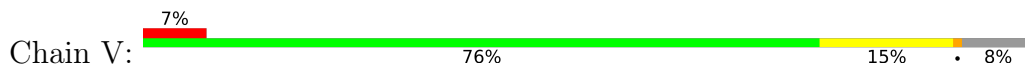
- Molecule 5: CRISPR system Cascade subunit CasB



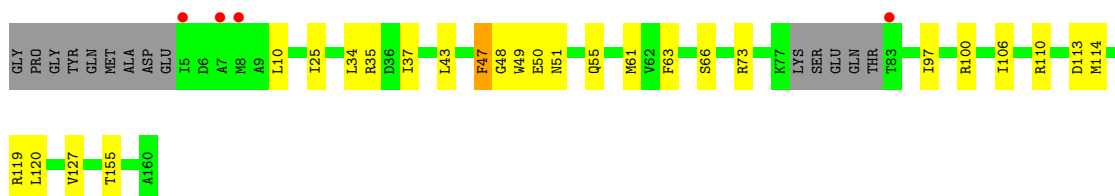
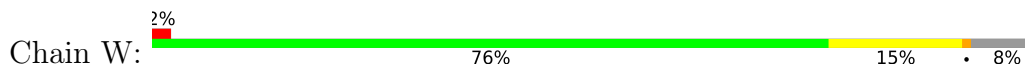
- Molecule 5: CRISPR system Cascade subunit CasB



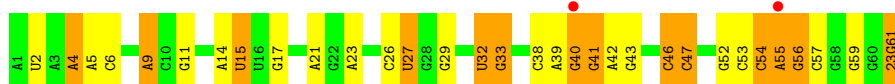
• Molecule 5: CRISPR system Cascade subunit CasB



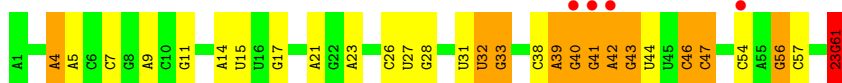
• Molecule 5: CRISPR system Cascade subunit CasB



• Molecule 6: crRNA



• Molecule 6: crRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.99Å 244.80Å 426.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.73 – 3.20 49.73 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.73-3.20) 97.1 (49.73-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 3.19Å)	Xtrriage
Refinement program	PHENIX (1.10pre_2089: ???)	Depositor
R, R_{free}	0.212 , 0.250 0.213 , 0.250	Depositor DCC
R_{free} test set	2000 reflections (1.09%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtrriage
Anisotropy	0.741	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	53308	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 23G, ZN

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	0/1554	0.79	1/2108 (0.0%)
1	M	0.29	0/1379	0.76	0/1878
2	B	0.31	0/2716	0.79	7/3681 (0.2%)
2	C	0.26	0/2712	0.67	0/3674
2	D	0.27	0/2717	0.68	0/3679
2	E	0.25	0/2791	0.65	0/3773
2	F	0.26	0/2790	0.70	0/3775
2	G	0.27	0/2794	0.68	0/3780
2	N	0.29	0/2586	0.75	3/3519 (0.1%)
2	O	0.26	0/2587	0.68	0/3512
2	P	0.26	0/2689	0.66	1/3648 (0.0%)
2	Q	0.26	0/2748	0.67	0/3716
2	R	0.25	0/2730	0.66	1/3690 (0.0%)
2	S	0.26	0/2678	0.68	0/3631
3	H	0.29	0/1756	0.75	3/2387 (0.1%)
3	T	0.29	0/1758	0.75	3/2391 (0.1%)
4	I	0.31	0/3883	0.77	4/5286 (0.1%)
4	U	0.30	0/3799	0.75	1/5181 (0.0%)
5	J	0.32	0/1240	0.78	4/1685 (0.2%)
5	K	0.32	0/1287	0.77	4/1739 (0.2%)
5	V	0.31	0/1185	0.75	1/1612 (0.1%)
5	W	0.31	0/1259	0.75	4/1702 (0.2%)
6	L	0.15	0/1423	0.43	0/2216
6	X	0.15	0/1423	0.41	0/2216
All	All	0.27	0/54484	0.70	37/74479 (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
2	B	0	1

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	W	47	PHE	N-CA-C	7.46	121.64	112.23
5	K	47	PHE	N-CA-C	7.23	120.58	111.69
2	B	327	GLY	N-CA-C	6.84	119.80	111.93
2	N	66	ILE	N-CA-C	-6.62	107.42	113.71
2	N	97	GLY	N-CA-C	-6.55	94.30	113.30
3	T	17	GLY	N-CA-C	6.43	119.33	111.93
5	K	110	ARG	CB-CA-C	-6.33	109.27	116.54
3	H	17	GLY	N-CA-C	6.31	119.19	111.93
4	I	202	GLU	CA-C-N	6.12	132.71	121.70
4	I	202	GLU	C-N-CA	6.12	132.71	121.70
2	B	95	LEU	N-CA-C	6.04	120.26	113.01
5	V	110	ARG	CB-CA-C	-6.03	109.61	116.54
2	B	14	SER	CA-C-N	5.90	127.22	119.84
2	B	14	SER	C-N-CA	5.90	127.22	119.84
5	W	110	ARG	CB-CA-C	-5.90	109.75	116.54
2	B	96	SER	N-CA-C	5.83	120.78	113.43
1	A	32	ASP	N-CA-C	5.82	117.62	111.28
4	I	221	ILE	N-CA-C	5.51	112.57	107.56
2	R	66	ILE	N-CA-C	-5.46	108.17	113.53
3	H	25	ARG	CA-C-N	5.45	125.91	120.52
3	H	25	ARG	C-N-CA	5.45	125.91	120.52
5	W	37	ILE	CA-C-N	5.41	124.75	118.85
5	W	37	ILE	C-N-CA	5.41	124.75	118.85
5	J	110	ARG	CB-CA-C	-5.40	110.33	116.54
2	B	338	ASP	CA-C-N	5.26	127.35	120.25
2	B	338	ASP	C-N-CA	5.26	127.35	120.25
4	U	29	CYS	N-CA-C	5.26	119.38	112.92
2	N	65	THR	N-CA-C	5.23	115.44	108.38
3	T	25	ARG	CA-C-N	5.22	125.69	120.52
3	T	25	ARG	C-N-CA	5.22	125.69	120.52
5	J	37	ILE	CA-C-N	5.17	124.49	118.85
5	J	37	ILE	C-N-CA	5.17	124.49	118.85
2	P	66	ILE	N-CA-C	-5.10	108.53	113.53
4	I	205	THR	N-CA-C	5.04	117.47	109.96
5	J	47	PHE	N-CA-C	5.03	119.44	112.45
5	K	37	ILE	CA-C-N	5.01	124.31	118.85
5	K	37	ILE	C-N-CA	5.01	124.31	118.85

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	110	ALA	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1523	0	1551	17	0
1	M	1354	0	1291	15	0
2	B	2673	0	2583	48	0
2	C	2670	0	2561	34	0
2	D	2674	0	2583	28	0
2	E	2748	0	2701	32	0
2	F	2746	0	2693	33	0
2	G	2749	0	2670	45	0
2	N	2544	0	2348	36	0
2	O	2546	0	2371	32	0
2	P	2645	0	2510	29	0
2	Q	2706	0	2636	39	0
2	R	2688	0	2624	33	0
2	S	2634	0	2532	40	0
3	H	1715	0	1694	14	0
3	T	1716	0	1688	25	0
4	I	3792	0	3716	58	0
4	U	3709	0	3571	51	0
5	J	1215	0	1168	19	0
5	K	1263	0	1260	19	0
5	V	1161	0	1116	13	0
5	W	1235	0	1232	12	0
6	L	1300	0	659	19	0
6	X	1300	0	659	23	0
7	I	1	0	0	0	0
7	U	1	0	0	0	0
All	All	53308	0	50417	616	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 6.

All (616) 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)
6:X:61:23G:O4'	6:X:61:23G:C4'	1.67	1.24
6:L:61:23G:O4'	6:L:61:23G:C4'	1.66	1.21
1:A:8:ILE:O	1:A:49:GLY:HA3	1.72	0.89
1:M:151:GLY:HA3	1:M:154:LYS:H	1.41	0.85
4:I:290:LYS:H	4:I:291:GLY:HA3	1.46	0.80
2:G:96:SER:HB2	2:G:98:LYS:H	1.47	0.78
6:L:40:G:H1'	6:L:41:G:H5'	1.65	0.77
4:U:473:PRO:HG3	5:W:106:ILE:HD11	1.67	0.77
4:I:101:MET:O	4:I:235:GLN:NE2	2.18	0.75
2:E:20:ARG:NH2	6:L:23:A:OP2	2.19	0.75
4:U:13:PRO:HD2	4:U:17:GLY:HA3	1.69	0.75
2:Q:2:SER:O	2:Q:244:ARG:NH2	2.18	0.74
2:C:185:ALA:HB2	2:D:271:ALA:HB3	1.70	0.73
1:M:85:TYR:HB2	1:M:197:ALA:HB3	1.70	0.73
2:F:1:MET:HB3	2:F:284:SER:HA	1.71	0.73
4:U:99:PRO:HB2	4:U:102:GLN:HG3	1.70	0.72
6:X:40:G:H1'	6:X:41:G:H5'	1.71	0.72
2:N:133:ASN:HB2	2:N:134:LEU:HA	1.71	0.72
4:I:13:PRO:HD2	4:I:17:GLY:HA3	1.72	0.72
2:G:168:THR:OG1	3:H:90:GLY:O	2.08	0.72
2:F:20:ARG:NH2	6:L:17:G:OP2	2.23	0.72
3:H:82:LEU:O	3:H:109:GLU:HA	1.89	0.71
2:Q:20:ARG:NH2	6:X:23:A:OP2	2.23	0.71
2:E:25:MET:HE3	5:K:119:ARG:HD3	1.73	0.70
1:M:102:ARG:NH1	6:X:44:U:O2	2.24	0.70
2:N:10:LEU:HB2	2:N:278:MET:HB3	1.73	0.69
5:K:44:VAL:HG13	5:K:49:TRP:HB2	1.75	0.68
2:P:73:ASP:OD1	2:P:77:GLN:NE2	2.25	0.68
2:Q:40:SER:OG	2:Q:42:GLN:OE1	2.12	0.68
2:Q:25:MET:HE3	5:W:119:ARG:HD3	1.75	0.67
2:B:2:SER:OG	2:B:244:ARG:NH2	2.27	0.67
2:O:132:ASP:H	2:O:133:ASN:HA	1.60	0.67
5:K:19:ASN:OD1	5:K:69:LYS:NZ	2.27	0.66
1:A:34:ALA:HB1	1:A:35:ARG:HA	1.78	0.66
2:B:10:LEU:HB2	2:B:278:MET:HB3	1.77	0.66
4:U:315:VAL:O	4:U:325:ASN:ND2	2.27	0.66
2:S:30:ILE:HD12	3:T:80:THR:HG21	1.77	0.66
2:S:2:SER:O	2:S:244:ARG:NH2	2.30	0.65
2:C:4:PHE:HB2	2:C:284:SER:O	1.97	0.65
2:O:25:MET:HE3	5:V:119:ARG:HE	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:20:ARG:NH2	6:X:17:G:OP2	2.30	0.64
2:S:301:LYS:HD2	2:S:307:PRO:HB3	1.80	0.64
4:I:57:ILE:HD11	4:I:229:VAL:HG13	1.79	0.64
4:U:57:ILE:HD11	4:U:229:VAL:HG13	1.78	0.64
2:S:202:ALA:HB3	2:S:213:HIS:HB3	1.80	0.64
3:T:22:GLU:OE2	4:U:360:ARG:NH2	2.32	0.63
2:S:244:ARG:NH1	2:S:360:ASN:OD1	2.31	0.62
3:T:143:THR:OG1	3:T:149:ARG:NH1	2.32	0.62
2:S:336:ASP:HB3	2:S:337:VAL:HA	1.82	0.62
2:B:110:ALA:HB1	2:B:111:VAL:HA	1.82	0.62
4:I:173:THR:O	4:I:347:MET:HA	1.99	0.62
5:K:152:PHE:O	5:K:156:THR:OG1	2.18	0.61
4:U:173:THR:O	4:U:347:MET:HA	1.99	0.61
2:G:179:ASP:OD1	6:L:5:A:O2'	2.17	0.61
2:P:1:MET:HB3	2:P:284:SER:HA	1.82	0.61
2:F:252:THR:HG21	2:F:358:ARG:HG3	1.81	0.61
2:Q:320:ALA:HA	2:Q:325:LEU:HB2	1.81	0.61
1:A:145:ARG:HG3	2:B:25:MET:HE3	1.83	0.61
2:B:18:LEU:HD13	2:B:39:ILE:HD11	1.82	0.61
2:S:179:ASP:OD2	3:T:48:ARG:NH2	2.34	0.61
2:N:58:ILE:HG22	2:N:158:VAL:HG21	1.83	0.60
4:U:346:ILE:HG22	4:U:364:VAL:HG12	1.83	0.60
2:G:61:SER:HB3	2:G:158:VAL:HG21	1.83	0.60
2:C:155:GLN:OE1	2:C:246:GLN:NE2	2.34	0.60
2:G:71:LEU:HD22	2:G:111:VAL:HG22	1.83	0.60
4:I:290:LYS:N	4:I:291:GLY:HA3	2.16	0.60
2:Q:209:GLN:O	6:X:28:G:N2	2.34	0.60
2:G:336:ASP:HB3	2:G:337:VAL:HA	1.84	0.60
2:E:64:ARG:HA	2:E:112:THR:O	2.01	0.60
5:J:106:ILE:HD12	5:J:145:ARG:HB3	1.82	0.60
5:J:113:ASP:OD1	5:J:114:MET:N	2.35	0.60
1:M:8:ILE:O	1:M:49:GLY:HA3	2.00	0.60
2:B:268:ARG:NH1	2:B:274:ASN:O	2.33	0.60
2:N:37:VAL:HG23	2:N:193:VAL:HG21	1.82	0.60
5:V:73:ARG:HB2	5:V:127:VAL:HG12	1.84	0.60
2:S:256:HIS:HB2	2:S:354:LYS:HD3	1.84	0.60
2:N:185:ALA:HB2	2:O:271:ALA:HB3	1.83	0.59
2:S:179:ASP:OD1	6:X:5:A:O2'	2.20	0.59
5:K:113:ASP:OD1	5:K:114:MET:N	2.35	0.59
2:B:12:SER:HA	2:B:222:GLY:O	2.01	0.59
5:V:113:ASP:OD1	5:V:114:MET:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:120:GLY:HA3	4:U:360:ARG:HH22	1.66	0.59
2:F:185:ALA:HB2	2:G:271:ALA:HB3	1.84	0.59
4:I:47:ALA:HB2	4:I:146:ILE:HD13	1.83	0.59
2:G:179:ASP:OD2	3:H:48:ARG:NH2	2.36	0.59
2:N:309:ILE:O	2:N:313:ASN:ND2	2.35	0.58
2:F:173:THR:HG23	2:F:174:GLU:HG3	1.85	0.58
2:B:22:ASP:OD1	5:J:27:ARG:NH2	2.37	0.58
2:B:249:GLU:O	2:B:252:THR:OG1	2.21	0.58
3:H:143:THR:OG1	3:H:149:ARG:NH1	2.36	0.58
2:E:5:ILE:HG23	2:E:230:ILE:HB	1.86	0.58
2:S:64:ARG:HG3	2:S:65:THR:HG23	1.84	0.58
2:O:317:ASP:O	2:O:321:ASN:ND2	2.36	0.57
4:U:105:GLY:N	4:U:240:GLU:OE2	2.37	0.57
5:J:73:ARG:HB2	5:J:127:VAL:HG12	1.86	0.57
2:G:201:THR:HA	2:G:213:HIS:O	2.04	0.57
2:N:49:ARG:O	2:N:61:SER:OG	2.21	0.57
4:U:351:ARG:NH1	4:U:359:GLU:OE1	2.37	0.57
4:U:2:ASN:HB3	4:U:5:ILE:HG22	1.86	0.57
2:R:2:SER:HA	2:R:283:PHE:HB3	1.87	0.57
6:X:42:A:O2'	6:X:43:G:O5'	2.23	0.57
2:D:185:ALA:HB2	2:E:271:ALA:HB3	1.87	0.57
2:Q:64:ARG:HA	2:Q:112:THR:O	2.05	0.57
2:E:19:ASN:ND2	2:E:40:SER:H	2.03	0.56
2:O:214:LEU:HD11	6:X:39:A:N6	2.20	0.56
2:P:2:SER:OG	2:P:244:ARG:NH2	2.37	0.56
2:S:315:TYR:O	2:S:319:VAL:HB	2.06	0.56
5:W:49:TRP:O	5:W:51:ASN:N	2.37	0.56
2:G:202:ALA:HB3	2:G:213:HIS:HB3	1.88	0.56
4:I:488:LYS:NZ	2:Q:132:ASP:OD2	2.39	0.56
5:J:107:ARG:HH12	5:K:36:ASP:HB3	1.70	0.56
2:Q:202:ALA:HB3	2:Q:213:HIS:HB3	1.88	0.56
5:W:113:ASP:OD1	5:W:114:MET:N	2.39	0.56
2:B:99:SER:OG	2:B:101:ASP:OD1	2.22	0.55
2:G:20:ARG:NH2	6:L:11:G:OP2	2.40	0.55
4:I:343:LEU:HD21	4:I:345:LEU:HD12	1.88	0.55
2:S:288:LEU:HD11	3:T:156:PRO:HG3	1.88	0.55
2:R:69:ALA:HB2	2:R:106:ILE:H	1.70	0.55
2:O:185:ALA:HB2	2:P:271:ALA:HB3	1.88	0.55
5:V:28:VAL:O	5:V:118:ARG:NH2	2.39	0.55
4:I:108:ALA:HB3	4:I:265:LEU:HD22	1.89	0.55
2:G:256:HIS:HB2	2:G:354:LYS:HD3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:MET:HG2	2:B:176:GLY:HA3	1.88	0.55
2:F:64:ARG:HA	2:F:112:THR:O	2.06	0.55
2:P:1:MET:HG2	2:P:285:ASP:H	1.72	0.55
2:B:167:ALA:HB3	2:B:173:THR:HA	1.89	0.55
2:D:207:GLN:HE21	2:D:209:GLN:HB3	1.71	0.54
1:M:95:THR:HG22	1:M:113:ARG:HG2	1.88	0.54
5:J:102:ILE:O	5:J:106:ILE:HG12	2.06	0.54
2:Q:201:THR:HA	2:Q:213:HIS:O	2.08	0.54
2:R:249:GLU:O	2:R:252:THR:OG1	2.24	0.54
1:A:8:ILE:HD11	1:A:23:LEU:HG	1.89	0.54
5:K:106:ILE:HG23	5:K:145:ARG:HB3	1.88	0.54
2:S:329:ALA:HB3	2:S:344:VAL:HG12	1.89	0.54
2:G:320:ALA:HA	2:G:325:LEU:HD23	1.89	0.54
2:C:95:LEU:HD22	2:C:172:MET:HE2	1.90	0.54
2:D:296:LYS:HG3	2:E:302:ASP:HB3	1.90	0.54
2:F:341:THR:O	2:F:344:VAL:HG12	2.07	0.54
2:N:12:SER:HA	2:N:222:GLY:O	2.08	0.54
4:U:434:VAL:O	4:U:438:VAL:HG13	2.08	0.54
2:E:111:VAL:HG21	2:F:202:ALA:HB1	1.89	0.54
2:R:70:GLN:N	2:R:70:GLN:OE1	2.41	0.54
2:C:2:SER:OG	2:C:244:ARG:NH2	2.39	0.54
2:G:240:GLY:HA2	2:G:241:GLY:C	2.33	0.54
2:N:268:ARG:NH1	2:N:274:ASN:O	2.41	0.54
2:S:318:ARG:HG3	2:S:319:VAL:HG23	1.90	0.54
4:U:47:ALA:HB2	4:U:146:ILE:HD13	1.89	0.54
2:B:36:ARG:NH2	2:B:294:PHE:O	2.35	0.53
4:I:143:CYS:HB3	4:I:253:CYS:SG	2.47	0.53
4:I:194:ARG:NE	4:I:333:GLN:HG3	2.23	0.53
2:Q:185:ALA:HB2	2:R:271:ALA:HB3	1.90	0.53
1:A:83:PRO:HB2	1:A:199:LEU:HD21	1.89	0.53
4:I:174:THR:HB	4:I:345:LEU:HD21	1.90	0.53
4:I:351:ARG:NH1	4:I:359:GLU:OE1	2.41	0.53
2:P:256:HIS:HB2	2:P:354:LYS:HD3	1.91	0.53
2:Q:132:ASP:H	2:Q:133:ASN:HA	1.73	0.53
2:N:305:LEU:O	2:N:309:ILE:HG12	2.09	0.53
2:P:1:MET:HE1	2:P:325:LEU:HD22	1.91	0.53
2:F:192:GLN:NE2	5:K:109:ASP:OD2	2.42	0.53
2:O:205:ASP:O	2:O:206:LEU:HB2	2.08	0.53
4:I:167:ARG:HH12	4:I:173:THR:HG22	1.74	0.52
1:A:1:MET:HE3	1:A:74:VAL:HG23	1.92	0.52
2:E:173:THR:HG23	2:E:174:GLU:HG2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:151:GLN:HA	4:I:155:ALA:HB3	1.91	0.52
2:Q:157:GLY:O	2:Q:159:ASP:N	2.42	0.52
2:D:214:LEU:O	5:J:100:ARG:NH2	2.42	0.52
2:N:18:LEU:HD22	2:N:39:ILE:HD11	1.91	0.52
4:U:226:ILE:O	4:U:230:ARG:HB3	2.10	0.52
2:E:309:ILE:HG21	2:E:337:VAL:HG21	1.90	0.52
2:N:23:MET:HE1	5:V:24:GLN:HA	1.92	0.52
2:F:41:SER:HB2	2:F:184:ILE:HG23	1.91	0.52
2:G:316:TRP:O	2:G:320:ALA:HB2	2.09	0.52
1:A:32:ASP:N	1:A:33:ALA:HA	2.25	0.52
2:B:49:ARG:O	2:B:61:SER:OG	2.25	0.52
2:C:115:VAL:HG23	2:C:118:GLU:HB2	1.91	0.52
2:F:5:ILE:HG23	2:F:230:ILE:HB	1.92	0.52
2:R:9:VAL:HB	2:R:226:ARG:HB2	1.90	0.52
1:A:113:ARG:NH2	6:L:59:G:O6	2.38	0.52
5:J:28:VAL:O	5:J:118:ARG:NH2	2.43	0.52
4:U:101:MET:HE1	4:U:149:PHE:CD1	2.45	0.52
2:B:66:ILE:HA	2:B:110:ALA:HB3	1.91	0.51
2:C:9:VAL:HG22	2:C:279:VAL:HG22	1.92	0.51
2:Q:39:ILE:HB	2:Q:187:ALA:HB3	1.92	0.51
4:U:174:THR:HB	4:U:345:LEU:HD21	1.92	0.51
2:B:269:THR:HG23	2:B:270:TYR:HD1	1.74	0.51
4:U:343:LEU:HD21	4:U:345:LEU:HD12	1.93	0.51
5:J:146:GLN:O	5:J:150:GLU:HG3	2.11	0.51
2:G:100:VAL:C	2:G:102:GLU:HB3	2.34	0.51
5:J:29:SER:OG	5:J:33:GLU:OE1	2.27	0.51
6:L:54:C:H4'	6:L:55:A:OP2	2.09	0.51
2:O:325:LEU:HD23	2:O:327:GLY:H	1.75	0.51
2:D:210:GLY:HA2	2:D:211:SER:C	2.36	0.51
2:Q:115:VAL:HG23	2:Q:118:GLU:HB2	1.91	0.51
2:C:323:TYR:OH	2:D:276:ALA:O	2.28	0.51
2:B:1:MET:HB3	2:B:284:SER:HA	1.91	0.51
2:C:256:HIS:HB2	2:C:354:LYS:HD3	1.93	0.51
4:I:2:ASN:HB3	4:I:5:ILE:HG12	1.93	0.51
2:Q:111:VAL:HG21	2:R:202:ALA:HB1	1.93	0.51
2:S:61:SER:HB3	2:S:158:VAL:HG21	1.93	0.51
4:U:409:LYS:O	4:U:478:THR:OG1	2.23	0.51
2:C:201:THR:HG22	2:C:214:LEU:HG	1.93	0.51
2:E:94:LEU:HB3	2:E:171:MET:HE2	1.92	0.51
4:I:434:VAL:O	4:I:438:VAL:HG13	2.11	0.51
3:T:51:THR:HG23	3:T:202:ILE:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:73:ARG:HB2	5:W:127:VAL:HG12	1.93	0.51
2:C:19:ASN:ND2	2:C:40:SER:H	2.09	0.50
2:D:30:ILE:O	2:E:221:SER:OG	2.29	0.50
2:E:282:ASN:OD1	2:E:326:ASN:ND2	2.43	0.50
2:R:216:THR:HG21	5:W:100:ARG:HG3	1.93	0.50
4:U:353:ASN:O	4:U:356:SER:OG	2.28	0.50
2:R:22:ASP:HB3	2:S:199:TRP:CD2	2.46	0.50
4:U:7:ASN:HB2	4:U:21:ILE:HG22	1.93	0.50
2:C:155:GLN:HG2	2:C:239:LEU:HD22	1.93	0.50
2:D:148:ALA:O	2:D:152:VAL:HG23	2.11	0.50
2:G:112:THR:HG23	2:G:238:ASN:HA	1.93	0.50
2:S:240:GLY:HA2	2:S:241:GLY:C	2.36	0.50
4:I:409:LYS:O	4:I:478:THR:OG1	2.20	0.50
5:K:102:ILE:O	5:K:106:ILE:HG12	2.11	0.50
6:L:56:G:O2'	6:L:57:C:H5'	2.11	0.50
5:W:10:LEU:HD23	5:W:61:MET:HE2	1.92	0.50
2:G:318:ARG:HG3	2:G:319:VAL:HG23	1.92	0.50
2:N:115:VAL:HG11	2:N:157:GLY:HA3	1.94	0.50
2:P:323:TYR:OH	2:Q:276:ALA:O	2.30	0.50
3:T:123:THR:HG23	3:T:125:HIS:N	2.27	0.50
4:U:101:MET:HE1	4:U:149:PHE:HD1	1.75	0.50
4:U:170:THR:HG21	4:U:352:ASN:HB2	1.92	0.50
2:G:316:TRP:O	2:G:320:ALA:CB	2.59	0.50
4:I:142:GLY:O	4:I:146:ILE:HG13	2.12	0.50
2:Q:288:LEU:HD22	2:Q:325:LEU:HD11	1.93	0.50
3:H:51:THR:HG23	3:H:202:ILE:HG22	1.93	0.50
4:I:68:ARG:NH1	4:I:337:ILE:O	2.45	0.50
2:P:341:THR:O	2:P:343:GLN:N	2.40	0.50
2:B:252:THR:HG22	2:B:357:VAL:HB	1.94	0.50
2:P:69:ALA:HB2	2:P:106:ILE:H	1.77	0.50
4:U:307:TRP:HA	4:U:310:ILE:HG13	1.94	0.50
2:R:185:ALA:HB2	2:S:271:ALA:HB3	1.94	0.49
2:F:21:ASP:N	2:F:25:MET:O	2.44	0.49
4:I:143:CYS:CB	4:I:253:CYS:SG	3.00	0.49
2:N:249:GLU:O	2:N:252:THR:OG1	2.23	0.49
2:O:42:GLN:HG2	6:X:31:U:H2'	1.94	0.49
4:U:142:GLY:O	4:U:146:ILE:HG13	2.12	0.49
2:O:42:GLN:HB3	6:X:31:U:H3'	1.94	0.49
2:R:21:ASP:N	2:R:25:MET:O	2.46	0.49
2:B:97:GLY:N	2:B:169:SER:O	2.46	0.49
4:U:277:TRP:HZ3	4:U:279:HIS:CD2	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:76:ARG:NH1	2:F:102:GLU:OE1	2.43	0.49
2:E:22:ASP:OD1	5:K:101:ARG:NH2	2.45	0.49
2:G:199:TRP:CH2	2:G:214:LEU:HD22	2.48	0.49
2:N:335:SER:O	2:N:337:VAL:N	2.40	0.49
2:R:1:MET:HB3	2:R:284:SER:HA	1.93	0.49
2:F:288:LEU:HD21	2:F:290:MET:HE3	1.95	0.49
2:F:67:HIS:CD2	2:G:207:GLN:HG2	2.48	0.48
5:J:150:GLU:O	5:J:154:LEU:HB2	2.12	0.48
2:O:16:SER:OG	2:O:17:CYS:N	2.46	0.48
2:O:249:GLU:O	2:O:252:THR:OG1	2.25	0.48
2:Q:5:ILE:HG23	2:Q:230:ILE:HB	1.94	0.48
2:G:167:ALA:N	6:L:6:C:O2'	2.45	0.48
2:N:274:ASN:OD1	2:N:274:ASN:N	2.46	0.48
2:Q:100:VAL:HG12	2:Q:106:ILE:HD11	1.95	0.48
2:B:153:ASN:OD1	2:B:156:GLN:NE2	2.46	0.48
2:G:149:ALA:HB1	2:G:170:GLY:HA3	1.94	0.48
4:I:216:LYS:O	4:I:219:GLU:HB2	2.14	0.48
1:A:151:GLY:HA2	1:A:152:ASP:C	2.36	0.48
2:B:37:VAL:HG23	2:B:193:VAL:HG21	1.95	0.48
5:K:97:ILE:HD12	5:K:120:LEU:HD22	1.95	0.48
2:P:69:ALA:HB1	2:P:104:GLU:HA	1.94	0.48
2:B:96:SER:H	2:B:97:GLY:HA2	1.78	0.48
2:G:96:SER:HB2	2:G:98:LYS:N	2.24	0.48
4:I:290:LYS:N	4:I:291:GLY:CA	2.76	0.48
5:W:35:ARG:NH2	5:W:55:GLN:OE1	2.46	0.48
2:D:256:HIS:HB2	2:D:354:LYS:HD3	1.96	0.48
1:A:10:ARG:HD2	1:A:46:THR:HG21	1.96	0.48
2:B:30:ILE:O	2:C:221:SER:OG	2.32	0.48
4:I:30:SER:OG	4:I:32:ASP:OD1	2.30	0.48
2:F:22:ASP:HB3	2:G:199:TRP:CD2	2.49	0.48
2:G:165:ARG:O	6:L:6:C:O2'	2.22	0.48
2:D:280:MET:HE1	2:D:316:TRP:CE2	2.48	0.48
2:R:295:GLU:OE1	2:S:304:PHE:N	2.43	0.48
2:S:116:VAL:O	2:S:120:ALA:HB2	2.14	0.48
3:T:89:LEU:HA	3:T:90:GLY:HA2	1.62	0.48
2:C:41:SER:HB2	2:C:184:ILE:HG23	1.95	0.47
2:F:72:ARG:HD3	2:F:100:VAL:HG13	1.96	0.47
2:F:144:LYS:NZ	2:F:174:GLU:HB3	2.28	0.47
4:U:245:ILE:HG12	4:U:246:GLY:H	1.79	0.47
5:V:38:PRO:HA	5:V:41:TYR:HD2	1.79	0.47
2:B:151:ARG:NH2	2:B:175:LEU:O	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:476:ILE:HA	4:I:479:LEU:HG	1.96	0.47
2:N:172:MET:O	2:N:176:GLY:N	2.37	0.47
5:W:47:PHE:N	5:W:48:GLY:HA2	2.30	0.47
2:C:19:ASN:ND2	2:C:27:LYS:HD2	2.30	0.47
2:C:132:ASP:N	2:C:133:ASN:HA	2.29	0.47
4:I:36:LEU:HD11	4:I:181:LEU:HD13	1.96	0.47
1:M:97:LEU:HD23	1:M:111:ARG:HG2	1.96	0.47
2:E:185:ALA:HB2	2:F:271:ALA:HB3	1.95	0.47
4:I:3:LEU:HB2	4:I:91:PHE:HB3	1.96	0.47
2:B:4:PHE:HB2	2:B:284:SER:O	2.15	0.47
2:D:132:ASP:N	2:D:133:ASN:HA	2.29	0.47
2:C:1:MET:HB3	2:C:284:SER:HA	1.96	0.47
4:I:119:ALA:O	4:I:360:ARG:NH2	2.48	0.47
1:M:86:PHE:HA	1:M:195:SER:O	2.14	0.47
2:O:20:ARG:NH1	2:O:24:ASN:OD1	2.48	0.47
2:P:6:ASN:HB2	2:P:282:ASN:ND2	2.30	0.47
2:R:64:ARG:HA	2:R:112:THR:O	2.14	0.47
3:T:148:ARG:HG2	6:X:4:A:H5'	1.96	0.47
2:B:108:ALA:C	2:B:110:ALA:H	2.22	0.47
2:F:249:GLU:O	2:F:252:THR:OG1	2.33	0.47
2:B:110:ALA:HB1	2:B:111:VAL:CA	2.45	0.47
2:B:274:ASN:OD1	2:B:274:ASN:N	2.45	0.47
2:G:75:LEU:HD13	2:G:119:ILE:HD13	1.96	0.47
2:N:269:THR:HG23	2:N:270:TYR:HD1	1.80	0.47
5:W:97:ILE:HD12	5:W:120:LEU:HD22	1.97	0.47
2:C:249:GLU:O	2:C:252:THR:OG1	2.26	0.47
2:G:88:ILE:O	2:G:91:THR:OG1	2.30	0.47
6:X:56:G:O2'	6:X:57:C:H5'	2.14	0.47
2:B:248:LEU:O	2:B:252:THR:HG23	2.15	0.46
2:D:2:SER:OG	2:D:244:ARG:NH2	2.48	0.46
5:K:106:ILE:HD12	5:K:145:ARG:HB3	1.97	0.46
2:N:69:ALA:O	2:N:72:ARG:HG2	2.15	0.46
2:P:249:GLU:O	2:P:252:THR:OG1	2.21	0.46
3:H:123:THR:HG23	3:H:125:HIS:N	2.31	0.46
4:I:268:LYS:NZ	2:R:132:ASP:OD2	2.44	0.46
2:R:252:THR:HG22	2:R:357:VAL:HB	1.97	0.46
2:O:123:CYS:HA	2:O:126:VAL:HG12	1.96	0.46
4:I:307:TRP:HA	4:I:310:ILE:HG13	1.96	0.46
2:P:185:ALA:HB2	2:Q:271:ALA:HB3	1.96	0.46
2:N:39:ILE:HB	2:N:187:ALA:HB3	1.98	0.46
2:O:156:GLN:HA	2:O:157:GLY:HA2	1.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:236:GLN:NE2	2:S:242:ALA:O	2.46	0.46
4:U:447:ILE:O	4:U:451:ARG:HG3	2.15	0.46
2:E:285:ASP:OD2	2:E:285:ASP:N	2.37	0.46
2:F:72:ARG:NH2	2:F:103:ALA:O	2.40	0.46
5:K:32:ASP:O	5:K:35:ARG:HB2	2.16	0.46
2:F:39:ILE:HB	2:F:187:ALA:HB3	1.98	0.46
2:S:91:THR:HG21	2:S:123:CYS:HA	1.98	0.46
4:U:226:ILE:HD11	4:U:277:TRP:CE2	2.51	0.46
5:J:52:PRO:HA	5:J:55:GLN:HG3	1.98	0.46
5:V:10:LEU:HD23	5:V:61:MET:HE2	1.98	0.46
4:I:446:VAL:HA	4:I:449:ASP:OD2	2.16	0.45
2:P:27:LYS:NZ	2:Q:198:ASP:OD1	2.44	0.45
2:R:64:ARG:HG2	2:R:113:PRO:HB3	1.97	0.45
2:S:71:LEU:HD22	2:S:111:VAL:HG22	1.97	0.45
2:E:180:GLY:HA3	2:E:181:ALA:HA	1.67	0.45
2:G:30:ILE:HD12	3:H:80:THR:HG21	1.98	0.45
5:J:150:GLU:HG2	5:K:41:TYR:CE1	2.51	0.45
2:N:248:LEU:O	2:N:252:THR:HG23	2.16	0.45
5:V:105:LEU:HD22	5:V:120:LEU:HD12	1.97	0.45
2:E:22:ASP:HB3	2:F:214:LEU:HD22	1.99	0.45
2:E:39:ILE:HB	2:E:187:ALA:HB3	1.99	0.45
3:H:148:ARG:HG2	6:L:4:A:H5''	1.98	0.45
2:P:21:ASP:N	2:P:25:MET:O	2.50	0.45
2:S:286:MET:HA	2:S:287:PRO:HD3	1.86	0.45
5:W:25:ILE:HG23	5:W:34:LEU:HD11	1.99	0.45
2:C:30:ILE:O	2:D:221:SER:OG	2.34	0.45
2:C:39:ILE:HB	2:C:187:ALA:HB3	1.98	0.45
4:I:208:GLN:O	4:I:230:ARG:NH1	2.43	0.45
4:I:235:GLN:HA	4:I:236:PRO:HD3	1.81	0.45
4:U:232:LEU:HD12	4:U:277:TRP:HH2	1.82	0.45
5:V:63:PHE:O	5:V:66:SER:OG	2.26	0.45
2:B:305:LEU:O	2:B:309:ILE:HG13	2.16	0.45
2:D:69:ALA:HB2	2:D:106:ILE:H	1.82	0.45
2:G:166:MET:C	2:G:168:THR:H	2.24	0.45
4:I:243:ASP:HA	4:I:244:PRO:HD3	1.79	0.45
4:I:474:LYS:HE2	4:I:474:LYS:HB3	1.74	0.45
5:K:151:ASP:O	5:K:155:THR:OG1	2.26	0.45
6:L:32:U:H2'	6:L:33:G:H4'	1.98	0.45
2:E:97:GLY:HA2	2:E:98:LYS:HA	1.67	0.45
2:F:76:ARG:HH12	2:F:102:GLU:CD	2.24	0.45
1:M:116:LEU:HD13	1:M:121:GLU:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:HIS:HB2	2:B:219:PHE:HB3	1.98	0.45
2:E:4:PHE:HB2	2:E:284:SER:O	2.17	0.45
4:I:99:PRO:HG2	4:I:102:GLN:HB2	1.99	0.45
3:T:205:PRO:HA	3:T:206:ARG:HA	1.59	0.45
2:D:21:ASP:N	2:D:25:MET:O	2.46	0.45
5:J:153:VAL:HG21	5:K:38:PRO:HB3	1.98	0.45
2:Q:252:THR:HG21	2:Q:358:ARG:HG3	1.98	0.45
2:D:252:THR:HG22	2:D:357:VAL:HB	1.99	0.45
2:G:180:GLY:HA3	2:G:181:ALA:HA	1.73	0.45
2:B:36:ARG:HD3	2:B:189:THR:O	2.17	0.44
3:H:197:ARG:NH1	4:I:38:LEU:O	2.50	0.44
5:K:25:ILE:HG23	5:K:34:LEU:HD11	1.98	0.44
2:D:39:ILE:HB	2:D:187:ALA:HB3	2.00	0.44
2:G:67:HIS:HB2	2:G:70:GLN:HG3	1.99	0.44
2:Q:30:ILE:O	2:R:221:SER:OG	2.34	0.44
3:T:108:ARG:NH2	6:X:7:C:O2	2.50	0.44
4:U:112:THR:HG21	4:U:266:LYS:HE2	2.00	0.44
2:D:20:ARG:NH2	6:L:29:G:OP2	2.50	0.44
2:N:64:ARG:HA	2:N:112:THR:O	2.17	0.44
3:T:16:TRP:CG	3:T:31:PRO:HA	2.53	0.44
3:T:82:LEU:HB2	3:T:110:TYR:HB2	1.99	0.44
2:C:305:LEU:O	2:C:309:ILE:HG12	2.17	0.44
4:U:45:LEU:HD23	4:U:154:GLN:HE22	1.83	0.44
6:X:32:U:H2'	6:X:33:G:H4'	2.00	0.44
1:A:99:ASN:OD1	1:A:100:GLN:N	2.50	0.44
4:I:180:ASP:OD1	4:I:181:LEU:N	2.51	0.44
3:H:205:PRO:HA	3:H:206:ARG:HA	1.57	0.44
2:E:252:THR:HG22	2:E:357:VAL:HB	1.98	0.44
2:G:160:ILE:HG22	2:G:178:VAL:HG11	1.99	0.44
4:I:3:LEU:O	4:I:8:TRP:NE1	2.50	0.44
4:I:80:PHE:CE2	4:I:84:ILE:HD13	2.53	0.44
2:P:252:THR:HG22	2:P:357:VAL:HB	2.00	0.44
2:R:155:GLN:OE1	2:R:246:GLN:NE2	2.48	0.44
1:A:24:TRP:CH2	1:A:34:ALA:HB3	2.53	0.44
2:B:108:ALA:O	2:B:110:ALA:N	2.49	0.44
2:C:123:CYS:HA	2:C:126:VAL:HG12	2.00	0.44
5:K:73:ARG:HB2	5:K:127:VAL:HG12	1.99	0.44
2:N:109:ASP:OD2	2:N:169:SER:OG	2.31	0.44
2:N:252:THR:HG22	2:N:357:VAL:HB	2.00	0.44
2:P:65:THR:HG21	2:Q:206:LEU:HD12	1.98	0.44
2:S:20:ARG:NH2	6:X:11:G:OP2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:75:LEU:HD22	2:S:119:ILE:HD11	2.00	0.44
2:S:194:ASP:HB3	4:U:471:HIS:CD2	2.53	0.44
2:O:21:ASP:N	2:O:25:MET:O	2.49	0.44
2:S:199:TRP:CH2	2:S:214:LEU:HD22	2.53	0.44
3:T:32:THR:HB	3:T:198:ASP:HB2	1.98	0.44
4:U:35:ARG:HD2	4:U:35:ARG:HA	1.74	0.44
4:I:235:GLN:HG2	4:I:237:ALA:H	1.82	0.43
5:K:52:PRO:HA	5:K:55:GLN:HG3	2.00	0.43
2:R:100:VAL:HA	2:R:106:ILE:HD12	1.98	0.43
2:S:158:VAL:HG12	2:S:239:LEU:HD11	1.99	0.43
2:B:7:ILE:HB	2:B:228:ALA:HB3	2.00	0.43
2:F:342:ALA:HA	2:F:343:GLN:HA	1.57	0.43
3:T:82:LEU:O	3:T:109:GLU:HA	2.18	0.43
4:U:368:ASN:O	4:U:371:TRP:HD1	2.01	0.43
2:E:305:LEU:O	2:E:309:ILE:HG12	2.19	0.43
2:F:283:PHE:HB2	2:F:328:ALA:HB1	2.01	0.43
2:G:241:GLY:HA3	2:G:242:ALA:HB2	2.00	0.43
4:I:208:GLN:HA	4:I:209:PRO:HD3	1.89	0.43
2:Q:113:PRO:HG2	2:Q:165:ARG:HD3	2.00	0.43
2:B:132:ASP:H	2:B:133:ASN:HA	1.82	0.43
2:B:296:LYS:HG3	2:C:302:ASP:HB3	2.00	0.43
2:C:84:ASP:HB3	2:C:87:ILE:HG12	2.01	0.43
2:E:21:ASP:N	2:E:25:MET:O	2.52	0.43
2:F:22:ASP:HA	6:L:15:U:H5	1.83	0.43
2:O:97:GLY:HA2	2:O:98:LYS:HA	1.59	0.43
3:T:25:ARG:HH21	4:U:130:VAL:HB	1.83	0.43
4:U:141:GLY:O	4:U:144:THR:HG22	2.19	0.43
5:V:25:ILE:HG23	5:V:34:LEU:HD11	1.99	0.43
2:D:249:GLU:O	2:D:252:THR:OG1	2.25	0.43
2:E:148:ALA:O	2:E:152:VAL:HG23	2.18	0.43
2:S:201:THR:HA	2:S:213:HIS:O	2.18	0.43
4:U:151:GLN:HA	4:U:155:ALA:HB3	2.01	0.43
6:X:46:C:C2'	6:X:47:C:H5'	2.49	0.43
2:S:179:ASP:OD1	2:S:179:ASP:N	2.50	0.43
4:U:243:ASP:HA	4:U:244:PRO:HD3	1.85	0.43
2:S:241:GLY:HA3	2:S:242:ALA:HB2	1.99	0.43
4:U:235:GLN:HA	4:U:236:PRO:HD3	1.80	0.43
5:V:151:ASP:O	5:V:155:THR:OG1	2.33	0.43
2:B:292:ASN:HD21	2:C:274:ASN:HB3	1.83	0.43
3:H:38:GLY:HA3	6:L:2:U:O4'	2.19	0.43
4:I:377:VAL:O	4:I:381:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:114:VAL:HB	6:X:43:G:H2'	2.01	0.43
1:A:86:PHE:HA	1:A:195:SER:O	2.19	0.43
2:B:235:LEU:HD23	2:B:247:ALA:HB1	2.01	0.43
2:C:10:LEU:HB2	2:C:278:MET:HE2	2.00	0.43
2:D:115:VAL:HG11	2:D:157:GLY:HA3	1.99	0.43
2:D:252:THR:HG21	2:D:358:ARG:HG3	2.00	0.43
2:D:347:MET:HE3	2:D:352:GLN:HB3	2.01	0.43
3:T:130:ILE:HD12	3:T:133:LEU:HD12	2.01	0.43
2:D:277:ASP:CG	2:D:305:LEU:HD21	2.45	0.42
2:E:115:VAL:HG23	2:E:118:GLU:HB2	2.00	0.42
2:F:111:VAL:HG21	2:G:202:ALA:HB1	2.00	0.42
4:I:245:ILE:HD11	4:I:260:ARG:NH2	2.34	0.42
2:P:248:LEU:HD23	2:P:357:VAL:O	2.19	0.42
4:U:245:ILE:N	4:U:260:ARG:O	2.46	0.42
3:H:16:TRP:CG	3:H:31:PRO:HA	2.53	0.42
2:P:111:VAL:HG21	2:Q:202:ALA:HB1	2.00	0.42
2:Q:97:GLY:HA3	2:Q:98:LYS:HD2	2.01	0.42
2:C:111:VAL:HG21	2:D:202:ALA:HB1	2.01	0.42
2:C:148:ALA:O	2:C:152:VAL:HG23	2.19	0.42
2:D:70:GLN:HB2	2:E:206:LEU:HD13	2.01	0.42
4:I:245:ILE:HD11	4:I:260:ARG:HH2	1.85	0.42
2:N:309:ILE:HG22	2:N:313:ASN:HD21	1.84	0.42
4:U:185:VAL:O	4:U:189:VAL:HG23	2.19	0.42
1:A:8:ILE:O	1:A:49:GLY:CA	2.56	0.42
2:B:121:TRP:O	2:B:125:GLN:HG2	2.20	0.42
2:G:22:ASP:HA	6:L:9:A:N7	2.33	0.42
2:N:235:LEU:HD23	2:N:247:ALA:HB1	2.01	0.42
2:N:251:ALA:O	2:N:255:VAL:HG23	2.20	0.42
3:T:31:PRO:HD2	3:T:65:VAL:HG11	1.99	0.42
2:E:30:ILE:O	2:F:221:SER:OG	2.37	0.42
4:I:40:ARG:NH2	4:I:119:ALA:O	2.51	0.42
2:S:10:LEU:HB2	2:S:278:MET:HE3	2.01	0.42
2:E:274:ASN:HA	2:E:275:PRO:HD3	1.91	0.42
4:I:247:ILE:HG13	4:I:258:ASN:HA	2.00	0.42
4:I:447:ILE:O	4:I:451:ARG:HG3	2.18	0.42
2:R:23:MET:HE3	4:U:474:LYS:HG3	2.02	0.42
3:T:190:HIS:CE1	3:T:216:ILE:HG23	2.55	0.42
2:N:58:ILE:CG2	2:N:158:VAL:HG21	2.48	0.42
2:N:292:ASN:HD21	2:O:274:ASN:HB3	1.85	0.42
2:Q:76:ARG:HH22	2:Q:101:ASP:HA	1.85	0.42
3:H:146:LEU:HA	3:H:147:GLY:HA2	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:118:ARG:HA	5:J:121:LEU:HD12	2.02	0.42
2:O:9:VAL:HG22	2:O:279:VAL:HG22	2.01	0.42
2:Q:345:LYS:HE3	2:Q:345:LYS:HB2	1.85	0.42
3:T:211:ARG:HG2	3:T:212:GLU:H	1.85	0.42
4:U:138:ALA:HB1	4:U:260:ARG:HH21	1.84	0.42
2:G:315:TYR:CE1	2:G:319:VAL:HG21	2.55	0.42
2:B:54:TYR:CD2	2:B:58:ILE:HD12	2.54	0.42
4:I:138:ALA:HB1	4:I:260:ARG:HH21	1.84	0.42
5:J:51:ASN:HA	5:J:52:PRO:HD3	1.88	0.42
2:P:304:PHE:O	2:P:308:SER:OG	2.33	0.42
2:Q:10:LEU:HB2	2:Q:278:MET:HE2	2.02	0.42
2:R:67:HIS:HB3	2:R:70:GLN:OE1	2.20	0.42
2:S:46:ARG:NH2	3:T:89:LEU:HD11	2.34	0.42
2:S:338:ASP:OD1	2:S:339:PRO:HD2	2.20	0.42
6:X:41:G:O2'	6:X:42:A:H5'	2.19	0.42
6:X:42:A:HO2'	6:X:43:G:P	2.43	0.42
2:B:45:LYS:O	2:B:49:ARG:HG3	2.19	0.41
2:C:244:ARG:O	2:C:248:LEU:HD12	2.20	0.41
2:F:337:VAL:C	2:F:339:PRO:HD3	2.45	0.41
2:G:305:LEU:O	2:G:309:ILE:HG12	2.20	0.41
4:I:36:LEU:CD1	4:I:181:LEU:HD13	2.49	0.41
5:J:154:LEU:HD23	5:J:154:LEU:HA	1.85	0.41
2:O:113:PRO:HB2	2:O:160:ILE:HD11	2.01	0.41
4:U:56:GLN:HA	4:U:189:VAL:HG13	2.01	0.41
2:B:5:ILE:CG2	2:B:230:ILE:HB	2.50	0.41
2:B:19:ASN:ND2	2:B:27:LYS:HD2	2.36	0.41
2:O:93:ALA:HA	2:O:97:GLY:HA2	2.02	0.41
2:O:305:LEU:O	2:O:309:ILE:HG12	2.20	0.41
2:Q:252:THR:HG22	2:Q:357:VAL:HB	2.02	0.41
2:R:304:PHE:O	2:R:308:SER:OG	2.30	0.41
4:U:177:ARG:HA	4:U:184:THR:HG23	2.01	0.41
4:U:236:PRO:HB3	4:U:271:PHE:HZ	1.85	0.41
2:B:180:GLY:HA3	2:B:181:ALA:HA	1.79	0.41
2:E:212:ALA:HB2	6:L:27:U:H3	1.85	0.41
2:G:173:THR:HG23	2:G:176:GLY:H	1.85	0.41
1:M:99:ASN:N	6:X:44:U:O4	2.38	0.41
2:R:354:LYS:O	2:R:358:ARG:HG3	2.21	0.41
2:S:292:ASN:H	3:T:154:THR:HG21	1.85	0.41
4:I:7:ASN:HB3	4:I:21:ILE:HG22	2.02	0.41
2:Q:1:MET:HA	2:Q:285:ASP:N	2.35	0.41
2:B:2:SER:O	2:B:3:ASN:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:22:ASP:OD1	2:C:22:ASP:N	2.50	0.41
2:E:314:GLN:HA	2:E:340:ILE:HD11	2.02	0.41
2:G:84:ASP:HB2	2:G:87:ILE:HD13	2.02	0.41
2:Q:45:LYS:O	2:Q:49:ARG:HG3	2.20	0.41
4:U:80:PHE:CZ	4:U:84:ILE:HD13	2.56	0.41
2:G:6:ASN:ND2	2:G:284:SER:OG	2.50	0.41
4:I:39:PRO:HG3	4:I:252:CYS:O	2.21	0.41
2:P:40:SER:HB2	2:P:42:GLN:OE1	2.20	0.41
2:S:315:TYR:CE1	2:S:319:VAL:HG21	2.55	0.41
3:T:14:GLN:HA	3:T:146:LEU:O	2.20	0.41
1:A:93:ILE:HG12	1:A:185:PRO:HG2	2.01	0.41
2:D:19:ASN:OD1	2:D:27:LYS:HD2	2.21	0.41
2:G:204:ASP:HB3	2:G:207:GLN:HG3	2.01	0.41
2:N:306:GLN:OE1	2:N:336:ASP:HA	2.21	0.41
2:R:40:SER:HB2	2:R:42:GLN:OE1	2.20	0.41
4:U:180:ASP:OD1	4:U:181:LEU:N	2.53	0.41
1:A:30:ARG:HA	1:A:31:PRO:HA	1.66	0.41
2:B:66:ILE:HD12	2:B:110:ALA:O	2.21	0.41
2:F:286:MET:HE1	2:G:261:GLU:HA	2.03	0.41
2:B:256:HIS:HB2	2:B:354:LYS:HD3	2.01	0.41
2:B:347:MET:HA	2:B:348:PRO:HD3	1.88	0.41
2:C:5:ILE:HG23	2:C:230:ILE:HB	2.02	0.41
2:F:305:LEU:O	2:F:309:ILE:HG12	2.21	0.41
2:G:325:LEU:HD13	2:G:325:LEU:HA	1.87	0.41
4:I:231:GLY:HA3	4:I:277:TRP:CZ2	2.55	0.41
1:M:83:PRO:HB2	1:M:199:LEU:HD11	2.03	0.41
1:M:110:LYS:NZ	6:X:46:C:H5 ⁷	2.35	0.41
1:M:140:HIS:HB2	2:N:219:PHE:HB3	2.03	0.41
2:N:262:VAL:HB	2:N:266:LYS:O	2.19	0.41
2:N:278:MET:HE3	2:N:331:GLN:HE21	1.86	0.41
2:O:63:LEU:HD11	2:O:71:LEU:HD13	2.01	0.41
2:O:76:ARG:NE	2:O:85:GLN:OE1	2.53	0.41
2:O:252:THR:HG22	2:O:357:VAL:HB	2.02	0.41
2:P:4:PHE:HB2	2:P:284:SER:O	2.21	0.41
2:P:30:ILE:O	2:Q:221:SER:OG	2.36	0.41
2:Q:305:LEU:O	2:Q:309:ILE:HG12	2.21	0.41
2:R:148:ALA:O	2:R:152:VAL:HG23	2.20	0.41
2:R:235:LEU:HD23	2:R:247:ALA:HB1	2.02	0.41
2:C:16:SER:HB3	2:C:272:ALA:HB2	2.03	0.41
3:H:31:PRO:HD2	3:H:65:VAL:HG11	2.03	0.41
2:O:70:GLN:HB2	2:P:206:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:148:ALA:O	2:P:152:VAL:HG23	2.21	0.41
2:Q:1:MET:N	2:Q:285:ASP:OD1	2.53	0.41
2:R:68:LEU:HD11	2:R:108:ALA:HB2	2.03	0.41
3:T:123:THR:HG23	3:T:125:HIS:H	1.86	0.41
1:M:87:ARG:HA	1:M:163:PHE:O	2.21	0.40
2:N:65:THR:OG1	2:N:66:ILE:N	2.54	0.40
2:F:252:THR:HG22	2:F:357:VAL:HB	2.03	0.40
2:G:75:LEU:HD22	2:G:119:ILE:HD11	2.02	0.40
4:I:213:LYS:HA	4:I:214:PRO:HD3	1.87	0.40
4:I:244:PRO:HG3	4:I:261:TYR:CE2	2.56	0.40
2:O:9:VAL:HB	2:O:226:ARG:HB2	2.02	0.40
2:P:248:LEU:O	2:P:252:THR:HG23	2.21	0.40
2:R:244:ARG:HE	2:R:360:ASN:ND2	2.19	0.40
2:S:342:ALA:O	2:S:344:VAL:HG22	2.20	0.40
2:C:18:LEU:HB3	2:C:263:PRO:HG2	2.04	0.40
4:I:185:VAL:O	4:I:189:VAL:HG23	2.22	0.40
4:I:298:LEU:HD21	4:I:309:GLN:HE21	1.86	0.40
6:L:46:C:C2'	6:L:47:C:H5'	2.50	0.40
1:M:142:ILE:HB	1:M:162:CYS:HB3	2.03	0.40
2:Q:97:GLY:HA2	2:Q:98:LYS:HA	1.70	0.40
5:V:41:TYR:O	5:V:45:GLN:HB2	2.22	0.40
2:C:354:LYS:O	2:C:358:ARG:HG3	2.22	0.40
2:D:65:THR:OG1	2:D:66:ILE:N	2.55	0.40
5:J:145:ARG:O	5:J:148:LEU:HB3	2.21	0.40
2:N:288:LEU:HD22	2:O:275:PRO:HG3	2.02	0.40
2:N:329:ALA:HB3	2:N:344:VAL:HG12	2.03	0.40
2:O:19:ASN:ND2	2:O:40:SER:H	2.19	0.40
2:O:30:ILE:O	2:P:221:SER:OG	2.34	0.40
2:O:84:ASP:H	2:O:87:ILE:HD12	1.86	0.40
2:O:354:LYS:O	2:O:358:ARG:HG3	2.21	0.40
2:P:75:LEU:HD12	2:P:92:LEU:HD11	2.04	0.40
2:Q:249:GLU:O	2:Q:252:THR:OG1	2.26	0.40
2:R:9:VAL:HG22	2:R:279:VAL:HG22	2.03	0.40
2:R:286:MET:HE1	2:S:261:GLU:HA	2.03	0.40
2:S:185:ALA:HB2	3:T:152:PRO:HG3	2.03	0.40
4:U:73:ASN:HA	4:U:74:PRO:HD3	1.95	0.40
5:V:37:ILE:HD12	5:V:40:PHE:H	1.87	0.40
5:W:63:PHE:O	5:W:66:SER:OG	2.36	0.40
6:X:40:G:C6	6:X:41:G:C6	3.08	0.40
2:E:45:LYS:O	2:E:49:ARG:HG3	2.22	0.40
5:J:63:PHE:O	5:J:66:SER:OG	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:92:LEU:HD23	2:R:92:LEU:HA	1.90	0.40
4:U:143:CYS:SG	4:U:252:CYS:HB3	2.61	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	197/199 (99%)	190 (96%)	7 (4%)	0	100	100
1	M	188/199 (94%)	181 (96%)	7 (4%)	0	100	100
2	B	353/363 (97%)	327 (93%)	25 (7%)	1 (0%)	36	68
2	C	350/363 (96%)	332 (95%)	17 (5%)	1 (0%)	36	68
2	D	351/363 (97%)	339 (97%)	12 (3%)	0	100	100
2	E	358/363 (99%)	344 (96%)	13 (4%)	1 (0%)	36	68
2	F	361/363 (99%)	341 (94%)	19 (5%)	1 (0%)	36	68
2	G	360/363 (99%)	335 (93%)	24 (7%)	1 (0%)	36	68
2	N	352/363 (97%)	322 (92%)	30 (8%)	0	100	100
2	O	345/363 (95%)	328 (95%)	16 (5%)	1 (0%)	36	68
2	P	355/363 (98%)	330 (93%)	24 (7%)	1 (0%)	36	68
2	Q	353/363 (97%)	343 (97%)	10 (3%)	0	100	100
2	R	351/363 (97%)	336 (96%)	14 (4%)	1 (0%)	36	68
2	S	349/363 (96%)	328 (94%)	19 (5%)	2 (1%)	21	56
3	H	217/224 (97%)	210 (97%)	7 (3%)	0	100	100
3	T	217/224 (97%)	210 (97%)	7 (3%)	0	100	100
4	I	490/502 (98%)	468 (96%)	21 (4%)	1 (0%)	43	73
4	U	488/502 (97%)	467 (96%)	19 (4%)	2 (0%)	30	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	J	154/165 (93%)	151 (98%)	3 (2%)	0	100	100
5	K	150/165 (91%)	148 (99%)	2 (1%)	0	100	100
5	V	148/165 (90%)	147 (99%)	0	1 (1%)	18	52
5	W	147/165 (89%)	144 (98%)	2 (1%)	1 (1%)	18	52
All	All	6634/6866 (97%)	6321 (95%)	298 (4%)	15 (0%)	43	73

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	I	202	GLU
4	U	165	GLY
4	U	369	GLN
5	W	50	GLU
2	B	110	ALA
2	C	100	VAL
2	E	100	VAL
2	O	207	GLN
2	S	240	GLY
2	S	342	ALA
2	G	342	ALA
2	R	324	GLY
5	V	48	GLY
2	F	340	ILE
2	P	324	GLY

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	160/170 (94%)	156 (98%)	4 (2%)	42	69
1	M	125/170 (74%)	124 (99%)	1 (1%)	73	82
2	B	269/298 (90%)	269 (100%)	0	100	100
2	C	267/298 (90%)	264 (99%)	3 (1%)	65	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	271/298 (91%)	267 (98%)	4 (2%)	57	76
2	E	282/298 (95%)	277 (98%)	5 (2%)	51	74
2	F	282/298 (95%)	278 (99%)	4 (1%)	59	77
2	G	282/298 (95%)	272 (96%)	10 (4%)	32	64
2	N	231/298 (78%)	228 (99%)	3 (1%)	61	78
2	O	238/298 (80%)	235 (99%)	3 (1%)	61	78
2	P	254/298 (85%)	252 (99%)	2 (1%)	73	82
2	Q	274/298 (92%)	271 (99%)	3 (1%)	65	79
2	R	272/298 (91%)	271 (100%)	1 (0%)	84	86
2	S	264/298 (89%)	255 (97%)	9 (3%)	32	64
3	H	183/192 (95%)	181 (99%)	2 (1%)	65	79
3	T	183/192 (95%)	182 (100%)	1 (0%)	81	85
4	I	396/426 (93%)	393 (99%)	3 (1%)	73	82
4	U	377/426 (88%)	371 (98%)	6 (2%)	55	75
5	J	118/141 (84%)	118 (100%)	0	100	100
5	K	132/141 (94%)	130 (98%)	2 (2%)	57	76
5	V	110/141 (78%)	108 (98%)	2 (2%)	51	74
5	W	128/141 (91%)	126 (98%)	2 (2%)	55	75
All	All	5098/5716 (89%)	5028 (99%)	70 (1%)	59	77

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	TYR
1	A	46	THR
1	A	96	ILE
1	A	109	ILE
2	C	248	LEU
2	C	290	MET
2	C	337	VAL
2	D	19	ASN
2	D	155	GLN
2	D	248	LEU
2	D	288	LEU
2	E	5	ILE
2	E	85	GLN

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Mol	Chain	Res	Type
2	E	214	LEU
2	E	285	ASP
2	E	326	ASN
2	F	5	ILE
2	F	106	ILE
2	F	290	MET
2	F	337	VAL
2	G	116	VAL
2	G	119	ILE
2	G	158	VAL
2	G	171	MET
2	G	172	MET
2	G	179	ASP
2	G	207	GLN
2	G	258	LEU
2	G	279	VAL
2	G	325	LEU
3	H	146	LEU
3	H	154	THR
4	I	57	ILE
4	I	101	MET
4	I	493	LEU
5	K	155	THR
5	K	156	THR
1	M	46	THR
2	N	92	LEU
2	N	134	LEU
2	N	158	VAL
2	O	96	SER
2	O	205	ASP
2	O	248	LEU
2	P	282	ASN
2	P	362	GLU
2	Q	23	MET
2	Q	288	LEU
2	Q	325	LEU
2	R	344	VAL
2	S	73	ASP
2	S	119	ILE
2	S	126	VAL
2	S	158	VAL
2	S	179	ASP

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Mol	Chain	Res	Type
2	S	229	ASN
2	S	258	LEU
2	S	301	LYS
2	S	325	LEU
3	T	154	THR
4	U	7	ASN
4	U	57	ILE
4	U	102	GLN
4	U	221	ILE
4	U	406	LYS
4	U	493	LEU
5	V	43	LEU
5	V	155	THR
5	W	43	LEU
5	W	155	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	100	GLN
1	A	159	GLN
2	B	57	ASN
2	B	156	GLN
2	B	292	ASN
2	B	306	GLN
2	B	313	ASN
2	C	13	HIS
2	C	19	ASN
2	C	57	ASN
2	C	77	GLN
2	C	217	GLN
2	C	282	ASN
2	C	292	ASN
2	C	306	GLN
2	D	3	ASN
2	D	6	ASN
2	D	13	HIS
2	D	207	GLN
2	D	229	ASN
2	D	234	GLN
2	D	282	ASN

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Mol	Chain	Res	Type
2	E	19	ASN
2	E	207	GLN
2	E	217	GLN
2	E	234	GLN
2	E	267	GLN
2	F	3	ASN
2	F	13	HIS
2	F	217	GLN
2	F	236	GLN
2	F	274	ASN
2	F	282	ASN
2	G	67	HIS
2	G	274	ASN
2	G	282	ASN
2	G	292	ASN
3	H	18	GLN
3	H	173	ASN
4	I	25	GLN
4	I	56	GLN
4	I	98	HIS
4	I	135	GLN
4	I	150	ASN
4	I	309	GLN
4	I	426	GLN
4	I	464	GLN
5	J	24	GLN
5	J	116	GLN
5	K	56	GLN
5	K	104	GLN
5	K	116	GLN
5	K	157	ASN
1	M	108	ASN
1	M	140	HIS
2	N	229	ASN
2	N	234	GLN
2	N	292	ASN
2	N	313	ASN
2	N	331	GLN
2	N	360	ASN
2	O	13	HIS
2	O	57	ASN
2	O	217	GLN

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Mol	Chain	Res	Type
2	O	274	ASN
2	P	8	HIS
2	P	217	GLN
2	P	229	ASN
2	P	234	GLN
2	P	236	GLN
2	P	282	ASN
2	Q	19	ASN
2	Q	67	HIS
2	Q	125	GLN
2	Q	236	GLN
2	Q	274	ASN
2	Q	360	ASN
2	R	3	ASN
2	R	125	GLN
2	R	229	ASN
2	R	234	GLN
2	R	274	ASN
2	S	13	HIS
2	S	326	ASN
3	T	18	GLN
3	T	173	ASN
3	T	190	HIS
4	U	98	HIS
4	U	309	GLN
4	U	426	GLN
4	U	464	GLN
5	V	54	HIS
5	V	56	GLN
5	V	74	HIS
5	W	104	GLN
5	W	123	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	L	60/61 (98%)	22 (36%)	1 (1%)
6	X	60/61 (98%)	20 (33%)	1 (1%)
All	All	120/122 (98%)	42 (35%)	2 (1%)

All (42) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	L	4	A
6	L	9	A
6	L	14	A
6	L	15	U
6	L	21	A
6	L	26	C
6	L	27	U
6	L	32	U
6	L	33	G
6	L	38	C
6	L	39	A
6	L	40	G
6	L	41	G
6	L	42	A
6	L	43	G
6	L	46	C
6	L	47	C
6	L	52	G
6	L	53	C
6	L	54	C
6	L	55	A
6	L	56	G
6	X	4	A
6	X	9	A
6	X	14	A
6	X	15	U
6	X	21	A
6	X	26	C
6	X	27	U
6	X	32	U
6	X	33	G
6	X	38	C
6	X	39	A
6	X	40	G
6	X	41	G
6	X	42	A
6	X	43	G
6	X	46	C
6	X	47	C
6	X	54	C
6	X	56	G
6	X	61	23G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	L	54	C
6	X	42	A

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	23G	X	61	6	24,29,30	4.13	14 (58%)	34,45,48	2.67	14 (41%)
6	23G	L	61	6	24,29,30	3.95	14 (58%)	34,45,48	2.62	14 (41%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	23G	X	61	6	-	2/7/35/36	0/4/4/4
6	23G	L	61	6	-	2/7/35/36	0/4/4/4

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	X	61	23G	O4'-C4'	10.19	1.67	1.45
6	L	61	23G	O4'-C4'	9.77	1.66	1.45
6	X	61	23G	C3'-C4'	-8.89	1.29	1.52
6	L	61	23G	C3'-C4'	-8.84	1.30	1.52
6	X	61	23G	C2-N2	6.93	1.50	1.34
6	L	61	23G	C2-N2	6.84	1.50	1.34
6	X	61	23G	C4-N3	6.78	1.49	1.34
6	L	61	23G	C4-N3	6.75	1.49	1.34
6	X	61	23G	C2-N3	5.61	1.46	1.33
6	L	61	23G	C2-N3	5.42	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	X	61	23G	PC-OC2	5.40	1.69	1.50
6	X	61	23G	O4'-C1'	-3.59	1.33	1.42
6	L	61	23G	O4'-C1'	-3.47	1.34	1.42
6	X	61	23G	C3'-C2'	3.09	1.59	1.53
6	L	61	23G	PC-OC1	3.03	1.69	1.55
6	L	61	23G	C3'-C2'	2.99	1.59	1.53
6	L	61	23G	O6-C6	-2.84	1.18	1.23
6	X	61	23G	O6-C6	-2.77	1.18	1.23
6	X	61	23G	O2'-C2'	-2.56	1.27	1.46
6	L	61	23G	O2'-C2'	-2.56	1.27	1.46
6	X	61	23G	C5-C6	2.55	1.53	1.44
6	L	61	23G	C2-N1	2.50	1.43	1.37
6	X	61	23G	C2-N1	2.43	1.43	1.37
6	L	61	23G	C5-C6	2.40	1.53	1.44
6	L	61	23G	C5-N7	-2.35	1.34	1.39
6	X	61	23G	C5-N7	-2.34	1.34	1.39
6	L	61	23G	C6-N1	2.25	1.43	1.38
6	X	61	23G	C6-N1	2.15	1.42	1.38

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	61	23G	C1'-N9-C8	-7.10	106.55	126.73
6	X	61	23G	C1'-N9-C8	-6.99	106.88	126.73
6	X	61	23G	C1'-N9-C4	6.26	144.98	126.49
6	L	61	23G	C1'-N9-C4	6.06	144.40	126.49
6	X	61	23G	C5-C4-N3	-5.96	118.91	128.39
6	L	61	23G	C5-C4-N3	-5.23	120.07	128.39
6	X	61	23G	C2-N3-C4	4.78	120.54	112.30
6	L	61	23G	C2-N3-C4	4.41	119.89	112.30
6	X	61	23G	C2-N1-C6	-3.62	118.55	125.11
6	L	61	23G	N9-C8-N7	-3.54	106.84	113.40
6	X	61	23G	N9-C4-N3	3.40	132.75	125.95
6	X	61	23G	N9-C8-N7	-3.36	107.17	113.40
6	L	61	23G	C2-N1-C6	-3.29	119.15	125.11
6	L	61	23G	N9-C4-N3	3.17	132.29	125.95
6	X	61	23G	C5-C6-N1	2.95	120.77	113.25
6	L	61	23G	O3'-PC-OC2	-2.87	108.17	115.76
6	L	61	23G	C5-C6-N1	2.83	120.46	113.25
6	X	61	23G	O2'-PC-OC2	-2.75	108.50	115.76
6	L	61	23G	O6-C6-C5	-2.74	119.31	126.53
6	X	61	23G	C8-N7-C5	2.63	108.94	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	X	61	23G	O6-C6-C5	-2.59	119.70	126.53
6	X	61	23G	O3'-PC-OC2	-2.55	109.03	115.76
6	L	61	23G	C8-N7-C5	2.45	108.62	104.26
6	L	61	23G	C4'-O4'-C1'	-2.38	104.21	109.47
6	L	61	23G	C5'-C4'-C3'	-2.13	107.28	114.38
6	X	61	23G	C4-C5-N7	-2.06	107.41	110.67
6	L	61	23G	O2'-PC-OC2	-2.05	110.35	115.76
6	X	61	23G	O4'-C4'-C3'	2.00	109.14	104.92

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	X	61	23G	O4'-C4'-C5'-O5'
6	L	61	23G	O4'-C4'-C5'-O5'
6	X	61	23G	C3'-C4'-C5'-O5'
6	L	61	23G	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	X	61	23G	1	0
6	L	61	23G	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	199/199 (100%)	0.53	12 (6%) 27 17	40, 79, 126, 149	0
1	M	192/199 (96%)	1.03	24 (12%) 8 6	73, 117, 146, 164	0
2	B	357/363 (98%)	0.47	24 (6%) 24 15	34, 71, 131, 174	0
2	C	356/363 (98%)	0.17	8 (2%) 62 42	29, 59, 113, 158	0
2	D	355/363 (97%)	0.21	11 (3%) 51 32	21, 54, 120, 151	0
2	E	362/363 (99%)	-0.04	12 (3%) 49 30	19, 42, 87, 122	0
2	F	363/363 (100%)	0.05	14 (3%) 43 27	16, 39, 100, 135	0
2	G	362/363 (99%)	0.05	11 (3%) 52 33	15, 42, 103, 132	0
2	N	356/363 (98%)	0.82	33 (9%) 14 9	63, 100, 148, 183	0
2	O	351/363 (96%)	0.60	27 (7%) 19 13	52, 82, 122, 166	0
2	P	359/363 (98%)	0.54	23 (6%) 25 16	47, 78, 138, 164	0
2	Q	359/363 (98%)	0.28	16 (4%) 38 24	36, 60, 107, 134	0
2	R	357/363 (98%)	0.29	15 (4%) 40 25	33, 61, 102, 143	0
2	S	353/363 (97%)	0.36	21 (5%) 28 18	34, 63, 116, 135	0
3	H	219/224 (97%)	0.13	2 (0%) 81 64	22, 46, 82, 107	0
3	T	219/224 (97%)	0.47	7 (3%) 50 31	37, 68, 109, 136	0
4	I	494/502 (98%)	0.23	15 (3%) 52 33	24, 54, 96, 131	0
4	U	492/502 (98%)	0.63	35 (7%) 22 14	33, 82, 123, 154	0
5	J	156/165 (94%)	0.41	6 (3%) 44 27	39, 74, 122, 152	0
5	K	154/165 (93%)	0.12	2 (1%) 75 55	23, 51, 94, 148	0
5	V	152/165 (92%)	0.72	12 (7%) 18 12	61, 94, 129, 141	0
5	W	151/165 (91%)	0.25	4 (2%) 57 37	34, 66, 102, 119	0
6	L	60/61 (98%)	-0.03	2 (3%) 49 30	29, 52, 95, 138	0
6	X	60/61 (98%)	0.15	4 (6%) 24 15	41, 71, 137, 157	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	6838/6988 (97%)	0.36	340 (4%) 34 22	15, 67, 125, 183	0

All (340) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Q	338	ASP	5.8
2	R	338	ASP	5.7
4	U	252	CYS	5.6
2	N	101	ASP	4.5
5	V	7	ALA	4.1
3	T	94	ASP	4.0
2	B	265	ALA	4.0
2	S	337	VAL	4.0
2	B	269	THR	4.0
2	F	134	LEU	3.9
2	S	343	GLN	3.8
4	I	237	ALA	3.8
2	N	265	ALA	3.7
2	O	335	SER	3.6
1	A	32	ASP	3.6
4	U	228	PHE	3.6
1	M	36	ASP	3.6
2	Q	214	LEU	3.6
2	E	213	HIS	3.5
2	O	213	HIS	3.4
2	R	1	MET	3.4
2	R	179	ASP	3.4
2	F	132	ASP	3.4
2	E	208	GLU	3.4
2	F	210	GLY	3.4
2	B	208	GLU	3.4
2	Q	101	ASP	3.4
5	J	24	GLN	3.4
2	S	209	GLN	3.3
2	C	136	ASP	3.3
2	B	273	PHE	3.3
4	I	258	ASN	3.2
2	C	99	SER	3.2
2	F	209	GLN	3.2
2	B	172	MET	3.2
5	J	32	ASP	3.2
2	D	214	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
2	R	135	ASP	3.2
4	U	200	PRO	3.2
2	P	335	SER	3.2
2	B	297	ALA	3.2
5	V	77	LYS	3.1
2	N	302	ASP	3.1
2	F	340	ILE	3.1
4	U	210	THR	3.1
2	N	333	SER	3.1
2	B	325	LEU	3.0
5	J	8	MET	3.0
2	B	21	ASP	3.0
1	A	35	ARG	3.0
2	C	42	GLN	3.0
2	B	362	GLU	3.0
2	N	325	LEU	3.0
4	U	63	ASP	3.0
2	S	170	GLY	3.0
2	Q	343	GLN	3.0
4	U	56	GLN	3.0
1	M	27	PHE	2.9
2	O	147	ILE	2.9
4	U	53	CYS	2.9
5	V	111	THR	2.9
2	N	2	SER	2.9
2	R	210	GLY	2.9
5	V	33	GLU	2.9
2	E	1	MET	2.9
2	G	99	SER	2.9
2	O	288	LEU	2.9
5	V	8	MET	2.9
2	S	169	SER	2.8
2	S	211	SER	2.8
2	R	21	ASP	2.8
5	V	76	ASP	2.8
2	P	213	HIS	2.8
2	C	62	SER	2.8
2	N	84	ASP	2.8
2	N	269	THR	2.8
2	P	341	THR	2.8
2	P	206	LEU	2.8
1	M	152	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
4	U	322	GLU	2.8
6	L	55	A	2.8
6	X	42	A	2.8
2	E	214	LEU	2.8
3	T	219	GLY	2.8
4	U	127	CYS	2.8
2	R	344	VAL	2.8
1	A	95	THR	2.8
5	V	157	ASN	2.7
1	M	37	PHE	2.7
2	B	16	SER	2.7
2	Q	163	SER	2.7
5	V	86	SER	2.7
2	O	21	ASP	2.7
2	N	229	ASN	2.7
4	I	320	GLN	2.7
2	G	139	LEU	2.7
2	N	208	GLU	2.7
2	O	174	GLU	2.7
2	N	338	ASP	2.7
4	I	414	SER	2.7
2	S	21	ASP	2.7
4	U	433	ASP	2.7
1	M	76	PHE	2.7
2	G	327	GLY	2.7
2	Q	335	SER	2.7
1	A	152	ASP	2.7
2	B	196	ASP	2.7
2	G	136	ASP	2.7
5	V	32	ASP	2.7
2	C	208	GLU	2.6
2	O	110	ALA	2.6
1	M	147	GLN	2.6
2	P	343	GLN	2.6
2	Q	210	GLY	2.6
4	U	138	ALA	2.6
1	M	20	HIS	2.6
2	F	138	LYS	2.6
2	N	103	ALA	2.6
2	R	363	ALA	2.6
4	U	122	SER	2.6
1	M	171	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
2	N	60	GLU	2.6
1	A	36	ASP	2.6
2	F	135	ASP	2.6
2	G	241	GLY	2.6
4	U	110	ASP	2.6
4	U	120	GLY	2.6
1	M	38	LEU	2.6
2	O	214	LEU	2.6
2	D	208	GLU	2.6
2	O	208	GLU	2.6
2	S	2	SER	2.5
2	B	134	LEU	2.5
2	C	133	ASN	2.5
2	F	337	VAL	2.5
2	Q	133	ASN	2.5
5	J	49	TRP	2.5
2	C	211	SER	2.5
4	I	56	GLN	2.5
2	O	183	SER	2.5
2	P	2	SER	2.5
2	B	338	ASP	2.5
2	N	73	ASP	2.5
2	Q	204	ASP	2.5
2	D	23	MET	2.5
2	S	141	LYS	2.5
1	M	186	ALA	2.5
2	S	342	ALA	2.5
5	K	8	MET	2.5
6	X	54	C	2.5
2	B	132	ASP	2.5
2	N	21	ASP	2.5
2	N	198	ASP	2.5
2	O	136	ASP	2.5
2	F	327	GLY	2.5
2	N	335	SER	2.4
4	U	115	GLU	2.4
1	M	28	PRO	2.4
1	M	185	PRO	2.4
2	D	210	GLY	2.4
4	I	159	GLY	2.4
2	N	69	ALA	2.4
1	A	50	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	P	214	LEU	2.4
4	U	321	ASN	2.4
1	A	33	ALA	2.4
2	E	212	ALA	2.4
2	O	167	ALA	2.4
2	B	278	MET	2.4
2	C	109	ASP	2.4
2	G	337	VAL	2.4
2	O	196	ASP	2.4
1	A	101	LYS	2.4
2	B	23	MET	2.4
2	Q	98	LYS	2.4
3	T	192	LEU	2.4
6	X	41	G	2.4
2	O	133	ASN	2.4
1	M	98	ASP	2.4
2	P	277	ASP	2.4
2	Q	21	ASP	2.4
2	R	212	ALA	2.4
4	U	318	ILE	2.4
2	E	99	SER	2.4
1	M	170	ASN	2.3
4	I	353	ASN	2.3
5	K	32	ASP	2.3
2	S	172	MET	2.3
2	N	334	LEU	2.3
2	S	174	GLU	2.3
2	F	341	THR	2.3
3	H	219	GLY	2.3
4	I	157	GLY	2.3
4	U	254	GLY	2.3
5	W	5	ILE	2.3
2	D	1	MET	2.3
4	U	109	ASN	2.3
2	P	136	ASP	2.3
2	S	132	ASP	2.3
1	M	77	GLN	2.3
2	N	362	GLU	2.3
2	N	203	VAL	2.3
6	L	40	G	2.3
2	O	2	SER	2.3
2	O	168	THR	2.3

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Mol	Chain	Res	Type	RSRZ
2	Q	212	ALA	2.3
2	P	1	MET	2.3
2	O	277	ASP	2.3
2	R	362	GLU	2.3
3	T	175	GLU	2.3
2	G	340	ILE	2.3
4	I	156	PRO	2.3
2	D	173	THR	2.3
2	E	211	SER	2.3
4	U	282	SER	2.3
4	I	15	ASN	2.3
2	N	146	ASP	2.3
2	O	104	GLU	2.3
2	S	340	ILE	2.3
1	A	34	ALA	2.3
2	Q	1	MET	2.3
1	M	45	ASN	2.3
4	U	116	LYS	2.3
2	R	101	ASP	2.3
2	P	340	ILE	2.2
5	W	83	THR	2.2
4	U	225	SER	2.2
2	O	343	GLN	2.2
2	P	133	ASN	2.2
3	T	162	CYS	2.2
2	D	84	ASP	2.2
2	G	101	ASP	2.2
2	P	84	ASP	2.2
2	P	101	ASP	2.2
2	P	145	GLU	2.2
4	U	237	ALA	2.2
2	E	341	THR	2.2
4	U	103	THR	2.2
2	D	163	SER	2.2
2	O	209	GLN	2.2
4	U	207	ASN	2.2
2	P	87	ILE	2.2
2	Q	102	GLU	2.2
4	U	344	GLU	2.2
2	B	264	GLY	2.2
2	O	105	LYS	2.2
1	M	135	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	213	HIS	2.2
2	E	100	VAL	2.2
2	O	100	VAL	2.2
2	B	147	ILE	2.2
6	X	40	G	2.2
1	M	16	LEU	2.2
2	B	123	CYS	2.2
4	I	443	ALA	2.2
5	V	160	ALA	2.2
2	E	204	ASP	2.2
2	P	194	ASP	2.2
2	R	302	ASP	2.2
3	H	188	THR	2.2
5	J	111	THR	2.2
2	N	343	GLN	2.2
4	U	479	LEU	2.2
2	S	301	LYS	2.2
4	U	14	ARG	2.2
2	P	336	ASP	2.2
2	R	336	ASP	2.2
3	T	74	ASP	2.2
3	T	207	GLN	2.1
2	B	266	LYS	2.1
2	N	163	SER	2.1
2	O	62	SER	2.1
2	O	96	SER	2.1
5	J	86	SER	2.1
5	W	8	MET	2.1
2	D	60	GLU	2.1
2	P	362	GLU	2.1
2	Q	351	GLU	2.1
2	F	133	ASN	2.1
2	F	359	ASN	2.1
2	S	229	ASN	2.1
2	S	326	ASN	2.1
1	M	15	ASP	2.1
4	I	208	GLN	2.1
1	A	47	PRO	2.1
1	M	150	SER	2.1
2	S	324	GLY	2.1
4	U	274	ASN	2.1
2	N	17	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	N	277	ASP	2.1
2	N	266	LYS	2.1
5	V	5	ILE	2.1
2	P	85	GLN	2.1
2	R	207	GLN	2.1
4	I	165	GLY	2.1
2	B	335	SER	2.1
2	S	142	VAL	2.1
1	M	97	LEU	2.1
2	N	194	ASP	2.1
4	U	89	ASP	2.1
2	D	212	ALA	2.1
2	Q	363	ALA	2.1
5	W	7	ALA	2.1
2	N	267	GLN	2.1
2	E	210	GLY	2.1
2	P	339	PRO	2.1
4	I	202	GLU	2.1
2	G	169	SER	2.1
2	P	211	SER	2.1
4	U	26	SER	2.1
2	R	126	VAL	2.1
2	G	138	LYS	2.1
2	O	134	LEU	2.1
2	B	1	MET	2.1
2	F	21	ASP	2.1
2	N	179	ASP	2.1
2	B	207	GLN	2.1
1	A	31	PRO	2.1
2	N	158	VAL	2.0
2	F	211	SER	2.0
4	U	15	ASN	2.0
1	M	17	TYR	2.0
2	E	363	ALA	2.0
2	S	338	ASP	2.0
2	G	170	GLY	2.0
1	M	187	LYS	2.0
4	U	289	LYS	2.0
2	O	325	LEU	2.0
4	U	4	LEU	2.0
1	A	155	SER	2.0
1	M	132	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
4	I	352	ASN	2.0
2	O	131	ALA	2.0
4	U	96	ALA	2.0
2	B	336	ASP	2.0
2	N	136	ASP	2.0
2	N	159	ASP	2.0
2	S	339	PRO	2.0
5	V	42	ARG	2.0
2	P	66	ILE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	23G	X	61	26/27	0.84	0.14	59,94,132,137	0
6	23G	L	61	26/27	0.86	0.12	42,77,110,118	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	ZN	I	601	1/1	0.95	0.09	113,113,113,113	0
7	ZN	U	601	1/1	0.96	0.07	134,134,134,134	0

6.5 Other polymers [i](#)

There are no such residues in this entry.