



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:43 PM UTC

PDB ID : 2R7X / pdb_00002r7x
Title : Crystal Structure of Rotavirus SA11 VP1/RNA (UGUGACC)/GTP complex
Authors : Lu, X.; Harrison, S.C.; Tao, Y.J.; Patton, J.T.; Nibert, M.L.
Deposited on : 2007-09-10
Resolution : 2.80 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

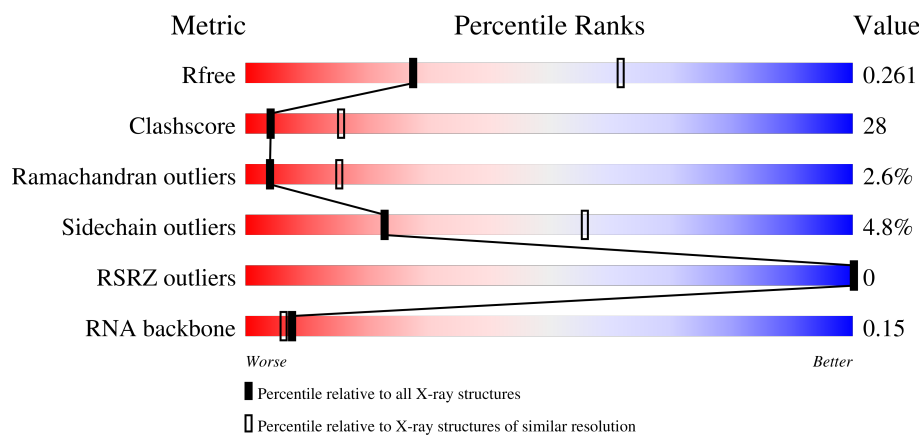
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)
RNA backbone	3983	1114 (3.00-2.60)

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	X	7	29% 29% 43%
1	Y	7	14% 43% 43%
2	A	1095	48% 43% 6% .
2	B	1095	49% 43% 6% ..

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 17744 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

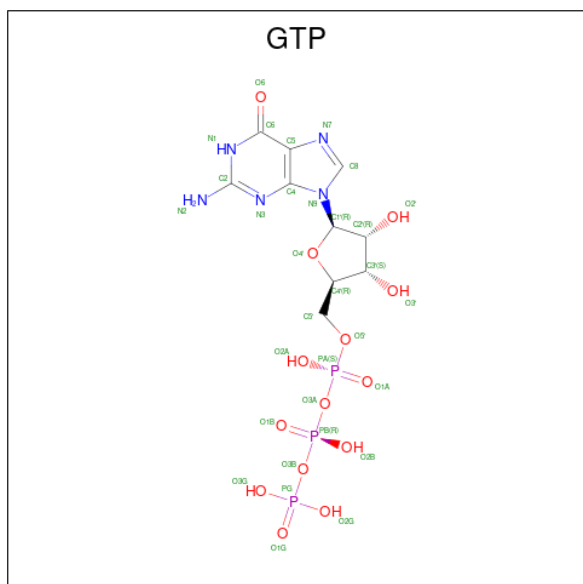
- Molecule 1 is a RNA chain called RNA (5'-R(*UP*GP*UP*GP*AP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	7	Total	C	N	O	P	0	0	0
			145	66	25	48	6			
1	Y	7	Total	C	N	O	P	0	0	0
			145	66	25	48	6			

- Molecule 2 is a protein called RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	1073	Total	C	N	O	S	0	0	0
			8695	5576	1447	1634	38			
2	B	1073	Total	C	N	O	S	0	0	0
			8695	5576	1447	1634	38			

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

3 Residue-property plots

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

- Molecule 1: RNA (5'-R(*UP*GP*UP*GP*AP*CP*C)-3')

Chain X: 



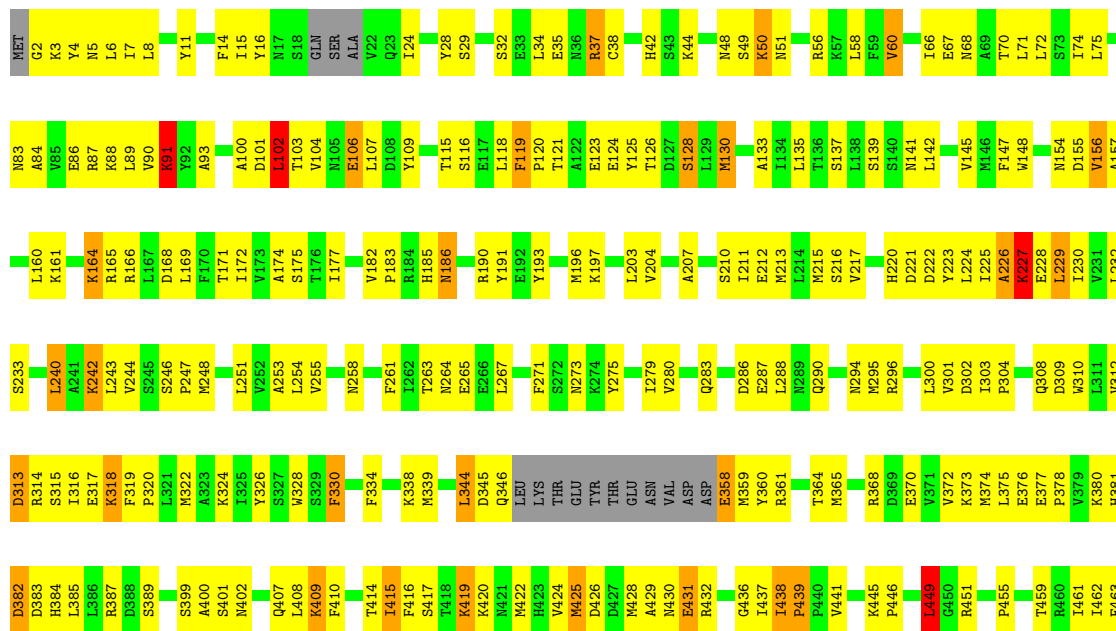
- Molecule 1: RNA (5'-R(*UP*GP*UP*GP*AP*CP*C)-3')

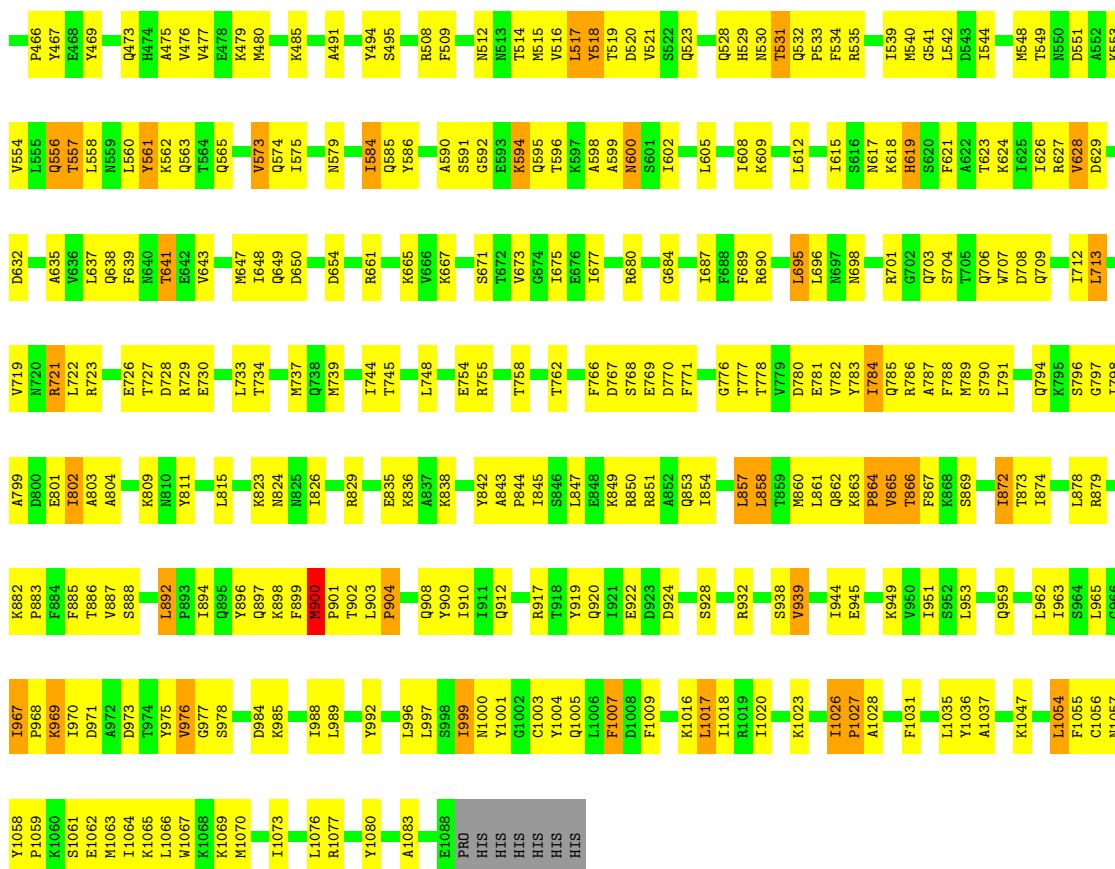
Chain Y: 



- Molecule 2: RNA-dependent RNA polymerase

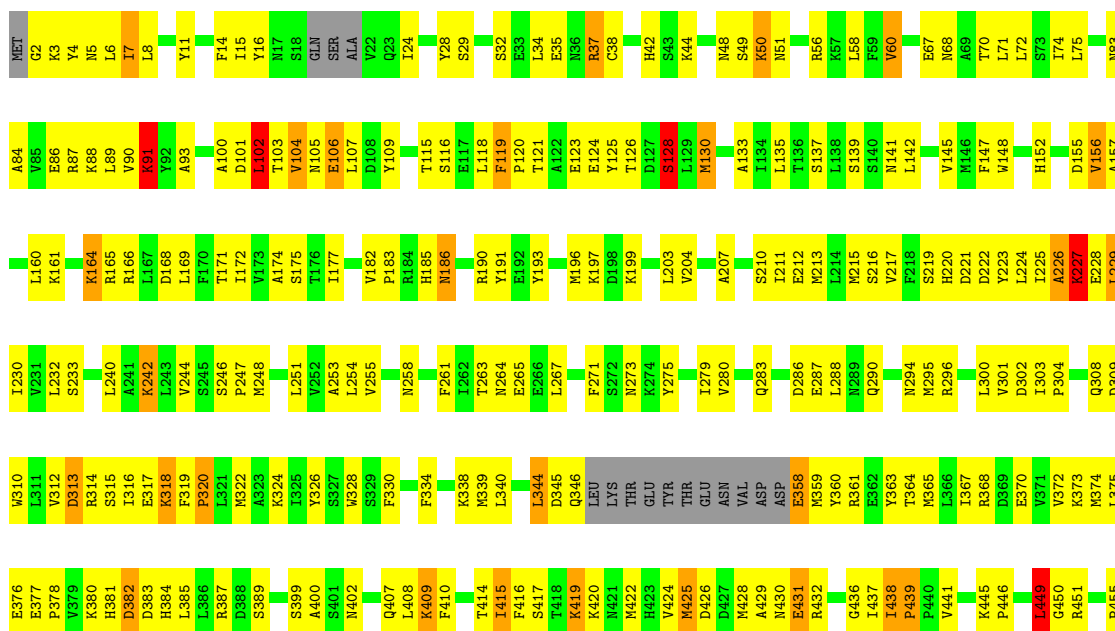
Chain A: 





- Molecule 2: RNA-dependent RNA polymerase

Chain B: 49% 43% 6% . .



[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.00Å 143.77Å 112.83Å 90.00° 90.65° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	83.1 (30.00-2.80) 80.8 (30.00-2.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.233 , 0.277 0.217 , 0.261	Depositor DCC
R_{free} test set	4650 reflections (8.06%)	wwPDB-VP
Wilson B-factor (Å ²)	55.4	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 23.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.358 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17744	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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: GTP

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	X	0.41	0/161	1.21	3/249 (1.2%)
1	Y	0.39	0/161	1.22	4/249 (1.6%)
2	A	0.49	0/8866	0.99	44/11985 (0.4%)
2	B	0.49	0/8866	0.99	45/11985 (0.4%)
All	All	0.49	0/18054	1.00	96/24468 (0.4%)

There are no bond length outliers.

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1026	ILE	CA-C-N	9.02	131.12	119.84
2	A	1026	ILE	C-N-CA	9.02	131.12	119.84
2	B	1026	ILE	CA-C-N	8.83	130.88	119.84
2	B	1026	ILE	C-N-CA	8.83	130.88	119.84
2	A	1020	ILE	N-CA-C	8.52	116.59	108.15
2	B	1020	ILE	N-CA-C	8.49	116.56	108.15
2	A	579	ASN	N-CA-C	-7.88	101.58	112.30
2	B	579	ASN	N-CA-C	-7.82	101.67	112.30
2	B	1058	TYR	CA-C-N	7.14	127.14	119.78
2	B	1058	TYR	C-N-CA	7.14	127.14	119.78
2	A	37	ARG	N-CA-C	-7.14	102.91	111.69
2	B	37	ARG	N-CA-C	-7.09	102.97	111.69
2	B	67	GLU	N-CA-C	7.00	118.69	111.14
2	A	1058	TYR	CA-C-N	6.99	126.98	119.78
2	A	1058	TYR	C-N-CA	6.99	126.98	119.78
2	A	67	GLU	N-CA-C	6.83	118.51	111.14
2	B	83	ASN	N-CA-C	-6.58	103.67	112.94
2	B	60	VAL	N-CA-C	-6.42	105.48	111.45
2	B	1004	TYR	N-CA-C	6.42	118.28	111.28
1	Y	1103	U	C2'-C3'-O3'	6.37	119.06	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1007	PHE	N-CA-C	6.37	119.48	110.50
2	A	83	ASN	N-CA-C	-6.32	104.03	112.94
2	B	119	PHE	CA-C-N	6.30	125.87	119.19
2	B	119	PHE	C-N-CA	6.30	125.87	119.19
2	A	1007	PHE	N-CA-C	6.28	119.36	110.50
2	B	449	LEU	N-CA-C	6.28	120.15	110.42
2	A	60	VAL	N-CA-C	-6.25	105.64	111.45
2	B	330	PHE	N-CA-C	6.19	119.00	111.82
2	A	449	LEU	N-CA-C	6.19	120.02	110.42
2	B	900	MET	CA-C-N	6.18	126.37	119.32
2	B	900	MET	C-N-CA	6.18	126.37	119.32
2	A	119	PHE	CA-C-N	6.18	125.74	119.19
2	A	119	PHE	C-N-CA	6.18	125.74	119.19
2	B	207	ALA	N-CA-C	-6.14	104.28	110.97
1	X	1103	U	C2'-C3'-O3'	6.08	118.62	109.50
2	A	1004	TYR	N-CA-C	5.97	117.79	111.28
2	B	438	ILE	CA-C-N	5.95	126.51	120.38
2	B	438	ILE	C-N-CA	5.95	126.51	120.38
2	A	594	LYS	N-CA-C	-5.94	105.11	112.90
2	A	902	THR	N-CA-C	5.93	118.70	111.82
2	A	438	ILE	CA-C-N	5.92	126.48	120.38
2	A	438	ILE	C-N-CA	5.92	126.48	120.38
2	B	713	LEU	N-CA-C	-5.90	104.54	110.97
2	A	445	LYS	CA-C-N	5.85	125.85	119.89
2	A	445	LYS	C-N-CA	5.85	125.85	119.89
2	A	494	TYR	N-CA-C	5.82	119.03	110.30
2	A	207	ALA	N-CA-C	-5.79	104.65	110.97
2	B	594	LYS	N-CA-C	-5.76	105.35	112.90
2	B	104	VAL	N-CA-C	5.75	118.28	111.09
2	B	902	THR	N-CA-C	5.74	118.48	111.82
2	B	494	TYR	N-CA-C	5.73	118.89	110.30
2	B	939	VAL	N-CA-C	-5.72	106.18	113.22
2	B	575	ILE	CB-CA-C	-5.68	105.66	110.94
2	B	739	MET	N-CA-C	5.65	118.98	111.75
2	A	900	MET	CA-C-N	5.65	126.90	119.84
2	A	900	MET	C-N-CA	5.65	126.90	119.84
2	A	1001	TYR	N-CA-C	5.62	118.86	110.14
2	A	68	ASN	N-CA-C	5.62	120.13	112.88
2	A	939	VAL	N-CA-C	-5.61	106.31	113.22
2	B	969	LYS	N-CA-C	5.60	117.07	111.07
2	A	104	VAL	N-CA-C	5.59	118.08	111.09
2	A	739	MET	N-CA-C	5.57	118.88	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	68	ASN	N-CA-C	5.54	120.03	112.88
2	A	475	ALA	N-CA-C	5.54	116.99	111.07
2	B	445	LYS	CA-C-N	5.49	125.49	119.89
2	B	445	LYS	C-N-CA	5.49	125.49	119.89
2	A	969	LYS	N-CA-C	5.47	116.92	111.07
2	A	216	SER	N-CA-C	-5.47	105.30	112.41
1	Y	1102	G	C2'-C3'-O3'	5.44	117.66	109.50
2	A	558	LEU	N-CA-C	-5.43	105.44	111.36
2	B	402	ASN	N-CA-C	-5.43	107.03	113.97
2	B	436	GLY	N-CA-C	-5.40	107.62	114.16
1	X	1102	G	C2'-C3'-O3'	5.38	117.57	109.50
2	A	32	SER	N-CA-C	5.33	117.51	111.11
2	B	32	SER	N-CA-C	5.33	117.51	111.11
2	B	216	SER	N-CA-C	-5.32	105.50	112.41
2	A	436	GLY	N-CA-C	-5.27	107.78	114.16
2	B	419	LYS	N-CA-C	5.26	117.94	110.10
2	A	713	LEU	N-CA-C	-5.24	105.26	110.97
1	Y	1101	U	C2'-C3'-O3'	5.24	117.35	109.50
2	B	475	ALA	N-CA-C	5.22	116.65	111.07
2	B	561	TYR	N-CA-C	-5.20	105.06	111.40
2	A	727	THR	N-CA-C	-5.20	100.77	109.24
2	A	967	ILE	CA-C-N	5.17	125.11	119.78
2	A	967	ILE	C-N-CA	5.17	125.11	119.78
2	A	419	LYS	N-CA-C	5.17	117.80	110.10
2	B	727	THR	N-CA-C	-5.15	100.85	109.24
2	B	1001	TYR	N-CA-C	5.15	118.12	110.14
2	A	561	TYR	N-CA-C	-5.13	105.14	111.40
1	X	1101	U	C2'-C3'-O3'	5.12	117.19	109.50
2	B	558	LEU	N-CA-C	-5.10	105.42	111.69
2	A	330	PHE	N-CA-C	5.10	118.76	112.54
2	B	7	ILE	N-CA-C	-5.10	106.29	112.76
2	A	402	ASN	N-CA-C	-5.09	107.46	113.97
2	B	891	HIS	N-CA-C	5.04	116.07	108.46
1	Y	1106	C	C5'-C4'-C3'	-5.03	108.46	116.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	145	0	77	18	0
1	Y	145	0	77	16	0
2	A	8695	0	8782	481	0
2	B	8695	0	8782	479	0
3	A	32	0	12	2	0
3	B	32	0	12	2	0
All	All	17744	0	17742	977	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 28.

All (977) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:865:VAL:HG13	2:A:866:THR:H	1.14	1.08
2:B:865:VAL:HG13	2:B:866:THR:H	1.14	1.08
2:B:734:THR:HA	2:B:737:MET:HE3	1.43	1.01
2:A:734:THR:HA	2:A:737:MET:HE3	1.44	1.00
2:B:520:ASP:HB3	2:B:667:LYS:HG2	1.45	0.98
2:A:520:ASP:HB3	2:A:667:LYS:HG2	1.46	0.97
2:B:186:ASN:ND2	2:B:190:ARG:H	1.65	0.95
2:A:186:ASN:ND2	2:A:190:ARG:H	1.67	0.93
1:X:1105:A:H5'	2:A:400:ALA:HB1	1.50	0.92
2:B:556:GLN:HE21	2:B:556:GLN:HA	1.36	0.90
2:A:556:GLN:HA	2:A:556:GLN:HE21	1.37	0.89
2:A:477:VAL:HA	2:A:480:MET:HE2	1.55	0.88
2:B:477:VAL:HA	2:B:480:MET:HE2	1.55	0.88
1:Y:1105:A:H5'	2:B:400:ALA:HB1	1.56	0.87
2:B:789:MET:HE2	2:B:1076:LEU:HD21	1.56	0.86
2:A:789:MET:HE2	2:A:1076:LEU:HD21	1.55	0.86
2:A:283:GLN:OE1	2:A:649:GLN:HG3	1.74	0.86
2:B:177:ILE:HD13	2:B:203:LEU:HD11	1.56	0.86
2:B:283:GLN:OE1	2:B:649:GLN:HG3	1.75	0.85
2:A:177:ILE:HD13	2:A:203:LEU:HD11	1.57	0.84
2:A:689:PHE:HB3	2:A:723:ARG:NH1	1.92	0.84
2:B:420:LYS:O	2:B:424:VAL:HG23	1.79	0.82
2:A:461:ILE:HD11	2:A:586:TYR:CZ	2.15	0.81
2:B:689:PHE:HB3	2:B:723:ARG:NH1	1.94	0.81
2:B:161:LYS:O	2:B:165:ARG:HG3	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:161:LYS:O	2:A:165:ARG:HG3	1.83	0.79
2:A:286:ASP:O	2:A:290:GLN:HG3	1.82	0.79
2:B:461:ILE:HD11	2:B:586:TYR:CZ	2.17	0.79
2:A:865:VAL:HG13	2:A:866:THR:N	1.95	0.79
2:B:865:VAL:HG13	2:B:866:THR:N	1.96	0.79
2:A:8:LEU:HD23	2:A:74:ILE:HD12	1.64	0.79
2:A:420:LYS:O	2:A:424:VAL:HG23	1.83	0.78
2:B:286:ASP:O	2:B:290:GLN:HG3	1.84	0.78
2:B:887:VAL:HG22	2:B:1054:LEU:HD11	1.64	0.78
2:B:120:PRO:HD2	2:B:124:GLU:OE2	1.83	0.77
2:A:120:PRO:HD2	2:A:124:GLU:OE2	1.83	0.77
2:B:515:MET:HE3	2:B:639:PHE:CE2	2.20	0.77
2:A:887:VAL:HG22	2:A:1054:LEU:HD11	1.65	0.77
2:A:477:VAL:HA	2:A:480:MET:CE	2.15	0.76
2:A:744:ILE:HG22	2:A:745:THR:HG23	1.67	0.76
2:A:515:MET:HE3	2:A:639:PHE:CE2	2.21	0.76
2:B:186:ASN:HD21	2:B:190:ARG:H	1.33	0.76
2:B:316:ILE:HD13	2:B:684:GLY:HA3	1.68	0.76
2:B:135:LEU:HD13	2:B:709:GLN:HE22	1.51	0.76
2:A:254:LEU:HD23	2:A:280:VAL:HG21	1.67	0.75
1:X:1103:U:HO2'	1:X:1104:G:C5'	1.98	0.75
2:B:8:LEU:HD23	2:B:74:ILE:HD12	1.68	0.75
2:A:598:ALA:O	2:A:602:ILE:HG13	1.87	0.75
2:B:477:VAL:HA	2:B:480:MET:CE	2.17	0.75
2:B:744:ILE:HG22	2:B:745:THR:HG23	1.69	0.74
2:B:254:LEU:HD23	2:B:280:VAL:HG21	1.67	0.74
2:B:312:VAL:HG23	2:B:313:ASP:OD2	1.86	0.74
2:B:428:MET:HE1	2:B:811:TYR:HD1	1.53	0.74
2:A:87:ARG:O	2:A:90:VAL:HG22	1.88	0.73
2:A:892:LEU:HD22	2:A:1017:LEU:HD11	1.70	0.73
2:B:165:ARG:HE	2:B:220:HIS:HA	1.53	0.73
2:A:190:ARG:HG2	2:A:701:ARG:NH2	2.04	0.73
2:B:190:ARG:HG2	2:B:701:ARG:NH2	2.04	0.72
2:A:135:LEU:HD13	2:A:709:GLN:HE22	1.55	0.72
2:A:316:ILE:HD13	2:A:684:GLY:HA3	1.71	0.72
2:A:66:ILE:CG2	2:B:894:ILE:HD11	2.19	0.72
2:A:312:VAL:HG23	2:A:313:ASP:OD2	1.88	0.72
2:A:165:ARG:HE	2:A:220:HIS:HA	1.54	0.72
2:A:186:ASN:HD21	2:A:190:ARG:H	1.37	0.72
2:B:87:ARG:O	2:B:90:VAL:HG22	1.90	0.72
2:A:509:PHE:CD2	2:A:624:LYS:HB3	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:959:GLN:HE21	2:A:976:VAL:HG11	1.54	0.71
2:B:892:LEU:HD22	2:B:1017:LEU:HD11	1.71	0.71
2:B:509:PHE:CD2	2:B:624:LYS:HB3	2.25	0.71
2:B:860:MET:HE3	2:B:860:MET:HA	1.72	0.71
2:A:428:MET:HE1	2:A:811:TYR:HD1	1.56	0.71
2:A:886:THR:HG22	2:B:512:ASN:ND2	2.06	0.71
2:A:860:MET:HA	2:A:860:MET:HE3	1.72	0.70
2:B:598:ALA:O	2:B:602:ILE:HG13	1.92	0.70
2:B:428:MET:CE	2:B:811:TYR:HD1	2.05	0.70
2:B:959:GLN:HE21	2:B:976:VAL:HG11	1.55	0.70
1:X:1105:A:H5'	2:A:400:ALA:CB	2.21	0.70
2:B:44:LYS:HB3	2:B:58:LEU:HD21	1.74	0.70
2:A:324:LYS:O	2:A:328:TRP:HD1	1.75	0.69
2:B:473:GLN:HG2	2:B:561:TYR:CE1	2.26	0.69
2:B:50:LYS:O	2:B:50:LYS:HG2	1.91	0.69
2:A:968:PRO:HG2	2:A:971:ASP:OD2	1.92	0.69
2:A:44:LYS:HB3	2:A:58:LEU:HD21	1.75	0.68
2:A:66:ILE:HG21	2:B:894:ILE:HD11	1.75	0.68
2:B:419:LYS:HB2	2:B:422:MET:HG3	1.74	0.68
2:A:102:LEU:HD22	2:A:102:LEU:H	1.59	0.68
2:A:473:GLN:HG2	2:A:561:TYR:CE1	2.28	0.68
1:Y:1105:A:H5'	2:B:400:ALA:CB	2.23	0.68
2:B:865:VAL:CG1	2:B:866:THR:H	1.97	0.68
2:B:324:LYS:O	2:B:328:TRP:HD1	1.77	0.67
2:B:102:LEU:H	2:B:102:LEU:HD22	1.60	0.67
2:A:865:VAL:CG1	2:A:866:THR:H	1.97	0.67
2:B:295:MET:HE1	2:B:303:ILE:CG2	2.24	0.67
2:A:951:ILE:HG12	2:A:985:LYS:HA	1.76	0.67
2:B:295:MET:O	2:B:300:LEU:HB2	1.94	0.67
2:A:428:MET:CE	2:A:811:TYR:HD1	2.08	0.67
2:A:532:GLN:HB2	2:A:533:PRO:HD3	1.77	0.67
2:A:155:ASP:O	2:A:160:LEU:HD13	1.95	0.67
2:A:975:TYR:O	2:A:977:GLY:N	2.28	0.67
2:A:409:LYS:HG3	2:A:414:THR:HG22	1.77	0.67
2:A:419:LYS:HB2	2:A:422:MET:HG3	1.76	0.67
2:B:295:MET:HE1	2:B:303:ILE:HG22	1.75	0.67
2:A:370:GLU:HG2	2:A:602:ILE:HG23	1.77	0.66
2:B:975:TYR:O	2:B:977:GLY:N	2.29	0.66
2:B:141:ASN:O	2:B:145:VAL:HG23	1.95	0.66
2:A:50:LYS:HG2	2:A:50:LYS:O	1.94	0.66
2:B:968:PRO:HG2	2:B:971:ASP:OD2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:963:ILE:HD11	2:A:969:LYS:HG2	1.78	0.66
2:B:778:THR:O	2:B:782:VAL:HG23	1.95	0.66
2:A:309:ASP:O	2:A:312:VAL:HG22	1.96	0.66
2:B:951:ILE:HG12	2:B:985:LYS:HA	1.77	0.65
2:A:191:TYR:CE2	2:A:204:VAL:HG11	2.31	0.65
2:B:744:ILE:HB	2:B:748:LEU:HD22	1.77	0.65
2:B:409:LYS:HG3	2:B:414:THR:HG22	1.79	0.65
2:A:361:ARG:O	2:A:365:MET:HG2	1.97	0.65
2:A:377:GLU:HB2	2:A:378:PRO:HD3	1.78	0.65
2:A:514:THR:HG22	2:A:638:GLN:HG3	1.77	0.65
2:B:370:GLU:HG2	2:B:602:ILE:HG23	1.78	0.65
2:A:473:GLN:OE1	2:A:595:GLN:HG2	1.95	0.65
2:A:477:VAL:HG21	2:A:594:LYS:HG3	1.78	0.65
2:A:687:ILE:HG23	2:A:900:MET:HG3	1.79	0.65
2:B:477:VAL:HG21	2:B:594:LYS:HG3	1.77	0.65
2:A:296:ARG:HH22	2:A:308:GLN:HE22	1.43	0.65
2:B:462:ILE:HG23	2:B:591:SER:O	1.97	0.65
2:B:532:GLN:HB2	2:B:533:PRO:HD3	1.79	0.65
2:B:963:ILE:HD11	2:B:969:LYS:HG2	1.78	0.65
2:B:155:ASP:O	2:B:160:LEU:HD13	1.97	0.65
2:B:361:ARG:O	2:B:365:MET:HG2	1.97	0.64
2:B:687:ILE:HG23	2:B:900:MET:HG3	1.80	0.64
2:A:135:LEU:HD22	2:A:709:GLN:HE21	1.63	0.64
2:B:296:ARG:HH22	2:B:308:GLN:HE22	1.44	0.64
2:B:898:LYS:HD3	2:B:908:GLN:HG2	1.79	0.64
2:A:898:LYS:HD3	2:A:908:GLN:HG2	1.79	0.64
1:Y:1106:C:H5'	1:Y:1107:C:OP2	1.98	0.64
2:A:744:ILE:HB	2:A:748:LEU:HD22	1.79	0.64
2:B:253:ALA:HB1	2:B:671:SER:HB2	1.78	0.64
2:B:473:GLN:OE1	2:B:595:GLN:HG2	1.97	0.64
2:A:319:PHE:N	2:A:320:PRO:CD	2.61	0.64
2:A:295:MET:HE1	2:A:303:ILE:CG2	2.28	0.64
2:B:539:ILE:HG23	2:B:562:LYS:HG3	1.80	0.63
2:A:126:THR:OG1	2:A:128:SER:HB3	1.98	0.63
2:A:539:ILE:HG23	2:A:562:LYS:HG3	1.80	0.63
2:B:309:ASP:O	2:B:312:VAL:HG22	1.97	0.63
2:B:377:GLU:HB2	2:B:378:PRO:HD3	1.80	0.63
2:A:141:ASN:O	2:A:145:VAL:HG23	1.98	0.63
2:B:191:TYR:CE2	2:B:204:VAL:HG11	2.33	0.63
2:B:319:PHE:N	2:B:320:PRO:CD	2.62	0.63
2:A:90:VAL:HG23	2:A:91:LYS:H	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:528:GLN:O	2:A:531:THR:HG22	1.98	0.63
2:B:528:GLN:O	2:B:531:THR:HG22	1.98	0.63
2:B:126:THR:OG1	2:B:128:SER:HB3	1.98	0.63
2:A:462:ILE:HG23	2:A:591:SER:O	1.99	0.63
2:A:145:VAL:HA	2:A:215:MET:HE2	1.80	0.63
2:A:253:ALA:HB1	2:A:671:SER:HB2	1.80	0.63
2:B:1059:PRO:O	2:B:1063:MET:HG3	1.98	0.63
2:A:3:LYS:O	2:A:7:ILE:HG12	1.99	0.63
2:B:687:ILE:CG2	2:B:900:MET:HG3	2.29	0.63
2:A:6:LEU:N	2:A:6:LEU:HD22	2.14	0.62
2:A:295:MET:HE1	2:A:303:ILE:HG22	1.80	0.62
2:B:90:VAL:HG23	2:B:91:LYS:H	1.64	0.62
2:A:623:THR:CG2	2:A:626:ILE:HG13	2.29	0.62
2:B:253:ALA:CB	2:B:671:SER:HB2	2.29	0.62
2:B:514:THR:HG22	2:B:638:GLN:HG3	1.81	0.62
2:A:1059:PRO:O	2:A:1063:MET:HG3	1.99	0.62
2:B:84:ALA:O	2:B:88:LYS:HG3	1.98	0.62
2:B:962:LEU:O	2:B:967:ILE:HB	2.00	0.62
2:A:137:SER:HB2	2:A:185:HIS:CD2	2.35	0.62
1:X:1106:C:H5'	1:X:1107:C:OP2	2.00	0.62
2:B:279:ILE:HG22	2:B:648:ILE:HD12	1.82	0.62
2:A:253:ALA:CB	2:A:671:SER:HB2	2.30	0.62
2:B:618:LYS:HD2	2:B:654:ASP:OD2	2.00	0.62
1:X:1103:U:HO2'	1:X:1104:G:H5''	1.65	0.61
2:A:261:PHE:CD2	2:A:899:PHE:HB3	2.35	0.61
2:A:242:LYS:O	2:A:246:SER:HB2	2.00	0.61
2:A:687:ILE:CG2	2:A:900:MET:HG3	2.30	0.61
2:A:777:THR:HG21	2:A:882:LYS:HE3	1.82	0.61
2:A:295:MET:O	2:A:300:LEU:HB2	2.00	0.61
2:A:618:LYS:HD2	2:A:654:ASP:OD2	2.01	0.61
2:B:3:LYS:O	2:B:7:ILE:HG12	2.01	0.61
2:B:777:THR:HG21	2:B:882:LYS:HE3	1.82	0.61
2:A:449:LEU:HD22	2:A:573:VAL:HG13	1.83	0.61
2:A:623:THR:HG21	2:A:626:ILE:HG13	1.82	0.61
2:B:6:LEU:N	2:B:6:LEU:HD22	2.16	0.61
2:B:115:THR:HB	2:B:197:LYS:HA	1.80	0.61
2:A:84:ALA:O	2:A:88:LYS:HG3	2.00	0.61
2:A:784:ILE:HD12	2:A:788:PHE:CE2	2.35	0.61
2:B:86:GLU:OE2	2:B:182:VAL:HB	2.00	0.61
2:B:623:THR:CG2	2:B:626:ILE:HG13	2.31	0.61
2:B:784:ILE:HD12	2:B:788:PHE:CE2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:708:ASP:O	2:A:712:ILE:HG13	2.01	0.61
2:B:145:VAL:HA	2:B:215:MET:HE2	1.82	0.60
2:B:169:LEU:HD21	2:B:227:LYS:HB2	1.83	0.60
2:B:520:ASP:HB2	2:B:667:LYS:HE2	1.83	0.60
2:A:627:ARG:HH11	2:A:627:ARG:HG2	1.66	0.60
2:A:962:LEU:O	2:A:967:ILE:HB	2.02	0.60
2:B:11:TYR:HA	2:B:147:PHE:CE1	2.36	0.60
2:B:261:PHE:CD2	2:B:899:PHE:HB3	2.36	0.60
2:B:556:GLN:HA	2:B:556:GLN:NE2	2.12	0.60
2:B:887:VAL:HG22	2:B:1054:LEU:CD1	2.31	0.60
1:Y:1105:A:C5'	2:B:400:ALA:HB1	2.32	0.60
2:A:796:SER:HB2	2:A:849:LYS:HE3	1.84	0.60
2:B:885:PHE:CE1	2:B:1056:CYS:HB2	2.37	0.60
2:B:417:SER:CB	2:B:422:MET:HE3	2.32	0.60
1:Y:1101:U:O4	2:B:415:ILE:HG13	2.02	0.59
2:A:778:THR:O	2:A:782:VAL:HG23	2.01	0.59
2:B:137:SER:HB2	2:B:185:HIS:CD2	2.38	0.59
2:A:446:PRO:HB2	2:A:574:GLN:HG3	1.83	0.59
2:B:485:LYS:HE2	2:B:495:SER:HA	1.84	0.59
2:B:860:MET:HE2	2:B:864:PRO:HG3	1.85	0.59
2:A:56:ARG:O	2:A:60:VAL:HG23	2.02	0.59
2:B:449:LEU:HD22	2:B:573:VAL:HG13	1.85	0.59
2:B:449:LEU:CD1	2:B:573:VAL:HG22	2.32	0.59
2:A:86:GLU:OE2	2:A:182:VAL:HB	2.02	0.59
2:B:242:LYS:O	2:B:246:SER:HB2	2.03	0.59
2:B:312:VAL:HG23	2:B:313:ASP:H	1.68	0.59
2:B:449:LEU:HD11	2:B:573:VAL:HG22	1.84	0.59
2:B:708:ASP:O	2:B:712:ILE:HG13	2.03	0.59
2:A:556:GLN:HA	2:A:556:GLN:NE2	2.14	0.59
2:A:860:MET:HE2	2:A:864:PRO:HG3	1.85	0.59
2:B:1000:ASN:C	2:B:1005:GLN:HB3	2.28	0.59
2:A:11:TYR:HA	2:A:147:PHE:CE1	2.38	0.58
2:A:882:LYS:HB3	2:A:883:PRO:HD3	1.83	0.58
2:A:115:THR:HB	2:A:197:LYS:HA	1.83	0.58
2:B:623:THR:HG21	2:B:626:ILE:HG13	1.84	0.58
2:B:748:LEU:C	2:B:748:LEU:HD23	2.27	0.58
2:A:703:GLN:CD	2:A:703:GLN:N	2.62	0.58
2:A:449:LEU:CD1	2:A:573:VAL:HG22	2.33	0.58
2:B:446:PRO:HB2	2:B:574:GLN:HG3	1.83	0.58
2:B:56:ARG:O	2:B:60:VAL:HG23	2.03	0.58
2:A:14:PHE:CE2	2:A:147:PHE:HB2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:133:ALA:HB1	2:A:701:ARG:HG3	1.85	0.58
2:A:748:LEU:HD23	2:A:748:LEU:C	2.28	0.58
2:B:591:SER:HB2	2:B:596:THR:HG21	1.86	0.58
2:B:794:GLN:HG2	2:B:853:GLN:OE1	2.03	0.58
2:B:798:ILE:O	2:B:802:ILE:HG22	2.04	0.58
2:A:279:ILE:HG22	2:A:648:ILE:HD12	1.86	0.58
2:A:476:VAL:O	2:A:480:MET:HG3	2.02	0.58
2:B:133:ALA:HB1	2:B:701:ARG:HG3	1.85	0.58
2:A:383:ASP:O	2:A:387:ARG:HG3	2.04	0.58
2:A:449:LEU:HD11	2:A:573:VAL:HG22	1.86	0.58
2:B:703:GLN:N	2:B:703:GLN:CD	2.62	0.58
1:X:1101:U:O4	2:A:415:ILE:HG13	2.04	0.57
2:B:530:ASN:O	2:B:533:PRO:HD2	2.04	0.57
2:A:886:THR:HG22	2:B:512:ASN:CG	2.29	0.57
2:A:887:VAL:HG22	2:A:1054:LEU:CD1	2.33	0.57
2:A:514:THR:CG2	2:A:638:GLN:HG3	2.34	0.57
2:A:959:GLN:NE2	2:A:976:VAL:HG11	2.19	0.57
2:B:627:ARG:HG2	2:B:627:ARG:HH11	1.69	0.57
2:A:244:VAL:HA	2:A:295:MET:HE3	1.86	0.57
2:B:882:LYS:HB3	2:B:883:PRO:HD3	1.85	0.57
2:A:621:PHE:CE1	2:A:637:LEU:HD13	2.40	0.57
2:B:14:PHE:CE2	2:B:147:PHE:HB2	2.40	0.57
2:B:135:LEU:HD22	2:B:709:GLN:HE21	1.69	0.57
2:B:796:SER:HB2	2:B:849:LYS:HE3	1.87	0.57
2:A:407:GLN:HE22	2:A:416:PHE:HB3	1.70	0.57
2:A:296:ARG:HH22	2:A:308:GLN:NE2	2.02	0.57
2:A:1000:ASN:C	2:A:1005:GLN:HB3	2.30	0.57
2:A:485:LYS:HE2	2:A:495:SER:HA	1.86	0.57
2:A:520:ASP:HB2	2:A:667:LYS:HE2	1.86	0.57
2:A:530:ASN:O	2:A:533:PRO:HD2	2.05	0.57
2:A:605:LEU:HD11	2:A:609:LYS:HE3	1.86	0.57
2:A:885:PHE:CE1	2:A:1056:CYS:HB2	2.40	0.57
2:B:605:LEU:HD11	2:B:609:LYS:HE3	1.86	0.57
1:X:1105:A:C5'	2:A:400:ALA:HB1	2.28	0.57
2:A:156:VAL:HG23	2:A:157:ALA:N	2.20	0.57
2:A:798:ILE:O	2:A:802:ILE:HG22	2.05	0.57
2:B:383:ASP:O	2:B:387:ARG:HG3	2.05	0.57
2:B:862:GLN:O	2:B:863:LYS:HB2	2.04	0.57
2:B:959:GLN:NE2	2:B:976:VAL:HG11	2.20	0.57
2:A:407:GLN:NE2	2:A:416:PHE:HB3	2.20	0.56
2:B:928:SER:O	2:B:932:ARG:HG3	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:LEU:C	2:B:75:LEU:HD23	2.31	0.56
2:A:169:LEU:HD21	2:A:227:LYS:HB2	1.87	0.56
2:A:794:GLN:HG2	2:A:853:GLN:OE1	2.05	0.56
2:A:997:LEU:HD12	2:A:1035:LEU:HD21	1.87	0.56
2:B:514:THR:CG2	2:B:638:GLN:HG3	2.35	0.56
2:B:621:PHE:CE1	2:B:637:LEU:HD13	2.41	0.56
2:B:860:MET:HE1	2:B:864:PRO:HA	1.87	0.56
2:B:894:ILE:O	2:B:894:ILE:HG13	2.05	0.56
2:A:860:MET:HE1	2:A:864:PRO:HA	1.87	0.56
2:A:928:SER:O	2:A:932:ARG:HG3	2.04	0.56
2:B:35:GLU:O	2:B:38:CYS:HB2	2.05	0.56
2:B:794:GLN:HG2	2:B:853:GLN:CD	2.30	0.56
2:A:945:GLU:HG2	2:A:992:TYR:CE1	2.39	0.56
2:B:244:VAL:HA	2:B:295:MET:HE3	1.87	0.56
2:B:892:LEU:CD2	2:B:1017:LEU:HD11	2.36	0.56
2:A:75:LEU:C	2:A:75:LEU:HD23	2.31	0.56
2:A:161:LYS:O	2:A:165:ARG:NH1	2.38	0.56
2:A:312:VAL:HG23	2:A:313:ASP:H	1.71	0.56
2:A:573:VAL:CG1	2:A:575:ILE:HG13	2.36	0.56
2:A:794:GLN:HG2	2:A:853:GLN:CD	2.31	0.56
2:B:312:VAL:HG23	2:B:313:ASP:N	2.21	0.56
2:B:466:PRO:HD2	2:B:469:TYR:CD2	2.41	0.56
2:B:476:VAL:O	2:B:480:MET:HG3	2.05	0.56
2:B:28:TYR:HD2	2:B:72:LEU:HB2	1.70	0.56
2:B:375:LEU:C	2:B:378:PRO:HD2	2.31	0.56
2:A:154:ASN:ND2	2:B:1019:ARG:HA	2.21	0.56
2:A:1016:LYS:O	2:A:1018:ILE:N	2.39	0.56
2:B:799:ALA:HB2	2:B:845:ILE:HD13	1.88	0.56
2:A:35:GLU:O	2:A:38:CYS:HB2	2.06	0.55
2:B:148:TRP:CZ3	2:B:166:ARG:HD2	2.41	0.55
2:A:591:SER:HB2	2:A:596:THR:HG21	1.89	0.55
2:A:862:GLN:O	2:A:863:LYS:HB2	2.05	0.55
2:B:518:TYR:H	2:B:518:TYR:HD2	1.52	0.55
2:A:66:ILE:HG22	2:B:894:ILE:HD11	1.88	0.55
2:A:799:ALA:HB2	2:A:845:ILE:HD13	1.88	0.55
2:B:161:LYS:O	2:B:165:ARG:NH1	2.38	0.55
2:A:417:SER:CB	2:A:422:MET:HE3	2.37	0.55
2:B:573:VAL:CG1	2:B:575:ILE:HG13	2.36	0.55
2:A:261:PHE:HD2	2:A:899:PHE:HB3	1.70	0.55
3:A:1111:GTP:O1B	3:A:1111:GTP:O3G	2.25	0.55
2:B:407:GLN:NE2	2:B:416:PHE:HB3	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:477:VAL:HG21	2:B:594:LYS:CG	2.36	0.55
2:B:438:ILE:HD12	2:B:563:GLN:HB3	1.88	0.55
2:B:261:PHE:HD2	2:B:899:PHE:HB3	1.71	0.55
2:B:695:LEU:HG	2:B:713:LEU:CD1	2.36	0.55
2:A:148:TRP:CZ3	2:A:166:ARG:HD2	2.42	0.55
2:A:1062:GLU:HA	2:A:1065:LYS:HD3	1.87	0.55
2:B:296:ARG:HH22	2:B:308:GLN:NE2	2.05	0.55
2:B:407:GLN:HE22	2:B:416:PHE:HB3	1.72	0.55
2:B:15:ILE:HG22	2:B:16:TYR:CD1	2.41	0.55
2:A:864:PRO:HA	2:A:867:PHE:HE2	1.71	0.54
2:B:945:GLU:HG2	2:B:992:TYR:CE1	2.41	0.54
2:B:1016:LYS:O	2:B:1018:ILE:N	2.39	0.54
2:A:477:VAL:HG21	2:A:594:LYS:CG	2.37	0.54
2:B:156:VAL:HG23	2:B:157:ALA:N	2.23	0.54
2:B:186:ASN:HD21	2:B:190:ARG:N	2.01	0.54
2:B:535:ARG:O	2:B:539:ILE:HG13	2.06	0.54
2:A:15:ILE:HG22	2:A:16:TYR:CD1	2.42	0.54
2:B:864:PRO:HA	2:B:867:PHE:HE2	1.72	0.54
2:B:619:HIS:ND1	2:B:619:HIS:N	2.56	0.54
2:B:165:ARG:HD3	2:B:223:TYR:CB	2.38	0.54
2:B:1062:GLU:HA	2:B:1065:LYS:HD3	1.88	0.54
2:A:945:GLU:HG2	2:A:992:TYR:HE1	1.72	0.54
2:B:399:SER:HB3	2:B:838:LYS:HB3	1.89	0.54
2:A:2:GLY:HA2	2:A:754:GLU:OE2	2.08	0.54
2:A:165:ARG:HD3	2:A:223:TYR:CB	2.38	0.54
2:A:165:ARG:HD3	2:A:223:TYR:HB2	1.90	0.54
2:B:2:GLY:HA2	2:B:754:GLU:OE2	2.08	0.54
2:B:116:SER:HB3	2:B:197:LYS:HG3	1.89	0.54
2:A:166:ARG:HD3	2:A:215:MET:SD	2.48	0.54
2:A:591:SER:HB2	2:A:596:THR:CG2	2.38	0.53
2:B:385:LEU:HD23	2:B:479:LYS:HE2	1.89	0.53
2:B:826:ILE:O	2:B:829:ARG:HG2	2.08	0.53
2:B:997:LEU:HD12	2:B:1035:LEU:HD21	1.90	0.53
2:A:992:TYR:O	2:A:996:LEU:HG	2.08	0.53
2:B:409:LYS:HB2	2:B:409:LYS:HZ2	1.73	0.53
2:B:992:TYR:O	2:B:996:LEU:HG	2.08	0.53
2:A:28:TYR:HD2	2:A:72:LEU:HB2	1.72	0.53
2:A:375:LEU:C	2:A:378:PRO:HD2	2.33	0.53
2:A:399:SER:HB3	2:A:838:LYS:HB3	1.90	0.53
2:A:438:ILE:HD12	2:A:563:GLN:HB3	1.90	0.53
2:A:467:TYR:C	2:A:467:TYR:CD1	2.87	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:523:GLN:HB2	2:A:665:LYS:O	2.08	0.53
2:A:695:LEU:HG	2:A:713:LEU:CD1	2.38	0.53
2:B:11:TYR:O	2:B:14:PHE:HB3	2.09	0.53
2:B:164:LYS:O	2:B:165:ARG:C	2.51	0.53
2:A:312:VAL:HG23	2:A:313:ASP:N	2.24	0.53
2:A:466:PRO:HD2	2:A:469:TYR:CD2	2.44	0.53
2:B:523:GLN:HB2	2:B:665:LYS:O	2.08	0.53
2:A:50:LYS:HB2	2:A:50:LYS:NZ	2.23	0.53
2:A:374:MET:HE2	2:A:480:MET:HB3	1.91	0.53
2:A:451:ARG:NH2	2:A:459:THR:HG21	2.24	0.53
2:A:882:LYS:HG3	2:A:1036:TYR:OH	2.09	0.53
1:Y:1103:U:O2'	1:Y:1104:G:O5'	2.27	0.53
2:A:437:ILE:O	2:A:439:PRO:HD3	2.09	0.53
2:A:894:ILE:O	2:A:894:ILE:HG13	2.08	0.53
2:B:4:TYR:HD1	2:B:733:LEU:HD22	1.73	0.53
2:B:835:GLU:OE1	2:B:838:LYS:HD2	2.09	0.53
2:B:917:ARG:HD3	2:B:1007:PHE:O	2.09	0.53
1:Y:1103:U:O2'	1:Y:1104:G:H5''	2.09	0.53
2:A:879:ARG:HG3	2:A:879:ARG:HH11	1.74	0.53
2:A:892:LEU:CD2	2:A:1017:LEU:HD11	2.36	0.53
2:B:632:ASP:OD2	2:B:677:ILE:HB	2.08	0.53
1:Y:1101:U:O2'	1:Y:1102:G:P	2.67	0.53
2:B:166:ARG:HD3	2:B:215:MET:SD	2.49	0.53
2:A:4:TYR:HD1	2:A:733:LEU:HD22	1.73	0.52
2:A:621:PHE:CD1	2:A:637:LEU:HD13	2.43	0.52
2:B:56:ARG:HG2	2:B:56:ARG:HH11	1.74	0.52
2:A:535:ARG:O	2:A:539:ILE:HG13	2.08	0.52
2:A:826:ILE:O	2:A:829:ARG:HG2	2.09	0.52
2:B:898:LYS:HD3	2:B:908:GLN:CG	2.39	0.52
2:B:811:TYR:CZ	2:B:815:LEU:HD11	2.45	0.52
2:B:50:LYS:HB2	2:B:50:LYS:NZ	2.24	0.52
2:B:287:GLU:HA	2:B:290:GLN:OE1	2.09	0.52
2:B:467:TYR:CD1	2:B:467:TYR:C	2.88	0.52
1:X:1101:U:O2'	1:X:1102:G:P	2.68	0.52
1:X:1103:U:O2'	1:X:1104:G:O5'	2.25	0.52
2:A:8:LEU:HA	2:A:737:MET:SD	2.49	0.52
2:A:385:LEU:HD23	2:A:479:LYS:HE2	1.90	0.52
2:A:874:ILE:O	2:A:878:LEU:HG	2.10	0.52
2:A:1018:ILE:HD12	2:A:1037:ALA:HB1	1.90	0.52
2:B:667:LYS:O	2:B:667:LYS:HG3	2.08	0.52
1:X:1102:G:H4'	1:X:1103:U:OP2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:ARG:HD3	2:B:223:TYR:HB2	1.92	0.52
2:A:116:SER:HA	2:A:119:PHE:O	2.09	0.52
2:A:186:ASN:HD21	2:A:190:ARG:N	2.04	0.52
2:A:409:LYS:HZ2	2:A:409:LYS:HB2	1.74	0.52
2:A:762:THR:HA	2:A:1077:ARG:O	2.10	0.52
2:B:301:VAL:C	2:B:304:PRO:HD2	2.34	0.52
2:B:518:TYR:CD2	2:B:518:TYR:N	2.77	0.52
2:B:591:SER:HB2	2:B:596:THR:CG2	2.39	0.52
2:B:945:GLU:HG2	2:B:992:TYR:HE1	1.74	0.52
2:A:641:THR:HG23	2:A:647:MET:HE1	1.91	0.52
2:B:387:ARG:HA	2:B:553:LYS:HB3	1.92	0.52
2:A:835:GLU:OE1	2:A:838:LYS:HD2	2.10	0.52
2:A:917:ARG:HD3	2:A:1007:PHE:O	2.10	0.52
2:B:516:VAL:HG21	2:B:675:ILE:CG2	2.40	0.52
2:B:882:LYS:HG3	2:B:1036:TYR:OH	2.10	0.52
2:B:116:SER:HA	2:B:119:PHE:O	2.09	0.51
2:A:116:SER:HB3	2:A:197:LYS:HG3	1.91	0.51
2:B:168:ASP:OD2	2:B:223:TYR:OH	2.21	0.51
2:B:556:GLN:HE21	2:B:556:GLN:CA	2.09	0.51
2:B:874:ILE:O	2:B:878:LEU:HG	2.10	0.51
2:A:619:HIS:ND1	2:A:619:HIS:N	2.59	0.51
2:B:879:ARG:HH11	2:B:879:ARG:HG3	1.75	0.51
2:B:762:THR:HA	2:B:1077:ARG:O	2.10	0.51
2:A:15:ILE:HG22	2:A:16:TYR:CE1	2.44	0.51
2:A:135:LEU:HD22	2:A:709:GLN:NE2	2.25	0.51
2:A:164:LYS:O	2:A:165:ARG:C	2.53	0.51
2:A:318:LYS:HB2	2:A:318:LYS:NZ	2.25	0.51
2:A:387:ARG:HA	2:A:553:LYS:HB3	1.92	0.51
2:B:15:ILE:HG22	2:B:16:TYR:CE1	2.44	0.51
2:A:28:TYR:CE2	2:A:70:THR:HB	2.46	0.51
2:A:56:ARG:HG2	2:A:56:ARG:HH11	1.76	0.51
2:A:168:ASP:OD2	2:A:223:TYR:OH	2.20	0.51
2:B:295:MET:HE2	2:B:300:LEU:HD13	1.93	0.51
2:A:776:GLY:HA3	2:A:785:GLN:NE2	2.26	0.51
2:A:811:TYR:CZ	2:A:815:LEU:HD11	2.46	0.51
2:B:621:PHE:CD1	2:B:637:LEU:HD13	2.45	0.51
2:B:776:GLY:HA3	2:B:785:GLN:NE2	2.26	0.51
2:A:11:TYR:O	2:A:14:PHE:HB3	2.11	0.51
2:B:437:ILE:O	2:B:439:PRO:HD3	2.11	0.51
2:B:900:MET:HE2	2:B:903:LEU:HG	1.91	0.51
2:A:287:GLU:HA	2:A:290:GLN:OE1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:428:MET:C	2:A:430:ASN:H	2.19	0.50
2:B:318:LYS:HB2	2:B:318:LYS:NZ	2.25	0.50
2:B:1000:ASN:O	2:B:1005:GLN:HB3	2.11	0.50
1:Y:1103:U:O2'	1:Y:1104:G:C5'	2.59	0.50
2:A:514:THR:HG22	2:A:638:GLN:CG	2.41	0.50
2:B:387:ARG:NH1	2:B:553:LYS:HG3	2.27	0.50
2:B:641:THR:HG23	2:B:647:MET:HE1	1.93	0.50
2:B:989:LEU:HD21	2:B:1070:MET:HE3	1.94	0.50
1:X:1103:U:O2'	1:X:1104:G:H5''	2.11	0.50
2:B:553:LYS:O	2:B:557:THR:HG23	2.11	0.50
2:A:381:HIS:O	2:A:382:ASP:C	2.54	0.50
2:A:516:VAL:HG21	2:A:675:ILE:CG2	2.42	0.50
2:B:29:SER:OG	2:B:34:LEU:HD23	2.11	0.50
2:B:428:MET:C	2:B:430:ASN:H	2.20	0.50
2:B:514:THR:HG22	2:B:638:GLN:CB	2.41	0.50
2:A:518:TYR:N	2:A:518:TYR:CD2	2.79	0.50
2:A:553:LYS:O	2:A:557:THR:HG23	2.11	0.50
2:A:898:LYS:HD3	2:A:908:GLN:CG	2.41	0.50
2:A:295:MET:HE2	2:A:300:LEU:HD13	1.94	0.50
2:B:8:LEU:HD13	2:B:737:MET:HG2	1.93	0.50
2:B:248:MET:HG2	2:B:326:TYR:CD1	2.47	0.50
2:B:28:TYR:CE2	2:B:70:THR:HB	2.47	0.50
2:A:193:TYR:CZ	2:A:197:LYS:HD2	2.47	0.50
2:A:667:LYS:HG3	2:A:667:LYS:O	2.10	0.50
2:A:853:GLN:HE21	2:A:853:GLN:HA	1.77	0.50
2:B:44:LYS:HB3	2:B:58:LEU:CD2	2.40	0.50
2:B:370:GLU:O	2:B:374:MET:HG3	2.12	0.50
2:B:680:ARG:HB3	2:B:689:PHE:CE1	2.47	0.50
2:B:8:LEU:HA	2:B:737:MET:SD	2.52	0.49
2:B:959:GLN:NE2	2:B:973:ASP:OD1	2.45	0.49
2:B:1018:ILE:HD12	2:B:1037:ALA:HB1	1.93	0.49
1:Y:1101:U:O2'	1:Y:1102:G:OP1	2.29	0.49
2:A:556:GLN:HE21	2:A:556:GLN:CA	2.09	0.49
2:B:899:PHE:O	2:B:901:PRO:HD3	2.11	0.49
2:A:210:SER:OG	2:A:230:ILE:HG23	2.13	0.49
2:A:248:MET:HG2	2:A:326:TYR:CD1	2.48	0.49
2:B:93:ALA:HB1	2:B:175:SER:HA	1.94	0.49
2:A:334:PHE:CE2	2:A:455:PRO:HD3	2.48	0.49
2:A:368:ARG:HG3	2:A:541:GLY:N	2.28	0.49
2:A:410:PHE:HE1	2:A:425:MET:HE2	1.76	0.49
2:B:193:TYR:CZ	2:B:197:LYS:HD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:90:VAL:HG23	2:A:91:LYS:N	2.27	0.49
2:A:102:LEU:HD22	2:A:102:LEU:N	2.25	0.49
2:B:643:VAL:HA	2:B:647:MET:SD	2.52	0.49
2:B:853:GLN:HE21	2:B:853:GLN:HA	1.78	0.49
2:A:857:LEU:O	2:A:861:LEU:HD13	2.12	0.49
2:A:29:SER:H	2:A:35:GLU:HG2	1.78	0.49
2:A:93:ALA:HB1	2:A:175:SER:HA	1.95	0.49
2:A:303:ILE:HB	2:A:304:PRO:HD3	1.92	0.49
2:A:461:ILE:HD11	2:A:586:TYR:CE1	2.47	0.49
2:B:90:VAL:HG23	2:B:91:LYS:N	2.27	0.49
2:B:313:ASP:OD2	2:B:313:ASP:N	2.35	0.49
2:B:485:LYS:HE2	2:B:495:SER:CA	2.42	0.49
2:B:650:ASP:O	2:B:654:ASP:OD1	2.31	0.49
2:A:789:MET:HE1	2:A:873:THR:HG21	1.95	0.49
2:A:853:GLN:HA	2:A:853:GLN:NE2	2.28	0.49
2:B:29:SER:H	2:B:35:GLU:HG2	1.78	0.49
2:B:102:LEU:HD22	2:B:102:LEU:N	2.25	0.49
2:B:853:GLN:HA	2:B:853:GLN:NE2	2.28	0.49
1:Y:1102:G:H4'	1:Y:1103:U:OP2	2.13	0.49
2:A:313:ASP:O	2:A:314:ARG:HB2	2.13	0.49
2:B:165:ARG:HE	2:B:220:HIS:CA	2.24	0.49
2:B:358:GLU:OE2	2:B:359:MET:HG3	2.12	0.49
2:B:857:LEU:O	2:B:861:LEU:HD13	2.12	0.49
1:X:1103:U:O2'	1:X:1104:G:C5'	2.60	0.49
2:A:139:SER:O	2:A:142:LEU:HB2	2.13	0.49
2:A:251:LEU:HD22	2:A:310:TRP:CZ3	2.48	0.49
2:A:857:LEU:C	2:A:857:LEU:HD23	2.37	0.49
2:B:437:ILE:N	2:B:437:ILE:HD12	2.28	0.48
2:A:8:LEU:CD2	2:A:74:ILE:HD12	2.38	0.48
2:A:8:LEU:HD13	2:A:737:MET:HG2	1.95	0.48
2:A:100:ALA:O	2:A:102:LEU:HD22	2.13	0.48
2:A:370:GLU:O	2:A:374:MET:HG3	2.13	0.48
2:B:212:GLU:HB2	2:B:696:LEU:HD12	1.94	0.48
2:A:165:ARG:NE	2:A:220:HIS:HA	2.23	0.48
2:A:368:ARG:HD3	2:A:540:MET:HE2	1.95	0.48
2:A:514:THR:HG22	2:A:638:GLN:CB	2.43	0.48
2:A:650:ASP:O	2:A:654:ASP:OD1	2.32	0.48
2:A:959:GLN:NE2	2:A:973:ASP:OD1	2.46	0.48
2:B:381:HIS:O	2:B:382:ASP:C	2.56	0.48
1:X:1101:U:O2'	1:X:1102:G:OP1	2.30	0.48
2:A:109:TYR:HA	2:A:118:LEU:CD2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:419:LYS:HB2	2:A:422:MET:CG	2.41	0.48
2:B:5:ASN:CG	2:B:71:LEU:HD23	2.39	0.48
2:B:165:ARG:NE	2:B:220:HIS:HA	2.24	0.48
2:B:514:THR:HG22	2:B:638:GLN:CG	2.43	0.48
2:A:44:LYS:HB3	2:A:58:LEU:CD2	2.41	0.48
2:A:193:TYR:CE2	2:A:197:LYS:HD2	2.49	0.48
2:A:229:LEU:O	2:A:233:SER:HB3	2.13	0.48
2:B:251:LEU:HD22	2:B:310:TRP:CZ3	2.48	0.48
2:B:419:LYS:HB2	2:B:422:MET:CG	2.41	0.48
2:B:967:ILE:N	2:B:967:ILE:HD12	2.28	0.48
2:A:364:THR:OG1	2:A:533:PRO:HB3	2.12	0.48
2:B:4:TYR:CD1	2:B:733:LEU:HD22	2.49	0.48
2:A:4:TYR:CD1	2:A:733:LEU:HD22	2.49	0.48
2:A:358:GLU:OE2	2:A:359:MET:HG3	2.13	0.48
2:A:842:TYR:CE2	2:A:844:PRO:HB2	2.49	0.48
2:B:89:LEU:HD11	2:B:174:ALA:HA	1.95	0.48
2:B:101:ASP:C	2:B:101:ASP:OD1	2.56	0.48
2:B:221:ASP:O	2:B:225:ILE:HG13	2.13	0.48
2:B:344:LEU:O	2:B:346:GLN:N	2.46	0.48
2:B:461:ILE:HD11	2:B:586:TYR:CE1	2.48	0.48
2:A:168:ASP:O	2:A:171:THR:HB	2.13	0.48
2:A:313:ASP:OD2	2:A:313:ASP:N	2.36	0.48
2:A:437:ILE:HD12	2:A:437:ILE:N	2.29	0.48
2:A:632:ASP:OD2	2:A:677:ILE:HB	2.13	0.48
2:A:1000:ASN:O	2:A:1005:GLN:HB3	2.13	0.48
2:B:786:ARG:HD3	2:B:869:SER:CB	2.43	0.48
2:B:842:TYR:CE2	2:B:844:PRO:HB2	2.49	0.48
2:A:843:ALA:HB3	2:A:844:PRO:HD3	1.95	0.48
2:A:887:VAL:HG12	2:A:888:SER:N	2.28	0.48
2:B:145:VAL:CG2	2:B:211:ILE:HG23	2.44	0.48
2:B:303:ILE:HB	2:B:304:PRO:HD3	1.94	0.48
2:B:451:ARG:NH2	2:B:459:THR:HG21	2.29	0.48
2:A:101:ASP:OD1	2:A:101:ASP:C	2.57	0.47
2:A:872:ILE:HD11	2:A:1069:LYS:HE3	1.95	0.47
2:A:899:PHE:O	2:A:901:PRO:HD3	2.13	0.47
2:A:999:ILE:HD11	2:A:1009:PHE:CZ	2.49	0.47
2:B:84:ALA:HB1	2:B:88:LYS:NZ	2.28	0.47
2:B:364:THR:OG1	2:B:533:PRO:HB3	2.12	0.47
2:A:84:ALA:HB1	2:A:88:LYS:NZ	2.28	0.47
2:A:539:ILE:HA	2:A:542:LEU:HD12	1.95	0.47
2:A:860:MET:C	2:A:862:GLN:H	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:ASP:O	2:B:171:THR:HB	2.14	0.47
2:A:165:ARG:HE	2:A:220:HIS:CA	2.25	0.47
2:A:430:ASN:O	2:A:432:ARG:N	2.47	0.47
2:B:789:MET:HE1	2:B:873:THR:HG21	1.96	0.47
2:B:193:TYR:CE2	2:B:197:LYS:HD2	2.50	0.47
2:B:382:ASP:OD1	2:B:551:ASP:HB2	2.14	0.47
2:B:410:PHE:HE1	2:B:425:MET:HE2	1.79	0.47
2:A:344:LEU:O	2:A:346:GLN:N	2.47	0.47
2:A:382:ASP:OD1	2:A:551:ASP:HB2	2.14	0.47
2:A:485:LYS:HE2	2:A:495:SER:CA	2.44	0.47
2:A:605:LEU:HD12	2:A:605:LEU:O	2.15	0.47
2:A:627:ARG:HG2	2:A:627:ARG:NH1	2.29	0.47
2:A:729:ARG:HE	2:A:770:ASP:CG	2.23	0.47
2:B:338:LYS:O	2:B:339:MET:C	2.58	0.47
2:B:860:MET:C	2:B:862:GLN:H	2.21	0.47
2:A:518:TYR:H	2:A:518:TYR:HD2	1.60	0.47
2:B:313:ASP:O	2:B:314:ARG:HB2	2.15	0.47
2:B:771:PHE:HB3	2:B:1003:CYS:SG	2.55	0.47
2:A:786:ARG:HD3	2:A:869:SER:CB	2.44	0.47
2:B:886:THR:OG1	2:B:1055:PHE:HB3	2.14	0.47
2:A:48:ASN:N	2:A:48:ASN:HD22	2.13	0.47
2:A:89:LEU:HD11	2:A:174:ALA:HA	1.96	0.47
2:A:338:LYS:O	2:A:339:MET:C	2.58	0.47
2:A:804:ALA:HA	2:A:809:LYS:HE3	1.96	0.47
2:B:368:ARG:HG3	2:B:541:GLY:N	2.30	0.47
2:B:539:ILE:HA	2:B:542:LEU:HD12	1.96	0.47
2:A:34:LEU:O	2:A:37:ARG:HB2	2.15	0.47
2:A:387:ARG:NH1	2:A:553:LYS:HG3	2.30	0.47
2:B:56:ARG:HG2	2:B:56:ARG:NH1	2.30	0.47
2:B:226:ALA:O	2:B:227:LYS:C	2.58	0.47
2:B:430:ASN:O	2:B:432:ARG:N	2.48	0.47
2:B:729:ARG:HE	2:B:770:ASP:CG	2.23	0.47
2:A:967:ILE:HD12	2:A:967:ILE:N	2.30	0.46
2:B:101:ASP:OD1	2:B:103:THR:HB	2.15	0.46
2:B:109:TYR:HA	2:B:118:LEU:CD2	2.45	0.46
2:B:229:LEU:O	2:B:233:SER:HB3	2.15	0.46
2:B:368:ARG:HD3	2:B:540:MET:HE2	1.97	0.46
2:A:29:SER:OG	2:A:34:LEU:HD23	2.15	0.46
2:A:680:ARG:HB3	2:A:689:PHE:CE1	2.50	0.46
2:A:796:SER:HB3	2:A:799:ALA:HB3	1.96	0.46
2:A:1018:ILE:HD12	2:A:1037:ALA:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:THR:O	2:B:172:ILE:C	2.58	0.46
2:B:804:ALA:HA	2:B:809:LYS:HE3	1.95	0.46
2:A:212:GLU:HB2	2:A:696:LEU:HD12	1.96	0.46
2:A:886:THR:OG1	2:A:1055:PHE:HB3	2.14	0.46
2:A:1067:TRP:O	2:A:1070:MET:HB2	2.15	0.46
2:B:49:SER:C	2:B:51:ASN:H	2.22	0.46
2:B:517:LEU:C	2:B:517:LEU:CD2	2.88	0.46
2:A:145:VAL:CG2	2:A:211:ILE:HG23	2.46	0.46
2:A:290:GLN:O	2:A:294:ASN:ND2	2.48	0.46
2:A:301:VAL:C	2:A:304:PRO:HD2	2.39	0.46
2:A:903:LEU:C	2:A:904:PRO:O	2.57	0.46
2:B:374:MET:HE2	2:B:480:MET:HB3	1.98	0.46
2:B:515:MET:HG2	2:B:639:PHE:HE2	1.80	0.46
2:B:796:SER:HB3	2:B:799:ALA:HB3	1.96	0.46
2:B:887:VAL:HG12	2:B:888:SER:N	2.30	0.46
2:B:271:PHE:CZ	2:B:273:ASN:HA	2.50	0.46
2:B:584:ILE:HD12	2:B:585:GLN:O	2.16	0.46
2:B:843:ALA:HB3	2:B:844:PRO:HD3	1.97	0.46
2:B:1018:ILE:HD12	2:B:1037:ALA:CB	2.46	0.46
2:B:295:MET:HE1	2:B:303:ILE:HG21	1.96	0.46
2:B:389:SER:OG	2:B:557:THR:HG21	2.16	0.46
2:B:734:THR:CA	2:B:737:MET:HE3	2.30	0.46
2:A:148:TRP:HB3	2:A:215:MET:HE1	1.97	0.46
2:A:515:MET:HG2	2:A:639:PHE:HE2	1.81	0.46
2:B:485:LYS:HE2	2:B:495:SER:C	2.40	0.46
2:B:903:LEU:C	2:B:904:PRO:O	2.57	0.46
2:A:5:ASN:CG	2:A:71:LEU:HD23	2.41	0.46
2:A:246:SER:N	2:A:247:PRO:CD	2.78	0.46
2:A:326:TYR:HE2	2:A:690:ARG:HB2	1.81	0.46
2:A:429:ALA:C	2:A:430:ASN:OD1	2.59	0.46
2:A:485:LYS:HE2	2:A:495:SER:C	2.40	0.46
2:A:643:VAL:HA	2:A:647:MET:SD	2.55	0.46
2:B:326:TYR:HE2	2:B:690:ARG:HB2	1.81	0.46
2:B:721:ARG:HD2	2:B:726:GLU:HG3	1.97	0.46
2:B:999:ILE:HD11	2:B:1009:PHE:CZ	2.51	0.46
2:A:56:ARG:HG2	2:A:56:ARG:NH1	2.31	0.46
2:B:48:ASN:HD22	2:B:48:ASN:N	2.14	0.46
2:B:89:LEU:HD11	2:B:174:ALA:CB	2.46	0.46
2:B:896:TYR:HB2	2:B:912:GLN:HA	1.98	0.46
3:B:1111:GTP:O1B	3:B:1111:GTP:O3G	2.34	0.46
2:B:438:ILE:HD11	2:B:560:LEU:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:857:LEU:C	2:B:857:LEU:HD23	2.40	0.46
2:A:221:ASP:O	2:A:225:ILE:HG13	2.16	0.45
2:B:210:SER:OG	2:B:230:ILE:HG23	2.17	0.45
2:A:49:SER:C	2:A:51:ASN:H	2.22	0.45
2:A:228:GLU:OE2	2:A:302:ASP:HB2	2.16	0.45
2:A:326:TYR:CE2	2:A:690:ARG:HB2	2.52	0.45
2:A:430:ASN:C	2:A:432:ARG:H	2.23	0.45
2:A:997:LEU:HD12	2:A:1035:LEU:CD2	2.46	0.45
2:B:11:TYR:CZ	2:B:15:ILE:HG13	2.52	0.45
2:B:28:TYR:CZ	2:B:784:ILE:HG12	2.50	0.45
2:B:130:MET:HE2	2:B:196:MET:HE2	1.97	0.45
2:A:89:LEU:HD11	2:A:174:ALA:CB	2.46	0.45
2:B:387:ARG:NH1	2:B:387:ARG:HB3	2.31	0.45
2:B:1067:TRP:O	2:B:1070:MET:HB2	2.15	0.45
2:A:11:TYR:CZ	2:A:15:ILE:HG13	2.51	0.45
2:B:135:LEU:HD22	2:B:709:GLN:NE2	2.30	0.45
2:A:217:VAL:HG13	2:A:223:TYR:N	2.31	0.45
2:A:430:ASN:C	2:A:432:ARG:N	2.74	0.45
2:A:703:GLN:CD	2:A:703:GLN:H	2.23	0.45
2:B:322:MET:N	2:B:322:MET:HE2	2.31	0.45
2:B:797:GLY:O	2:B:801:GLU:HG3	2.17	0.45
2:A:171:THR:O	2:A:172:ILE:C	2.60	0.45
2:A:217:VAL:HG13	2:A:222:ASP:CB	2.47	0.45
2:A:438:ILE:HD11	2:A:560:LEU:HB3	1.97	0.45
2:A:721:ARG:HD2	2:A:726:GLU:HG3	1.98	0.45
2:A:758:THR:HG22	2:A:766:PHE:O	2.16	0.45
2:A:984:ASP:O	2:A:988:ILE:HG12	2.17	0.45
2:B:339:MET:CE	2:B:449:LEU:HB3	2.46	0.45
2:B:556:GLN:NE2	2:B:556:GLN:CA	2.75	0.45
2:B:596:THR:O	2:B:600:ASN:HB2	2.16	0.45
2:A:130:MET:HE2	2:A:196:MET:HE2	1.98	0.45
2:A:182:VAL:HA	2:A:183:PRO:HD3	1.80	0.45
2:A:612:LEU:HD23	2:A:615:ILE:HD11	1.98	0.45
2:A:896:TYR:HB2	2:A:912:GLN:HA	1.99	0.45
2:A:1026:ILE:HA	2:A:1027:PRO:HD2	1.59	0.45
2:B:217:VAL:HG13	2:B:222:ASP:CB	2.47	0.45
2:B:334:PHE:CE2	2:B:455:PRO:HD3	2.52	0.45
2:B:872:ILE:HD11	2:B:1069:LYS:HE3	1.98	0.45
2:B:999:ILE:HD12	2:B:999:ILE:HA	1.77	0.45
2:A:441:VAL:HG13	2:A:469:TYR:OH	2.17	0.45
2:B:34:LEU:O	2:B:37:ARG:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:1101:U:HO2'	1:Y:1102:G:P	2.40	0.45
2:A:322:MET:HE2	2:A:322:MET:N	2.32	0.45
2:A:374:MET:CE	2:A:480:MET:HB3	2.47	0.45
2:A:797:GLY:O	2:A:801:GLU:HG3	2.17	0.45
2:A:803:ALA:HB1	2:A:836:LYS:HE3	1.99	0.45
2:A:959:GLN:HE21	2:A:973:ASP:HA	1.82	0.45
2:B:217:VAL:HG13	2:B:223:TYR:N	2.31	0.45
2:B:326:TYR:CE2	2:B:690:ARG:HB2	2.52	0.45
2:B:584:ILE:HD12	2:B:585:GLN:C	2.42	0.45
2:B:605:LEU:HB2	2:B:628:VAL:HG11	1.99	0.45
2:B:959:GLN:HE21	2:B:973:ASP:HA	1.82	0.45
2:B:963:ILE:CD1	2:B:969:LYS:HG2	2.46	0.45
2:B:1026:ILE:HA	2:B:1027:PRO:HD2	1.58	0.45
2:A:271:PHE:CZ	2:A:273:ASN:HA	2.52	0.44
2:A:584:ILE:HD12	2:A:585:GLN:O	2.17	0.44
2:A:975:TYR:C	2:A:977:GLY:N	2.75	0.44
2:B:161:LYS:C	2:B:165:ARG:NH1	2.75	0.44
2:B:627:ARG:HG2	2:B:627:ARG:NH1	2.31	0.44
2:B:84:ALA:HB1	2:B:88:LYS:HZ1	1.83	0.44
2:B:125:TYR:CG	2:B:126:THR:N	2.85	0.44
2:B:148:TRP:HB3	2:B:215:MET:HE1	1.98	0.44
2:B:246:SER:N	2:B:247:PRO:CD	2.80	0.44
2:B:429:ALA:C	2:B:430:ASN:OD1	2.60	0.44
2:B:430:ASN:C	2:B:432:ARG:H	2.24	0.44
2:B:703:GLN:CD	2:B:703:GLN:H	2.24	0.44
2:A:900:MET:HE2	2:A:903:LEU:HG	1.97	0.44
2:A:999:ILE:HD12	2:A:999:ILE:HA	1.79	0.44
2:B:100:ALA:O	2:B:102:LEU:HD22	2.17	0.44
2:B:186:ASN:ND2	2:B:186:ASN:C	2.75	0.44
2:B:380:LYS:HE3	2:B:548:MET:CE	2.48	0.44
2:A:734:THR:CA	2:A:737:MET:HE3	2.32	0.44
2:A:963:ILE:CD1	2:A:969:LYS:HG2	2.46	0.44
1:X:1102:G:O2'	1:X:1103:U:P	2.75	0.44
1:X:1105:A:C6	2:A:462:ILE:HD13	2.52	0.44
2:A:28:TYR:CZ	2:A:784:ILE:HG12	2.52	0.44
2:A:161:LYS:C	2:A:165:ARG:NH1	2.76	0.44
2:A:186:ASN:ND2	2:A:186:ASN:C	2.75	0.44
2:A:226:ALA:O	2:A:227:LYS:C	2.61	0.44
2:B:182:VAL:HA	2:B:183:PRO:HD3	1.80	0.44
2:B:975:TYR:C	2:B:977:GLY:N	2.76	0.44
2:A:8:LEU:HD12	2:A:737:MET:SD	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:255:VAL:HG11	2:A:316:ILE:HD13	2.00	0.44
2:A:322:MET:HE2	2:A:322:MET:HA	2.00	0.44
2:A:596:THR:O	2:A:600:ASN:HB2	2.17	0.44
2:B:784:ILE:HG22	2:B:785:GLN:N	2.33	0.44
2:A:919:TYR:CD1	2:A:919:TYR:C	2.96	0.44
2:B:139:SER:O	2:B:142:LEU:HB2	2.18	0.44
1:Y:1105:A:C6	2:B:462:ILE:HD13	2.53	0.44
2:A:125:TYR:CG	2:A:126:THR:N	2.86	0.44
2:A:924:ASP:C	2:A:944:ILE:HD13	2.43	0.44
2:B:135:LEU:HD13	2:B:709:GLN:NE2	2.26	0.44
2:B:8:LEU:CD2	2:B:74:ILE:HD12	2.42	0.43
2:B:408:LEU:O	2:B:414:THR:HA	2.17	0.43
2:B:450:GLY:O	2:B:462:ILE:N	2.50	0.43
2:B:1070:MET:O	2:B:1073:ILE:HG13	2.18	0.43
2:A:186:ASN:C	2:A:186:ASN:HD22	2.25	0.43
2:A:410:PHE:CE1	2:A:425:MET:HE2	2.52	0.43
2:A:949:LYS:O	2:A:953:LEU:HG	2.19	0.43
2:B:126:THR:HG23	2:B:126:THR:O	2.18	0.43
2:B:228:GLU:OE2	2:B:302:ASP:HB2	2.18	0.43
2:B:719:VAL:HG12	2:B:723:ARG:HD2	2.00	0.43
1:X:1102:G:N1	2:A:190:ARG:HD3	2.33	0.43
2:A:295:MET:HE1	2:A:303:ILE:HG21	1.99	0.43
2:A:387:ARG:NH1	2:A:387:ARG:HB3	2.33	0.43
2:B:213:MET:O	2:B:217:VAL:HG23	2.19	0.43
2:B:430:ASN:C	2:B:432:ARG:N	2.75	0.43
2:B:605:LEU:O	2:B:605:LEU:HD12	2.18	0.43
2:B:780:ASP:O	2:B:783:TYR:HB3	2.18	0.43
2:B:962:LEU:C	2:B:967:ILE:HB	2.43	0.43
2:B:992:TYR:CE1	2:B:996:LEU:HD21	2.53	0.43
2:A:334:PHE:CD2	2:A:455:PRO:HD3	2.53	0.43
2:A:556:GLN:NE2	2:A:556:GLN:CA	2.77	0.43
2:A:962:LEU:C	2:A:967:ILE:HB	2.43	0.43
2:A:1028:ALA:O	2:A:1031:PHE:HB3	2.18	0.43
2:B:8:LEU:HD12	2:B:737:MET:SD	2.58	0.43
2:A:123:GLU:N	2:A:123:GLU:CD	2.77	0.43
2:A:264:ASN:O	2:A:267:LEU:N	2.49	0.43
2:A:783:TYR:CZ	2:A:864:PRO:HB2	2.53	0.43
2:B:186:ASN:C	2:B:186:ASN:HD22	2.25	0.43
2:B:612:LEU:HD23	2:B:615:ILE:HD11	2.00	0.43
2:A:517:LEU:CD2	2:A:517:LEU:C	2.91	0.43
2:A:989:LEU:HD21	2:A:1070:MET:HE3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:380:LYS:HE3	2:B:548:MET:HE2	2.01	0.43
2:B:491:ALA:HB3	2:B:629:ASP:HB2	2.00	0.43
2:B:748:LEU:C	2:B:748:LEU:CD2	2.92	0.43
2:A:584:ILE:HD12	2:A:585:GLN:C	2.44	0.43
2:A:771:PHE:HB3	2:A:1003:CYS:SG	2.59	0.43
2:A:784:ILE:HG22	2:A:785:GLN:N	2.34	0.43
2:B:803:ALA:HB1	2:B:836:LYS:HE3	2.01	0.43
2:B:863:LYS:HB2	2:B:863:LYS:HE3	1.80	0.43
1:Y:1102:G:N1	2:B:190:ARG:HD3	2.33	0.43
2:A:897:GLN:OE1	2:A:897:GLN:N	2.40	0.43
2:B:301:VAL:O	2:B:304:PRO:HD2	2.18	0.43
2:B:632:ASP:CG	2:B:677:ILE:HB	2.43	0.43
2:B:984:ASP:O	2:B:988:ILE:HG12	2.19	0.43
1:X:1103:U:O2'	1:X:1104:G:P	2.76	0.43
2:A:101:ASP:OD1	2:A:103:THR:HB	2.19	0.43
2:A:186:ASN:HD22	2:A:186:ASN:N	2.16	0.43
2:A:608:ILE:HD11	2:A:635:ALA:HB2	2.00	0.43
2:A:748:LEU:C	2:A:748:LEU:CD2	2.92	0.43
2:A:787:ALA:O	2:A:790:SER:HB3	2.19	0.43
2:B:919:TYR:CD1	2:B:919:TYR:C	2.97	0.43
2:A:24:ILE:O	2:A:24:ILE:HG22	2.19	0.43
2:A:240:LEU:O	2:A:243:LEU:HB2	2.19	0.43
2:A:380:LYS:HE3	2:A:548:MET:CE	2.49	0.43
2:B:123:GLU:N	2:B:123:GLU:CD	2.77	0.43
2:A:1066:LEU:O	2:A:1069:LYS:N	2.52	0.42
2:B:315:SER:C	2:B:317:GLU:N	2.76	0.42
2:B:360:TYR:OH	2:B:529:HIS:HB3	2.19	0.42
2:B:428:MET:HE1	2:B:811:TYR:CD1	2.43	0.42
2:A:408:LEU:O	2:A:414:THR:HA	2.19	0.42
2:A:519:THR:HG22	2:A:521:VAL:HG13	2.02	0.42
2:B:7:ILE:HG22	2:B:7:ILE:O	2.19	0.42
2:B:186:ASN:HD22	2:B:186:ASN:N	2.16	0.42
2:B:728:ASP:OD1	2:B:730:GLU:HB2	2.19	0.42
2:B:1061:SER:O	2:B:1064:ILE:HG22	2.19	0.42
2:A:177:ILE:HD13	2:A:203:LEU:CD1	2.38	0.42
2:A:534:PHE:CZ	2:A:599:ALA:HB1	2.54	0.42
2:A:780:ASP:O	2:A:783:TYR:HB3	2.19	0.42
2:A:854:ILE:O	2:A:858:LEU:HB2	2.19	0.42
2:A:975:TYR:C	2:A:977:GLY:H	2.27	0.42
2:A:1016:LYS:C	2:A:1018:ILE:H	2.27	0.42
2:B:177:ILE:HD13	2:B:203:LEU:CD1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:255:VAL:HG11	2:B:316:ILE:HD13	2.01	0.42
2:B:258:ASN:OD1	2:B:275:TYR:HD1	2.02	0.42
2:A:7:ILE:O	2:A:7:ILE:HG22	2.20	0.42
2:A:544:ILE:O	2:A:548:MET:HG3	2.19	0.42
2:B:164:LYS:O	2:B:166:ARG:N	2.53	0.42
2:B:783:TYR:CZ	2:B:864:PRO:HB2	2.55	0.42
1:Y:1102:G:O2'	1:Y:1103:U:P	2.77	0.42
2:A:863:LYS:HB2	2:A:863:LYS:HE3	1.81	0.42
2:B:264:ASN:O	2:B:267:LEU:N	2.50	0.42
2:B:375:LEU:O	2:B:378:PRO:HD2	2.19	0.42
2:B:949:LYS:O	2:B:953:LEU:HG	2.20	0.42
2:A:339:MET:CE	2:A:449:LEU:HB3	2.49	0.42
2:A:1026:ILE:HG12	2:A:1026:ILE:O	2.20	0.42
2:A:1047:LYS:HE3	2:A:1047:LYS:HB2	1.76	0.42
2:B:449:LEU:HA	2:B:449:LEU:HD12	1.77	0.42
2:B:706:GLN:O	2:B:707:TRP:C	2.60	0.42
2:B:854:ILE:O	2:B:858:LEU:HB2	2.19	0.42
2:A:6:LEU:C	2:A:8:LEU:N	2.76	0.42
2:B:340:LEU:HD13	2:B:575:ILE:HG21	2.02	0.42
2:B:544:ILE:O	2:B:548:MET:HG3	2.20	0.42
2:B:997:LEU:HD12	2:B:1035:LEU:CD2	2.49	0.42
2:A:689:PHE:HB3	2:A:723:ARG:HH12	1.75	0.42
2:A:781:GLU:O	2:A:785:GLN:HG3	2.20	0.42
2:A:1061:SER:O	2:A:1064:ILE:HG22	2.20	0.42
2:B:722:LEU:HD21	2:B:771:PHE:CE1	2.54	0.42
2:B:735:LYS:O	2:B:739:MET:HG3	2.19	0.42
2:B:823:LYS:HG2	2:B:824:ASN:N	2.34	0.42
2:B:1016:LYS:C	2:B:1018:ILE:H	2.28	0.42
1:X:1104:G:H5'	2:A:401:SER:HB2	2.01	0.42
2:A:109:TYR:HA	2:A:118:LEU:HD22	2.01	0.42
2:A:491:ALA:HB3	2:A:629:ASP:HB2	2.01	0.42
2:A:1080:TYR:O	2:A:1083:ALA:HB3	2.19	0.42
2:B:255:VAL:CG1	2:B:316:ILE:HB	2.50	0.42
2:B:584:ILE:HD12	2:B:585:GLN:N	2.35	0.42
2:B:897:GLN:OE1	2:B:897:GLN:N	2.42	0.42
2:A:133:ALA:O	2:A:698:ASN:HB2	2.19	0.42
2:A:164:LYS:O	2:A:166:ARG:N	2.53	0.42
2:A:563:GLN:HA	2:A:563:GLN:NE2	2.34	0.42
2:A:719:VAL:HG12	2:A:723:ARG:HD2	2.02	0.42
2:A:823:LYS:HG2	2:A:824:ASN:N	2.34	0.42
2:A:847:LEU:O	2:A:851:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1070:MET:O	2:A:1073:ILE:HG13	2.20	0.42
2:B:374:MET:CE	2:B:480:MET:HB3	2.50	0.42
2:B:519:THR:HG22	2:B:521:VAL:HG13	2.02	0.42
2:A:255:VAL:CG1	2:A:316:ILE:HB	2.50	0.41
2:A:425:MET:O	2:A:426:ASP:C	2.63	0.41
2:A:847:LEU:HD23	2:A:850:ARG:NH1	2.34	0.41
2:B:425:MET:O	2:B:426:ASP:C	2.63	0.41
2:B:534:PHE:CZ	2:B:599:ALA:HB1	2.54	0.41
2:B:758:THR:HG22	2:B:766:PHE:O	2.20	0.41
2:B:975:TYR:C	2:B:977:GLY:H	2.28	0.41
2:A:106:GLU:O	2:A:107:LEU:C	2.62	0.41
2:A:232:LEU:CD2	2:A:300:LEU:HG	2.50	0.41
2:A:449:LEU:HA	2:A:449:LEU:HD12	1.76	0.41
2:A:920:GLN:OE1	2:A:920:GLN:HA	2.20	0.41
2:A:992:TYR:CE1	2:A:996:LEU:HD21	2.55	0.41
2:B:104:VAL:HG23	2:B:105:ASN:ND2	2.34	0.41
2:B:924:ASP:C	2:B:944:ILE:HD13	2.46	0.41
2:A:70:THR:HG21	2:A:755:ARG:HG2	2.02	0.41
2:A:213:MET:O	2:A:217:VAL:HG23	2.21	0.41
2:A:723:ARG:NH2	3:A:1111:GTP:O3B	2.37	0.41
2:A:796:SER:OG	2:A:845:ILE:HG23	2.21	0.41
2:B:6:LEU:C	2:B:8:LEU:N	2.76	0.41
2:B:842:TYR:CZ	2:B:844:PRO:HG2	2.54	0.41
2:A:258:ASN:OD1	2:A:275:TYR:HD1	2.04	0.41
2:A:322:MET:HE2	2:A:322:MET:CA	2.50	0.41
2:A:360:TYR:OH	2:A:529:HIS:HB3	2.20	0.41
2:A:704:SER:HB2	2:A:708:ASP:CB	2.50	0.41
2:B:363:TYR:CZ	2:B:367:ILE:HD11	2.56	0.41
2:B:384:HIS:HE2	2:B:938:SER:C	2.28	0.41
2:B:626:ILE:C	2:B:627:ARG:HG2	2.45	0.41
2:B:661:ARG:HA	2:B:661:ARG:HD2	1.82	0.41
2:B:667:LYS:O	2:B:667:LYS:CG	2.69	0.41
2:B:680:ARG:HB3	2:B:689:PHE:HE1	1.85	0.41
2:B:920:GLN:OE1	2:B:920:GLN:HA	2.20	0.41
2:B:1047:LYS:HE3	2:B:1047:LYS:HB2	1.75	0.41
2:B:1080:TYR:O	2:B:1083:ALA:HB3	2.20	0.41
2:A:410:PHE:HE1	2:A:425:MET:CE	2.32	0.41
2:A:415:ILE:HG23	2:A:416:PHE:N	2.35	0.41
2:A:516:VAL:HG21	2:A:675:ILE:HG21	2.01	0.41
2:A:767:ASP:C	2:A:769:GLU:H	2.28	0.41
2:B:372:VAL:O	2:B:373:LYS:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:608:ILE:HD11	2:B:635:ALA:HB2	2.02	0.41
2:A:103:THR:O	2:A:103:THR:HG22	2.21	0.41
2:A:315:SER:C	2:A:317:GLU:N	2.78	0.41
2:A:477:VAL:HG11	2:A:594:LYS:HG3	2.03	0.41
2:A:661:ARG:HA	2:A:661:ARG:HD2	1.83	0.41
2:A:767:ASP:O	2:A:769:GLU:N	2.53	0.41
2:B:232:LEU:CD2	2:B:300:LEU:HG	2.50	0.41
2:B:573:VAL:HG12	2:B:575:ILE:HG13	2.02	0.41
2:B:612:LEU:CD2	2:B:637:LEU:HD11	2.50	0.41
2:B:796:SER:OG	2:B:845:ILE:HG23	2.21	0.41
2:B:860:MET:O	2:B:862:GLN:N	2.44	0.41
2:B:880:ASP:O	2:B:883:PRO:HD2	2.20	0.41
2:A:265:GLU:C	2:A:267:LEU:H	2.29	0.41
2:A:389:SER:OG	2:A:557:THR:HG21	2.20	0.41
2:A:573:VAL:HG12	2:A:575:ILE:HG13	2.02	0.41
2:A:584:ILE:HD12	2:A:585:GLN:N	2.36	0.41
2:A:853:GLN:HE21	2:A:853:GLN:CA	2.33	0.41
2:A:967:ILE:HA	2:A:968:PRO:HD2	1.89	0.41
2:B:70:THR:HG21	2:B:755:ARG:HG2	2.02	0.41
2:B:441:VAL:HG13	2:B:469:TYR:OH	2.21	0.41
2:B:786:ARG:HD3	2:B:869:SER:OG	2.20	0.41
2:B:950:VAL:O	2:B:958:ILE:HG12	2.21	0.41
2:A:126:THR:O	2:A:126:THR:HG23	2.21	0.41
2:A:384:HIS:HE2	2:A:938:SER:C	2.28	0.41
2:A:617:ASN:N	2:A:617:ASN:HD22	2.17	0.41
2:A:706:GLN:O	2:A:707:TRP:C	2.62	0.41
2:A:722:LEU:HD21	2:A:771:PHE:CE1	2.55	0.41
2:A:965:LEU:HB2	2:A:967:ILE:HD13	2.03	0.41
2:A:1023:LYS:NZ	2:A:1057:ASN:HA	2.36	0.41
2:B:213:MET:SD	2:B:229:LEU:HD23	2.61	0.41
2:B:290:GLN:O	2:B:294:ASN:ND2	2.54	0.41
2:B:449:LEU:HD11	2:B:573:VAL:CG2	2.49	0.41
2:B:900:MET:HB3	2:B:903:LEU:CD1	2.50	0.41
2:B:965:LEU:HB2	2:B:967:ILE:HD13	2.03	0.41
2:A:212:GLU:CB	2:A:696:LEU:HD12	2.51	0.41
2:A:254:LEU:CD2	2:A:280:VAL:HG21	2.44	0.41
2:A:288:LEU:HD12	2:A:288:LEU:O	2.20	0.41
2:A:330:PHE:CE1	2:A:690:ARG:CZ	3.04	0.41
2:A:463:PHE:CZ	2:A:590:ALA:HB3	2.56	0.41
2:A:605:LEU:HB2	2:A:628:VAL:HG11	2.03	0.41
2:A:744:ILE:HD11	2:A:858:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:288:LEU:O	2:B:288:LEU:HD12	2.20	0.41
2:B:322:MET:HE2	2:B:322:MET:HA	2.03	0.41
2:B:516:VAL:HG21	2:B:675:ILE:HG21	2.01	0.41
2:B:781:GLU:O	2:B:785:GLN:HG3	2.21	0.41
2:B:1020:ILE:O	2:B:1020:ILE:HG22	2.20	0.41
2:A:102:LEU:H	2:A:102:LEU:CD2	2.30	0.41
2:A:539:ILE:HD11	2:A:565:GLN:O	2.20	0.41
2:A:1016:LYS:C	2:A:1018:ILE:N	2.79	0.41
2:B:103:THR:O	2:B:103:THR:HG22	2.21	0.41
2:B:183:PRO:HG3	2:B:199:LYS:HD3	2.02	0.41
2:B:254:LEU:CD2	2:B:280:VAL:HG21	2.44	0.41
2:A:428:MET:HE1	2:A:811:TYR:CD1	2.46	0.40
2:A:783:TYR:CE2	2:A:864:PRO:HB2	2.56	0.40
2:A:860:MET:C	2:A:862:GLN:N	2.79	0.40
2:A:959:GLN:CD	2:A:973:ASP:OD1	2.64	0.40
2:B:24:ILE:O	2:B:24:ILE:HG22	2.21	0.40
2:B:219:SER:O	2:B:222:ASP:HB2	2.21	0.40
2:B:607:LEU:O	2:B:610:THR:HB	2.21	0.40
2:B:723:ARG:NH2	3:B:1111:GTP:O3B	2.49	0.40
2:A:429:ALA:O	2:A:430:ASN:OD1	2.40	0.40
2:A:728:ASP:OD1	2:A:730:GLU:HB2	2.21	0.40
2:A:887:VAL:CG1	2:A:888:SER:N	2.84	0.40
2:B:109:TYR:HA	2:B:118:LEU:HD22	2.03	0.40
2:B:152:HIS:CD2	2:B:155:ASP:OD2	2.75	0.40
2:B:165:ARG:HB3	2:B:223:TYR:HB2	2.03	0.40
2:B:212:GLU:CB	2:B:696:LEU:HD12	2.51	0.40
2:B:787:ALA:O	2:B:790:SER:HB3	2.22	0.40
2:B:860:MET:C	2:B:862:GLN:N	2.79	0.40
2:B:967:ILE:HA	2:B:968:PRO:HD2	1.90	0.40
2:A:372:VAL:O	2:A:373:LYS:C	2.65	0.40
2:A:549:THR:HG21	2:A:554:VAL:HG11	2.04	0.40
2:A:909:TYR:O	2:A:910:ILE:C	2.65	0.40
2:B:751:PHE:HA	2:B:752:PRO:HD3	1.87	0.40
2:B:959:GLN:CD	2:B:973:ASP:OD1	2.65	0.40
2:A:165:ARG:HB3	2:A:223:TYR:HB2	2.04	0.40
2:A:324:LYS:O	2:A:328:TRP:CD1	2.64	0.40
2:A:632:ASP:CG	2:A:677:ILE:HB	2.46	0.40
2:A:1066:LEU:O	2:A:1067:TRP:C	2.65	0.40
2:B:847:LEU:O	2:B:851:ARG:HG3	2.21	0.40
2:B:853:GLN:HE21	2:B:853:GLN:CA	2.33	0.40
1:Y:1103:U:O2'	1:Y:1104:G:P	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:135:LEU:HD13	2:A:709:GLN:NE2	2.29	0.40
2:A:860:MET:O	2:A:862:GLN:N	2.45	0.40
2:B:106:GLU:O	2:B:107:LEU:C	2.64	0.40
2:B:217:VAL:HG13	2:B:222:ASP:HB3	2.04	0.40
2:B:265:GLU:C	2:B:267:LEU:H	2.30	0.40
2:B:344:LEU:C	2:B:346:GLN:N	2.79	0.40
2:B:554:VAL:O	2:B:558:LEU:HB2	2.21	0.40
2:B:847:LEU:HD23	2:B:850:ARG:NH1	2.35	0.40
2:B:1066:LEU:O	2:B:1069:LYS:N	2.54	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	
2	A	1067/1095 (97%)	915 (86%)	124 (12%)	28 (3%)	4	15
2	B	1067/1095 (97%)	919 (86%)	120 (11%)	28 (3%)	4	15
All	All	2134/2190 (97%)	1834 (86%)	244 (11%)	56 (3%)	4	15

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	866	THR
2	A	976	VAL
2	A	978	SER
2	B	866	THR
2	B	976	VAL
2	B	978	SER
2	A	106	GLU
2	A	128	SER
2	A	226	ALA

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Mol	Chain	Res	Type
2	A	345	ASP
2	A	864	PRO
2	A	865	VAL
2	A	1017	LEU
2	B	106	GLU
2	B	128	SER
2	B	345	ASP
2	B	864	PRO
2	B	865	VAL
2	B	1017	LEU
2	A	91	LYS
2	A	431	GLU
2	A	592	GLY
2	A	768	SER
2	B	91	LYS
2	B	226	ALA
2	B	431	GLU
2	B	592	GLY
2	A	240	LEU
2	A	376	GLU
2	A	382	ASP
2	A	425	MET
2	A	439	PRO
2	A	1027	PRO
2	B	227	LYS
2	B	240	LEU
2	B	376	GLU
2	B	382	ASP
2	B	425	MET
2	B	768	SER
2	B	1027	PRO
2	A	42	HIS
2	A	102	LEU
2	A	164	LYS
2	A	227	LYS
2	A	531	THR
2	B	42	HIS
2	B	102	LEU
2	B	164	LYS
2	B	439	PRO
2	B	508	ARG
2	A	508	ARG

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Mol	Chain	Res	Type
2	A	904	PRO
2	B	531	THR
2	B	964	SER
2	B	904	PRO
2	A	673	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	
2	A	974/996 (98%)	928 (95%)	46 (5%)	23	57
2	B	974/996 (98%)	926 (95%)	48 (5%)	22	55
All	All	1948/1992 (98%)	1854 (95%)	94 (5%)	23	56

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	50	LYS
2	A	91	LYS
2	A	102	LEU
2	A	121	THR
2	A	130	MET
2	A	156	VAL
2	A	186	ASN
2	A	224	LEU
2	A	227	LYS
2	A	229	LEU
2	A	242	LYS
2	A	263	THR
2	A	313	ASP
2	A	318	LYS
2	A	344	LEU
2	A	358	GLU
2	A	409	LYS
2	A	415	ILE

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Mol	Chain	Res	Type
2	A	431	GLU
2	A	449	LEU
2	A	512	ASN
2	A	517	LEU
2	A	518	TYR
2	A	556	GLN
2	A	557	THR
2	A	573	VAL
2	A	584	ILE
2	A	600	ASN
2	A	619	HIS
2	A	628	VAL
2	A	641	THR
2	A	695	LEU
2	A	721	ARG
2	A	784	ILE
2	A	791	LEU
2	A	802	ILE
2	A	857	LEU
2	A	858	LEU
2	A	872	ILE
2	A	892	LEU
2	A	900	MET
2	A	922	GLU
2	A	939	VAL
2	A	970	ILE
2	A	999	ILE
2	A	1054	LEU
2	B	50	LYS
2	B	91	LYS
2	B	102	LEU
2	B	121	THR
2	B	128	SER
2	B	130	MET
2	B	156	VAL
2	B	186	ASN
2	B	224	LEU
2	B	227	LYS
2	B	229	LEU
2	B	242	LYS
2	B	263	THR
2	B	313	ASP

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Mol	Chain	Res	Type
2	B	318	LYS
2	B	320	PRO
2	B	344	LEU
2	B	358	GLU
2	B	409	LYS
2	B	415	ILE
2	B	431	GLU
2	B	449	LEU
2	B	512	ASN
2	B	517	LEU
2	B	518	TYR
2	B	556	GLN
2	B	557	THR
2	B	573	VAL
2	B	584	ILE
2	B	600	ASN
2	B	619	HIS
2	B	628	VAL
2	B	641	THR
2	B	695	LEU
2	B	721	ARG
2	B	784	ILE
2	B	791	LEU
2	B	802	ILE
2	B	858	LEU
2	B	872	ILE
2	B	892	LEU
2	B	900	MET
2	B	922	GLU
2	B	939	VAL
2	B	970	ILE
2	B	996	LEU
2	B	999	ILE
2	B	1054	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	36	ASN
2	A	48	ASN
2	A	143	ASN
2	A	152	HIS

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Mol	Chain	Res	Type
2	A	154	ASN
2	A	186	ASN
2	A	220	HIS
2	A	289	ASN
2	A	294	ASN
2	A	308	GLN
2	A	407	GLN
2	A	512	ASN
2	A	528	GLN
2	A	530	ASN
2	A	556	GLN
2	A	563	GLN
2	A	565	GLN
2	A	617	ASN
2	A	646	GLN
2	A	653	ASN
2	A	698	ASN
2	A	706	GLN
2	A	709	GLN
2	A	760	ASN
2	A	794	GLN
2	A	840	ASN
2	A	853	GLN
2	A	895	GLN
2	A	908	GLN
2	A	959	GLN
2	B	36	ASN
2	B	48	ASN
2	B	143	ASN
2	B	152	HIS
2	B	186	ASN
2	B	220	HIS
2	B	289	ASN
2	B	294	ASN
2	B	308	GLN
2	B	407	GLN
2	B	512	ASN
2	B	528	GLN
2	B	530	ASN
2	B	556	GLN
2	B	563	GLN
2	B	565	GLN

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Mol	Chain	Res	Type
2	B	604	ASN
2	B	617	ASN
2	B	638	GLN
2	B	646	GLN
2	B	653	ASN
2	B	698	ASN
2	B	709	GLN
2	B	760	ASN
2	B	794	GLN
2	B	840	ASN
2	B	853	GLN
2	B	895	GLN
2	B	908	GLN
2	B	959	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	7/7 (100%)	4 (57%)	3 (42%)
1	Y	7/7 (100%)	4 (57%)	3 (42%)
All	All	14/14 (100%)	8 (57%)	6 (42%)

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	1102	G
1	X	1103	U
1	X	1104	G
1	X	1105	A
1	Y	1102	G
1	Y	1103	U
1	Y	1104	G
1	Y	1105	A

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1101	U
1	X	1102	G
1	X	1103	U
1	Y	1101	U

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Mol	Chain	Res	Type
1	Y	1102	G
1	Y	1103	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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	$\# Z > 2$
3	GTP	B	1111	-	33,34,34	2.86	9 (27%)	50,54,54	3.28	18 (36%)
3	GTP	A	1111	-	33,34,34	2.67	8 (24%)	50,54,54	3.22	17 (34%)

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
3	GTP	B	1111	-	-	3/22/38/38	0/3/3/3
3	GTP	A	1111	-	-	2/22/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1111	GTP	PB-O3B	10.08	1.70	1.59
3	A	1111	GTP	PB-O3B	9.75	1.70	1.59
3	B	1111	GTP	PA-O3A	8.29	1.68	1.59
3	A	1111	GTP	PA-O3A	7.45	1.67	1.59
3	B	1111	GTP	PB-O3A	5.79	1.65	1.59
3	A	1111	GTP	PB-O3A	4.78	1.64	1.59
3	B	1111	GTP	PG-O1G	-4.01	1.38	1.50
3	A	1111	GTP	PG-O1G	-3.69	1.39	1.50
3	B	1111	GTP	C2'-C1'	-2.69	1.45	1.53
3	A	1111	GTP	C2'-C1'	-2.45	1.45	1.53
3	A	1111	GTP	PG-O2G	2.43	1.63	1.54
3	B	1111	GTP	PG-O2G	2.31	1.63	1.54
3	B	1111	GTP	C5-N7	-2.15	1.34	1.39
3	A	1111	GTP	C2'-C3'	2.14	1.59	1.53
3	B	1111	GTP	C2'-C3'	2.07	1.59	1.53
3	A	1111	GTP	C5-N7	-2.05	1.35	1.39
3	B	1111	GTP	O4'-C1'	-2.05	1.37	1.42

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1111	GTP	O3G-PG-O1G	-11.70	65.25	110.83
3	A	1111	GTP	O3G-PG-O1G	-11.67	65.36	110.83
3	A	1111	GTP	O2G-PG-O1G	-9.50	73.83	110.83
3	B	1111	GTP	O2G-PG-O1G	-9.14	75.20	110.83
3	B	1111	GTP	O4'-C4'-C5'	-9.11	80.14	109.33
3	A	1111	GTP	O4'-C4'-C5'	-8.47	82.19	109.33
3	B	1111	GTP	O3G-PG-O2G	5.62	128.87	107.80
3	A	1111	GTP	O3G-PG-O2G	5.47	128.31	107.80
3	B	1111	GTP	C5-C4-N3	-5.14	120.20	128.39
3	A	1111	GTP	C5-C4-N3	-5.06	120.34	128.39
3	A	1111	GTP	C2-N3-C4	5.03	120.96	112.30
3	B	1111	GTP	C2-N3-C4	4.91	120.75	112.30
3	B	1111	GTP	N9-C4-N3	4.44	134.83	125.95
3	A	1111	GTP	N9-C4-N3	4.39	134.73	125.95
3	A	1111	GTP	O2G-PG-O3B	4.32	119.12	104.64
3	B	1111	GTP	O4'-C4'-C3'	-4.29	96.64	105.15
3	B	1111	GTP	C2'-C1'-N9	4.13	124.76	113.25
3	B	1111	GTP	O2G-PG-O3B	3.99	118.00	104.64
3	A	1111	GTP	O4'-C4'-C3'	-3.93	97.36	105.15
3	A	1111	GTP	C2'-C1'-N9	3.86	124.00	113.25
3	B	1111	GTP	C2'-C3'-C4'	2.98	108.37	102.61
3	B	1111	GTP	C8-N7-C5	2.71	109.09	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1111	GTP	C2'-C3'-C4'	2.67	107.76	102.61
3	A	1111	GTP	C8-N7-C5	2.61	108.91	104.26
3	B	1111	GTP	C5'-C4'-C3'	2.54	124.36	115.21
3	A	1111	GTP	O3A-PB-O1B	-2.52	103.12	110.70
3	B	1111	GTP	O6-C6-C5	-2.44	120.09	126.53
3	B	1111	GTP	C2-N1-C6	-2.43	120.70	125.11
3	A	1111	GTP	O6-C6-C5	-2.36	120.30	126.53
3	A	1111	GTP	C5'-C4'-C3'	2.33	123.59	115.21
3	A	1111	GTP	C2-N1-C6	-2.32	120.91	125.11
3	B	1111	GTP	O3A-PB-O1B	-2.32	103.74	110.70
3	B	1111	GTP	O2'-C2'-C1'	2.05	117.16	110.10
3	B	1111	GTP	C5-C6-N1	2.04	118.45	113.25
3	A	1111	GTP	O2'-C2'-C1'	2.02	117.05	110.10

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1111	GTP	O4'-C4'-C5'-O5'
3	A	1111	GTP	O4'-C4'-C5'-O5'
3	B	1111	GTP	C5'-O5'-PA-O1A
3	A	1111	GTP	PB-O3B-PG-O1G
3	B	1111	GTP	PB-O3B-PG-O1G

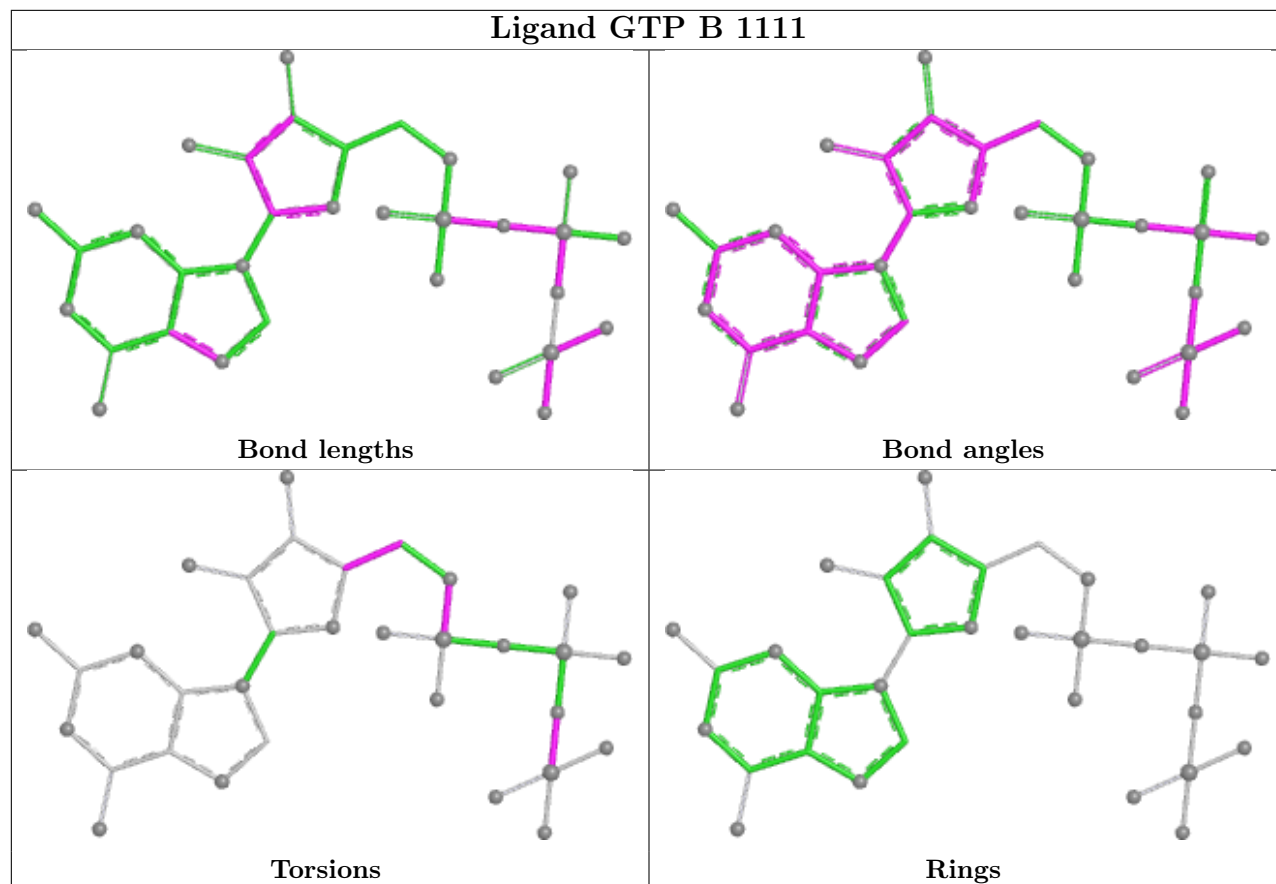
There are no ring outliers.

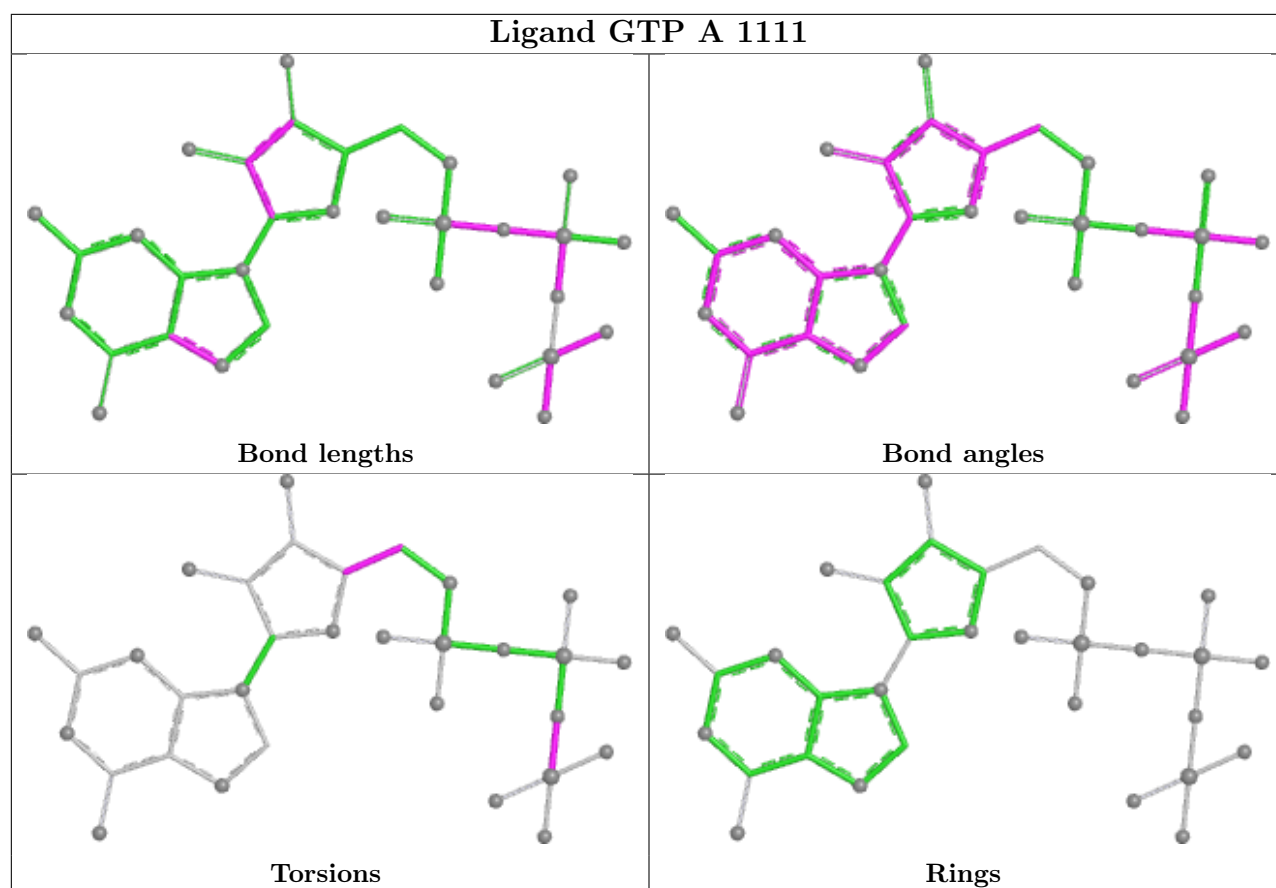
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1111	GTP	2	0
3	A	1111	GTP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.





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	X	7/7 (100%)	-1.77	0 100 100	47, 60, 73, 77	0
1	Y	7/7 (100%)	-1.69	0 100 100	47, 59, 72, 77	0
2	A	1073/1095 (97%)	-1.55	0 100 100	15, 49, 79, 120	0
2	B	1073/1095 (97%)	-1.54	0 100 100	17, 50, 80, 121	0
All	All	2160/2204 (98%)	-1.55	0 100 100	15, 50, 79, 121	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

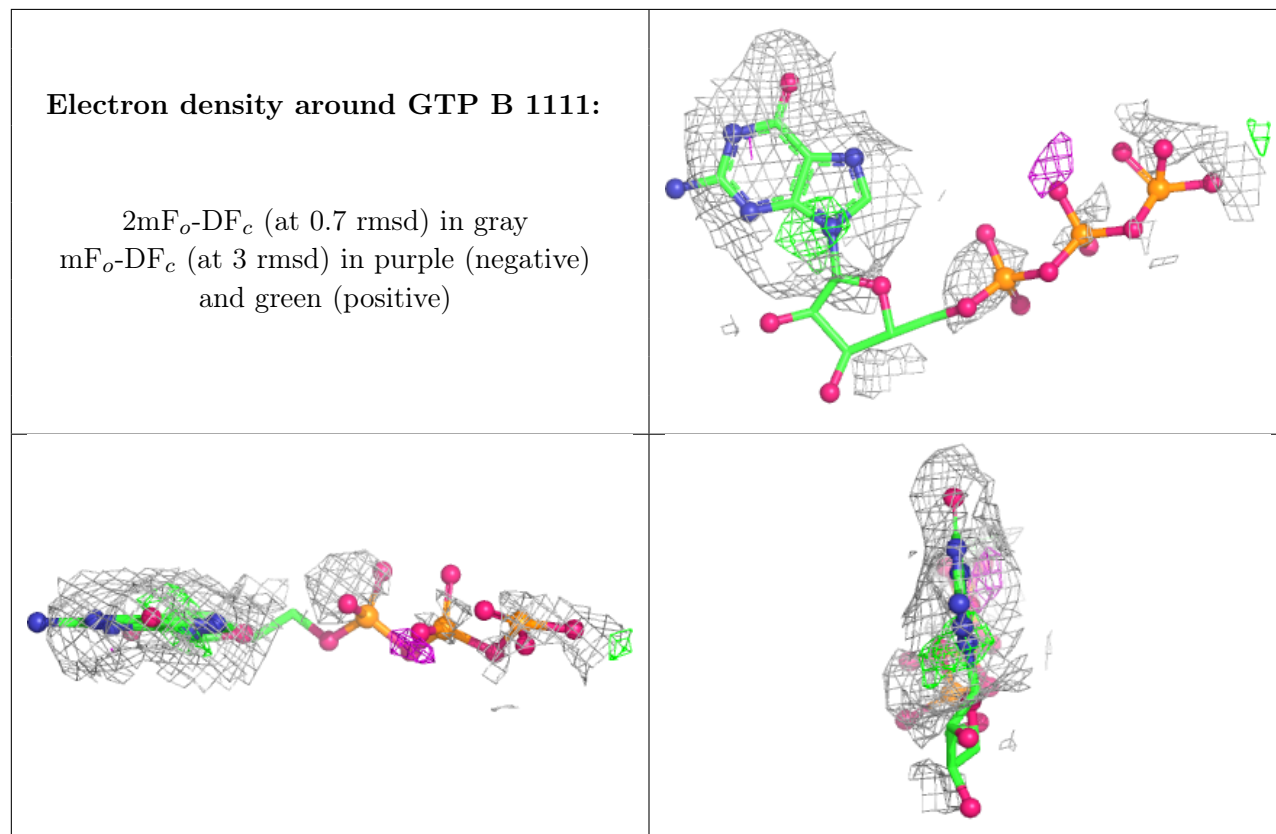
6.4 Ligands [i](#)

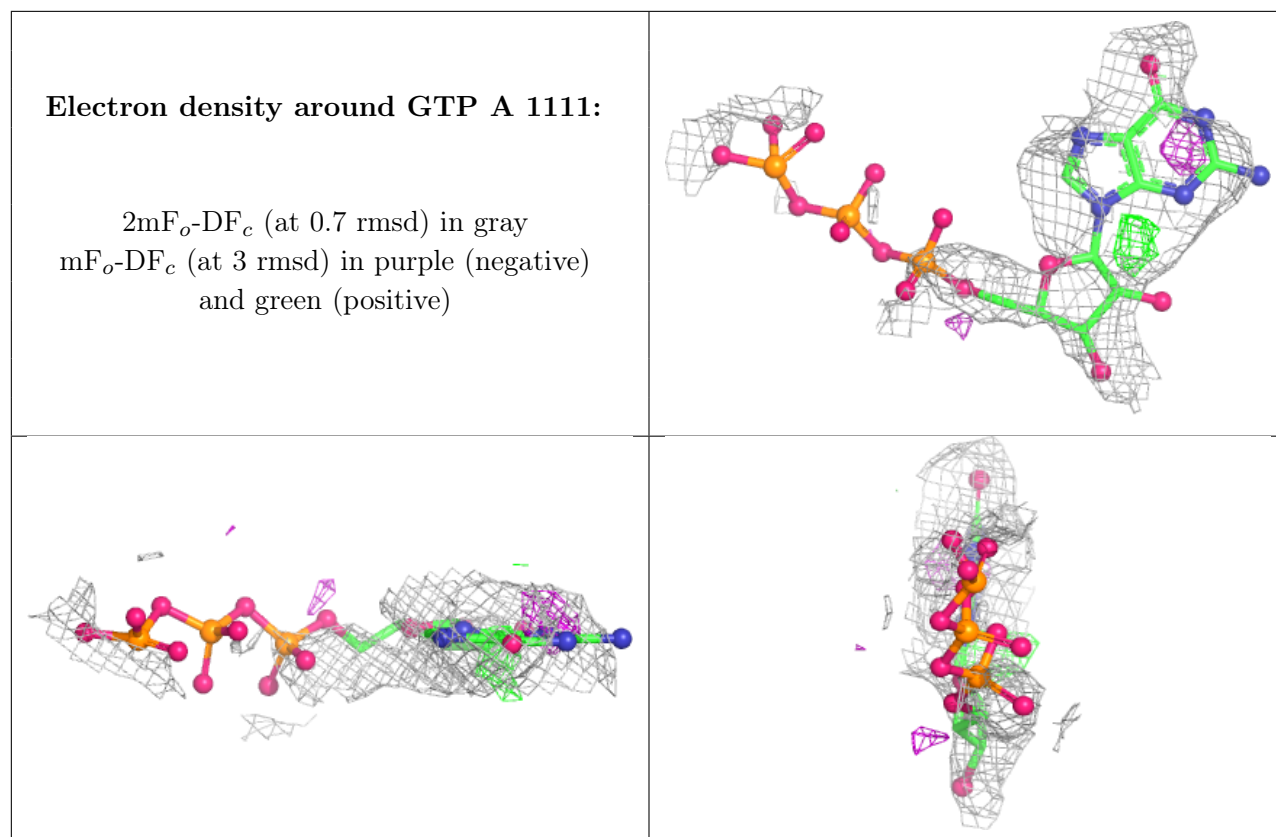
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GTP	B	1111	32/32	0.94	0.08	112,142,150,150	0
3	GTP	A	1111	32/32	0.95	0.09	107,137,145,145	0

The following is a graphical depiction of the model fit to experimental electron density of all

instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.