



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:13 PM GMT

PDB ID : 3A6P
Title : Crystal structure of Exportin-5:RanGTP:pre-miRNAcomplex
Authors : Okada, C.; Yamashita, E.; Lee, S.J.; Shibata, S.; Katahira, J.; Nakagawa, A.;
Yoneda, Y.; Tsukihara, T.
Deposited on : 2009-09-07
Resolution : 2.92 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

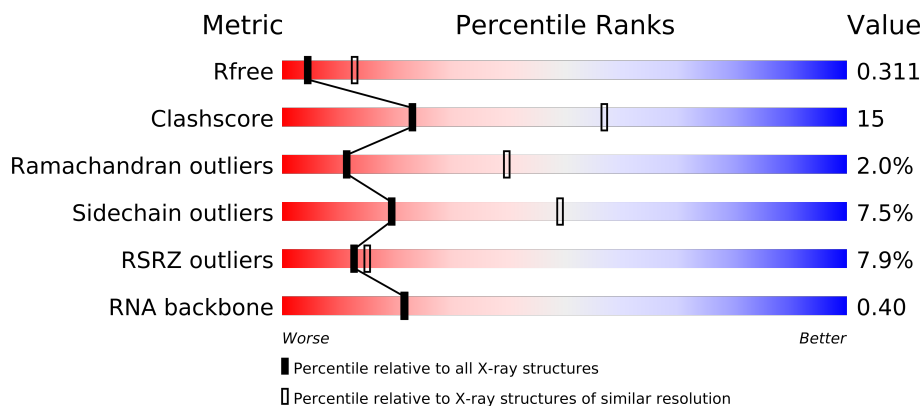
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.92 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}	66092	1172 (2.94-2.90)
Clashscore	79885	1461 (2.94-2.90)
Ramachandran outliers	78287	1419 (2.94-2.90)
Sidechain outliers	78261	1421 (2.94-2.90)
RSRZ outliers	66119	1173 (2.94-2.90)
RNA backbone	1838	1003 (3.42-2.42)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1204	
1	F	1204	
2	B	13	
2	G	13	
3	C	216	
3	H	216	
4	D	24	
4	I	24	
5	E	24	
5	J	24	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 22052 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Exportin-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1072	Total	C	N	O	S	0	0	0
			8570	5480	1442	1574	74			
1	F	1072	Total	C	N	O	S	0	0	0
			8570	5480	1442	1574	74			

- Molecule 2 is a protein called 13-mer peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	13	Total	C	N	O	0	0	0
			66	39	13	14			
2	G	13	Total	C	N	O	0	0	0
			66	39	13	14			

- Molecule 3 is a protein called GTP-binding nuclear protein Ran.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	170	Total	C	N	O	S	0	0	0
			1386	900	244	238	4			
3	H	170	Total	C	N	O	S	0	0	0
			1386	900	244	238	4			

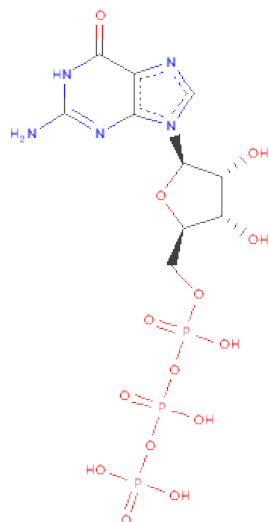
- Molecule 4 is a RNA chain called pre-microRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	22	Total	C	N	O	P	0	0	0
			466	211	88	147	20			
4	I	22	Total	C	N	O	P	0	0	0
			466	211	88	147	20			

- Molecule 5 is a RNA chain called pre-microRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	24	Total	C	N	O	P	0	0	0
			505	226	84	172	23			
5	J	24	Total	C	N	O	P	0	0	0
			505	226	84	172	23			

- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
6	H	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

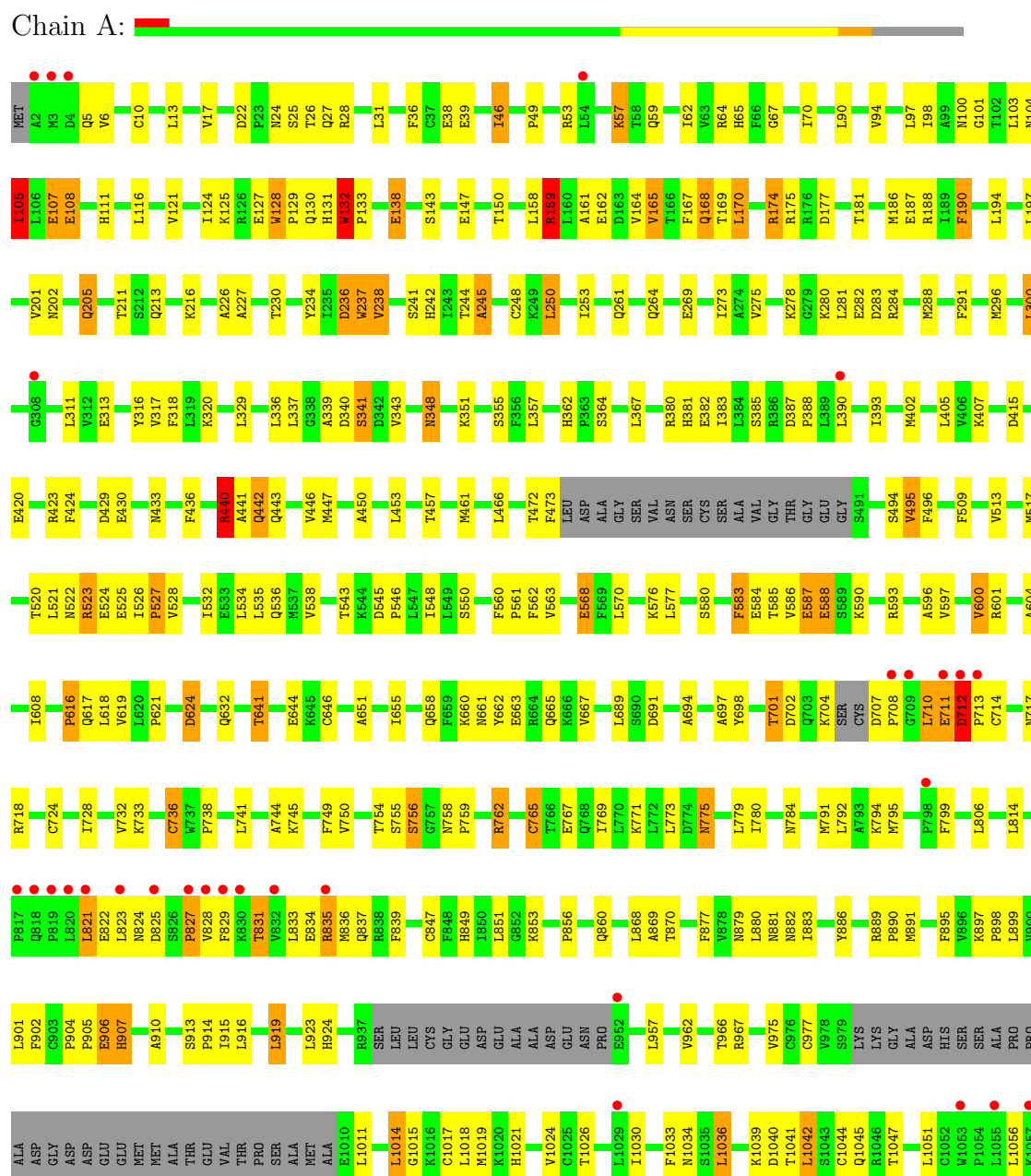
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

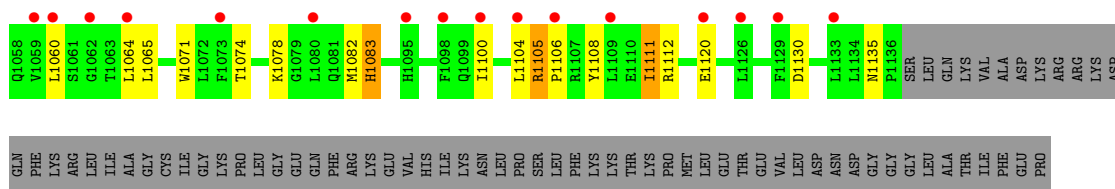
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	1	Total	Mg	0	0
			1	1		
7	C	1	Total	Mg	0	0
			1	1		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

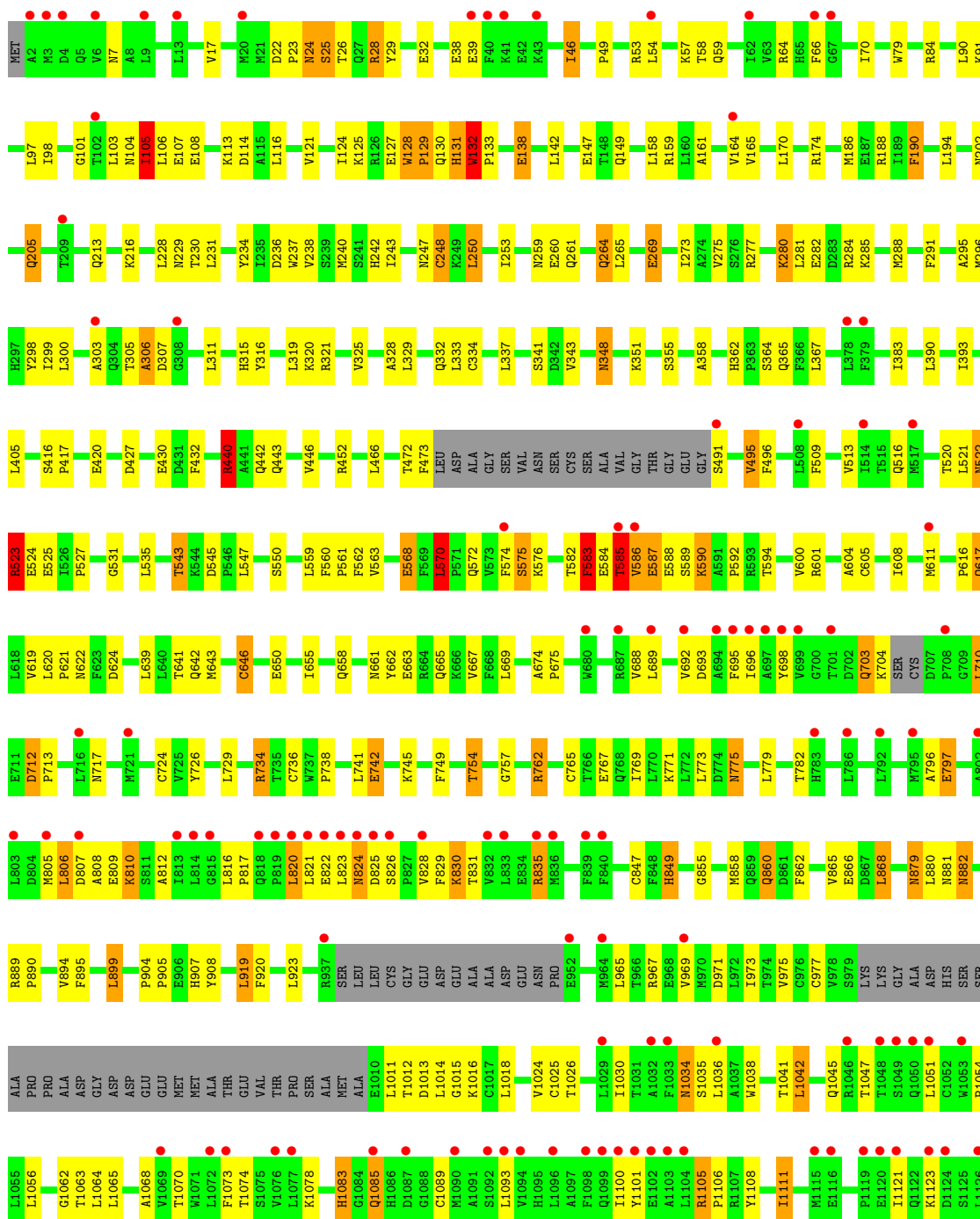
• Molecule 1: Exportin-5

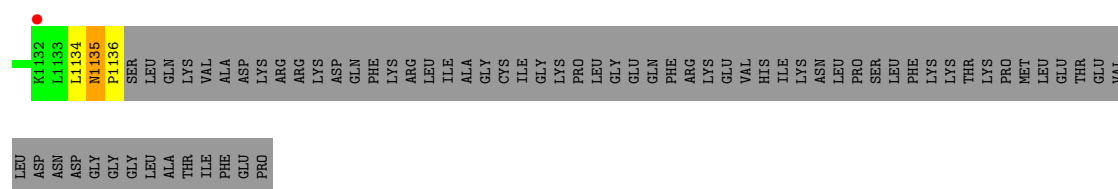




• Molecule 1: Exportin-5

Chain F:





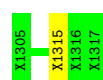
- Molecule 2: 13-mer peptide

Chain B:

There are no outlier residues recorded for this chain.

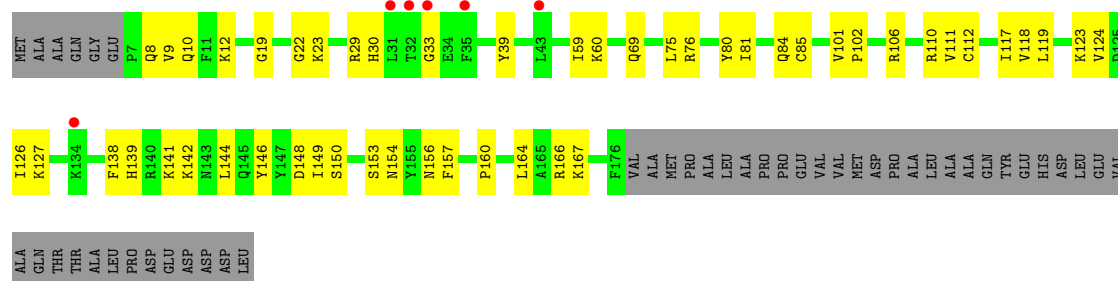
- Molecule 2: 13-mer peptide

Chain G:



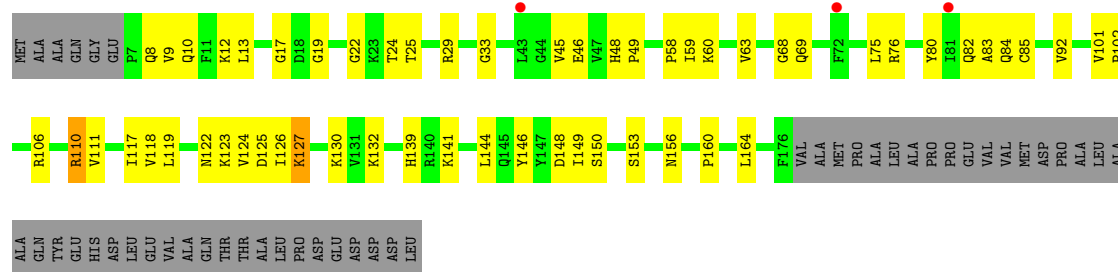
- Molecule 3: GTP-binding nuclear protein Ran

Chain C:



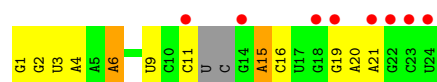
- Molecule 3: GTP-binding nuclear protein Ran

Chain H:



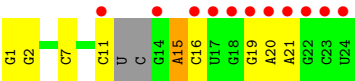
- Molecule 4: pre-microRNA

Chain D:



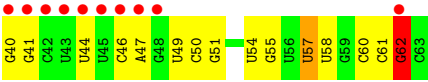
- Molecule 4: pre-microRNA

Chain I: 



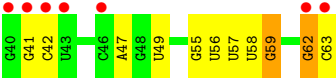
• Molecule 5: pre-microRNA

Chain E: 



• Molecule 5: pre-microRNA

Chain J: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.16Å 304.67Å 89.23Å 90.00° 110.79° 90.00°	Depositor
Resolution (Å)	39.84 – 2.92 62.93 – 2.92	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.84-2.92) 98.2 (62.93-2.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.20 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.247 , 0.312 0.249 , 0.311	Depositor DCC
R_{free} test set	3827 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	69.5	Xtriage
Anisotropy	0.745	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 48.0	EDS
Estimated twinning fraction	0.031 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 74910 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	22052	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.06	12/8738 (0.1%)	1.00	23/11831 (0.2%)
1	F	0.88	8/8738 (0.1%)	0.86	7/11831 (0.1%)
3	C	0.87	0/1421	0.82	0/1918
3	H	0.84	0/1421	0.83	0/1918
4	D	1.25	3/521 (0.6%)	1.76	12/809 (1.5%)
4	I	1.11	0/521	1.68	9/809 (1.1%)
5	E	1.23	2/562 (0.4%)	1.75	17/874 (1.9%)
5	J	1.06	0/562	1.51	6/874 (0.7%)
All	All	0.98	25/22484 (0.1%)	1.03	74/30864 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	TRP	CG-CD2	14.20	1.67	1.43
1	A	237	TRP	CZ3-CH2	13.24	1.61	1.40
1	A	165	VAL	CA-CB	9.13	1.74	1.54
1	A	237	TRP	CG-CD1	-8.79	1.24	1.36
4	D	1	G	N9-C8	-8.53	1.31	1.37
1	A	646	CYS	CB-SG	-6.75	1.70	1.82
1	A	132	TRP	CB-CG	6.58	1.62	1.50
1	A	237	TRP	CD2-CE2	-6.42	1.33	1.41
1	F	280	LYS	CE-NZ	6.41	1.65	1.49
1	A	765	CYS	CB-SG	-6.19	1.71	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	646	CYS	CB-SG	-5.88	1.72	1.81
4	D	1	G	N7-C5	-5.70	1.35	1.39
4	D	4	A	N7-C5	-5.60	1.35	1.39
1	A	238	VAL	CB-CG1	5.56	1.64	1.52
1	F	605	CYS	CB-SG	-5.38	1.73	1.81
5	E	61	C	C5-C6	-5.34	1.30	1.34
5	E	55	G	C5-C4	-5.32	1.34	1.38
1	F	1025	CYS	CB-SG	-5.23	1.73	1.81
1	A	580	SER	CB-OG	-5.20	1.35	1.42
1	F	585	THR	CA-CB	5.19	1.66	1.53
1	A	237	TRP	CD1-NE1	5.14	1.46	1.38
1	F	724	CYS	CB-SG	-5.07	1.73	1.81
1	A	107	GLU	CG-CD	5.06	1.59	1.51
1	F	334	CYS	CB-SG	-5.01	1.73	1.81
1	F	847	CYS	CB-SG	-5.01	1.73	1.81

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1	G	O4'-C1'-N9	11.60	117.48	108.20
1	A	237	TRP	CD1-NE1-CE2	10.62	118.56	109.00
4	I	2	G	C5-C6-O6	-10.20	122.48	128.60
1	A	237	TRP	CG-CD1-NE1	-10.03	100.07	110.10
4	D	1	G	C4-C5-N7	-9.08	107.17	110.80
1	A	237	TRP	CD1-CG-CD2	8.98	113.48	106.30
4	I	2	G	N1-C6-O6	8.97	125.28	119.90
1	A	736	CYS	CA-CB-SG	-8.64	98.44	114.00
1	A	237	TRP	CE2-CD2-CE3	8.59	129.01	118.70
1	F	570	LEU	CB-CG-CD1	-8.43	96.67	111.00
1	A	237	TRP	CH2-CZ2-CE2	-8.28	109.12	117.40
1	A	237	TRP	CB-CG-CD1	-8.22	116.31	127.00
1	A	64	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	A	128	TRP	C-N-CD	7.47	144.09	128.40
5	E	60	C	O4'-C1'-N1	7.45	114.16	108.20
4	D	1	G	N3-C4-C5	-7.40	124.90	128.60
1	F	440	ARG	NE-CZ-NH1	7.38	123.99	120.30
5	E	62	G	C3'-C2'-C1'	7.11	107.19	101.50
1	A	170	LEU	CA-CB-CG	6.93	131.24	115.30
5	E	55	G	N1-C6-O6	-6.91	115.76	119.90
4	I	1	G	C5-C6-N1	6.87	114.93	111.50
1	A	64	ARG	NE-CZ-NH1	6.83	123.71	120.30
5	E	62	G	P-O3'-C3'	6.67	127.70	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	62	G	C4'-C3'-C2'	-6.59	96.01	102.60
1	A	646	CYS	CA-CB-SG	-6.59	102.13	114.00
1	A	237	TRP	CE2-CD2-CG	-6.55	102.06	107.30
5	E	61	C	N3-C4-C5	6.53	124.51	121.90
1	F	646	CYS	CA-CB-SG	-6.50	102.30	114.00
4	D	1	G	O4'-C1'-N9	6.33	113.27	108.20
4	D	1	G	C5-N7-C8	6.31	107.46	104.30
1	A	159	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	A	174	ARG	NE-CZ-NH1	6.28	123.44	120.30
4	I	1	G	N3-C4-C5	-6.21	125.50	128.60
4	I	1	G	C3'-C2'-C1'	-6.18	96.56	101.50
1	F	710	LEU	CA-CB-CG	6.15	129.44	115.30
1	F	669	LEU	CB-CG-CD1	-6.14	100.56	111.00
5	E	54	U	P-O3'-C3'	-6.00	112.50	119.70
5	J	42	C	O4'-C1'-N1	5.98	112.98	108.20
4	D	1	G	C6-N1-C2	-5.96	121.52	125.10
4	D	3	U	C2-N3-C4	-5.96	123.43	127.00
5	E	50	C	N3-C4-C5	5.94	124.28	121.90
5	E	51	G	C8-N9-C4	-5.87	104.05	106.40
4	D	2	G	P-O3'-C3'	5.81	126.67	119.70
5	E	46	C	O4'-C1'-N1	5.78	112.83	108.20
4	I	15	A	O4'-C1'-N9	5.77	112.82	108.20
1	A	821	LEU	CA-CB-CG	5.75	128.51	115.30
4	I	7	C	O4'-C1'-N1	5.73	112.78	108.20
1	A	132	TRP	CA-CB-CG	5.61	124.36	113.70
5	J	62	G	C4'-C3'-C2'	-5.57	97.03	102.60
1	A	237	TRP	CG-CD2-CE3	-5.55	128.90	133.90
5	E	55	G	C5-C6-N1	5.43	114.22	111.50
1	F	816	LEU	CA-CB-CG	5.43	127.78	115.30
1	F	440	ARG	NE-CZ-NH2	-5.42	117.59	120.30
4	D	1	G	N1-C6-O6	-5.41	116.65	119.90
5	E	61	C	P-O3'-C3'	-5.41	113.21	119.70
1	A	710	LEU	CA-CB-CG	5.38	127.67	115.30
5	J	42	C	C6-N1-C2	-5.36	118.16	120.30
1	A	440	ARG	NE-CZ-NH1	5.35	122.97	120.30
4	I	1	G	C2-N3-C4	5.34	114.57	111.90
4	D	1	G	N9-C4-C5	5.29	107.52	105.40
4	D	3	U	O4'-C1'-N1	5.28	112.43	108.20
4	D	15	A	O4'-C1'-N9	5.27	112.41	108.20
5	E	49	U	O4'-C1'-N1	5.24	112.39	108.20
5	E	61	C	C2-N3-C4	-5.22	117.29	119.90
1	A	128	TRP	C-N-CA	-5.19	100.19	122.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	357	LEU	CB-CG-CD1	-5.16	102.23	111.00
5	E	55	G	C6-N1-C2	-5.12	122.03	125.10
5	J	62	G	C3'-C2'-C1'	5.09	105.57	101.50
5	J	59	G	P-O3'-C3'	-5.08	113.61	119.70
4	D	6	A	C2-N3-C4	5.05	113.13	110.60
5	J	57	U	O4'-C1'-N1	5.05	112.24	108.20
5	E	57	U	O4'-C1'-N1	5.04	112.23	108.20
5	E	58	U	N1-C2-O2	5.04	126.33	122.80
1	A	883	ILE	CG1-CB-CG2	-5.01	100.38	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	583	PHE	Peptide

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8570	0	8664	292	0
1	F	8570	0	8664	267	0
2	B	66	0	15	0	0
2	G	66	0	15	1	0
3	C	1386	0	1408	34	0
3	H	1386	0	1408	40	0
4	D	466	0	242	1	0
4	I	466	0	242	0	0
5	E	505	0	258	5	0
5	J	505	0	258	6	0
6	C	32	0	12	9	0
6	H	32	0	12	7	0
7	C	1	0	0	0	0
7	H	1	0	0	0	0
All	All	22052	0	21198	630	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (630) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:105:ILE:CG1	1:A:105:ILE:CD1	1.78	1.57
1:A:543:THR:HG22	1:A:545:ASP:H	1.17	1.09
1:F:495:VAL:O	1:F:496:PHE:CD1	2.15	0.99
1:A:168:GLN:HB2	1:A:175:ARG:HD2	1.41	0.99
1:A:545:ASP:OD2	1:A:548:ILE:HG12	1.63	0.99
1:F:905:PRO:HA	1:F:908:TYR:CD1	2.02	0.95
1:A:495:VAL:HG12	1:A:496:PHE:N	1.80	0.93
1:A:697:ALA:HA	1:A:702:ASP:OD1	1.72	0.90
1:F:1035:SER:HA	1:F:1038:TRP:CD1	2.07	0.90
1:A:362:HIS:CD2	1:A:364:SER:H	1.90	0.89
1:A:661:ASN:H	1:A:665:GLN:HE21	1.21	0.88
1:A:405:LEU:HD23	1:A:440:ARG:HD2	1.56	0.85
1:F:236:ASP:HA	1:F:277:ARG:HD2	1.59	0.84
1:F:205:GLN:HE21	1:F:205:GLN:HA	1.42	0.83
1:A:754:THR:HG22	1:A:756:SER:H	1.41	0.83
3:C:123:LYS:HG2	6:C:1177:GTP:C6	2.13	0.83
1:F:79:TRP:HZ3	1:F:90:LEU:HD23	1.42	0.83
1:F:240:MET:HA	1:F:243:ILE:HD13	1.60	0.83
1:A:593:ARG:NH1	1:A:601:ARG:NH1	2.27	0.82
1:A:495:VAL:HG12	1:A:496:PHE:H	1.40	0.82
1:F:1105:ARG:HA	1:F:1111:ILE:HG13	1.61	0.82
1:A:661:ASN:H	1:A:665:GLN:NE2	1.77	0.81
1:F:905:PRO:HA	1:F:908:TYR:CE1	2.16	0.81
1:A:733:LYS:HG3	1:A:853:LYS:HE3	1.64	0.80
1:A:104:ASN:C	1:A:105:ILE:HG13	2.02	0.80
1:F:584:GLU:O	1:F:586:VAL:N	2.16	0.79
1:A:205:GLN:HE21	1:A:205:GLN:HA	1.47	0.79
1:F:305:THR:O	1:F:315:HIS:NE2	2.15	0.79
1:A:168:GLN:HB2	1:A:175:ARG:CD	2.14	0.77
1:A:186:MET:CE	1:A:190:PHE:HD1	1.96	0.77
1:F:521:LEU:HD22	1:F:525:GLU:HB3	1.65	0.77
1:F:583:PHE:HD1	1:F:584:GLU:H	1.32	0.76
1:F:698:TYR:CE2	1:F:717:ASN:HB3	2.20	0.76
1:A:1039:LYS:O	1:A:1039:LYS:HG2	1.86	0.76
1:F:186:MET:CE	1:F:190:PHE:HD1	1.99	0.76
1:A:440:ARG:HG2	1:A:440:ARG:HH11	1.51	0.76
1:F:1018:LEU:HD22	1:F:1024:VAL:HG11	1.68	0.76
1:A:494:SER:HB3	1:A:545:ASP:OD1	1.85	0.75
1:F:977:CYS:HA	1:F:1012:THR:OG1	1.87	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:226:ALA:O	1:A:230:THR:HG22	1.86	0.74
1:A:495:VAL:CG1	1:A:496:PHE:N	2.50	0.74
1:F:281:LEU:HA	1:F:284:ARG:HG3	1.70	0.74
1:F:574:PHE:HE2	1:F:611:MET:CE	2.01	0.74
1:F:105:ILE:HD12	1:F:106:LEU:H	1.52	0.73
1:F:641:THR:HG22	1:F:643:MET:H	1.52	0.73
1:A:543:THR:HG22	1:A:545:ASP:N	1.98	0.73
1:A:186:MET:HE2	1:A:190:PHE:CD1	2.23	0.73
1:A:186:MET:HE2	1:A:190:PHE:HD1	1.54	0.72
1:A:1018:LEU:HD22	1:A:1024:VAL:HG11	1.70	0.72
3:H:117:ILE:HB	3:H:144:LEU:HD22	1.71	0.71
1:F:560:PHE:N	1:F:561:PRO:HD2	2.05	0.71
1:F:1105:ARG:N	1:F:1106:PRO:HD2	2.06	0.71
1:A:835:ARG:HE	1:A:835:ARG:HA	1.55	0.70
1:F:574:PHE:HE2	1:F:611:MET:HE3	1.56	0.70
1:F:570:LEU:HD13	1:F:622:ASN:ND2	2.07	0.69
1:F:440:ARG:HA	1:F:443:GLN:HB3	1.74	0.69
1:A:641:THR:HG22	1:A:644:GLU:H	1.57	0.69
1:F:495:VAL:HG22	1:F:824:ASN:HD21	1.58	0.69
1:A:1047:THR:HG23	1:A:1051:LEU:HD23	1.74	0.69
1:A:27:GLN:HE21	1:A:31:LEU:HD11	1.58	0.69
1:A:336:LEU:HB3	1:A:343:VAL:HG21	1.74	0.69
1:A:616:PRO:HB2	1:A:658:GLN:HG3	1.75	0.68
1:F:821:LEU:HD21	1:F:828:VAL:HG23	1.74	0.68
1:A:202:ASN:O	1:A:205:GLN:HB2	1.94	0.68
1:F:333:LEU:HD11	1:F:337:LEU:HG	1.76	0.67
1:A:164:VAL:HG13	1:A:165:VAL:HG23	1.74	0.67
1:F:383:ILE:N	1:F:383:ILE:HD12	2.09	0.67
1:A:362:HIS:HD2	1:A:364:SER:H	1.43	0.67
1:A:596:ALA:HB2	1:A:823:LEU:HB3	1.77	0.67
1:F:560:PHE:N	1:F:561:PRO:CD	2.59	0.66
1:F:689:LEU:HD22	1:F:779:LEU:HB2	1.78	0.66
1:F:574:PHE:CE2	1:F:611:MET:CE	2.79	0.65
1:F:213:GLN:HG2	1:F:216:LYS:HB2	1.78	0.65
3:C:29:ARG:HG2	3:C:157:PHE:HE2	1.61	0.65
1:F:879:ASN:ND2	1:F:882:ASN:HB2	2.12	0.65
1:F:650:GLU:OE1	1:F:734:ARG:NH1	2.27	0.65
3:H:123:LYS:HG2	6:H:1177:GTP:C5	2.31	0.65
1:F:754:THR:O	1:F:757:GLY:N	2.29	0.65
1:A:907:HIS:HB3	1:A:910:ALA:HB3	1.79	0.65
1:A:62:ILE:HD12	1:A:62:ILE:H	1.60	0.65
1:A:724:CYS:O	1:A:728:ILE:HG13	1.97	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:662:TYR:CE1	1:A:762:ARG:HG2	2.32	0.64
1:F:521:LEU:HD22	1:F:525:GLU:CB	2.27	0.64
1:F:186:MET:HE3	1:F:190:PHE:HD1	1.61	0.64
1:A:560:PHE:N	1:A:561:PRO:HD2	2.12	0.64
1:F:97:LEU:HD23	1:F:101:GLY:HA3	1.78	0.64
1:F:129:PRO:CG	1:F:174:ARG:HH22	2.11	0.64
1:F:1047:THR:HG23	1:F:1051:LEU:HD23	1.80	0.64
3:C:29:ARG:HG2	3:C:157:PHE:CE2	2.32	0.64
1:F:762:ARG:HG3	1:F:762:ARG:HH11	1.63	0.63
1:F:247:ASN:O	1:F:248:CYS:HB2	1.96	0.63
1:A:835:ARG:HH22	5:E:62:G:H5"	1.63	0.63
1:A:655:ILE:O	1:A:658:GLN:HB2	1.98	0.63
1:A:698:TYR:CE2	1:A:717:ASN:HB3	2.33	0.62
1:A:701:THR:HG22	1:A:799:PHE:CB	2.29	0.62
1:F:127:GLU:HB2	1:F:131:HIS:HB2	1.81	0.62
1:A:583:PHE:CE2	1:A:588:GLU:HG3	2.34	0.62
1:F:835:ARG:HE	1:F:835:ARG:HA	1.64	0.62
1:F:616:PRO:HB2	1:F:658:GLN:HG3	1.80	0.62
1:F:108:GLU:HB3	1:F:113:LYS:HE3	1.82	0.62
1:A:128:TRP:O	1:A:129:PRO:C	2.34	0.62
1:A:689:LEU:HD22	1:A:779:LEU:HB2	1.82	0.62
1:F:1074:THR:HG22	1:F:1078:LYS:HE3	1.82	0.62
1:F:619:VAL:HG23	1:F:655:ILE:HD13	1.81	0.62
1:F:164:VAL:HG13	1:F:165:VAL:HG23	1.81	0.62
1:A:707:ASP:HB3	1:A:710:LEU:HB3	1.82	0.61
1:F:570:LEU:HD22	1:F:574:PHE:CZ	2.35	0.61
3:C:117:ILE:HB	3:C:144:LEU:HD22	1.81	0.61
1:F:124:ILE:HG23	1:F:128:TRP:HB2	1.82	0.61
1:A:440:ARG:HA	1:A:443:GLN:HB3	1.83	0.61
1:A:339:ALA:O	1:A:341:SER:N	2.34	0.61
1:A:906:GLU:N	1:A:906:GLU:OE1	2.31	0.61
1:A:754:THR:HB	1:A:758:ASN:H	1.66	0.61
3:C:85:CYS:HB2	3:C:164:LEU:HD22	1.83	0.61
3:C:123:LYS:HG2	6:C:1177:GTP:C5	2.36	0.60
1:F:583:PHE:HD1	1:F:584:GLU:N	2.00	0.60
1:A:889:ARG:HB3	1:A:890:PRO:HD3	1.82	0.60
1:A:701:THR:HG22	1:A:799:PHE:HB2	1.82	0.60
1:F:889:ARG:HB3	1:F:890:PRO:HD3	1.82	0.60
1:A:1018:LEU:HB3	1:A:1024:VAL:HG11	1.82	0.60
1:A:162:GLU:OE1	3:C:106:ARG:HD3	2.02	0.60
1:A:313:GLU:O	1:A:317:VAL:HG23	2.01	0.60
1:F:619:VAL:CG2	1:F:655:ILE:HD13	2.31	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:H:149:ILE:HG22	3:H:156:ASN:HB2	1.82	0.60
1:F:620:LEU:N	1:F:621:PRO:CD	2.64	0.60
1:A:313:GLU:HG3	1:A:424:PHE:CZ	2.37	0.59
1:A:550:SER:HB2	1:A:600:VAL:CG1	2.32	0.59
1:F:26:THR:HG22	1:F:28:ARG:H	1.66	0.59
1:A:754:THR:HG22	1:A:756:SER:N	2.16	0.59
1:A:593:ARG:NH1	1:A:601:ARG:HH11	1.97	0.59
3:H:123:LYS:HG2	6:H:1177:GTP:C6	2.37	0.59
1:A:822:GLU:HG3	1:A:824:ASN:H	1.66	0.59
1:A:814:LEU:HD21	1:A:957:LEU:HA	1.84	0.59
3:C:150:SER:HB3	3:C:153:SER:HB3	1.85	0.59
1:F:1083:HIS:HB3	1:F:1089:CYS:SG	2.43	0.59
1:A:385:SER:HB2	1:A:453:LEU:HD11	1.85	0.58
1:F:1105:ARG:NH1	1:F:1134:LEU:HD11	2.18	0.58
1:F:205:GLN:NE2	1:F:205:GLN:HA	2.16	0.58
3:H:22:GLY:HA2	6:H:1177:GTP:H5"	1.85	0.58
1:A:597:VAL:O	1:A:601:ARG:HG3	2.03	0.58
1:A:128:TRP:O	1:A:128:TRP:CD1	2.56	0.58
1:F:616:PRO:HB2	1:F:658:GLN:CG	2.33	0.58
1:A:641:THR:HB	1:A:644:GLU:CD	2.24	0.57
1:A:711:GLU:O	1:A:713:PRO:HD2	2.04	0.57
3:C:29:ARG:HE	3:C:154:ASN:HD21	1.51	0.57
1:A:587:GLU:OE2	1:A:590:LYS:HB2	2.04	0.57
1:F:362:HIS:CD2	1:F:364:SER:H	2.21	0.57
1:F:585:THR:O	1:F:586:VAL:C	2.42	0.57
1:F:509:PHE:O	1:F:513:VAL:HG23	2.05	0.57
1:A:593:ARG:NH1	1:A:601:ARG:HH12	2.03	0.57
3:C:39:TYR:CD1	6:C:1177:GTP:H5"	2.39	0.57
1:F:738:PRO:HD3	1:F:749:PHE:CE1	2.39	0.57
1:A:619:VAL:HG23	1:A:655:ILE:HG23	1.87	0.57
1:F:260:GLU:O	1:F:264:GLN:HG3	2.04	0.57
1:F:828:VAL:HG12	1:F:830:LYS:NZ	2.20	0.56
1:F:765:CYS:O	1:F:769:ILE:HG12	2.04	0.56
3:H:9:VAL:O	3:H:10:GLN:HB3	2.04	0.56
1:A:775:ASN:HD22	1:A:775:ASN:H	1.52	0.56
3:C:9:VAL:HG21	3:C:59:ILE:HD12	1.86	0.56
1:A:543:THR:HG21	1:A:548:ILE:HB	1.86	0.56
1:F:749:PHE:O	1:F:762:ARG:HD3	2.04	0.56
3:C:80:TYR:HB2	3:C:111:VAL:HG11	1.86	0.56
1:A:616:PRO:HA	1:A:619:VAL:HG22	1.87	0.56
1:A:583:PHE:HD1	1:A:584:GLU:H	1.51	0.56
1:F:452:ARG:HG3	1:F:520:THR:HG21	1.87	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:300:LEU:HG	1:A:355:SER:HB2	1.86	0.56
1:F:186:MET:HE3	1:F:190:PHE:CD1	2.38	0.56
1:F:642:GLN:HB2	5:J:63:C:OP2	2.05	0.56
1:A:316:TYR:CE2	1:A:320:LYS:HD2	2.41	0.56
1:A:821:LEU:HD23	1:A:827:PRO:HG2	1.87	0.56
1:F:807:ASP:N	1:F:807:ASP:OD1	2.38	0.56
1:F:495:VAL:HG22	1:F:824:ASN:ND2	2.21	0.56
1:F:543:THR:HG22	1:F:545:ASP:H	1.71	0.56
1:F:495:VAL:C	1:F:496:PHE:CD1	2.79	0.55
1:A:617:GLN:HE21	1:A:618:LEU:H	1.53	0.55
1:F:586:VAL:O	1:F:587:GLU:HB2	2.06	0.55
3:C:9:VAL:CG2	3:C:59:ILE:HD12	2.36	0.55
1:F:158:LEU:HD13	1:F:230:THR:HA	1.88	0.55
1:F:1035:SER:HA	1:F:1038:TRP:NE1	2.22	0.55
1:F:616:PRO:HD2	1:F:617:GLN:OE1	2.05	0.55
3:H:150:SER:HB3	3:H:153:SER:HB3	1.88	0.55
1:F:161:ALA:HB2	1:F:234:TYR:CZ	2.41	0.55
1:F:604:ALA:O	1:F:608:ILE:HG12	2.07	0.55
1:F:472:THR:HG22	1:F:473:PHE:H	1.69	0.55
1:F:662:TYR:CE1	1:F:762:ARG:HG2	2.41	0.55
1:A:701:THR:HB	1:A:795:MET:HG2	1.89	0.55
1:F:617:GLN:CD	1:F:617:GLN:H	2.10	0.55
1:F:194:LEU:HD11	1:F:253:ILE:HD12	1.87	0.55
1:A:624:ASP:OD1	1:A:624:ASP:N	2.36	0.55
3:C:22:GLY:HA2	6:C:1177:GTP:O1A	2.07	0.55
1:F:337:LEU:CD2	1:F:343:VAL:O	2.54	0.55
1:F:269:GLU:HG2	1:F:321:ARG:HH11	1.72	0.55
1:A:236:ASP:HB3	1:A:273:ILE:CG2	2.37	0.55
1:F:860:GLN:CD	1:F:860:GLN:H	2.09	0.55
1:F:333:LEU:CD1	1:F:337:LEU:HG	2.36	0.54
1:A:132:TRP:HH2	1:A:138:GLU:HG2	1.72	0.54
1:A:663:GLU:O	1:A:667:VAL:HG23	2.07	0.54
1:A:583:PHE:CZ	1:A:588:GLU:HA	2.42	0.54
1:A:128:TRP:C	1:A:128:TRP:CD1	2.79	0.54
1:A:919:LEU:HD22	1:A:923:LEU:HD11	1.90	0.54
1:A:791:MET:HA	1:A:794:LYS:HD3	1.90	0.54
1:A:616:PRO:HB2	1:A:658:GLN:CG	2.37	0.54
1:A:213:GLN:HE21	1:A:216:LYS:HD3	1.73	0.54
1:A:288:MET:CE	1:A:288:MET:HA	2.37	0.54
1:A:17:VAL:HG23	3:C:75:LEU:HD21	1.90	0.54
1:F:967:ARG:HH21	1:F:1042:LEU:HB2	1.73	0.54
1:F:661:ASN:H	1:F:665:GLN:NE2	2.06	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:765:CYS:O	1:A:769:ILE:HG12	2.07	0.54
1:A:177:ASP:O	1:A:181:THR:OG1	2.25	0.53
1:F:742:GLU:OE2	1:F:745:LYS:HE3	2.08	0.53
1:A:523:ARG:HB3	1:A:523:ARG:HH11	1.74	0.53
1:A:897:LYS:HB3	1:A:898:PRO:HD3	1.89	0.53
1:F:1011:LEU:HD13	1:F:1054:PRO:HB2	1.89	0.53
1:F:703:GLN:O	1:F:704:LYS:HG3	2.08	0.53
1:A:407:LYS:HA	1:A:436:PHE:CZ	2.44	0.53
1:F:1018:LEU:HB3	1:F:1024:VAL:HG11	1.89	0.53
1:A:814:LEU:HD11	1:A:957:LEU:HB2	1.90	0.53
1:A:821:LEU:HD21	1:A:828:VAL:HG23	1.90	0.53
1:A:1064:LEU:HD13	1:A:1104:LEU:HD21	1.90	0.53
1:A:593:ARG:HD2	1:A:597:VAL:HG12	1.91	0.53
1:A:234:TYR:O	1:A:238:VAL:HG13	2.09	0.53
1:F:132:TRP:N	1:F:133:PRO:CD	2.72	0.53
1:A:311:LEU:HD21	1:A:424:PHE:CD1	2.44	0.53
3:C:119:LEU:HD23	3:C:139:HIS:HB3	1.91	0.53
1:F:572:GLN:O	1:F:575:SER:HB2	2.09	0.53
1:A:767:GLU:O	1:A:771:LYS:HG3	2.09	0.53
1:F:895:PHE:O	1:F:899:LEU:HB2	2.09	0.53
1:F:712:ASP:CB	1:F:713:PRO:CD	2.87	0.53
1:F:704:LYS:HD2	1:F:797:GLU:OE1	2.09	0.52
1:A:827:PRO:O	1:A:829:PHE:CD1	2.63	0.52
1:F:754:THR:C	1:F:757:GLY:H	2.12	0.52
1:A:440:ARG:CG	1:A:440:ARG:HH11	2.20	0.52
1:A:165:VAL:HG11	1:A:237:TRP:CD2	2.45	0.52
1:F:306:ALA:HA	1:F:319:LEU:HD11	1.90	0.52
1:A:97:LEU:HD23	1:A:101:GLY:HA3	1.91	0.52
3:H:22:GLY:HA2	6:H:1177:GTP:C5'	2.39	0.52
1:F:97:LEU:HA	1:F:101:GLY:HA3	1.92	0.52
1:F:416:SER:HB2	1:F:417:PRO:HD2	1.90	0.52
1:A:584:GLU:O	1:A:586:VAL:HG22	2.09	0.52
1:A:586:VAL:O	1:A:587:GLU:HB2	2.09	0.52
1:A:300:LEU:HD12	1:A:351:LYS:HB3	1.92	0.52
1:A:711:GLU:HG3	1:A:718:ARG:HH22	1.74	0.51
1:A:780:ILE:HD11	1:A:847:CYS:HB3	1.92	0.51
1:A:704:LYS:O	1:A:708:PRO:HA	2.11	0.51
1:F:821:LEU:HD21	1:F:828:VAL:CG2	2.40	0.51
1:F:124:ILE:CG2	1:F:128:TRP:HB2	2.40	0.51
1:A:1033:PHE:HA	1:A:1036:LEU:HD22	1.91	0.51
1:F:311:LEU:HD22	1:F:420:GLU:HG3	1.92	0.51
3:C:29:ARG:HE	3:C:154:ASN:ND2	2.08	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:767:GLU:O	1:F:771:LYS:HG3	2.11	0.51
1:F:582:THR:O	1:F:601:ARG:NH2	2.44	0.51
1:F:205:GLN:HE21	1:F:205:GLN:CA	2.16	0.51
1:A:617:GLN:NE2	1:A:618:LEU:H	2.08	0.51
1:A:791:MET:O	1:A:794:LYS:HB2	2.11	0.51
1:A:472:THR:HG22	1:A:473:PHE:H	1.74	0.51
1:F:440:ARG:HH11	1:F:440:ARG:HG2	1.74	0.51
1:A:269:GLU:O	1:A:273:ILE:HG13	2.11	0.51
1:A:577:LEU:HB3	1:A:608:ILE:HD11	1.92	0.51
1:A:775:ASN:N	1:A:775:ASN:ND2	2.59	0.50
1:A:618:LEU:O	1:A:621:PRO:HD2	2.11	0.50
1:F:46:ILE:C	1:F:49:PRO:HD2	2.32	0.50
1:A:745:LYS:HA	1:A:750:VAL:HG12	1.93	0.50
3:H:12:LYS:HD3	3:H:82:GLN:O	2.12	0.50
1:F:570:LEU:CD2	1:F:574:PHE:CZ	2.94	0.50
1:F:1051:LEU:O	1:F:1054:PRO:HD2	2.10	0.50
1:A:236:ASP:HB3	1:A:273:ILE:HG22	1.94	0.50
1:A:90:LEU:O	1:A:94:VAL:HG23	2.12	0.50
3:H:119:LEU:HD23	3:H:139:HIS:HB3	1.94	0.50
1:F:240:MET:HA	1:F:243:ILE:CD1	2.36	0.50
1:F:442:GLN:O	1:F:446:VAL:HG23	2.11	0.50
1:A:694:ALA:O	1:A:697:ALA:HB3	2.12	0.50
1:F:1101:TYR:O	1:F:1105:ARG:HB2	2.12	0.50
1:F:574:PHE:CD2	1:F:611:MET:HE1	2.46	0.50
1:F:7:ASN:HA	1:F:53:ARG:NH1	2.27	0.50
3:C:146:TYR:OH	3:C:148:ASP:HB3	2.12	0.50
1:A:125:LYS:HB3	1:A:170:LEU:HD21	1.94	0.50
1:A:161:ALA:HB2	1:A:234:TYR:CZ	2.47	0.49
3:H:146:TYR:OH	3:H:148:ASP:HB3	2.12	0.49
1:F:919:LEU:HD22	1:F:923:LEU:HD11	1.93	0.49
1:A:164:VAL:CG1	1:A:165:VAL:HG23	2.41	0.49
1:A:121:VAL:HG21	1:A:159:ARG:HB3	1.93	0.49
1:A:67:GLY:HA2	1:A:70:ILE:HD12	1.93	0.49
1:F:383:ILE:N	1:F:383:ILE:CD1	2.75	0.49
1:A:728:ILE:O	1:A:732:VAL:HG23	2.12	0.49
3:H:118:VAL:HG11	3:H:160:PRO:HB3	1.93	0.49
1:A:158:LEU:HD13	1:A:230:THR:HA	1.94	0.49
1:F:234:TYR:O	1:F:238:VAL:HG13	2.13	0.49
1:A:1014:LEU:HA	1:A:1017:CYS:HB3	1.94	0.49
1:F:186:MET:HB3	1:F:242:HIS:CE1	2.48	0.49
1:F:1073:PHE:HD1	1:F:1100:ILE:HG21	1.78	0.49
3:H:123:LYS:HB3	3:H:126:ILE:HD12	1.95	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:149:ILE:HG22	3:C:156:ASN:HB2	1.95	0.49
1:A:382:GLU:HA	1:A:382:GLU:OE1	2.12	0.49
1:A:339:ALA:C	1:A:341:SER:H	2.17	0.49
1:F:321:ARG:O	1:F:325:VAL:HG23	2.13	0.49
1:A:1033:PHE:HA	1:A:1036:LEU:CD2	2.43	0.49
1:A:107:GLU:O	1:A:108:GLU:CB	2.61	0.49
1:F:692:VAL:O	1:F:696:ILE:HG12	2.13	0.48
1:F:194:LEU:HD13	1:F:250:LEU:HD23	1.94	0.48
1:F:570:LEU:HD22	1:F:574:PHE:HZ	1.78	0.48
1:A:550:SER:HB2	1:A:600:VAL:HG13	1.95	0.48
1:F:495:VAL:O	1:F:496:PHE:HD1	1.85	0.48
1:F:1108:TYR:HB2	1:F:1111:ILE:HD11	1.95	0.48
1:F:583:PHE:CD1	1:F:584:GLU:N	2.78	0.48
1:A:234:TYR:HA	1:A:237:TRP:NE1	2.29	0.48
1:F:822:GLU:HB3	1:F:825:ASP:HB2	1.95	0.48
1:A:754:THR:CG2	1:A:755:SER:N	2.76	0.48
1:A:127:GLU:O	1:A:132:TRP:HB2	2.14	0.48
1:F:904:PRO:HG2	1:F:907:HIS:HD2	1.79	0.48
1:F:762:ARG:NH1	1:F:762:ARG:HG3	2.27	0.48
1:F:104:ASN:HB2	1:F:107:GLU:OE1	2.14	0.48
1:F:264:GLN:NE2	1:F:265:LEU:H	2.12	0.48
1:F:269:GLU:O	1:F:273:ILE:HG13	2.12	0.48
1:F:710:LEU:HG	1:F:712:ASP:OD2	2.14	0.48
1:F:923:LEU:HD13	1:F:969:VAL:HG13	1.96	0.48
1:A:525:GLU:OE1	1:A:525:GLU:N	2.46	0.48
1:A:534:LEU:O	1:A:538:VAL:HG23	2.14	0.48
1:F:365:GLN:HG3	1:F:432:PHE:HE1	1.79	0.48
1:A:919:LEU:HD22	1:A:923:LEU:CD1	2.44	0.48
3:H:17:GLY:O	3:H:68:GLY:HA3	2.13	0.48
1:F:22:ASP:HB3	1:F:25:SER:HB2	1.96	0.48
1:F:202:ASN:O	1:F:205:GLN:HB2	2.13	0.48
3:H:19:GLY:HA2	6:H:1177:GTP:O1G	2.14	0.48
1:A:441:ALA:HB2	5:E:57:U:H1'	1.96	0.48
1:F:142:LEU:O	1:F:149:GLN:HB3	2.13	0.48
1:A:806:LEU:HA	1:A:837:GLN:HE21	1.78	0.48
1:F:1026:THR:HG22	1:F:1030:ILE:HD11	1.96	0.47
3:C:29:ARG:O	3:C:33:GLY:N	2.47	0.47
1:F:754:THR:O	1:F:757:GLY:HA2	2.14	0.47
3:C:12:LYS:HE2	3:C:81:ILE:O	2.14	0.47
1:A:10:CYS:SG	1:A:53:ARG:HD2	2.53	0.47
1:F:806:LEU:O	1:F:810:LYS:HG3	2.15	0.47
1:A:1105:ARG:N	1:A:1106:PRO:HD2	2.29	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:775:ASN:ND2	1:A:775:ASN:H	2.12	0.47
1:A:1108:TYR:HB2	1:A:1111:ILE:HD11	1.95	0.47
3:C:39:TYR:HD1	6:C:1177:GTP:H5''	1.78	0.47
1:F:305:THR:O	1:F:307:ASP:N	2.47	0.47
3:H:13:LEU:HD23	3:H:63:VAL:HG22	1.96	0.47
1:F:522:ASN:O	1:F:524:GLU:N	2.48	0.47
1:A:280:LYS:HE2	1:A:282:GLU:OE2	2.14	0.47
1:A:167:PHE:O	1:A:168:GLN:C	2.52	0.47
1:A:362:HIS:CD2	1:A:364:SER:N	2.72	0.47
3:C:123:LYS:HB3	3:C:126:ILE:HD12	1.97	0.47
1:A:523:ARG:HB3	1:A:523:ARG:NH1	2.29	0.47
1:A:1044:CYS:HB3	1:A:1083:HIS:NE2	2.29	0.47
1:F:849:HIS:HA	1:F:894:VAL:HG13	1.96	0.47
3:H:132:LYS:HE2	5:J:49:U:P	2.55	0.47
1:A:526:ILE:HA	1:A:527:PRO:HD2	1.54	0.47
1:F:98:ILE:HG12	1:F:116:LEU:HD11	1.96	0.47
1:F:550:SER:HB2	1:F:600:VAL:HG12	1.97	0.47
1:F:865:VAL:HB	1:F:868:LEU:HG	1.97	0.47
1:A:891:MET:O	1:A:895:PHE:HB3	2.15	0.47
1:A:62:ILE:H	1:A:62:ILE:CD1	2.26	0.47
1:A:906:GLU:CD	1:A:906:GLU:H	2.18	0.47
1:F:1105:ARG:N	1:F:1106:PRO:CD	2.77	0.46
1:A:904:PRO:HA	1:A:905:PRO:HD3	1.69	0.46
1:F:291:PHE:HA	1:F:296:MET:HE3	1.97	0.46
1:A:381:HIS:CD2	1:A:383:ILE:H	2.34	0.46
1:F:574:PHE:CE2	1:F:611:MET:HE1	2.49	0.46
3:H:25:THR:OG1	6:H:1177:GTP:H5'	2.14	0.46
1:F:904:PRO:HG2	1:F:907:HIS:CD2	2.50	0.46
1:A:46:ILE:C	1:A:49:PRO:HD2	2.34	0.46
1:A:738:PRO:HD2	1:A:749:PHE:CD1	2.50	0.46
1:A:291:PHE:HA	1:A:296:MET:CE	2.45	0.46
1:A:967:ARG:HH21	1:A:1042:LEU:HB2	1.81	0.46
3:C:124:VAL:HG11	3:C:148:ASP:HB2	1.98	0.46
1:A:831:THR:HB	1:A:834:GLU:HB2	1.97	0.46
1:F:563:VAL:HG11	1:F:570:LEU:HG	1.97	0.46
1:A:532:ILE:O	1:A:536:GLN:HG3	2.15	0.46
1:F:663:GLU:O	1:F:667:VAL:HG23	2.16	0.46
1:F:568:GLU:HG3	1:F:568:GLU:H	1.27	0.46
1:F:495:VAL:C	1:F:496:PHE:HD1	2.18	0.46
1:A:691:ASP:HB3	1:A:694:ALA:HB3	1.98	0.46
1:F:1101:TYR:CE2	1:F:1105:ARG:HG3	2.51	0.46
1:F:754:THR:O	1:F:757:GLY:CA	2.62	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:619:VAL:HG21	1:F:655:ILE:CD1	2.45	0.46
1:A:264:GLN:HB2	1:A:318:PHE:CE1	2.50	0.46
1:A:977:CYS:O	1:A:1011:LEU:HA	2.14	0.46
1:A:977:CYS:HB3	1:A:1015:GLY:HA2	1.98	0.46
1:F:364:SER:HB3	1:F:367:LEU:HB2	1.97	0.46
3:H:132:LYS:HE2	5:J:49:U:OP1	2.15	0.46
1:A:98:ILE:HG12	1:A:116:LEU:HD11	1.97	0.46
1:A:835:ARG:HH12	5:E:62:G:H5''	1.81	0.46
1:F:348:ASN:HD22	1:F:351:LYS:HD3	1.80	0.46
1:F:977:CYS:HA	1:F:1012:THR:HG1	1.78	0.46
1:A:835:ARG:NH2	5:E:62:G:H5''	2.31	0.46
1:A:632:GLN:HG2	1:F:639:LEU:CD1	2.46	0.46
1:A:390:LEU:O	1:A:393:ILE:HG22	2.16	0.46
1:A:143:SER:OG	1:A:150:THR:HG23	2.16	0.46
1:A:543:THR:CG2	1:A:545:ASP:HB3	2.45	0.46
1:F:165:VAL:HG11	1:F:237:TRP:CE2	2.51	0.46
1:A:522:ASN:O	1:A:524:GLU:N	2.49	0.46
3:H:48:HIS:HA	3:H:49:PRO:HD3	1.79	0.46
1:A:494:SER:HB3	1:A:545:ASP:CG	2.36	0.46
1:F:828:VAL:O	1:F:830:LYS:NZ	2.48	0.46
1:F:889:ARG:HG2	1:F:889:ARG:HH11	1.79	0.46
1:F:362:HIS:HD2	1:F:364:SER:H	1.63	0.46
1:A:522:ASN:C	1:A:524:GLU:H	2.19	0.46
5:J:55:G:H2'	5:J:56:U:C6	2.51	0.46
1:F:809:GLU:O	1:F:812:ALA:HB3	2.16	0.46
1:A:754:THR:HG22	1:A:755:SER:N	2.32	0.45
1:A:187:GLU:HA	1:A:242:HIS:HD2	1.81	0.45
3:H:80:TYR:N	3:H:80:TYR:CD1	2.84	0.45
1:A:495:VAL:HG13	1:A:496:PHE:HD1	1.81	0.45
1:A:593:ARG:HH12	1:A:601:ARG:HH12	1.64	0.45
1:A:593:ARG:HH12	1:A:601:ARG:NH1	2.07	0.45
1:A:94:VAL:O	1:A:97:LEU:HB2	2.16	0.45
1:F:1026:THR:HG22	1:F:1030:ILE:CD1	2.47	0.45
1:A:568:GLU:HG3	1:A:568:GLU:H	1.17	0.45
1:F:1085:GLN:HE22	3:H:130:LYS:HE2	1.82	0.45
1:A:205:GLN:HE21	1:A:205:GLN:CA	2.19	0.45
3:C:118:VAL:HG11	3:C:160:PRO:HB3	1.97	0.45
1:A:563:VAL:HG11	1:A:570:LEU:HG	1.97	0.45
1:A:244:THR:HA	1:A:248:CYS:SG	2.56	0.45
3:C:19:GLY:HA2	6:C:1177:GTP:O2G	2.17	0.45
3:H:8:GLN:HB3	3:H:58:PRO:O	2.16	0.45
1:F:736:CYS:O	1:F:736:CYS:SG	2.75	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:194:LEU:HD11	1:A:253:ILE:HD12	1.97	0.45
1:A:429:ASP:N	1:A:429:ASP:OD2	2.49	0.45
1:F:104:ASN:O	1:F:105:ILE:C	2.55	0.45
1:F:620:LEU:N	1:F:621:PRO:HD2	2.32	0.45
1:F:1065:LEU:O	1:F:1068:ALA:HB3	2.16	0.45
1:A:509:PHE:O	1:A:513:VAL:HG23	2.17	0.45
3:C:22:GLY:HA2	6:C:1177:GTP:PA	2.57	0.45
1:A:129:PRO:HD2	1:A:174:ARG:HH22	1.82	0.45
1:A:103:LEU:HB2	1:A:108:GLU:HB2	1.98	0.45
1:A:526:ILE:HG22	1:A:562:PHE:HE2	1.82	0.45
1:A:457:THR:O	1:A:461:MET:HG3	2.16	0.45
1:A:495:VAL:HG23	1:A:824:ASN:ND2	2.32	0.45
1:F:291:PHE:HA	1:F:296:MET:CE	2.47	0.45
1:F:295:ALA:O	1:F:299:ILE:HG12	2.17	0.45
1:F:390:LEU:O	1:F:393:ILE:HG22	2.17	0.45
1:A:420:GLU:O	1:A:423:ARG:HB2	2.17	0.45
1:F:264:GLN:HG3	1:F:264:GLN:H	1.52	0.45
3:H:124:VAL:HG11	3:H:148:ASP:HB2	1.98	0.45
1:F:547:LEU:HD21	1:F:823:LEU:HD13	1.98	0.45
5:J:58:U:H2'	5:J:59:G:H8	1.82	0.45
1:F:828:VAL:HG12	1:F:830:LYS:HZ3	1.82	0.44
1:A:560:PHE:N	1:A:561:PRO:CD	2.79	0.44
1:A:129:PRO:CD	1:A:174:ARG:HH22	2.30	0.44
1:A:1064:LEU:O	1:A:1065:LEU:C	2.54	0.44
1:F:965:LEU:O	1:F:969:VAL:HG23	2.17	0.44
1:A:593:ARG:HD2	1:A:597:VAL:CG1	2.46	0.44
1:F:129:PRO:HG2	1:F:174:ARG:HH22	1.79	0.44
1:F:1036:LEU:HD22	1:F:1093:LEU:HD21	1.98	0.44
3:H:101:VAL:N	3:H:102:PRO:CD	2.80	0.44
1:F:54:LEU:O	1:F:64:ARG:HA	2.17	0.44
1:A:618:LEU:HD12	1:A:618:LEU:HA	1.82	0.44
1:A:744:ALA:O	1:A:749:PHE:HB2	2.17	0.44
1:F:125:LYS:HD2	1:F:170:LEU:HD21	1.98	0.44
1:A:281:LEU:HD12	1:A:281:LEU:HA	1.82	0.44
1:F:303:ALA:O	1:F:306:ALA:HB3	2.17	0.44
1:A:1074:THR:HG22	1:A:1078:LYS:HE3	1.98	0.44
1:F:430:GLU:OE1	1:F:430:GLU:N	2.50	0.44
1:A:521:LEU:HD22	1:A:525:GLU:CB	2.47	0.44
1:A:194:LEU:HD13	1:A:250:LEU:HD23	1.99	0.44
5:J:58:U:C2	5:J:59:G:C8	3.06	0.44
1:A:869:ALA:HA	1:A:915:ILE:HD11	2.00	0.44
1:F:588:GLU:HB2	1:F:589:SER:H	1.50	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:84:ARG:HE	1:F:84:ARG:HB3	1.53	0.44
1:F:186:MET:O	1:F:190:PHE:HB2	2.18	0.44
1:F:855:GLY:HA2	1:F:862:PHE:HD2	1.82	0.44
1:A:186:MET:CE	1:A:190:PHE:CD1	2.84	0.44
1:F:1070:THR:O	1:F:1074:THR:OG1	2.34	0.44
1:F:858:MET:HB2	1:F:862:PHE:HB2	2.00	0.44
1:A:916:LEU:HD23	1:A:916:LEU:HA	1.87	0.44
1:A:105:ILE:CD1	1:A:105:ILE:CB	2.86	0.43
1:A:651:ALA:O	1:A:655:ILE:HG13	2.18	0.43
1:F:889:ARG:HB3	1:F:890:PRO:CD	2.45	0.43
1:F:91:LYS:HE3	1:F:132:TRP:CH2	2.53	0.43
1:F:865:VAL:O	1:F:866:GLU:C	2.56	0.43
1:A:442:GLN:O	1:A:446:VAL:HG23	2.18	0.43
1:F:592:PRO:HG3	1:F:829:PHE:HE1	1.83	0.43
3:H:150:SER:CB	3:H:153:SER:HB3	2.48	0.43
1:A:526:ILE:O	1:A:528:VAL:N	2.50	0.43
1:F:1105:ARG:HG2	1:F:1111:ILE:HG13	2.00	0.43
1:F:128:TRP:O	1:F:129:PRO:C	2.56	0.43
1:A:632:GLN:HG2	1:F:639:LEU:HD11	2.00	0.43
3:H:85:CYS:HB2	3:H:164:LEU:HD22	2.00	0.43
1:A:1056:LEU:HD23	1:A:1056:LEU:HA	1.74	0.43
1:F:1108:TYR:O	1:F:1111:ILE:HG12	2.18	0.43
1:A:913:SER:HB3	1:A:914:PRO:CD	2.48	0.43
1:F:775:ASN:H	1:F:775:ASN:HD22	1.65	0.43
1:A:313:GLU:HG3	1:A:424:PHE:HZ	1.80	0.43
1:A:550:SER:HB2	1:A:600:VAL:HG12	1.99	0.43
1:A:563:VAL:CG1	1:A:570:LEU:HG	2.49	0.43
1:F:259:ASN:ND2	1:F:298:TYR:HD2	2.17	0.43
1:A:430:GLU:OE1	1:A:430:GLU:N	2.50	0.43
3:C:30:HIS:CE1	3:C:157:PHE:O	2.71	0.43
1:F:362:HIS:CD2	1:F:367:LEU:HD12	2.54	0.43
1:F:452:ARG:HG3	1:F:520:THR:CG2	2.48	0.43
1:F:1030:ILE:O	1:F:1034:ASN:HB2	2.19	0.43
1:A:596:ALA:HB2	1:A:823:LEU:CB	2.46	0.43
3:H:29:ARG:O	3:H:33:GLY:HA2	2.19	0.43
3:C:110:ARG:HD3	3:C:110:ARG:HA	1.85	0.43
1:A:162:GLU:HB3	1:A:167:PHE:CE1	2.54	0.43
1:F:1105:ARG:HH11	1:F:1134:LEU:HD11	1.82	0.43
3:H:80:TYR:HB2	3:H:111:VAL:HG11	1.99	0.43
1:F:1015:GLY:O	1:F:1016:LYS:C	2.56	0.43
1:A:387:ASP:HA	1:A:388:PRO:HD3	1.84	0.43
1:F:570:LEU:HD13	1:F:622:ASN:HD21	1.83	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:807:ASP:HA	1:F:810:LYS:HD3	2.00	0.43
1:F:522:ASN:O	1:F:523:ARG:C	2.57	0.43
1:A:447:MET:O	1:A:450:ALA:HB3	2.18	0.43
1:A:186:MET:O	1:A:190:PHE:HB2	2.19	0.43
1:F:1135:ASN:HB2	1:F:1136:PRO:HD3	2.01	0.43
1:F:121:VAL:HG21	1:F:159:ARG:HB3	2.01	0.43
1:F:1101:TYR:CZ	1:F:1105:ARG:HG3	2.54	0.42
1:F:661:ASN:H	1:F:665:GLN:HE21	1.65	0.42
1:A:291:PHE:HA	1:A:296:MET:HE1	1.99	0.42
1:A:856:PRO:HB3	1:A:902:PHE:CD2	2.53	0.42
1:F:574:PHE:CE2	1:F:611:MET:HE3	2.43	0.42
3:H:24:THR:N	6:H:1177:GTP:O1A	2.52	0.42
1:F:920:PHE:CE2	1:F:973:ILE:HG12	2.55	0.42
1:F:17:VAL:HG23	3:H:75:LEU:HD21	1.99	0.42
1:F:689:LEU:O	1:F:782:THR:OG1	2.30	0.42
1:F:587:GLU:HG2	1:F:590:LYS:HB2	2.01	0.42
1:A:27:GLN:HE21	1:A:31:LEU:CD1	2.30	0.42
1:F:821:LEU:HD11	1:F:828:VAL:CG2	2.50	0.42
1:A:1112:ARG:HD2	1:A:1130:ASP:OD2	2.20	0.42
1:F:452:ARG:HB2	1:F:516:GLN:NE2	2.34	0.42
1:A:1100:ILE:O	1:A:1104:LEU:HB2	2.20	0.42
1:A:5:GLN:HG2	1:A:6:VAL:N	2.35	0.42
3:H:45:VAL:HG22	3:H:46:GLU:N	2.34	0.42
1:A:1019:MET:C	1:A:1021:HIS:H	2.23	0.42
1:F:585:THR:O	1:F:587:GLU:N	2.53	0.42
1:A:710:LEU:HG	1:A:712:ASP:OD2	2.19	0.42
1:F:1036:LEU:O	1:F:1083:HIS:NE2	2.52	0.42
1:A:236:ASP:HB3	1:A:273:ILE:HG21	2.01	0.42
1:F:703:GLN:H	1:F:796:ALA:HB3	1.85	0.42
1:A:22:ASP:HB3	1:A:25:SER:HB3	2.02	0.42
3:H:106:ARG:O	3:H:110:ARG:HB2	2.20	0.42
1:A:165:VAL:HG21	1:A:237:TRP:CH2	2.54	0.42
1:A:658:GLN:C	1:A:660:LYS:N	2.73	0.42
1:A:821:LEU:HD21	1:A:828:VAL:CG2	2.50	0.42
1:F:355:SER:O	1:F:358:ALA:HB3	2.20	0.42
3:H:92:VAL:HG22	3:H:122:ASN:O	2.20	0.42
1:A:405:LEU:CD2	1:A:440:ARG:HD2	2.40	0.42
3:H:126:ILE:O	3:H:127:LYS:C	2.58	0.42
1:F:835:ARG:NE	1:F:835:ARG:HA	2.33	0.42
1:F:132:TRP:HH2	1:F:138:GLU:HG2	1.85	0.42
1:A:741:LEU:HD11	1:A:759:PRO:HG3	2.02	0.42
1:F:228:LEU:O	1:F:229:ASN:C	2.57	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:316:TYR:CE2	1:F:320:LYS:HD2	2.54	0.42
1:A:244:THR:O	1:A:245:ALA:C	2.58	0.42
1:F:646:CYS:SG	1:F:726:TYR:HB3	2.60	0.42
1:A:197:LEU:HD13	1:A:227:ALA:HB3	2.01	0.42
1:F:729:LEU:O	1:F:729:LEU:HD23	2.19	0.42
1:F:288:MET:HA	1:F:288:MET:CE	2.50	0.42
1:A:132:TRP:N	1:A:133:PRO:CD	2.83	0.41
1:A:472:THR:HG22	1:A:473:PHE:N	2.34	0.41
3:H:12:LYS:HD3	3:H:83:ALA:HA	2.02	0.41
1:A:13:LEU:HD23	1:A:36:PHE:HE2	1.84	0.41
1:A:962:VAL:O	1:A:966:THR:OG1	2.34	0.41
1:A:665:GLN:H	1:A:665:GLN:HG3	1.66	0.41
1:A:835:ARG:NE	1:A:835:ARG:HA	2.28	0.41
1:A:65:HIS:CD2	1:A:111:HIS:HD2	2.37	0.41
1:A:1030:ILE:HA	1:A:1071:TRP:HH2	1.84	0.41
3:C:39:TYR:HE1	6:C:1177:GTP:O3B	2.02	0.41
1:F:164:VAL:CG1	1:F:165:VAL:HG23	2.48	0.41
1:F:303:ALA:O	1:F:306:ALA:CB	2.68	0.41
1:A:745:LYS:HA	1:A:750:VAL:CG1	2.50	0.41
1:A:563:VAL:H	1:A:563:VAL:HG23	1.63	0.41
1:A:901:LEU:HD21	1:A:975:VAL:HG12	2.02	0.41
1:F:806:LEU:HD12	1:F:808:ALA:HB3	2.02	0.41
1:A:545:ASP:HA	1:A:546:PRO:HD3	1.87	0.41
1:F:1111:ILE:H	1:F:1111:ILE:HG12	1.62	0.41
3:H:9:VAL:CG2	3:H:59:ILE:HD12	2.51	0.41
3:H:125:ASP:HB3	3:H:153:SER:HB2	2.01	0.41
1:A:127:GLU:HB2	1:A:131:HIS:HB2	2.02	0.41
1:A:738:PRO:CD	1:A:749:PHE:CE1	3.03	0.41
3:C:138:PHE:CZ	3:C:142:LYS:HG3	2.55	0.41
5:E:40:G:H2'	5:E:40:G:N3	2.36	0.41
1:A:57:LYS:H	1:A:57:LYS:HG2	1.58	0.41
1:F:328:ALA:O	1:F:332:GLN:HG2	2.21	0.41
1:F:1062:GLY:O	1:F:1063:THR:C	2.59	0.41
1:F:165:VAL:HG11	1:F:237:TRP:CD2	2.55	0.41
1:A:711:GLU:HG2	1:A:714:CYS:HB2	2.02	0.41
3:H:9:VAL:HG21	3:H:59:ILE:HD12	2.02	0.41
1:A:604:ALA:O	1:A:608:ILE:HG12	2.21	0.41
1:A:877:PHE:HB3	1:A:880:LEU:HD11	2.02	0.41
1:A:913:SER:HB3	1:A:914:PRO:HD3	2.02	0.41
3:H:110:ARG:HA	3:H:110:ARG:HD3	1.83	0.41
1:F:66:PHE:CE2	1:F:70:ILE:HD11	2.56	0.41
3:C:23:LYS:NZ	6:C:1177:GTP:O2G	2.44	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:280:LYS:HB3	1:A:283:ASP:OD1	2.21	0.41
1:F:282:GLU:HA	1:F:285:LYS:HE3	2.02	0.41
1:A:836:MET:O	1:A:839:PHE:HB3	2.21	0.41
1:F:674:ALA:N	1:F:675:PRO:CD	2.83	0.41
1:F:559:LEU:C	1:F:561:PRO:HD2	2.40	0.41
1:A:799:PHE:HA	1:A:833:LEU:HD13	2.03	0.41
1:A:362:HIS:CD2	1:A:367:LEU:HD12	2.56	0.41
1:F:236:ASP:OD1	1:F:236:ASP:N	2.52	0.41
1:A:201:VAL:O	1:A:205:GLN:HG2	2.21	0.41
1:A:698:TYR:CD2	1:A:717:ASN:HB3	2.56	0.41
1:A:584:GLU:O	1:A:586:VAL:N	2.54	0.41
1:F:616:PRO:CB	1:F:658:GLN:HG3	2.47	0.41
1:F:1026:THR:O	1:F:1030:ILE:HG13	2.21	0.41
1:A:291:PHE:O	1:A:348:ASN:HB2	2.21	0.41
1:A:402:MET:SD	1:A:461:MET:HE2	2.61	0.41
1:F:114:ASP:OD1	1:F:159:ARG:NH1	2.53	0.41
1:F:688:VAL:O	1:F:695:PHE:HB2	2.21	0.41
1:A:337:LEU:HD12	1:A:337:LEU:HA	1.83	0.41
1:F:655:ILE:HG21	1:F:655:ILE:HD13	1.76	0.41
1:F:26:THR:HB	1:F:29:TYR:CD1	2.56	0.41
1:A:877:PHE:CZ	1:A:895:PHE:HE2	2.39	0.41
1:A:380:ARG:CZ	4:D:9:U:H4'	2.50	0.41
1:A:190:PHE:HE1	1:A:234:TYR:HB3	1.87	0.40
1:A:313:GLU:OE2	3:C:167:LYS:NZ	2.54	0.40
1:F:550:SER:HB2	1:F:600:VAL:CG1	2.51	0.40
1:A:851:LEU:HD23	1:A:851:LEU:HA	1.91	0.40
1:A:168:GLN:HG3	1:A:168:GLN:O	2.21	0.40
1:A:205:GLN:NE2	1:A:205:GLN:HA	2.26	0.40
1:A:1018:LEU:HB3	1:A:1024:VAL:CG1	2.51	0.40
1:A:897:LYS:HB3	1:A:898:PRO:CD	2.51	0.40
1:F:1121:ILE:HD12	2:G:1315:UNK:O	2.21	0.40
1:F:24:ASN:OD1	1:F:24:ASN:N	2.53	0.40
1:F:128:TRP:O	1:F:130:GLN:N	2.55	0.40
1:F:7:ASN:HA	1:F:53:ARG:HH12	1.86	0.40
1:A:1026:THR:HG22	1:A:1030:ILE:HD11	2.02	0.40
1:F:971:ASP:O	1:F:975:VAL:HG23	2.21	0.40
3:C:101:VAL:N	3:C:102:PRO:CD	2.84	0.40
1:F:1064:LEU:HB2	1:F:1108:TYR:OH	2.21	0.40
1:F:337:LEU:HD21	1:F:343:VAL:O	2.21	0.40
1:A:97:LEU:HD23	1:A:97:LEU:HA	1.81	0.40
1:A:517:MET:CG	1:A:521:LEU:HD12	2.50	0.40
1:A:124:ILE:HD13	1:A:124:ILE:HG21	1.91	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:1056:LEU:HD23	1:F:1056:LEU:HA	1.82	0.40
1:A:879:ASN:OD1	1:A:882:ASN:ND2	2.53	0.40
1:F:531:GLY:HA3	1:F:562:PHE:CE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	1062/1204 (88%)	965 (91%)	73 (7%)	24 (2%)	10	35
1	F	1062/1204 (88%)	948 (89%)	92 (9%)	22 (2%)	11	38
3	C	168/216 (78%)	154 (92%)	11 (6%)	3 (2%)	13	43
3	H	168/216 (78%)	152 (90%)	15 (9%)	1 (1%)	33	75
All	All	2460/2840 (87%)	2219 (90%)	191 (8%)	50 (2%)	11	40

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	GLU
1	A	211	THR
1	A	245	ALA
1	A	340	ASP
1	A	712	ASP
3	C	127	LYS
1	F	128	TRP
1	F	306	ALA
1	F	523	ARG
1	F	585	THR
1	F	712	ASP
3	H	127	LYS
1	A	100	ASN
1	A	168	GLN
1	A	495	VAL

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Mol	Chain	Res	Type
1	A	523	ARG
1	A	527	PRO
1	A	587	GLU
1	A	1060	LEU
1	A	1120	GLU
1	F	103	LEU
1	F	805	MET
1	F	1083	HIS
1	A	585	THR
1	A	616	PRO
1	A	831	THR
1	A	886	TYR
1	A	1083	HIS
3	C	10	GLN
1	F	248	CYS
1	F	586	VAL
1	F	587	GLU
1	F	594	THR
1	F	820	LEU
1	F	1135	ASN
1	A	348	ASN
1	A	588	GLU
1	A	1135	ASN
3	C	8	GLN
1	F	105	ILE
1	A	105	ILE
1	A	241	SER
1	F	132	TRP
1	A	827	PRO
1	F	23	PRO
1	F	46	ILE
1	F	129	PRO
1	F	527	PRO
1	F	817	PRO
1	F	495	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	967/1073 (90%)	895 (93%)	72 (7%)	20	50
1	F	967/1073 (90%)	885 (92%)	82 (8%)	15	42
3	C	150/185 (81%)	143 (95%)	7 (5%)	36	75
3	H	150/185 (81%)	144 (96%)	6 (4%)	42	80
All	All	2234/2516 (89%)	2067 (92%)	167 (8%)	19	49

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	26	THR
1	A	28	ARG
1	A	38	GLU
1	A	39	GLU
1	A	46	ILE
1	A	57	LYS
1	A	59	GLN
1	A	105	ILE
1	A	130	GLN
1	A	132	TRP
1	A	138	GLU
1	A	147	GLU
1	A	159	ARG
1	A	169	THR
1	A	188	ARG
1	A	190	PHE
1	A	205	GLN
1	A	236	ASP
1	A	250	LEU
1	A	261	GLN
1	A	275	VAL
1	A	278	LYS
1	A	284	ARG
1	A	300	LEU
1	A	329	LEU
1	A	341	SER
1	A	415	ASP
1	A	433	ASN
1	A	440	ARG
1	A	442	GLN
1	A	466	LEU
1	A	520	THR

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Mol	Chain	Res	Type
1	A	535	LEU
1	A	568	GLU
1	A	576	LYS
1	A	583	PHE
1	A	600	VAL
1	A	624	ASP
1	A	641	THR
1	A	701	THR
1	A	711	GLU
1	A	712	ASP
1	A	736	CYS
1	A	756	SER
1	A	762	ARG
1	A	773	LEU
1	A	775	ASN
1	A	784	ASN
1	A	792	LEU
1	A	825	ASP
1	A	835	ARG
1	A	849	HIS
1	A	860	GLN
1	A	868	LEU
1	A	870	THR
1	A	881	ASN
1	A	899	LEU
1	A	906	GLU
1	A	907	HIS
1	A	919	LEU
1	A	924	HIS
1	A	1014	LEU
1	A	1034	ASN
1	A	1036	LEU
1	A	1040	ASP
1	A	1041	THR
1	A	1042	LEU
1	A	1045	GLN
1	A	1082	MET
1	A	1105	ARG
1	A	1111	ILE
3	C	60	LYS
3	C	69	GLN
3	C	76	ARG

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Mol	Chain	Res	Type
3	C	84	GLN
3	C	112	CYS
3	C	141	LYS
3	C	166	ARG
1	F	24	ASN
1	F	25	SER
1	F	28	ARG
1	F	32	GLU
1	F	38	GLU
1	F	39	GLU
1	F	57	LYS
1	F	58	THR
1	F	59	GLN
1	F	105	ILE
1	F	131	HIS
1	F	132	TRP
1	F	138	GLU
1	F	147	GLU
1	F	188	ARG
1	F	190	PHE
1	F	205	GLN
1	F	231	LEU
1	F	250	LEU
1	F	261	GLN
1	F	264	GLN
1	F	269	GLU
1	F	275	VAL
1	F	280	LYS
1	F	300	LEU
1	F	329	LEU
1	F	341	SER
1	F	348	ASN
1	F	405	LEU
1	F	427	ASP
1	F	440	ARG
1	F	466	LEU
1	F	491	SER
1	F	522	ASN
1	F	523	ARG
1	F	535	LEU
1	F	543	THR
1	F	568	GLU

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Mol	Chain	Res	Type
1	F	570	LEU
1	F	575	SER
1	F	576	LYS
1	F	583	PHE
1	F	590	LYS
1	F	617	GLN
1	F	624	ASP
1	F	693	ASP
1	F	703	GLN
1	F	734	ARG
1	F	741	LEU
1	F	742	GLU
1	F	754	THR
1	F	762	ARG
1	F	773	LEU
1	F	775	ASN
1	F	797	GLU
1	F	806	LEU
1	F	810	LYS
1	F	820	LEU
1	F	824	ASN
1	F	826	SER
1	F	830	LYS
1	F	831	THR
1	F	835	ARG
1	F	849	HIS
1	F	860	GLN
1	F	868	LEU
1	F	879	ASN
1	F	880	LEU
1	F	881	ASN
1	F	882	ASN
1	F	899	LEU
1	F	919	LEU
1	F	1013	ASP
1	F	1014	LEU
1	F	1034	ASN
1	F	1041	THR
1	F	1042	LEU
1	F	1045	GLN
1	F	1085	GLN
1	F	1105	ARG

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Mol	Chain	Res	Type
1	F	1111	ILE
1	F	1123	LYS
3	H	60	LYS
3	H	69	GLN
3	H	76	ARG
3	H	84	GLN
3	H	110	ARG
3	H	141	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	65	HIS
1	A	69	GLN
1	A	73	HIS
1	A	80	ASN
1	A	111	HIS
1	A	130	GLN
1	A	149	GLN
1	A	168	GLN
1	A	173	GLN
1	A	179	GLN
1	A	202	ASN
1	A	205	GLN
1	A	213	GLN
1	A	242	HIS
1	A	362	HIS
1	A	381	HIS
1	A	442	GLN
1	A	469	GLN
1	A	617	GLN
1	A	636	ASN
1	A	657	ASN
1	A	665	GLN
1	A	703	GLN
1	A	775	ASN
1	A	784	ASN
1	A	837	GLN
1	A	879	ASN
1	A	882	ASN
1	A	907	HIS

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Mol	Chain	Res	Type
1	A	935	ASN
1	A	1021	HIS
1	A	1058	GLN
3	C	30	HIS
3	C	143	ASN
3	C	156	ASN
3	C	173	ASN
1	F	65	HIS
1	F	111	HIS
1	F	149	GLN
1	F	173	GLN
1	F	179	GLN
1	F	185	ASN
1	F	200	ASN
1	F	202	ASN
1	F	205	GLN
1	F	242	HIS
1	F	247	ASN
1	F	259	ASN
1	F	264	GLN
1	F	362	HIS
1	F	442	GLN
1	F	469	GLN
1	F	516	GLN
1	F	622	ASN
1	F	628	ASN
1	F	636	ASN
1	F	657	ASN
1	F	665	GLN
1	F	775	ASN
1	F	784	ASN
1	F	837	GLN
1	F	860	GLN
1	F	879	ASN
1	F	907	HIS
1	F	935	ASN
1	F	1045	GLN
1	F	1058	GLN
1	F	1085	GLN
3	H	143	ASN
3	H	156	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	D	20/24 (83%)	7 (35%)	0
4	I	20/24 (83%)	6 (30%)	0
5	E	23/24 (95%)	4 (17%)	0
5	J	23/24 (95%)	3 (13%)	0
All	All	86/96 (89%)	20 (23%)	0

All (20) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	D	6	A
4	D	11	C
4	D	15	A
4	D	16	C
4	D	19	G
4	D	20	A
4	D	21	A
5	E	41	G
5	E	44	U
5	E	47	A
5	E	62	G
4	I	11	C
4	I	15	A
4	I	16	C
4	I	19	G
4	I	20	A
4	I	21	A
5	J	41	G
5	J	47	A
5	J	62	G

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	GTP	C	1177	7	34,34,34	1.23	2 (5%)	51,54,54	2.20	12 (23%)
6	GTP	H	1177	7	34,34,34	1.02	1 (2%)	51,54,54	2.99	14 (27%)

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	GTP	C	1177	7	-	0/22/38/38	0/1/3/3
6	GTP	H	1177	7	-	0/22/38/38	0/1/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1177	GTP	C2-N3	5.46	1.40	1.33
6	H	1177	GTP	C2-N3	3.50	1.37	1.33
6	C	1177	GTP	C2-N1	2.12	1.40	1.36

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	1177	GTP	C6-C5-N7	-15.70	132.03	134.14
6	C	1177	GTP	C6-C5-N7	-8.47	133.00	134.14
6	H	1177	GTP	O4'-C1'-N9	7.56	115.47	108.44
6	C	1177	GTP	PB-O3B-PG	-5.51	115.51	131.68
6	C	1177	GTP	O3A-PB-O3B	-4.40	92.72	101.66
6	C	1177	GTP	PA-O3A-PB	-3.94	120.14	131.68
6	H	1177	GTP	C5-C4-N3	-3.76	120.49	125.94
6	H	1177	GTP	PB-O3B-PG	-3.60	121.12	131.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	1177	GTP	O3A-PA-O5'	-3.60	87.31	103.41
6	C	1177	GTP	C5-C4-N3	-3.44	120.96	125.94
6	C	1177	GTP	C2-N3-C4	3.38	119.85	115.09
6	H	1177	GTP	N3-C4-N9	3.33	131.80	126.91
6	C	1177	GTP	O4'-C1'-N9	-3.31	105.36	108.44
6	C	1177	GTP	N3-C4-N9	3.19	131.58	126.91
6	H	1177	GTP	O2G-PG-O3B	3.05	119.59	105.14
6	C	1177	GTP	O3G-PG-O2G	2.97	119.17	107.61
6	H	1177	GTP	C2-N3-C4	2.97	119.26	115.09
6	H	1177	GTP	C3'-C2'-C1'	2.85	105.36	100.91
6	H	1177	GTP	C2'-C1'-N9	-2.73	106.26	113.27
6	H	1177	GTP	O3G-PG-O1G	2.70	119.26	110.44
6	C	1177	GTP	C4'-O4'-C1'	2.52	112.49	109.75
6	C	1177	GTP	C4-C5-N7	-2.41	107.46	109.52
6	H	1177	GTP	PA-O3A-PB	-2.33	124.84	131.68
6	H	1177	GTP	C5'-C4'-C3'	-2.31	105.96	115.21
6	C	1177	GTP	O3'-C3'-C4'	-2.24	104.47	111.08
6	H	1177	GTP	O2A-PA-O3A	2.22	115.69	105.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1072/1204 (89%)	0.22	46 (4%) 34 40	32, 76, 127, 156	0
1	F	1072/1204 (89%)	0.59	113 (10%) 7 8	59, 94, 143, 162	0
2	B	0/13	-	-	-	-
2	G	0/13	-	-	-	-
3	C	170/216 (78%)	0.34	6 (3%) 42 49	59, 90, 115, 127	0
3	H	170/216 (78%)	0.28	3 (1%) 65 75	64, 88, 111, 122	0
4	D	22/24 (91%)	1.67	8 (36%) 1 1	62, 126, 220, 227	0
4	I	22/24 (91%)	2.48	11 (50%) 0 0	71, 191, 259, 263	0
5	E	24/24 (100%)	1.67	10 (41%) 1 0	78, 118, 205, 210	0
5	J	24/24 (100%)	2.65	7 (29%) 1 1	121, 170, 256, 271	0
All	All	2576/2962 (86%)	0.46	204 (7%) 13 15	32, 86, 141, 271	0

All (204) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	J	40	G	14.9
1	F	823	LEU	11.0
1	F	819	PRO	9.9
1	F	820	LEU	9.5
1	F	4	ASP	8.9
1	A	3	MET	8.0
1	F	821	LEU	7.9
4	I	23	C	7.2
5	J	41	G	6.9
5	J	42	C	6.7
1	F	818	GLN	6.4
1	F	2	ALA	6.4
1	F	1072	LEU	6.3
1	F	1077	LEU	6.1

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Mol	Chain	Res	Type	RSRZ
1	F	840	PHE	5.8
1	A	4	ASP	5.7
1	F	1073	PHE	5.7
1	F	1100	ILE	5.7
1	A	1060	LEU	5.6
5	E	47	A	5.5
4	D	23	C	5.4
1	A	2	ALA	5.3
5	J	62	G	5.3
4	I	22	G	5.3
4	I	24	U	5.3
1	F	1090	MET	5.3
1	F	825	ASP	5.1
5	J	63	C	5.1
1	A	708	PRO	5.0
1	F	824	ASN	5.0
1	F	3	MET	4.9
4	D	14	G	4.9
1	F	822	GLU	4.5
1	A	823	LEU	4.5
1	A	1104	LEU	4.5
4	I	19	G	4.5
4	D	22	G	4.4
1	F	1033	PHE	4.4
1	F	699	VAL	4.3
5	E	40	G	4.3
5	J	46	C	4.3
1	F	786	LEU	4.3
1	F	1051	LEU	4.2
1	F	839	PHE	4.2
4	I	18	G	4.2
1	A	827	PRO	4.1
1	F	1116	GLU	4.1
1	A	1073	PHE	4.1
1	A	1098	PHE	4.1
1	F	692	VAL	4.1
1	A	819	PRO	4.0
5	E	43	U	4.0
5	J	43	U	3.9
4	I	16	C	3.9
4	D	19	G	3.9
4	I	21	A	3.9

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Mol	Chain	Res	Type	RSRZ
1	F	303	ALA	3.8
5	E	46	C	3.8
1	A	308	GLY	3.8
1	A	829	PHE	3.8
1	F	1094	VAL	3.7
1	F	1098	PHE	3.7
1	F	783	HIS	3.7
1	F	1132	LYS	3.7
1	A	1106	PRO	3.7
1	F	833	LEU	3.7
4	I	20	A	3.6
1	A	821	LEU	3.6
1	F	1046	ARG	3.6
1	F	687	ARG	3.6
1	F	1093	LEU	3.6
1	F	701	THR	3.5
1	A	820	LEU	3.5
1	F	1096	LEU	3.5
1	F	695	PHE	3.5
1	A	1120	GLU	3.4
1	A	832	VAL	3.4
1	A	828	VAL	3.3
3	C	32	THR	3.3
1	F	680	TRP	3.3
1	F	1115	MET	3.3
1	F	164	VAL	3.3
1	F	39	GLU	3.3
1	F	689	LEU	3.2
5	E	48	G	3.2
5	E	42	C	3.2
1	F	1049	SER	3.2
1	F	1085	GLN	3.2
4	D	24	U	3.2
1	A	713	PRO	3.2
1	F	708	PRO	3.2
1	F	102	THR	3.1
4	D	18	G	3.1
1	F	308	GLY	3.1
1	F	9	LEU	3.1
1	A	798	PRO	3.1
1	F	1036	LEU	3.0
1	F	1092	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	40	PHE	3.0
1	F	517	MET	3.0
1	F	43	LYS	3.0
3	H	43	LEU	3.0
1	F	828	VAL	2.9
4	D	21	A	2.9
1	F	1104	LEU	2.9
1	F	964	MET	2.9
1	F	1053	TRP	2.9
1	F	697	ALA	2.9
1	F	803	LEU	2.9
1	A	825	ASP	2.9
4	I	17	U	2.9
1	F	1119	PRO	2.8
1	F	1076	VAL	2.8
1	A	1100	ILE	2.8
1	F	813	ILE	2.8
1	F	1069	VAL	2.8
1	F	574	PHE	2.8
1	F	792	LEU	2.8
1	A	952	GLU	2.8
1	A	1055	LEU	2.8
1	F	54	LEU	2.8
4	D	11	C	2.8
1	A	1062	GLY	2.7
1	F	1048	THR	2.7
1	F	1087	ASP	2.7
1	F	378	LEU	2.7
1	F	6	VAL	2.7
1	F	13	LEU	2.7
1	F	1121	ILE	2.7
3	C	35	PHE	2.7
1	F	826	SER	2.7
5	E	45	U	2.7
3	C	31	LEU	2.7
5	E	44	U	2.7
1	A	712	ASP	2.7
1	F	491	SER	2.7
1	F	1123	LYS	2.7
3	C	33	GLY	2.7
1	F	937	ARG	2.6
1	A	830	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	1120	GLU	2.6
1	A	1053	TRP	2.6
1	A	1129	PHE	2.6
1	F	209	THR	2.6
1	F	66	PHE	2.6
1	F	41	LYS	2.6
1	F	795	MET	2.6
1	F	62	ILE	2.6
1	A	1109	LEU	2.5
1	F	807	ASP	2.5
5	E	41	G	2.5
1	F	721	MET	2.5
1	A	1080	LEU	2.4
1	F	836	MET	2.4
1	F	1124	ASP	2.4
1	A	1059	VAL	2.4
1	F	969	VAL	2.4
1	F	1103	ALA	2.4
1	F	67	GLY	2.4
1	F	815	GLY	2.4
1	A	54	LEU	2.4
1	F	585	THR	2.4
4	I	14	G	2.3
1	F	802	ALA	2.3
5	E	62	G	2.3
1	A	709	GLY	2.3
1	A	1064	LEU	2.3
1	A	1029	LEU	2.3
1	F	952	GLU	2.3
1	F	1050	GLN	2.3
1	F	696	ILE	2.3
1	F	814	LEU	2.2
1	A	817	PRO	2.2
3	H	72	PHE	2.2
1	A	1095	HIS	2.2
1	F	20	MET	2.2
1	F	694	ALA	2.2
1	A	1126	LEU	2.2
1	F	1029	LEU	2.2
3	H	81	ILE	2.2
3	C	134	LYS	2.2
1	F	379	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	43	LEU	2.2
1	F	508	LEU	2.2
1	F	1101	TYR	2.2
1	A	1057	LYS	2.2
1	F	832	VAL	2.2
4	I	11	C	2.2
1	F	586	VAL	2.1
1	F	716	LEU	2.1
1	F	1099	GLN	2.1
1	A	390	LEU	2.1
1	A	818	GLN	2.1
1	F	835	ARG	2.1
1	F	805	MET	2.1
1	F	1032	ALA	2.1
1	F	698	TYR	2.1
1	A	711	GLU	2.1
1	A	1133	LEU	2.1
1	F	1126	LEU	2.1
1	F	514	ILE	2.0
1	A	835	ARG	2.0
1	F	611	MET	2.0
1	F	1102	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	MG	H	1178	1/1	0.23	0.35	74,74,74,74	0
6	GTP	H	1177	32/32	0.19	-0.43	92,100,112,115	0
6	GTP	C	1177	32/32	0.18	-0.57	96,101,105,106	0
7	MG	C	1178	1/1	0.15	-3.03	85,85,85,85	0

6.5 Other polymers

There are no such residues in this entry.