



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2020 – 02:08 PM BST

PDB ID : 6UU2
Title : E. coli sigma-S transcription initiation complex with 3-nt RNA ("Old" crystal soaked with GTP and ATP for 30 minutes)
Authors : Zuo, Y.; De, S.; Steitz, T.A.
Deposited on : 2019-10-30
Resolution : 4.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

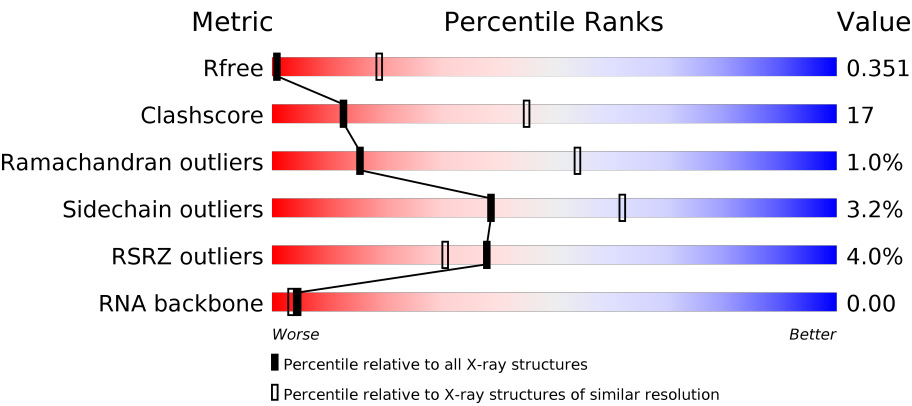
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1043 (5.00-3.80)
Clashscore	141614	1111 (5.00-3.80)
Ramachandran outliers	138981	1059 (5.00-3.80)
Sidechain outliers	138945	1041 (5.00-3.80)
RSRZ outliers	127900	1095 (5.08-3.70)
RNA backbone	3102	1058 (5.60-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	AAA	242	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>71%22%• 5%</div></div>
1	BBB	242	<div><div>5%</div><div><div></div><div></div><div></div><div></div></div><div>76%16%• 6%</div></div>
2	CCC	1342	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>71%28%•</div></div>
3	DDD	1407	<div><div>5%</div><div><div></div><div></div><div></div><div></div></div><div>67%27%• •</div></div>

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Mol	Chain	Length	Quality of chain
4	EEE	90	
5	FFF	336	
6	111	50	
7	222	50	
8	333	3	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	ZN	DDD	1502	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 28949 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	230	Total	C	N	O	S	0	0	0
			1787	1112	317	352	6			
1	BBB	228	Total	C	N	O	S	0	0	0
			1767	1100	312	349	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-6	ALA	-	expression tag	UNP A0A377D9Q8
AAA	-5	HIS	-	expression tag	UNP A0A377D9Q8
AAA	-4	HIS	-	expression tag	UNP A0A377D9Q8
AAA	-3	HIS	-	expression tag	UNP A0A377D9Q8
AAA	-2	HIS	-	expression tag	UNP A0A377D9Q8
AAA	-1	HIS	-	expression tag	UNP A0A377D9Q8
AAA	0	HIS	-	expression tag	UNP A0A377D9Q8
BBB	-6	ALA	-	expression tag	UNP A0A377D9Q8
BBB	-5	HIS	-	expression tag	UNP A0A377D9Q8
BBB	-4	HIS	-	expression tag	UNP A0A377D9Q8
BBB	-3	HIS	-	expression tag	UNP A0A377D9Q8
BBB	-2	HIS	-	expression tag	UNP A0A377D9Q8
BBB	-1	HIS	-	expression tag	UNP A0A377D9Q8
BBB	0	HIS	-	expression tag	UNP A0A377D9Q8

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	CCC	1340	Total	C	N	O	S	0	0	0
			10570	6631	1841	2055	43			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	DDD	1350	Total	C	N	O	S	0	0	0
			10478	6578	1867	1984	49			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	EEE	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

- Molecule 5 is a protein called RNA polymerase sigma factor RpoS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	FFF	277	Total	C	N	O	S	0	0	0
			2253	1411	415	423	4			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
FFF	2	GLY	SER	conflict	UNP P13445
FFF	33	GLU	GLN	conflict	UNP P13445
FFF	329	LEU	-	expression tag	UNP P13445
FFF	330	GLU	-	expression tag	UNP P13445
FFF	331	HIS	-	expression tag	UNP P13445
FFF	332	HIS	-	expression tag	UNP P13445
FFF	333	HIS	-	expression tag	UNP P13445
FFF	334	HIS	-	expression tag	UNP P13445
FFF	335	HIS	-	expression tag	UNP P13445
FFF	336	HIS	-	expression tag	UNP P13445

- Molecule 6 is a DNA chain called Synthetic DNA 50-MER (promoter non-template strand).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	111	31	Total	C	N	O	P	0	0	0
			638	303	117	187	31			

- Molecule 7 is a DNA chain called Synthetic DNA 50-MER (promoter template strand).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	222	35	Total	C	N	O	P	0	0	0
			716	342	132	208	34			

- Molecule 8 is a RNA chain called RNA 3-mer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	333	3	Total	C	N	O	P	0	0	0
			77	30	15	27	5			

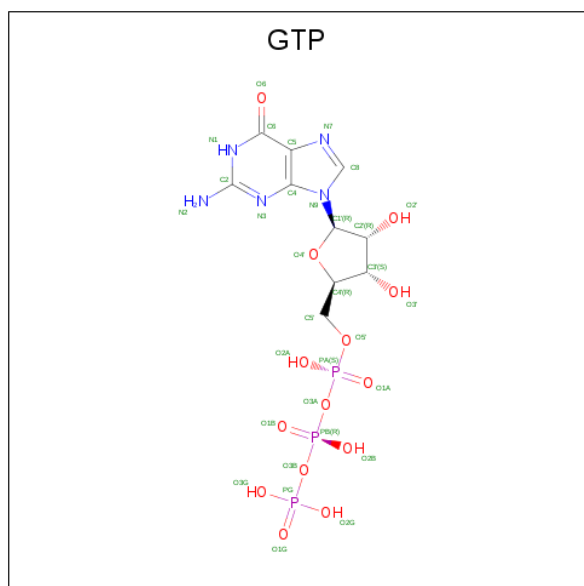
- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	CCC	1	Total	Mg	0	0
			1	1		
9	DDD	1	Total	Mg	0	0
			1	1		

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	DDD	2	Total	Zn	0	0
			2	2		

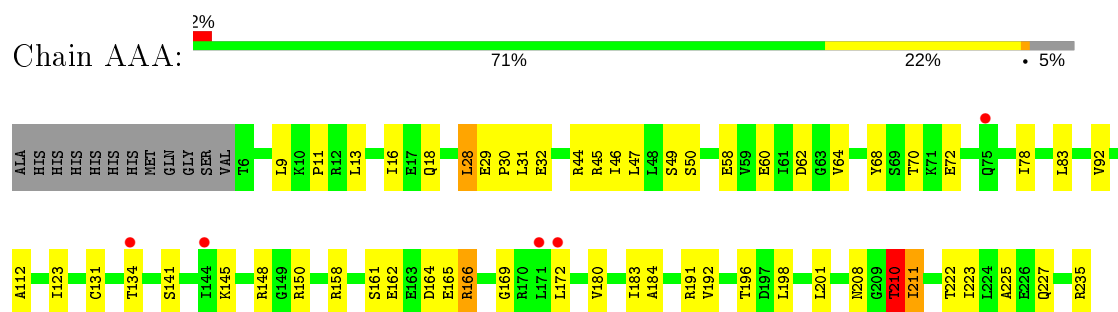
- Molecule 11 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



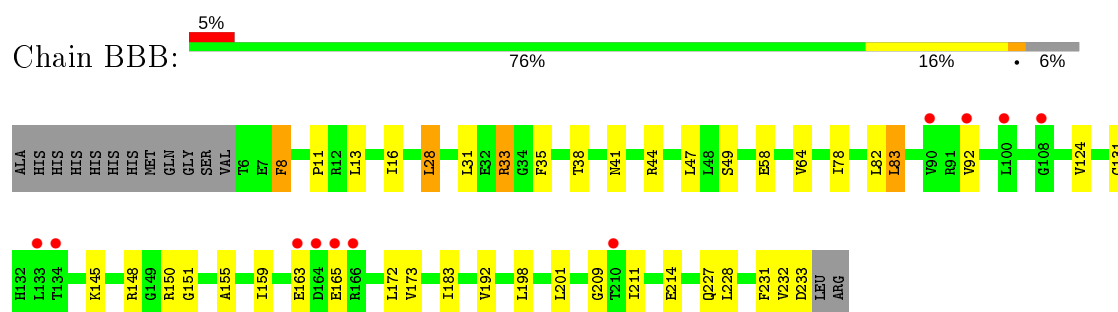
3 Residue-property plots [i](#)

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

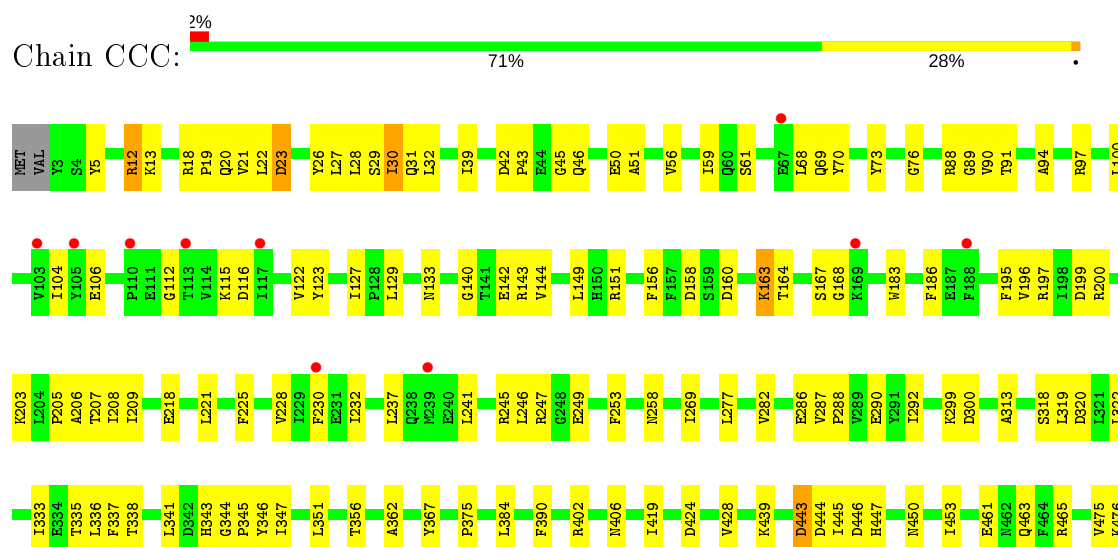
- Molecule 1: DNA-directed RNA polymerase subunit alpha

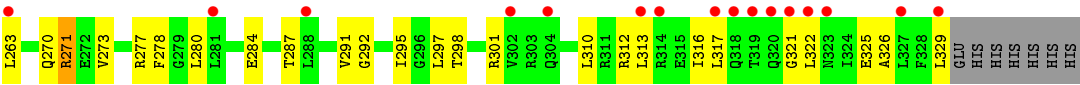


- Molecule 1: DNA-directed RNA polymerase subunit alpha

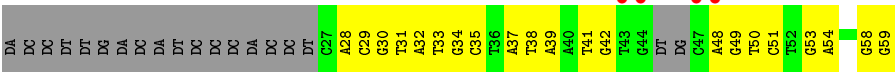
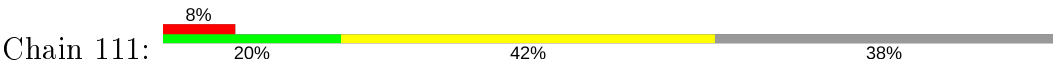


- Molecule 2: DNA-directed RNA polymerase subunit beta

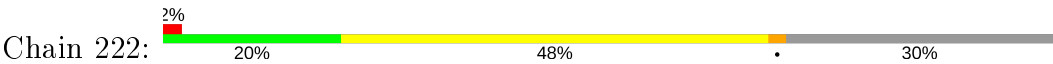




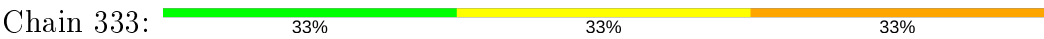
- Molecule 6: Synthetic DNA 50-MER (promoter non-template strand)



- Molecule 7: Synthetic DNA 50-MER (promoter template strand)



- Molecule 8: RNA 3-mer



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	131.47Å 153.23Å 229.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.70 – 4.40 49.68 – 4.40	Depositor EDS
% Data completeness (in resolution range)	96.8 (49.70-4.40) 96.9 (49.68-4.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 4.45Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.297 , 0.363 0.286 , 0.351	Depositor DCC
R_{free} test set	1380 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	199.6	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 280.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.32$, $\langle L^2 \rangle = 0.16$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	28949	wwPDB-VP
Average B, all atoms (Å ²)	324.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% 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, ZN, 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	AAA	0.65	0/1809	0.67	0/2450
1	BBB	0.65	0/1789	0.66	0/2425
2	CCC	0.64	0/10739	0.71	0/14489
3	DDD	0.65	0/10636	0.71	0/14362
4	EEE	0.63	0/629	0.70	0/847
5	FFF	0.67	0/2282	0.66	0/3076
6	111	0.31	0/714	0.62	0/1098
7	222	0.32	0/803	0.71	1/1238 (0.1%)
8	333	0.41	0/50	0.55	0/76
All	All	0.63	0/29451	0.70	1/40061 (0.0%)

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	222	22	DA	O5'-P-OP2	-5.87	100.41	105.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	210	THR	Peptide

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	AAA	1787	0	1813	53	0
1	BBB	1767	0	1789	43	0
2	CCC	10570	0	10582	403	0
3	DDD	10478	0	10690	429	0
4	EEE	627	0	634	12	0
5	FFF	2253	0	2297	133	0
6	111	638	0	351	55	0
7	222	716	0	396	50	0
8	333	77	0	34	8	0
9	CCC	1	0	0	0	0
9	DDD	1	0	0	0	0
10	DDD	2	0	0	2	0
11	DDD	32	0	12	5	0
All	All	28949	0	28598	959	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 17.

All (959) 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)
3:DDD:752:GLY:N	3:DDD:781:LYS:NZ	1.67	1.40
3:DDD:646:ILE:CG2	3:DDD:741:ALA:O	1.72	1.34
3:DDD:731:ARG:NH1	11:DDD:1504:GTP:O3G	1.71	1.22
3:DDD:752:GLY:CA	3:DDD:781:LYS:NZ	2.00	1.22
2:CCC:549:ASP:OD2	3:DDD:750:PRO:HB2	1.40	1.21
3:DDD:752:GLY:N	3:DDD:781:LYS:HZ1	1.25	1.20
2:CCC:26:TYR:O	2:CCC:29:SER:OG	1.59	1.20
2:CCC:868:SER:OG	2:CCC:944:ARG:N	1.75	1.17
3:DDD:646:ILE:HG22	3:DDD:647:PRO:HD2	1.14	1.13
2:CCC:549:ASP:OD2	3:DDD:750:PRO:CB	1.95	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:83:LEU:HD21	3:DDD:526:VAL:HB	1.22	1.11
3:DDD:750:PRO:O	3:DDD:781:LYS:HE3	1.51	1.11
3:DDD:527:LEU:HB2	3:DDD:550:VAL:HG13	1.13	1.10
3:DDD:752:GLY:CA	3:DDD:781:LYS:HZ1	1.64	1.09
3:DDD:752:GLY:HA2	3:DDD:781:LYS:HZ3	1.13	1.07
2:CCC:1284:ALA:HA	3:DDD:1357:ILE:HD12	1.37	1.06
3:DDD:752:GLY:HA2	3:DDD:781:LYS:NZ	1.67	1.05
1:AAA:50:SER:OG	1:BBB:35:PHE:HZ	1.40	1.04
2:CCC:1105:SER:HB2	3:DDD:731:ARG:HD2	1.36	1.04
3:DDD:697:MET:SD	3:DDD:737:ILE:HG22	1.99	1.03
6:111:54:DA:N6	7:222:9:DT:O4	1.92	1.03
3:DDD:744:ARG:HB3	3:DDD:759:ILE:HB	1.39	1.02
2:CCC:200:ARG:HD3	6:111:50:DT:O2	1.60	1.02
2:CCC:914:LYS:HG2	2:CCC:915:ASP:H	1.23	1.00
2:CCC:903:ARG:NH1	2:CCC:910:ALA:HB2	1.77	1.00
3:DDD:744:ARG:HG2	3:DDD:759:ILE:HD12	1.40	0.99
3:DDD:1133:ASP:O	3:DDD:1244:GLN:NE2	1.97	0.98
2:CCC:228:VAL:HB	2:CCC:335:THR:OG1	1.63	0.98
3:DDD:752:GLY:H	3:DDD:781:LYS:HZ2	1.01	0.98
2:CCC:205:PRO:O	2:CCC:208:ILE:HG22	1.64	0.97
1:AAA:72:GLU:OE2	2:CCC:726:TYR:OH	1.81	0.97
3:DDD:646:ILE:HG23	3:DDD:741:ALA:O	0.80	0.96
2:CCC:903:ARG:CZ	2:CCC:910:ALA:HB2	1.95	0.95
3:DDD:294:ASN:ND2	5:FFF:121:GLU:OE2	2.00	0.95
3:DDD:750:PRO:HA	3:DDD:781:LYS:CG	1.97	0.95
2:CCC:870:ILE:HB	2:CCC:944:ARG:HG2	1.46	0.94
3:DDD:744:ARG:HB3	3:DDD:759:ILE:CB	1.98	0.94
2:CCC:1238:LEU:O	2:CCC:1242:LYS:HG2	1.69	0.93
3:DDD:744:ARG:HB3	3:DDD:759:ILE:CG2	1.99	0.93
3:DDD:646:ILE:CG2	3:DDD:647:PRO:HD2	1.99	0.92
1:BBB:83:LEU:HD21	3:DDD:526:VAL:CB	2.01	0.91
3:DDD:839:VAL:O	3:DDD:864:LEU:HD12	1.70	0.90
2:CCC:905:ILE:HG13	5:FFF:310:LEU:HD22	1.53	0.90
1:AAA:134:THR:HB	2:CCC:773:LEU:HD22	1.53	0.90
3:DDD:746:LEU:H	3:DDD:746:LEU:HD12	1.35	0.90
3:DDD:646:ILE:HG23	3:DDD:741:ALA:C	1.92	0.89
3:DDD:325:LYS:HE2	3:DDD:330:MET:HG3	1.55	0.89
3:DDD:752:GLY:N	3:DDD:781:LYS:HZ2	1.53	0.89
1:AAA:70:THR:OG1	2:CCC:729:ALA:HB3	1.74	0.88
3:DDD:334:LYS:NZ	7:222:14:DC:OP2	2.08	0.86
3:DDD:381:ILE:HD11	3:DDD:412:LEU:HD13	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:560:PRO:HB2	3:DDD:776:THR:HG21	1.54	0.86
3:DDD:791:ALA:HA	7:222:13:DA:C8	2.11	0.85
1:AAA:50:SER:HG	1:BBB:35:PHE:HZ	0.87	0.85
2:CCC:142:GLU:OE1	2:CCC:515:MET:HE1	1.75	0.85
2:CCC:133:ASN:O	2:CCC:527:LYS:NZ	2.09	0.84
2:CCC:903:ARG:NH1	2:CCC:910:ALA:CB	2.41	0.84
3:DDD:527:LEU:HB2	3:DDD:550:VAL:CG1	2.04	0.83
2:CCC:1287:LEU:HD23	3:DDD:1357:ILE:HD11	1.58	0.83
2:CCC:549:ASP:OD2	3:DDD:750:PRO:HB3	1.77	0.83
2:CCC:914:LYS:HG2	2:CCC:915:ASP:N	1.93	0.82
3:DDD:749:LYS:O	3:DDD:781:LYS:HD2	1.80	0.82
3:DDD:744:ARG:CB	3:DDD:759:ILE:CG2	2.58	0.82
2:CCC:967:LEU:HD21	2:CCC:1021:LEU:HD13	1.60	0.82
3:DDD:261:ALA:HA	5:FFF:220:THR:O	1.81	0.81
2:CCC:241:LEU:CD2	2:CCC:277:LEU:HD21	2.11	0.80
5:FFF:189:LEU:O	5:FFF:191:HIS:N	2.15	0.80
2:CCC:1145:ILE:HG22	2:CCC:1161:LEU:HD11	1.63	0.80
3:DDD:744:ARG:CB	3:DDD:759:ILE:HG21	2.11	0.80
3:DDD:481:ARG:NH1	4:EEE:3:ARG:O	2.15	0.79
3:DDD:325:LYS:HE2	3:DDD:330:MET:CG	2.12	0.78
3:DDD:749:LYS:HB3	3:DDD:750:PRO:HD2	1.64	0.78
5:FFF:160:ASN:HD21	5:FFF:169:ILE:CD1	1.97	0.78
3:DDD:748:ALA:HB2	3:DDD:754:ILE:HG13	1.63	0.78
3:DDD:134:ASP:HB3	3:DDD:159:ILE:HD11	1.65	0.77
1:AAA:222:THR:OG1	1:BBB:233:ASP:HB2	1.85	0.77
5:FFF:164:THR:HB	5:FFF:219:ILE:HD12	1.67	0.77
1:AAA:50:SER:OG	1:BBB:35:PHE:CZ	2.28	0.77
3:DDD:393:THR:CG2	5:FFF:322:LEU:HD21	2.15	0.76
3:DDD:645:VAL:O	3:DDD:741:ALA:HB1	1.86	0.76
5:FFF:273:VAL:HG13	5:FFF:291:VAL:HG11	1.67	0.76
2:CCC:812:PHE:HB2	3:DDD:357:VAL:HG11	1.68	0.75
3:DDD:750:PRO:HA	3:DDD:781:LYS:CD	2.16	0.75
3:DDD:839:VAL:HG13	3:DDD:882:VAL:HG11	1.68	0.75
7:222:21:DG:H4'	7:222:22:DA:H5'	1.69	0.74
2:CCC:241:LEU:HD21	2:CCC:277:LEU:HD21	1.67	0.74
2:CCC:26:TYR:HE2	2:CCC:32:LEU:HD12	1.52	0.74
2:CCC:868:SER:HB3	2:CCC:942:ASP:HB3	1.68	0.74
2:CCC:1107:MET:HE2	3:DDD:739:GLN:OE1	1.87	0.74
2:CCC:1287:LEU:CD2	3:DDD:1357:ILE:HD11	2.16	0.74
3:DDD:898:CYS:HG	10:DDD:1502:ZN:ZN	0.98	0.74
3:DDD:898:CYS:SG	10:DDD:1502:ZN:ZN	1.76	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:751:ASP:C	3:DDD:781:LYS:HZ1	1.91	0.74
1:AAA:49:SER:HB3	2:CCC:1083:GLU:OE2	1.87	0.74
5:FFF:234:LEU:O	5:FFF:238:LEU:HG	1.89	0.73
1:AAA:13:LEU:HD21	1:AAA:16:ILE:HD11	1.69	0.73
1:BBB:47:LEU:HD13	1:BBB:183:ILE:HD12	1.71	0.73
2:CCC:901:LEU:HD12	5:FFF:310:LEU:CD2	2.18	0.73
5:FFF:180:ARG:NH2	7:222:28:DG:OP2	2.21	0.73
1:BBB:13:LEU:HD21	1:BBB:16:ILE:HD11	1.69	0.73
2:CCC:1259:LEU:HD11	5:FFF:239:ALA:HB2	1.71	0.73
2:CCC:894:GLN:HE22	3:DDD:77:ARG:H	1.37	0.72
2:CCC:868:SER:CB	2:CCC:944:ARG:H	2.01	0.72
2:CCC:1305:TYR:CD1	5:FFF:250:THR:HG21	2.24	0.72
3:DDD:1075:ARG:HD2	3:DDD:1193:TRP:HB3	1.69	0.72
3:DDD:646:ILE:HG22	3:DDD:647:PRO:CD	2.08	0.72
3:DDD:706:VAL:HG13	3:DDD:715:LYS:HG3	1.69	0.72
7:222:15:DT:H5''	7:222:15:DT:H6	1.53	0.72
3:DDD:820:ILE:HG12	3:DDD:1227:HIS:CD2	2.25	0.72
3:DDD:964:LYS:NZ	3:DDD:1199:PHE:CE1	2.59	0.71
3:DDD:664:ILE:HD11	3:DDD:685:ILE:HD11	1.72	0.71
2:CCC:218:GLU:OE2	2:CCC:299:LYS:HD3	1.91	0.71
3:DDD:619:ILE:O	3:DDD:623:GLN:HG2	1.90	0.71
3:DDD:750:PRO:HA	3:DDD:781:LYS:HG3	1.71	0.70
7:222:21:DG:H4'	7:222:22:DA:C5'	2.21	0.70
2:CCC:1302:THR:HG22	5:FFF:246:PRO:HA	1.73	0.70
3:DDD:697:MET:CE	3:DDD:737:ILE:HG22	2.21	0.70
2:CCC:841:ARG:CZ	3:DDD:257:GLY:HA2	2.22	0.70
2:CCC:1301:ARG:NH1	5:FFF:243:GLU:OE2	2.24	0.70
3:DDD:848:VAL:HG21	3:DDD:880:VAL:HG13	1.74	0.70
3:DDD:79:LYS:CE	5:FFF:284:GLU:OE2	2.40	0.70
2:CCC:867:GLU:OE1	2:CCC:943:LYS:NZ	2.22	0.69
2:CCC:549:ASP:HB3	3:DDD:750:PRO:HG3	1.73	0.69
5:FFF:133:LYS:HE3	6:111:35:DC:O5'	1.92	0.69
3:DDD:173:GLY:O	3:DDD:175:GLU:N	2.26	0.69
2:CCC:186:PHE:CD2	2:CCC:196:VAL:HG22	2.28	0.69
3:DDD:548:VAL:HG12	3:DDD:550:VAL:HG22	1.74	0.69
2:CCC:463:GLN:HG3	2:CCC:505:PHE:HB2	1.75	0.69
2:CCC:563:THR:OG1	2:CCC:569:ILE:O	2.09	0.69
5:FFF:190:ASP:OD1	5:FFF:191:HIS:N	2.26	0.69
5:FFF:170:HIS:O	5:FFF:174:GLU:HG2	1.92	0.69
2:CCC:867:GLU:OE1	2:CCC:943:LYS:HD3	1.92	0.69
3:DDD:488:ASN:HD21	4:EEE:6:VAL:HG23	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:210:THR:HG22	1:AAA:211:ILE:N	2.07	0.68
2:CCC:806:PRO:HG2	3:DDD:632:ALA:O	1.93	0.68
2:CCC:318:SER:OG	2:CCC:320:ASP:OD1	2.11	0.68
1:AAA:158:ARG:HD2	1:AAA:172:LEU:HD11	1.76	0.68
5:FFF:149:TRP:HH2	6:111:35:DC:OP2	1.76	0.68
2:CCC:30:ILE:HD11	2:CCC:575:LEU:HD22	1.73	0.68
2:CCC:841:ARG:NH1	3:DDD:257:GLY:HA2	2.09	0.68
1:AAA:165:GLU:O	1:AAA:165:GLU:HG3	1.93	0.68
2:CCC:123:TYR:CZ	5:FFF:190:ASP:O	2.47	0.68
2:CCC:868:SER:HB2	2:CCC:944:ARG:HB2	1.74	0.67
3:DDD:750:PRO:HA	3:DDD:781:LYS:CB	2.24	0.67
2:CCC:539:THR:HB	2:CCC:542:ARG:HG3	1.74	0.67
3:DDD:754:ILE:N	3:DDD:754:ILE:HD12	2.10	0.67
1:AAA:158:ARG:HD2	1:AAA:172:LEU:HD21	1.76	0.67
3:DDD:392:THR:HG21	5:FFF:321:GLY:HA3	1.75	0.67
2:CCC:672:GLU:HG3	2:CCC:673:HIS:CD2	2.29	0.67
2:CCC:901:LEU:HD12	5:FFF:310:LEU:HD21	1.77	0.67
3:DDD:48:THR:O	3:DDD:50:LYS:N	2.25	0.67
2:CCC:46:GLN:HB2	2:CCC:51:ALA:HA	1.77	0.66
2:CCC:206:ALA:O	2:CCC:209:ILE:HG22	1.95	0.66
2:CCC:549:ASP:CG	3:DDD:750:PRO:HB3	2.15	0.66
2:CCC:559:CYS:HB2	2:CCC:662:SER:HB3	1.76	0.66
3:DDD:750:PRO:HA	3:DDD:781:LYS:HB2	1.78	0.66
2:CCC:1301:ARG:CD	5:FFF:246:PRO:HG3	2.25	0.66
2:CCC:199:ASP:OD2	6:111:48:DA:H2	1.79	0.66
3:DDD:342:LEU:HG	3:DDD:1352:ILE:HG23	1.77	0.66
2:CCC:1287:LEU:HD23	3:DDD:1357:ILE:CD1	2.26	0.66
2:CCC:525:THR:HG21	2:CCC:687:ARG:CD	2.26	0.66
2:CCC:156:PHE:CE2	2:CCC:158:ASP:HB2	2.30	0.66
1:AAA:184:ALA:HB2	2:CCC:1091:GLY:HA3	1.77	0.66
2:CCC:144:VAL:HB	2:CCC:526:HIS:CE1	2.31	0.66
2:CCC:200:ARG:O	2:CCC:200:ARG:HG2	1.96	0.65
2:CCC:577:VAL:HG23	2:CCC:661:VAL:O	1.95	0.65
2:CCC:88:ARG:NH2	2:CCC:1035:LYS:HB3	2.11	0.65
3:DDD:518:VAL:HG21	3:DDD:708:ASN:ND2	2.11	0.65
2:CCC:477:GLU:OE1	5:FFF:108:ARG:HD2	1.97	0.65
3:DDD:490:ILE:HD11	3:DDD:614:LEU:CD1	2.26	0.65
3:DDD:863:LEU:HD22	3:DDD:908:ILE:CG1	2.26	0.65
2:CCC:444:ASP:OD1	2:CCC:447:HIS:HB2	1.97	0.65
2:CCC:887:VAL:HB	2:CCC:913:VAL:CG1	2.27	0.65
3:DDD:709:ARG:NH1	3:DDD:709:ARG:HB3	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:425:ARG:NH2	8:333:16:G:O2'	2.30	0.65
2:CCC:812:PHE:CB	3:DDD:357:VAL:HG11	2.27	0.65
1:AAA:158:ARG:HB3	1:AAA:172:LEU:HD21	1.79	0.64
5:FFF:158:ILE:HG22	5:FFF:158:ILE:O	1.96	0.64
1:AAA:210:THR:O	1:AAA:211:ILE:C	2.35	0.64
2:CCC:618:GLN:HE21	3:DDD:769:VAL:HB	1.61	0.64
3:DDD:205:LEU:O	3:DDD:205:LEU:HD23	1.97	0.64
5:FFF:166:ARG:NH2	6:111:32:DA:OP2	2.30	0.64
2:CCC:1103:VAL:HG22	2:CCC:1111:GLN:NE2	2.13	0.64
2:CCC:549:ASP:CG	3:DDD:750:PRO:CB	2.65	0.64
2:CCC:576:SER:OG	2:CCC:659:GLN:O	2.11	0.64
2:CCC:828:PHE:HB3	2:CCC:1060:ILE:HG21	1.80	0.64
6:111:33:DT:H2''	6:111:34:DG:H5'	1.80	0.64
2:CCC:848:GLU:HG2	2:CCC:888:THR:HG22	1.80	0.64
2:CCC:1101:LEU:HD13	3:DDD:504:GLN:HG3	1.80	0.64
5:FFF:169:ILE:HG22	5:FFF:173:LYS:HD2	1.80	0.64
2:CCC:905:ILE:CG1	5:FFF:310:LEU:HD22	2.27	0.64
3:DDD:859:PRO:HG2	3:DDD:862:THR:HG21	1.80	0.64
1:AAA:47:LEU:HD13	1:AAA:183:ILE:HD12	1.81	0.63
3:DDD:746:LEU:N	3:DDD:746:LEU:HD12	2.11	0.63
2:CCC:183:TRP:CZ2	6:111:49:DG:C5	2.86	0.63
7:222:18:DT:H73	7:222:18:DT:OP2	1.99	0.63
2:CCC:196:VAL:HG23	2:CCC:206:ALA:HA	1.79	0.63
2:CCC:143:ARG:HH12	2:CCC:507:GLY:HA2	1.62	0.63
3:DDD:24:LEU:HD12	3:DDD:232:ASN:HB3	1.80	0.63
2:CCC:1105:SER:CB	3:DDD:731:ARG:HD2	2.21	0.63
3:DDD:735:ALA:HA	3:DDD:738:ARG:HD2	1.81	0.63
3:DDD:885:VAL:HG13	3:DDD:894:VAL:HG11	1.79	0.63
3:DDD:750:PRO:O	3:DDD:781:LYS:CE	2.40	0.63
2:CCC:871:VAL:O	2:CCC:944:ARG:NH2	2.31	0.63
3:DDD:863:LEU:HD22	3:DDD:908:ILE:HG13	1.80	0.63
5:FFF:160:ASN:HD21	5:FFF:169:ILE:HD13	1.64	0.63
6:111:54:DA:C6	7:222:9:DT:O4	2.51	0.63
3:DDD:1075:ARG:CZ	3:DDD:1193:TRP:CD2	2.82	0.63
5:FFF:222:VAL:HG12	5:FFF:235:LEU:HB2	1.81	0.63
2:CCC:69:GLN:O	2:CCC:100:LEU:HD12	1.99	0.62
3:DDD:298:MET:SD	5:FFF:117:LEU:HB3	2.38	0.62
2:CCC:245:ARG:HB3	2:CCC:337:PHE:CE1	2.33	0.62
2:CCC:560:PRO:CB	3:DDD:776:THR:HG21	2.28	0.62
7:222:20:DG:H2''	7:222:21:DG:H5'	1.82	0.62
2:CCC:967:LEU:HD21	2:CCC:1021:LEU:HD22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:390:PHE:HA	2:CCC:419:ILE:HG23	1.82	0.62
1:BBB:155:ALA:HB1	1:BBB:172:LEU:HD23	1.82	0.62
3:DDD:572:THR:HG22	3:DDD:593:ASN:OD1	2.00	0.62
5:FFF:160:ASN:HD21	5:FFF:169:ILE:HD11	1.65	0.62
1:BBB:64:VAL:HG13	1:BBB:78:ILE:HD13	1.82	0.62
2:CCC:183:TRP:CH2	6:111:49:DG:C4	2.88	0.62
3:DDD:620:PHE:CZ	3:DDD:624:ILE:HD11	2.35	0.62
3:DDD:791:ALA:HA	7:222:13:DA:H8	1.64	0.61
2:CCC:548:ARG:HA	2:CCC:570:GLY:HA3	1.82	0.61
5:FFF:298:THR:HG21	5:FFF:301:ARG:HD3	1.82	0.61
7:222:19:DA:O5'	7:222:19:DA:H8	1.82	0.61
3:DDD:1025:MET:HB2	3:DDD:1126:GLN:HE21	1.63	0.61
3:DDD:305:ALA:CB	3:DDD:316:ILE:HD12	2.30	0.61
3:DDD:750:PRO:HA	3:DDD:781:LYS:HD2	1.80	0.61
2:CCC:1273:MET:SD	7:222:14:DC:O4'	2.58	0.61
2:CCC:541:GLU:OE2	6:111:51:DC:N3	2.33	0.61
2:CCC:1005:GLU:HG2	2:CCC:1006:GLU:H	1.64	0.61
2:CCC:892:GLU:OE1	3:DDD:76:LYS:NZ	2.34	0.61
5:FFF:170:HIS:CD2	6:111:31:DT:H73	2.35	0.61
1:AAA:44:ARG:NH2	2:CCC:1215:GLY:O	2.34	0.61
3:DDD:1344:LEU:HD23	3:DDD:1349:GLU:HB3	1.82	0.61
2:CCC:1107:MET:CE	3:DDD:739:GLN:OE1	2.48	0.60
2:CCC:562:GLU:HG2	2:CCC:574:SER:HB2	1.82	0.60
2:CCC:56:VAL:HG12	2:CCC:59:ILE:HD11	1.81	0.60
2:CCC:868:SER:HG	2:CCC:944:ARG:N	1.94	0.60
3:DDD:1156:LEU:HD23	3:DDD:1209:VAL:HA	1.83	0.60
2:CCC:122:VAL:HG22	2:CCC:490:GLN:HB3	1.82	0.60
2:CCC:870:ILE:CB	2:CCC:944:ARG:HG2	2.28	0.60
3:DDD:819:GLY:O	3:DDD:1227:HIS:NE2	2.33	0.60
1:AAA:191:ARG:HG3	1:AAA:196:THR:HG22	1.83	0.60
2:CCC:550:VAL:HG21	3:DDD:776:THR:HG22	1.83	0.60
3:DDD:708:ASN:HB2	3:DDD:714:GLU:HB3	1.84	0.60
2:CCC:341:LEU:HD11	3:DDD:1043:GLY:HA2	1.84	0.59
2:CCC:870:ILE:O	2:CCC:944:ARG:NH1	2.35	0.59
3:DDD:22:ILE:HG22	3:DDD:1336:ALA:HA	1.84	0.59
1:AAA:58:GLU:HB2	1:AAA:145:LYS:HB3	1.84	0.59
2:CCC:590:PRO:HG3	2:CCC:605:TYR:CE2	2.37	0.59
2:CCC:894:GLN:HG3	3:DDD:69:GLU:OE2	2.02	0.59
2:CCC:799:ASN:HA	2:CCC:1231:TYR:HA	1.84	0.59
3:DDD:750:PRO:C	3:DDD:781:LYS:HE3	2.21	0.59
3:DDD:839:VAL:HG12	3:DDD:839:VAL:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:849:LEU:HA	3:DDD:857:LEU:HB3	1.84	0.59
5:FFF:322:LEU:HD22	5:FFF:326:ALA:HB2	1.83	0.59
1:BBB:11:PRO:HB2	1:BBB:28:LEU:HD12	1.84	0.59
1:AAA:45:ARG:NE	1:BBB:38:THR:OG1	2.30	0.59
2:CCC:1313:HIS:HB2	3:DDD:474:LEU:HG	1.84	0.59
2:CCC:453:ILE:HD12	2:CCC:587:LEU:HD21	1.85	0.59
2:CCC:68:LEU:HD12	2:CCC:475:VAL:HG11	1.85	0.59
3:DDD:1207:GLY:HA3	3:DDD:1224:ARG:HE	1.68	0.59
3:DDD:964:LYS:CE	3:DDD:1199:PHE:CE1	2.86	0.59
2:CCC:183:TRP:CZ2	6:111:49:DG:C4	2.91	0.59
3:DDD:826:ILE:HG21	3:DDD:992:LYS:O	2.03	0.59
3:DDD:1217:PRO:HA	3:DDD:1220:ILE:HD12	1.84	0.59
2:CCC:887:VAL:HB	2:CCC:913:VAL:HG13	1.84	0.59
3:DDD:739:GLN:HB3	3:DDD:744:ARG:HD2	1.85	0.59
7:222:22:DA:H1'	7:222:23:DT:H5'	1.84	0.58
1:BBB:58:GLU:HB2	1:BBB:145:LYS:HB3	1.85	0.58
2:CCC:868:SER:HB2	2:CCC:944:ARG:CB	2.33	0.58
3:DDD:809:VAL:HG22	3:DDD:915:ILE:HD11	1.84	0.58
3:DDD:869:CYS:O	3:DDD:873:GLU:OE1	2.21	0.58
3:DDD:645:VAL:O	3:DDD:741:ALA:CB	2.51	0.58
5:FFF:122:GLU:CD	5:FFF:157:ALA:HB1	2.23	0.58
1:AAA:64:VAL:HG13	1:AAA:78:ILE:HD13	1.85	0.58
2:CCC:61:SER:HB3	2:CCC:479:LEU:HB3	1.83	0.58
3:DDD:818:GLU:HB3	3:DDD:887:SER:HB2	1.85	0.58
5:FFF:147:THR:O	5:FFF:151:ARG:HG2	2.03	0.58
3:DDD:964:LYS:HD3	3:DDD:1199:PHE:HE1	1.69	0.58
3:DDD:362:ARG:NH2	3:DDD:619:ILE:HG12	2.19	0.58
2:CCC:200:ARG:CD	6:111:50:DT:O2	2.46	0.58
2:CCC:1287:LEU:HD23	3:DDD:1357:ILE:CG1	2.34	0.58
2:CCC:1301:ARG:HD3	5:FFF:246:PRO:HG3	1.84	0.58
3:DDD:744:ARG:HB2	3:DDD:759:ILE:HG21	1.85	0.58
2:CCC:390:PHE:HA	2:CCC:419:ILE:CG2	2.34	0.58
2:CCC:564:PRO:O	2:CCC:569:ILE:HA	2.03	0.58
3:DDD:820:ILE:HG12	3:DDD:1227:HIS:CG	2.39	0.58
3:DDD:739:GLN:O	3:DDD:763:PHE:HD2	1.87	0.58
2:CCC:30:ILE:HD11	2:CCC:575:LEU:CD2	2.33	0.57
2:CCC:810:TYR:HA	3:DDD:357:VAL:HG21	1.86	0.57
2:CCC:199:ASP:OD2	6:111:48:DA:C2	2.57	0.57
2:CCC:525:THR:HG21	2:CCC:687:ARG:HD3	1.85	0.57
3:DDD:57:PHE:O	3:DDD:98:ARG:NH2	2.37	0.57
5:FFF:98:ASN:HA	6:111:41:DT:O2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:1337:ILE:HG23	2:CCC:1337:ILE:O	2.04	0.57
2:CCC:807:TRP:CD1	2:CCC:817:LEU:HD22	2.39	0.57
3:DDD:189:LEU:O	3:DDD:192:MET:HG2	2.04	0.57
2:CCC:288:PRO:HB2	2:CCC:290:GLU:HG2	1.86	0.57
2:CCC:674:ASP:O	3:DDD:772:TYR:OH	2.19	0.57
3:DDD:393:THR:HG21	5:FFF:322:LEU:HD21	1.85	0.57
2:CCC:866:ASP:OD2	2:CCC:944:ARG:HB2	2.05	0.57
6:111:28:DA:N6	7:222:34:DG:O6	2.38	0.57
6:111:54:DA:H2	7:222:10:DC:O2	1.88	0.57
7:222:10:DC:H2'	7:222:11:DA:C8	2.39	0.57
6:111:51:DC:H6	6:111:51:DC:OP2	1.88	0.57
2:CCC:100:LEU:HD22	2:CCC:493:ILE:HD11	1.87	0.57
2:CCC:241:LEU:HD23	2:CCC:277:LEU:HD21	1.85	0.57
3:DDD:250:ARG:HD2	3:DDD:266:ASN:OD1	2.04	0.57
3:DDD:700:ASN:O	3:DDD:704:GLU:HG3	2.04	0.57
1:BBB:83:LEU:HD11	3:DDD:526:VAL:C	2.26	0.57
2:CCC:292:ILE:HD12	2:CCC:322:LEU:HD22	1.87	0.57
2:CCC:375:PRO:HG3	5:FFF:67:TYR:OH	2.05	0.57
2:CCC:42:ASP:O	2:CCC:50:GLU:HG2	2.04	0.56
1:BBB:124:VAL:HG11	1:BBB:209:GLY:HA3	1.87	0.56
3:DDD:79:LYS:HE3	5:FFF:284:GLU:OE2	2.03	0.56
3:DDD:839:VAL:HG12	3:DDD:864:LEU:HD12	1.86	0.56
2:CCC:31:GLN:HG3	2:CCC:527:LYS:HB3	1.88	0.56
3:DDD:746:LEU:HA	3:DDD:758:PRO:CB	2.36	0.56
2:CCC:19:PRO:HA	2:CCC:1156:ARG:HD2	1.86	0.56
5:FFF:87:ASP:OD2	5:FFF:90:SER:OG	2.11	0.56
2:CCC:241:LEU:HD21	2:CCC:277:LEU:CD2	2.34	0.56
5:FFF:133:LYS:HE3	6:111:35:DC:P	2.46	0.56
3:DDD:334:LYS:HE2	7:222:14:DC:OP1	2.05	0.56
2:CCC:200:ARG:HB2	6:111:50:DT:H3	1.69	0.56
2:CCC:975:ILE:HD13	2:CCC:998:LEU:HD21	1.87	0.56
3:DDD:949:SER:HB3	3:DDD:1019:ASN:HD22	1.71	0.56
5:FFF:169:ILE:CG2	5:FFF:173:LYS:HD2	2.35	0.56
2:CCC:443:ASP:N	2:CCC:443:ASP:OD1	2.39	0.56
3:DDD:843:VAL:CG2	3:DDD:897:HIS:O	2.54	0.56
3:DDD:518:VAL:O	3:DDD:520:ALA:N	2.39	0.56
2:CCC:253:PHE:CZ	2:CCC:287:VAL:HG12	2.41	0.55
2:CCC:1301:ARG:CG	5:FFF:246:PRO:HG3	2.36	0.55
2:CCC:1081:PRO:HB2	2:CCC:1083:GLU:OE1	2.05	0.55
3:DDD:115:TRP:CZ2	3:DDD:1329:THR:HG22	2.41	0.55
3:DDD:930:LEU:HB3	3:DDD:1134:ILE:HG13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FFF:262:TRP:CG	5:FFF:316:ILE:HG21	2.41	0.55
2:CCC:142:GLU:OE1	2:CCC:515:MET:CE	2.52	0.55
3:DDD:519:ASN:HA	3:DDD:523:GLU:HB2	1.89	0.55
3:DDD:705:THR:HG22	3:DDD:705:THR:O	2.06	0.55
3:DDD:393:THR:OG1	5:FFF:322:LEU:HD21	2.05	0.55
2:CCC:1234:LYS:HE2	2:CCC:1238:LEU:HD21	1.87	0.55
3:DDD:334:LYS:HZ3	7:222:14:DC:P	2.26	0.55
2:CCC:164:THR:OG1	2:CCC:167:SER:OG	2.24	0.55
2:CCC:967:LEU:HD21	2:CCC:1021:LEU:CD1	2.36	0.55
3:DDD:488:ASN:HD21	4:EEE:6:VAL:CG2	2.19	0.55
3:DDD:609:TYR:HA	3:DDD:617:THR:HG21	1.88	0.55
5:FFF:262:TRP:HB3	5:FFF:316:ILE:HG21	1.89	0.55
5:FFF:162:THR:HG21	7:222:26:DT:H3	1.72	0.55
2:CCC:1333:LEU:O	3:DDD:113:HIS:NE2	2.40	0.55
3:DDD:71:LEU:HG	3:DDD:90:VAL:HG21	1.89	0.55
3:DDD:848:VAL:HG11	3:DDD:880:VAL:HG13	1.89	0.55
3:DDD:1075:ARG:HD2	3:DDD:1193:TRP:CB	2.36	0.54
3:DDD:843:VAL:HG11	3:DDD:883:ARG:HD3	1.89	0.54
5:FFF:170:HIS:H	5:FFF:170:HIS:CD2	2.25	0.54
3:DDD:264:ASP:OD2	3:DDD:322:ARG:NH2	2.41	0.54
3:DDD:388:ARG:HB3	3:DDD:390:LEU:HD13	1.88	0.54
3:DDD:282:LEU:HD21	5:FFF:125:LEU:HD21	1.89	0.54
2:CCC:88:ARG:NH1	2:CCC:1040:ASP:OD1	2.40	0.54
3:DDD:807:LEU:HD11	3:DDD:894:VAL:HG13	1.88	0.54
3:DDD:1175:LEU:O	3:DDD:1187:GLU:HA	2.08	0.54
5:FFF:144:THR:HG1	6:111:39:DA:H8	1.55	0.54
7:222:21:DG:C4'	7:222:22:DA:H5'	2.38	0.54
2:CCC:901:LEU:CD1	5:FFF:310:LEU:CD2	2.86	0.54
2:CCC:901:LEU:HD13	5:FFF:278:PHE:CE2	2.42	0.54
3:DDD:849:LEU:HD11	3:DDD:853:THR:HA	1.90	0.54
3:DDD:903:LEU:H	3:DDD:903:LEU:HD12	1.73	0.54
5:FFF:122:GLU:OE1	5:FFF:157:ALA:HB3	2.08	0.54
6:111:53:DG:H1'	6:111:54:DA:H5'	1.89	0.54
1:AAA:158:ARG:CD	1:AAA:172:LEU:HD11	2.37	0.54
2:CCC:807:TRP:CZ3	2:CCC:1086:PRO:HG3	2.43	0.54
2:CCC:1285:TYR:HD2	3:DDD:1361:THR:HG21	1.73	0.54
3:DDD:134:ASP:CB	3:DDD:159:ILE:HD11	2.36	0.54
6:111:32:DA:C2	7:222:32:DA:C2	2.95	0.54
5:FFF:116:LEU:HA	5:FFF:119:LEU:HD12	1.89	0.54
6:111:37:DA:H4'	6:111:38:DT:OP1	2.07	0.54
1:AAA:9:LEU:O	1:BBB:227:GLN:NE2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:551:HIS:ND1	2:CCC:553:THR:OG1	2.36	0.54
6:111:28:DA:N7	6:111:29:DC:N4	2.56	0.54
5:FFF:145:TYR:CD1	6:111:37:DA:C5	2.96	0.53
2:CCC:228:VAL:CB	2:CCC:335:THR:OG1	2.48	0.53
1:AAA:11:PRO:HB3	1:AAA:31:LEU:HD23	1.90	0.53
3:DDD:689:ALA:O	3:DDD:693:VAL:HG23	2.08	0.53
3:DDD:744:ARG:HB2	3:DDD:759:ILE:CG2	2.36	0.53
3:DDD:367:GLY:HA3	3:DDD:448:GLN:HB2	1.89	0.53
2:CCC:1296:ASP:HB3	2:CCC:1321:GLU:H	1.73	0.53
2:CCC:344:GLY:HA3	2:CCC:346:TYR:CZ	2.43	0.53
3:DDD:1134:ILE:HD13	3:DDD:1244:GLN:HG3	1.89	0.53
1:AAA:11:PRO:HB2	1:AAA:28:LEU:HD12	1.90	0.53
2:CCC:1308:ILE:HG23	3:DDD:380:PHE:CE2	2.43	0.53
2:CCC:1101:LEU:O	3:DDD:731:ARG:HG2	2.09	0.53
2:CCC:550:VAL:HG21	3:DDD:776:THR:CG2	2.39	0.53
2:CCC:144:VAL:HB	2:CCC:526:HIS:HE1	1.73	0.53
2:CCC:638:SER:O	2:CCC:639:LYS:CG	2.56	0.53
3:DDD:644:MET:CE	3:DDD:740:LEU:HD13	2.38	0.53
3:DDD:646:ILE:HD11	3:DDD:764:ARG:HD3	1.90	0.53
5:FFF:169:ILE:HG22	5:FFF:173:LYS:CD	2.38	0.53
2:CCC:127:ILE:O	2:CCC:127:ILE:HG13	2.09	0.53
2:CCC:1251:TYR:OH	3:DDD:348:ASP:OD2	2.21	0.53
3:DDD:743:MET:HB2	3:DDD:760:THR:O	2.09	0.53
5:FFF:122:GLU:OE1	5:FFF:157:ALA:CB	2.57	0.53
5:FFF:152:GLN:HE22	5:FFF:156:ARG:HD3	1.73	0.52
2:CCC:549:ASP:CB	3:DDD:750:PRO:HG3	2.38	0.52
2:CCC:878:THR:HG22	2:CCC:879:GLY:N	2.24	0.52
3:DDD:1269:ALA:HB2	3:DDD:1275:LEU:HD23	1.90	0.52
11:DDD:1504:GTP:C4'	11:DDD:1504:GTP:O1A	2.57	0.52
3:DDD:843:VAL:HG21	3:DDD:897:HIS:HA	1.91	0.52
3:DDD:946:ALA:O	3:DDD:948:SER:N	2.43	0.52
2:CCC:207:THR:HG21	2:CCC:351:LEU:HG	1.91	0.52
3:DDD:435:GLN:HB2	3:DDD:457:TYR:OH	2.09	0.52
2:CCC:1136:GLN:O	2:CCC:1137:GLU:HB2	2.09	0.52
3:DDD:334:LYS:HA	3:DDD:339:ARG:HD2	1.92	0.52
3:DDD:464:ASP:OD1	8:333:16:G:H4'	2.09	0.52
3:DDD:515:ARG:HH22	3:DDD:718:SER:C	2.12	0.52
3:DDD:697:MET:CE	3:DDD:737:ILE:CG2	2.88	0.52
1:AAA:46:ILE:HG12	1:BBB:35:PHE:CE1	2.45	0.52
1:BBB:11:PRO:HB3	1:BBB:31:LEU:HD23	1.92	0.52
2:CCC:28:LEU:HD21	2:CCC:524:ILE:HG13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:166:ARG:NH2	2:CCC:863:SER:HB2	2.25	0.52
3:DDD:22:ILE:HD11	3:DDD:1319:PHE:CE1	2.45	0.52
3:DDD:620:PHE:CE2	3:DDD:624:ILE:HD11	2.45	0.52
2:CCC:1289:GLU:HG2	2:CCC:1294:LYS:HE3	1.92	0.52
2:CCC:89:GLY:HA2	2:CCC:140:GLY:HA3	1.91	0.52
3:DDD:672:LEU:C	3:DDD:672:LEU:HD13	2.31	0.52
2:CCC:1046:VAL:HG11	2:CCC:1049:ILE:HD11	1.91	0.52
3:DDD:1080:ILE:HB	3:DDD:1097:ALA:HB3	1.91	0.52
2:CCC:591:TYR:OH	2:CCC:637:ARG:NH2	2.43	0.51
1:AAA:47:LEU:HD13	1:AAA:183:ILE:CD1	2.40	0.51
2:CCC:1271:GLY:O	2:CCC:1275:VAL:HG23	2.10	0.51
2:CCC:660:VAL:HG21	3:DDD:773:PHE:HD2	1.76	0.51
1:BBB:64:VAL:CG1	1:BBB:78:ILE:HD13	2.41	0.51
3:DDD:122:SER:O	3:DDD:124:ILE:N	2.43	0.51
3:DDD:325:LYS:HE2	3:DDD:330:MET:HG2	1.92	0.51
3:DDD:59:ALA:HB3	3:DDD:71:LEU:HD11	1.92	0.51
3:DDD:584:PRO:HD3	3:DDD:620:PHE:CD1	2.46	0.51
5:FFF:221:SER:O	5:FFF:234:LEU:HD12	2.11	0.51
1:AAA:45:ARG:HD3	1:BBB:38:THR:HA	1.92	0.51
2:CCC:1157:GLN:HG3	2:CCC:1157:GLN:O	2.11	0.51
2:CCC:590:PRO:HB2	2:CCC:655:VAL:HG21	1.92	0.51
3:DDD:572:THR:CG2	3:DDD:593:ASN:OD1	2.58	0.51
4:EEE:41:GLU:HG3	4:EEE:43:ASN:H	1.75	0.51
2:CCC:1142:ARG:NH1	2:CCC:1161:LEU:O	2.43	0.51
3:DDD:1167:LYS:HB2	3:DDD:1174:ARG:HD2	1.91	0.51
11:DDD:1504:GTP:H4'	11:DDD:1504:GTP:O1A	2.11	0.51
1:AAA:64:VAL:CG1	1:AAA:78:ILE:HD13	2.41	0.51
1:AAA:225:ALA:HB2	1:BBB:228:LEU:HD13	1.93	0.51
2:CCC:782:VAL:HG21	2:CCC:792:GLY:CA	2.40	0.51
3:DDD:1152:GLU:O	3:DDD:1214:PRO:HD2	2.10	0.51
2:CCC:160:ASP:OD2	2:CCC:163:LYS:HB2	2.11	0.51
5:FFF:122:GLU:CD	5:FFF:157:ALA:CB	2.79	0.51
1:BBB:165:GLU:O	1:BBB:165:GLU:HG3	2.10	0.51
2:CCC:894:GLN:HE22	3:DDD:77:ARG:N	2.05	0.51
3:DDD:93:THR:HG22	3:DDD:94:GLN:H	1.76	0.51
5:FFF:70:LEU:HD11	6:111:41:DT:C5	2.46	0.51
2:CCC:402:ARG:HD2	2:CCC:406:ASN:HD21	1.76	0.51
3:DDD:857:LEU:HD21	3:DDD:875:ASN:HD22	1.76	0.51
5:FFF:158:ILE:HG22	7:222:26:DT:O2	2.11	0.51
2:CCC:696:ASP:O	2:CCC:795:ALA:HB1	2.11	0.50
3:DDD:680:ASN:ND2	3:DDD:1023:HIS:HB3	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:222:12:DG:O5'	7:222:12:DG:H8	1.94	0.50
3:DDD:487:THR:O	3:DDD:614:LEU:HD11	2.11	0.50
6:111:50:DT:OP1	6:111:50:DT:H4'	2.11	0.50
7:222:22:DA:O5'	7:222:22:DA:H2'	2.11	0.50
2:CCC:782:VAL:HG21	2:CCC:792:GLY:HA3	1.94	0.50
2:CCC:1223:ARG:NH2	3:DDD:721:SER:OG	2.43	0.50
2:CCC:477:GLU:OE1	5:FFF:108:ARG:CD	2.59	0.50
1:BBB:82:LEU:HD22	1:BBB:173:VAL:CG2	2.41	0.50
3:DDD:1271:SER:OG	3:DDD:1292:LEU:HD21	2.12	0.50
3:DDD:79:LYS:NZ	5:FFF:284:GLU:OE2	2.43	0.50
2:CCC:200:ARG:CG	2:CCC:200:ARG:O	2.54	0.50
3:DDD:334:LYS:HG2	3:DDD:339:ARG:HD2	1.92	0.50
3:DDD:823:THR:HB	3:DDD:824:PRO:HD2	1.93	0.50
5:FFF:149:TRP:CH2	6:111:35:DC:OP2	2.63	0.50
7:222:14:DC:O5'	7:222:14:DC:H6	1.94	0.50
1:BBB:92:VAL:O	1:BBB:148:ARG:NH2	2.45	0.50
3:DDD:1267:VAL:O	3:DDD:1268:ASN:CB	2.60	0.50
3:DDD:1364:ALA:CB	4:EEE:21:LEU:CD1	2.90	0.50
1:AAA:223:ILE:O	1:AAA:227:GLN:HG2	2.12	0.50
2:CCC:1305:TYR:CE1	5:FFF:250:THR:HG21	2.45	0.50
2:CCC:900:LYS:HE2	5:FFF:277:ARG:HH12	1.76	0.50
3:DDD:1292:LEU:O	3:DDD:1296:GLY:N	2.45	0.50
3:DDD:739:GLN:O	3:DDD:763:PHE:CD2	2.64	0.50
5:FFF:160:ASN:ND2	5:FFF:166:ARG:NH1	2.60	0.50
2:CCC:1301:ARG:HD3	5:FFF:246:PRO:CG	2.42	0.50
2:CCC:1273:MET:HG3	7:222:14:DC:H4'	1.94	0.50
7:222:5:DC:H1'	7:222:6:DG:H5'	1.94	0.50
6:111:54:DA:N1	7:222:9:DT:C4	2.80	0.50
2:CCC:1149:TYR:HB3	2:CCC:1159:VAL:CG1	2.42	0.50
3:DDD:1025:MET:CB	3:DDD:1126:GLN:HE21	2.24	0.50
3:DDD:1025:MET:HB2	3:DDD:1126:GLN:NE2	2.26	0.50
11:DDD:1504:GTP:O4'	8:333:16:G:O3'	2.19	0.50
3:DDD:555:TYR:CE2	3:DDD:565:ALA:HB2	2.47	0.50
5:FFF:140:PHE:CD1	6:111:37:DA:H2''	2.47	0.50
3:DDD:645:VAL:C	3:DDD:741:ALA:HB1	2.31	0.50
2:CCC:1302:THR:HG21	5:FFF:249:THR:HG21	1.93	0.50
1:BBB:82:LEU:HD22	1:BBB:173:VAL:HG22	1.94	0.49
2:CCC:68:LEU:HD12	2:CCC:475:VAL:CG1	2.41	0.49
3:DDD:748:ALA:HA	3:DDD:754:ILE:HA	1.94	0.49
2:CCC:618:GLN:CD	3:DDD:770:LEU:HD13	2.32	0.49
5:FFF:155:GLU:O	5:FFF:159:MET:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:593:ASN:OD1	3:DDD:593:ASN:O	2.30	0.49
3:DDD:754:ILE:N	3:DDD:754:ILE:CD1	2.75	0.49
5:FFF:140:PHE:CG	6:111:37:DA:H2'	2.47	0.49
2:CCC:104:ILE:HD12	2:CCC:116:ASP:HB2	1.94	0.49
3:DDD:123:ARG:HH22	3:DDD:1334:GLU:HG2	1.77	0.49
3:DDD:393:THR:HG21	5:FFF:322:LEU:HD11	1.95	0.49
3:DDD:601:ILE:O	3:DDD:604:MET:HB2	2.11	0.49
3:DDD:664:ILE:HD11	3:DDD:685:ILE:CD1	2.39	0.49
3:DDD:700:ASN:O	3:DDD:704:GLU:CG	2.61	0.49
3:DDD:743:MET:HE2	3:DDD:760:THR:HA	1.94	0.49
2:CCC:205:PRO:O	2:CCC:208:ILE:CG2	2.48	0.49
2:CCC:26:TYR:CE2	2:CCC:32:LEU:HD12	2.41	0.49
5:FFF:63:GLY:O	5:FFF:67:TYR:HD2	1.95	0.49
2:CCC:1146:GLN:HB2	2:CCC:1161:LEU:HD12	1.94	0.49
3:DDD:331:ILE:HD12	3:DDD:331:ILE:N	2.27	0.49
3:DDD:582:ILE:HG23	3:DDD:623:GLN:CB	2.43	0.49
3:DDD:700:ASN:O	3:DDD:704:GLU:HB2	2.12	0.49
2:CCC:1119:MET:HB2	2:CCC:1228:GLY:HA2	1.94	0.49
2:CCC:186:PHE:CE2	2:CCC:196:VAL:HG22	2.47	0.49
3:DDD:115:TRP:O	3:DDD:119:SER:HB3	2.12	0.49
3:DDD:750:PRO:HD3	3:DDD:777:HIS:HB3	1.95	0.49
5:FFF:119:LEU:CD2	5:FFF:158:ILE:HD11	2.42	0.49
5:FFF:234:LEU:O	5:FFF:238:LEU:CG	2.60	0.49
7:222:22:DA:O5'	7:222:22:DA:C2'	2.61	0.49
2:CCC:700:VAL:HG21	2:CCC:1114:GLU:CG	2.43	0.49
2:CCC:806:PRO:CG	3:DDD:632:ALA:O	2.60	0.49
2:CCC:424:ASP:O	2:CCC:428:VAL:HG23	2.12	0.49
3:DDD:378:LYS:N	3:DDD:379:PRO:HD2	2.28	0.49
3:DDD:697:MET:SD	3:DDD:737:ILE:CG2	2.88	0.49
3:DDD:75:TYR:HB2	3:DDD:92:VAL:HG21	1.95	0.49
2:CCC:1155:VAL:HG12	2:CCC:1157:GLN:O	2.13	0.49
2:CCC:898:GLU:OE2	5:FFF:280:LEU:HD13	2.13	0.49
2:CCC:812:PHE:CB	3:DDD:357:VAL:CG1	2.90	0.49
3:DDD:736:GLN:HA	3:DDD:736:GLN:HE21	1.78	0.49
5:FFF:126:GLY:HA3	5:FFF:153:THR:HG21	1.95	0.49
2:CCC:94:ALA:HB2	2:CCC:129:LEU:HD11	1.95	0.48
2:CCC:1268:GLN:OE1	3:DDD:352:ARG:HB3	2.12	0.48
2:CCC:439:LYS:O	2:CCC:439:LYS:HG3	2.13	0.48
2:CCC:716:ALA:HB3	2:CCC:784:ALA:HB3	1.94	0.48
3:DDD:268:LEU:HD13	3:DDD:306:LEU:HA	1.94	0.48
2:CCC:1315:MET:HB2	3:DDD:473:THR:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:805:MET:HE2	2:CCC:806:PRO:O	2.12	0.48
2:CCC:812:PHE:HB2	3:DDD:357:VAL:CG1	2.43	0.48
2:CCC:1287:LEU:HD21	3:DDD:1351:VAL:HG22	1.94	0.48
3:DDD:165:TYR:O	3:DDD:169:LEU:HB2	2.12	0.48
2:CCC:1077:SER:HA	3:DDD:356:THR:OG1	2.14	0.48
3:DDD:647:PRO:HG2	3:DDD:650:LYS:HB2	1.95	0.48
3:DDD:644:MET:HE2	3:DDD:740:LEU:HD13	1.94	0.48
2:CCC:1145:ILE:CG2	2:CCC:1161:LEU:HD11	2.40	0.48
2:CCC:230:PHE:N	2:CCC:333:ILE:O	2.35	0.48
3:DDD:1327:GLU:O	3:DDD:1331:VAL:HG23	2.13	0.48
6:111:58:DG:H2"	6:111:59:DG:C8	2.48	0.48
2:CCC:1244:HIS:CE1	2:CCC:1262:LYS:HA	2.48	0.48
1:AAA:68:TYR:O	2:CCC:756:TYR:CE2	2.66	0.48
3:DDD:1159:ILE:HA	3:DDD:1206:ARG:HG2	1.93	0.48
2:CCC:290:GLU:HA	2:CCC:319:LEU:HD21	1.95	0.48
3:DDD:850:LYS:HB2	3:DDD:851:PRO:HD2	1.95	0.48
3:DDD:868:TRP:O	3:DDD:872:LEU:HG	2.14	0.48
7:222:13:DA:H2'	7:222:14:DC:C6	2.49	0.48
3:DDD:1330:ARG:NH2	7:222:9:DT:O3'	2.46	0.48
2:CCC:564:PRO:CB	8:333:14:GTP:O1A	2.62	0.48
1:AAA:92:VAL:O	1:AAA:148:ARG:NH2	2.46	0.48
3:DDD:294:ASN:O	3:DDD:298:MET:CG	2.61	0.48
3:DDD:416:ILE:CD1	3:DDD:441:LEU:HD21	2.44	0.48
2:CCC:555:TYR:HA	3:DDD:773:PHE:CE2	2.49	0.48
5:FFF:156:ARG:HE	6:111:33:DT:C7	2.26	0.48
5:FFF:222:VAL:CG1	5:FFF:235:LEU:HB2	2.44	0.48
3:DDD:432:LEU:HD13	3:DDD:499:ILE:HG21	1.96	0.48
2:CCC:1264:GLN:HG3	5:FFF:237:ILE:HG23	1.96	0.48
1:BBB:163:GLU:HG3	1:BBB:163:GLU:O	2.14	0.48
2:CCC:1245:ALA:HB2	3:DDD:372:MET:HG3	1.95	0.48
2:CCC:705:GLU:HB3	2:CCC:794:LEU:H	1.78	0.48
2:CCC:714:VAL:HG21	2:CCC:787:PRO:HD2	1.96	0.48
5:FFF:122:GLU:OE2	5:FFF:157:ALA:HB1	2.13	0.48
3:DDD:615:LYS:HB2	3:DDD:616:PRO:HD3	1.95	0.48
5:FFF:158:ILE:CG2	5:FFF:158:ILE:O	2.62	0.48
6:111:49:DG:H2"	6:111:50:DT:H5"	1.96	0.47
3:DDD:1134:ILE:CD1	3:DDD:1244:GLN:HG3	2.44	0.47
3:DDD:803:VAL:CG2	3:DDD:1309:ILE:O	2.62	0.47
3:DDD:321:LYS:CG	3:DDD:321:LYS:O	2.62	0.47
2:CCC:241:LEU:HD11	2:CCC:246:LEU:HD11	1.96	0.47
2:CCC:76:GLY:O	2:CCC:94:ALA:HB1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:369:PRO:HB2	3:DDD:372:MET:HB2	1.96	0.47
3:DDD:750:PRO:C	3:DDD:781:LYS:CE	2.82	0.47
5:FFF:158:ILE:O	5:FFF:162:THR:CG2	2.62	0.47
7:222:22:DA:H2''	7:222:23:DT:O5'	2.14	0.47
3:DDD:708:ASN:HD22	3:DDD:714:GLU:HB3	1.78	0.47
3:DDD:848:VAL:HG11	3:DDD:880:VAL:HG22	1.97	0.47
7:222:16:DC:N3	8:333:14:GTP:N2	2.55	0.47
2:CCC:518:ASN:O	2:CCC:519:ASN:HB2	2.13	0.47
1:AAA:46:ILE:HG12	1:BBB:35:PHE:HE1	1.79	0.47
2:CCC:870:ILE:HD12	2:CCC:944:ARG:HB3	1.96	0.47
2:CCC:866:ASP:OD2	2:CCC:944:ARG:HD3	2.13	0.47
3:DDD:1134:ILE:O	3:DDD:1134:ILE:HG22	2.15	0.47
6:111:33:DT:C2'	6:111:34:DG:H5'	2.45	0.47
2:CCC:13:LYS:NZ	2:CCC:1149:TYR:O	2.48	0.47
2:CCC:901:LEU:HD13	5:FFF:278:PHE:HE2	1.79	0.47
2:CCC:525:THR:HG21	2:CCC:687:ARG:HD2	1.96	0.47
2:CCC:97:ARG:NH2	5:FFF:190:ASP:CB	2.78	0.47
3:DDD:863:LEU:HD22	3:DDD:908:ILE:HG12	1.96	0.47
3:DDD:1364:ALA:HB3	4:EEE:21:LEU:HD11	1.96	0.47
2:CCC:1172:LEU:O	2:CCC:1176:LEU:HG	2.15	0.47
6:111:29:DC:O2	7:222:34:DG:N2	2.42	0.47
5:FFF:156:ARG:HE	6:111:33:DT:H72	1.79	0.47
3:DDD:1078:LEU:HG	3:DDD:1101:LEU:HD11	1.96	0.47
3:DDD:282:LEU:CD2	5:FFF:125:LEU:HD21	2.45	0.47
5:FFF:263:LEU:HD11	5:FFF:280:LEU:HD23	1.96	0.47
2:CCC:123:TYR:CE1	5:FFF:190:ASP:O	2.67	0.47
3:DDD:839:VAL:O	3:DDD:864:LEU:CD1	2.52	0.47
1:BBB:31:LEU:CD1	1:BBB:201:LEU:HB2	2.45	0.47
2:CCC:1107:MET:HB3	3:DDD:763:PHE:CE2	2.50	0.47
2:CCC:156:PHE:CZ	2:CCC:445:ILE:HG13	2.50	0.47
3:DDD:973:LEU:CD2	3:DDD:1006:GLY:HA2	2.45	0.47
3:DDD:680:ASN:HD21	3:DDD:1023:HIS:CG	2.32	0.47
3:DDD:129:ASP:HB2	3:DDD:220:ARG:NH1	2.30	0.47
2:CCC:375:PRO:CG	5:FFF:67:TYR:OH	2.63	0.47
2:CCC:195:PHE:CG	2:CCC:203:LYS:HD3	2.50	0.46
3:DDD:680:ASN:ND2	3:DDD:1023:HIS:CG	2.84	0.46
3:DDD:802:ASP:OD1	3:DDD:1313:SER:HB2	2.15	0.46
3:DDD:839:VAL:HG13	3:DDD:882:VAL:CG1	2.42	0.46
6:111:31:DT:H2''	6:111:32:DA:H5'	1.97	0.46
5:FFF:100:ARG:HB3	6:111:42:DG:H5''	1.97	0.46
1:BBB:83:LEU:HD21	3:DDD:526:VAL:CG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:149:LEU:HB2	2:CCC:530:ILE:CG2	2.45	0.46
2:CCC:600:THR:HB	2:CCC:602:GLU:HG2	1.96	0.46
2:CCC:20:GLN:O	2:CCC:20:GLN:HG3	2.16	0.46
2:CCC:560:PRO:HB2	3:DDD:776:THR:CG2	2.35	0.46
2:CCC:901:LEU:HA	5:FFF:278:PHE:CZ	2.50	0.46
1:BBB:41:ASN:ND2	2:CCC:1217:THR:HA	2.31	0.46
2:CCC:1321:GLU:OE1	3:DDD:99:ARG:NH1	2.49	0.46
1:BBB:47:LEU:HD13	1:BBB:183:ILE:CD1	2.41	0.46
2:CCC:715:THR:HG22	2:CCC:786:GLY:H	1.81	0.46
3:DDD:826:ILE:CG2	3:DDD:992:LYS:O	2.64	0.46
2:CCC:1313:HIS:CD2	4:EEE:31:GLN:NE2	2.83	0.46
5:FFF:54:VAL:CG1	5:FFF:59:GLN:OE1	2.64	0.46
5:FFF:141:ARG:HB2	6:111:39:DA:OP2	2.16	0.46
2:CCC:914:LYS:CG	2:CCC:915:ASP:N	2.63	0.46
2:CCC:992:LEU:HB3	2:CCC:993:PRO:HD2	1.98	0.46
3:DDD:339:ARG:CZ	3:DDD:798:ARG:HH22	2.28	0.46
6:111:54:DA:N1	7:222:9:DT:O4	2.49	0.46
2:CCC:840:SER:OG	2:CCC:1048:LYS:HG2	2.15	0.46
2:CCC:237:LEU:HD23	2:CCC:287:VAL:HG23	1.98	0.46
3:DDD:749:LYS:HB3	3:DDD:750:PRO:CD	2.42	0.46
1:AAA:31:LEU:CD1	1:AAA:201:LEU:HB2	2.45	0.46
2:CCC:967:LEU:CD2	2:CCC:1021:LEU:HD22	2.45	0.46
2:CCC:533:LEU:HD21	2:CCC:571:LEU:HD13	1.98	0.46
2:CCC:800:MET:HE1	2:CCC:828:PHE:CE2	2.51	0.46
2:CCC:867:GLU:OE1	2:CCC:943:LYS:CE	2.63	0.46
2:CCC:97:ARG:NH2	5:FFF:190:ASP:HB3	2.31	0.46
3:DDD:1080:ILE:HD12	3:DDD:1115:ILE:HD11	1.98	0.46
3:DDD:1138:LEU:N	3:DDD:1139:PRO:CD	2.78	0.46
3:DDD:1164:SER:HB2	3:DDD:1176:VAL:O	2.16	0.46
3:DDD:1169:THR:OG1	3:DDD:1174:ARG:NH2	2.49	0.46
3:DDD:22:ILE:CD1	3:DDD:1319:PHE:CE1	2.99	0.46
3:DDD:731:ARG:HA	3:DDD:731:ARG:HD3	1.75	0.46
1:AAA:112:ALA:HB1	1:AAA:123:ILE:HG21	1.98	0.46
1:AAA:235:ARG:HB3	1:BBB:214:GLU:OE2	2.16	0.46
2:CCC:1103:VAL:HG22	2:CCC:1111:GLN:HE22	1.80	0.46
2:CCC:168:GLY:O	3:DDD:1065:ALA:HB1	2.16	0.46
2:CCC:696:ASP:HB3	2:CCC:798:GLN:HG2	1.98	0.46
3:DDD:385:LEU:HD23	3:DDD:411:ILE:CD1	2.46	0.46
3:DDD:750:PRO:CA	3:DDD:781:LYS:HD2	2.46	0.46
3:DDD:294:ASN:O	3:DDD:298:MET:HG3	2.15	0.45
3:DDD:68:TYR:CZ	3:DDD:78:LEU:HD21	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FFF:262:TRP:CG	5:FFF:316:ILE:CG2	2.99	0.45
5:FFF:80:ALA:HB1	5:FFF:136:PRO:HG3	1.98	0.45
1:AAA:60:GLU:HG3	1:AAA:169:GLY:O	2.16	0.45
2:CCC:59:ILE:CG2	2:CCC:476:LYS:HE3	2.46	0.45
11:DDD:1504:GTP:C3'	11:DDD:1504:GTP:O1A	2.64	0.45
3:DDD:186:GLN:HB2	3:DDD:238:ILE:HG13	1.97	0.45
3:DDD:813:ASP:OD1	3:DDD:883:ARG:NH2	2.44	0.45
3:DDD:261:ALA:CA	5:FFF:220:THR:O	2.59	0.45
6:111:29:DC:H2''	6:111:30:DG:OP2	2.17	0.45
2:CCC:21:VAL:HG21	2:CCC:592:ARG:CZ	2.47	0.45
2:CCC:811:ASN:HA	2:CCC:815:SER:O	2.16	0.45
3:DDD:905:ARG:NH1	3:DDD:910:ASN:OD1	2.49	0.45
3:DDD:975:ILE:CD1	3:DDD:997:VAL:HG11	2.46	0.45
2:CCC:901:LEU:HB2	5:FFF:278:PHE:CD2	2.51	0.45
2:CCC:337:PHE:HE2	2:CCC:343:HIS:CD2	2.34	0.45
2:CCC:674:ASP:O	3:DDD:772:TYR:CE1	2.69	0.45
3:DDD:839:VAL:CG1	3:DDD:882:VAL:HG11	2.43	0.45
3:DDD:958:ILE:HG23	3:DDD:982:LEU:HD11	1.99	0.45
2:CCC:144:VAL:HG23	2:CCC:515:MET:HB2	1.98	0.45
2:CCC:245:ARG:HD3	2:CCC:337:PHE:CD1	2.51	0.45
2:CCC:868:SER:OG	2:CCC:943:LYS:C	2.51	0.45
3:DDD:709:ARG:HB3	3:DDD:709:ARG:CZ	2.46	0.45
7:222:20:DG:C2'	7:222:21:DG:H5'	2.46	0.45
1:AAA:70:THR:OG1	2:CCC:729:ALA:CB	2.55	0.45
3:DDD:267:ASP:O	3:DDD:271:ARG:HG3	2.17	0.45
2:CCC:1313:HIS:CD2	4:EEE:31:GLN:HE22	2.34	0.45
5:FFF:178:TYR:CE2	5:FFF:212:MET:HG3	2.52	0.45
5:FFF:271:ARG:O	5:FFF:271:ARG:HG2	2.15	0.45
2:CCC:1281:TYR:CD2	3:DDD:484:MET:HE3	2.51	0.45
2:CCC:634:VAL:HG12	2:CCC:636:CYS:SG	2.56	0.45
2:CCC:867:GLU:OE1	2:CCC:943:LYS:CD	2.62	0.45
2:CCC:912:ASP:OD1	2:CCC:913:VAL:N	2.50	0.45
3:DDD:803:VAL:HG21	3:DDD:1309:ILE:O	2.16	0.45
3:DDD:490:ILE:O	3:DDD:499:ILE:HG22	2.16	0.45
5:FFF:247:GLU:O	5:FFF:250:THR:HG22	2.16	0.45
3:DDD:394:ILE:HD12	5:FFF:254:ASP:CB	2.46	0.45
2:CCC:338:THR:HB	2:CCC:345:PRO:HB3	1.98	0.45
2:CCC:461:GLU:OE2	2:CCC:465:ARG:NH2	2.50	0.45
2:CCC:533:LEU:HD23	2:CCC:538:LEU:O	2.17	0.45
3:DDD:395:LYS:HG2	5:FFF:329:LEU:HD12	1.98	0.45
3:DDD:703:THR:O	3:DDD:703:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:165:GLU:CG	1:BBB:165:GLU:O	2.64	0.45
2:CCC:685:MET:SD	2:CCC:1073:LYS:HG2	2.57	0.45
2:CCC:12:ARG:HG3	2:CCC:1181:PRO:HB2	1.99	0.45
2:CCC:933:VAL:HG11	2:CCC:945:ALA:HB2	1.98	0.45
3:DDD:452:LEU:HB3	3:DDD:500:ILE:HG23	1.99	0.45
2:CCC:942:ASP:O	2:CCC:946:LEU:HG	2.16	0.45
3:DDD:339:ARG:HA	3:DDD:343:LEU:HD12	1.99	0.45
3:DDD:843:VAL:CG1	3:DDD:883:ARG:HD3	2.47	0.45
3:DDD:843:VAL:HG21	3:DDD:897:HIS:O	2.17	0.45
1:BBB:83:LEU:HA	1:BBB:83:LEU:HD13	1.88	0.44
2:CCC:1210:ILE:CG2	2:CCC:1211:ARG:N	2.80	0.44
3:DDD:1036:ARG:HB3	3:DDD:1079:LYS:HB3	1.98	0.44
3:DDD:1364:ALA:O	3:DDD:1367:GLN:HG2	2.18	0.44
6:111:53:DG:N2	7:222:11:DA:C2	2.85	0.44
7:222:16:DC:H5"	7:222:16:DC:H6	1.81	0.44
2:CCC:564:PRO:HB3	8:333:14:GTP:PA	2.57	0.44
2:CCC:1313:HIS:CE1	3:DDD:380:PHE:HE2	2.34	0.44
2:CCC:518:ASN:O	2:CCC:691:PRO:HD3	2.17	0.44
3:DDD:1063:ASP:HB3	3:DDD:1103:GLY:HA3	1.98	0.44
3:DDD:120:LEU:HA	3:DDD:121:PRO:C	2.38	0.44
3:DDD:242:LEU:HD12	3:DDD:243:PRO:HD2	2.00	0.44
2:CCC:1276:TRP:HH2	3:DDD:798:ARG:HG2	1.81	0.44
3:DDD:1029:THR:HG22	3:DDD:1121:LEU:HD11	2.00	0.44
3:DDD:964:LYS:CD	3:DDD:1199:PHE:HE1	2.30	0.44
2:CCC:800:MET:HE2	2:CCC:800:MET:HB3	1.93	0.44
2:CCC:847:PRO:HB3	2:CCC:1047:LEU:HD11	1.99	0.44
2:CCC:870:ILE:HD12	2:CCC:944:ARG:CG	2.48	0.44
3:DDD:137:ARG:HD2	5:FFF:53:ARG:NH1	2.32	0.44
6:111:28:DA:C2	7:222:36:DG:N2	2.85	0.44
2:CCC:1151:LEU:HD22	2:CCC:1198:LEU:HD12	2.00	0.44
2:CCC:27:LEU:C	2:CCC:29:SER:H	2.21	0.44
3:DDD:125:GLY:HA2	3:DDD:135:ILE:HD11	1.99	0.44
5:FFF:176:ASN:OD1	7:222:26:DT:H71	2.18	0.44
2:CCC:549:ASP:CB	3:DDD:750:PRO:CB	2.95	0.44
2:CCC:839:VAL:HG13	2:CCC:839:VAL:O	2.18	0.44
2:CCC:903:ARG:NH1	2:CCC:910:ALA:HB3	2.28	0.44
2:CCC:812:PHE:HB3	3:DDD:357:VAL:CG1	2.48	0.44
2:CCC:700:VAL:HG21	2:CCC:1114:GLU:HG3	1.99	0.44
2:CCC:1182:ILE:HD11	2:CCC:1198:LEU:HD21	2.00	0.44
3:DDD:1050:THR:HG22	3:DDD:1051:ASP:N	2.33	0.44
6:111:31:DT:H1'	6:111:32:DA:H5"	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:700:VAL:HG12	2:CCC:1117:LEU:HD23	2.00	0.44
2:CCC:1296:ASP:O	2:CCC:1297:ASP:C	2.55	0.44
2:CCC:337:PHE:HE2	2:CCC:343:HIS:HD2	1.64	0.44
2:CCC:848:GLU:CG	2:CCC:888:THR:HG22	2.45	0.44
3:DDD:518:VAL:HG21	3:DDD:708:ASN:CG	2.38	0.44
3:DDD:749:LYS:O	3:DDD:781:LYS:NZ	2.44	0.44
3:DDD:741:ALA:O	3:DDD:762:ASN:ND2	2.50	0.44
2:CCC:1004:ASP:N	2:CCC:1004:ASP:OD1	2.51	0.44
2:CCC:277:LEU:HD12	2:CCC:282:VAL:HG21	2.00	0.44
2:CCC:905:ILE:HG23	5:FFF:310:LEU:O	2.18	0.44
2:CCC:1255:THR:O	2:CCC:1256:GLN:HB2	2.17	0.43
3:DDD:1207:GLY:HA3	3:DDD:1224:ARG:NE	2.32	0.43
3:DDD:519:ASN:CA	3:DDD:523:GLU:HB2	2.47	0.43
5:FFF:80:ALA:CB	5:FFF:136:PRO:HG3	2.48	0.43
2:CCC:197:ARG:HD3	2:CCC:200:ARG:HA	2.00	0.43
2:CCC:1287:LEU:O	2:CCC:1291:LEU:HG	2.18	0.43
2:CCC:221:LEU:HD22	2:CCC:336:LEU:CD1	2.49	0.43
2:CCC:993:PRO:HG2	2:CCC:996:ARG:HD2	2.00	0.43
3:DDD:321:LYS:O	3:DDD:321:LYS:HG3	2.18	0.43
3:DDD:357:VAL:HG12	3:DDD:461:PHE:CE2	2.54	0.43
3:DDD:385:LEU:CD2	3:DDD:411:ILE:HD12	2.48	0.43
1:AAA:164:ASP:OD1	1:AAA:165:GLU:N	2.45	0.43
2:CCC:671:LEU:HD23	2:CCC:1186:VAL:HG13	2.01	0.43
2:CCC:230:PHE:HB2	2:CCC:333:ILE:HB	2.00	0.43
2:CCC:453:ILE:HD12	2:CCC:587:LEU:CD2	2.48	0.43
2:CCC:548:ARG:HH11	2:CCC:570:GLY:H	1.67	0.43
3:DDD:460:ASP:OD1	3:DDD:460:ASP:N	2.48	0.43
3:DDD:746:LEU:HA	3:DDD:758:PRO:HB3	2.01	0.43
3:DDD:809:VAL:HG22	3:DDD:915:ILE:CD1	2.47	0.43
2:CCC:1176:LEU:HD22	2:CCC:1181:PRO:HD2	2.00	0.43
2:CCC:1308:ILE:HG23	3:DDD:380:PHE:CD2	2.53	0.43
1:AAA:68:TYR:O	2:CCC:756:TYR:CD2	2.71	0.43
3:DDD:140:TYR:OH	3:DDD:312:ARG:HD2	2.18	0.43
3:DDD:739:GLN:HG3	3:DDD:744:ARG:HA	2.00	0.43
3:DDD:644:MET:HE1	3:DDD:740:LEU:HD22	2.01	0.43
3:DDD:746:LEU:H	3:DDD:746:LEU:CD1	2.14	0.43
3:DDD:927:GLY:O	3:DDD:931:THR:OG1	2.35	0.43
5:FFF:229:ASP:HB2	5:FFF:231:GLU:HG2	2.01	0.43
2:CCC:199:ASP:CG	6:111:48:DA:C2	2.92	0.43
2:CCC:878:THR:CG2	2:CCC:879:GLY:N	2.80	0.43
3:DDD:223:LEU:O	3:DDD:227:PHE:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:646:ILE:HD13	3:DDD:762:ASN:HD21	1.83	0.43
2:CCC:905:ILE:HD11	5:FFF:313:LEU:HD23	2.01	0.43
7:222:22:DA:H1'	7:222:23:DT:C5'	2.48	0.43
2:CCC:1119:MET:HG2	2:CCC:1204:LEU:HD13	2.00	0.43
2:CCC:195:PHE:CD2	2:CCC:203:LYS:HD3	2.54	0.43
2:CCC:714:VAL:HG21	2:CCC:787:PRO:CD	2.49	0.43
2:CCC:905:ILE:HA	5:FFF:310:LEU:HB3	2.00	0.43
3:DDD:801:VAL:HA	3:DDD:920:ALA:CB	2.49	0.43
1:AAA:62:ASP:OD2	1:AAA:141:SER:HB3	2.18	0.42
1:AAA:192:VAL:CG2	1:AAA:198:LEU:HD12	2.49	0.42
1:BBB:192:VAL:HG23	1:BBB:198:LEU:HD12	2.01	0.42
2:CCC:1284:ALA:CA	3:DDD:1357:ILE:HD12	2.27	0.42
2:CCC:1075:VAL:HG11	3:DDD:354:VAL:HG11	2.00	0.42
3:DDD:709:ARG:CB	3:DDD:709:ARG:CZ	2.96	0.42
3:DDD:832:LYS:HB3	3:DDD:1242:ARG:HD3	2.01	0.42
5:FFF:287:THR:O	5:FFF:291:VAL:HG23	2.18	0.42
1:AAA:45:ARG:HE	1:BBB:38:THR:HG1	1.61	0.42
2:CCC:878:THR:CG2	2:CCC:879:GLY:H	2.33	0.42
3:DDD:123:ARG:HD3	3:DDD:123:ARG:HA	1.90	0.42
2:CCC:1240:ASP:OD1	3:DDD:445:LYS:HE3	2.18	0.42
5:FFF:170:HIS:CG	6:111:31:DT:H73	2.54	0.42
2:CCC:232:ILE:HD11	2:CCC:333:ILE:HD12	2.02	0.42
3:DDD:429:LEU:HD23	3:DDD:429:LEU:HA	1.92	0.42
3:DDD:745:GLY:O	3:DDD:759:ILE:N	2.43	0.42
2:CCC:550:VAL:CG2	3:DDD:776:THR:HG22	2.48	0.42
5:FFF:54:VAL:HG13	5:FFF:59:GLN:OE1	2.19	0.42
2:CCC:1149:TYR:HB3	2:CCC:1159:VAL:HG13	1.99	0.42
2:CCC:1220:GLN:HG2	2:CCC:1221:PHE:N	2.34	0.42
2:CCC:221:LEU:HD22	2:CCC:336:LEU:HD13	2.00	0.42
2:CCC:225:PHE:CE2	2:CCC:347:ILE:HB	2.55	0.42
2:CCC:549:ASP:HB3	3:DDD:750:PRO:CG	2.47	0.42
3:DDD:612:LEU:HB3	3:DDD:616:PRO:HG2	2.02	0.42
3:DDD:793:SER:OG	3:DDD:928:THR:HA	2.19	0.42
7:222:8:DG:H2''	7:222:9:DT:H5'	2.02	0.42
2:CCC:564:PRO:HB2	8:333:14:GTP:O1A	2.20	0.42
3:DDD:1364:ALA:CB	4:EEE:21:LEU:HD11	2.50	0.42
3:DDD:582:ILE:HG23	3:DDD:623:GLN:HB2	2.01	0.42
2:CCC:675:ASP:N	3:DDD:763:PHE:CE1	2.87	0.42
5:FFF:163:ARG:CD	5:FFF:167:LEU:HD12	2.49	0.42
2:CCC:1073:LYS:NZ	8:333:16:G:OP1	2.37	0.42
1:BBB:44:ARG:HA	1:BBB:183:ILE:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:1119:MET:HB2	2:CCC:1228:GLY:CA	2.49	0.42
2:CCC:1238:LEU:O	2:CCC:1242:LYS:CG	2.55	0.42
2:CCC:560:PRO:O	3:DDD:780:ARG:NH2	2.39	0.42
3:DDD:910:ASN:HB3	4:EEE:15:ASN:OD1	2.19	0.42
6:111:48:DA:OP2	6:111:48:DA:C8	2.73	0.42
2:CCC:196:VAL:CG2	2:CCC:206:ALA:HA	2.49	0.42
2:CCC:367:TYR:HA	2:CCC:384:LEU:CD2	2.49	0.42
2:CCC:648:ASP:N	2:CCC:648:ASP:OD1	2.51	0.42
2:CCC:22:LEU:HB3	2:CCC:655:VAL:HG11	2.02	0.42
3:DDD:342:LEU:HD12	3:DDD:342:LEU:HA	1.82	0.42
3:DDD:926:PRO:O	3:DDD:930:LEU:HG	2.19	0.42
5:FFF:218:ARG:HG2	7:222:24:DT:H73	2.01	0.42
2:CCC:1124:ILE:HD11	2:CCC:1198:LEU:HD11	2.01	0.42
2:CCC:300:ASP:OD1	2:CCC:313:ALA:N	2.48	0.42
2:CCC:61:SER:CB	2:CCC:479:LEU:HB3	2.50	0.42
2:CCC:984:VAL:O	2:CCC:984:VAL:HG13	2.20	0.42
3:DDD:1158:GLU:HA	3:DDD:1223:LEU:HD22	2.02	0.42
1:BBB:83:LEU:HD11	3:DDD:526:VAL:O	2.19	0.42
3:DDD:309:ASN:HB2	3:DDD:326:SER:HB3	2.01	0.42
2:CCC:1284:ALA:HA	3:DDD:1357:ILE:CD1	2.28	0.42
2:CCC:23:ASP:N	2:CCC:23:ASP:OD1	2.49	0.42
2:CCC:569:ILE:HD13	3:DDD:784:ALA:CA	2.50	0.42
2:CCC:548:ARG:CA	2:CCC:570:GLY:HA3	2.50	0.42
3:DDD:803:VAL:HG23	3:DDD:1313:SER:HB3	2.01	0.42
3:DDD:816:THR:HG22	3:DDD:818:GLU:H	1.85	0.42
5:FFF:317:LEU:HD23	5:FFF:322:LEU:HD12	2.01	0.42
1:AAA:222:THR:OG1	1:BBB:233:ASP:CB	2.63	0.41
2:CCC:1184:THR:HG23	2:CCC:1189:GLY:HA3	2.02	0.41
2:CCC:758:ARG:HG3	2:CCC:833:ILE:O	2.19	0.41
3:DDD:1217:PRO:HB2	3:DDD:1306:LEU:CD2	2.49	0.41
3:DDD:267:ASP:OD1	3:DDD:267:ASP:N	2.53	0.41
3:DDD:576:ARG:HD3	3:DDD:593:ASN:HA	2.01	0.41
3:DDD:609:TYR:CA	3:DDD:617:THR:HG21	2.50	0.41
3:DDD:843:VAL:O	3:DDD:883:ARG:HB2	2.20	0.41
5:FFF:99:LEU:O	5:FFF:102:VAL:HB	2.20	0.41
6:111:34:DG:C2	7:222:30:DA:C2	3.07	0.41
1:AAA:47:LEU:O	1:AAA:180:VAL:HG21	2.19	0.41
2:CCC:356:THR:HG21	2:CCC:362:ALA:HA	2.00	0.41
2:CCC:443:ASP:HB3	2:CCC:450:ASN:HD21	1.83	0.41
3:DDD:1087:ASP:N	3:DDD:1087:ASP:OD1	2.53	0.41
3:DDD:749:LYS:HE2	3:DDD:755:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FFF:317:LEU:CD2	5:FFF:322:LEU:HD12	2.50	0.41
7:222:16:DC:C5'	7:222:16:DC:H6	2.34	0.41
7:222:17:DG:C2'	7:222:18:DT:H5'	2.50	0.41
2:CCC:551:HIS:CE1	2:CCC:553:THR:HG1	2.30	0.41
3:DDD:572:THR:CG2	3:DDD:593:ASN:CG	2.89	0.41
1:BBB:8:PHE:O	1:BBB:8:PHE:CD1	2.74	0.41
2:CCC:638:SER:O	2:CCC:639:LYS:HG3	2.20	0.41
2:CCC:660:VAL:CG2	3:DDD:773:PHE:HD2	2.33	0.41
2:CCC:828:PHE:HB3	2:CCC:1060:ILE:CG2	2.46	0.41
2:CCC:854:ILE:HB	2:CCC:857:VAL:HG21	2.02	0.41
2:CCC:90:VAL:HG12	2:CCC:91:THR:N	2.36	0.41
3:DDD:800:LEU:HD22	3:DDD:1256:ILE:HG12	2.03	0.41
3:DDD:378:LYS:HE2	3:DDD:382:TYR:OH	2.21	0.41
3:DDD:438:GLU:HA	3:DDD:439:PRO:HD3	1.94	0.41
5:FFF:292:GLY:HA2	5:FFF:297:LEU:H	1.86	0.41
2:CCC:106:GLU:HG2	2:CCC:115:LYS:HD2	2.02	0.41
2:CCC:1277:ALA:HB3	3:DDD:434:ILE:HD12	2.02	0.41
2:CCC:1315:MET:HE2	2:CCC:1317:PRO:HB3	2.01	0.41
2:CCC:967:LEU:HD21	2:CCC:1021:LEU:CD2	2.50	0.41
3:DDD:140:TYR:OH	3:DDD:312:ARG:NH1	2.54	0.41
3:DDD:495:ASN:OD1	3:DDD:497:GLU:HB2	2.20	0.41
3:DDD:964:LYS:HD3	3:DDD:1199:PHE:CE1	2.52	0.41
7:222:9:DT:H1'	7:222:10:DC:H5'	2.01	0.41
7:222:16:DC:H3'	7:222:17:DG:H5''	2.02	0.41
1:AAA:158:ARG:HD2	1:AAA:172:LEU:CD1	2.48	0.41
1:AAA:158:ARG:HD2	1:AAA:172:LEU:CD2	2.49	0.41
1:AAA:83:LEU:HD13	1:AAA:83:LEU:HA	1.90	0.41
2:CCC:18:ARG:NH2	2:CCC:620:ASN:O	2.54	0.41
2:CCC:615:VAL:HA	2:CCC:638:SER:HB3	2.02	0.41
2:CCC:638:SER:O	2:CCC:639:LYS:HG2	2.20	0.41
3:DDD:288:PRO:HG3	5:FFF:92:ARG:HG2	2.03	0.41
2:CCC:1315:MET:SD	3:DDD:473:THR:HG21	2.60	0.41
3:DDD:478:LEU:HG	4:EEE:47:THR:HG23	2.01	0.41
3:DDD:614:LEU:HG	4:EEE:5:THR:HG23	2.03	0.41
6:111:51:DC:OP1	6:111:51:DC:H3'	2.21	0.41
2:CCC:1281:TYR:CE2	3:DDD:431:ARG:O	2.73	0.41
2:CCC:1301:ARG:HG3	2:CCC:1302:THR:N	2.36	0.41
2:CCC:160:ASP:CG	2:CCC:163:LYS:HB2	2.41	0.41
2:CCC:587:LEU:HA	2:CCC:587:LEU:HD23	1.81	0.41
2:CCC:663:VAL:O	2:CCC:666:SER:OG	2.36	0.41
1:AAA:70:THR:HG1	2:CCC:729:ALA:HB3	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:985:GLU:HB3	2:CCC:988:LYS:HB3	2.03	0.41
3:DDD:133:ARG:O	3:DDD:137:ARG:HG3	2.21	0.41
3:DDD:220:ARG:O	3:DDD:224:LEU:HG	2.21	0.41
3:DDD:426:ALA:HA	3:DDD:427:PRO:HA	1.81	0.41
3:DDD:750:PRO:CA	3:DDD:781:LYS:HB2	2.47	0.41
3:DDD:836:ARG:HB2	3:DDD:873:GLU:OE2	2.20	0.41
3:DDD:582:ILE:HD12	3:DDD:623:GLN:HB3	2.01	0.41
2:CCC:1149:TYR:CD1	2:CCC:1159:VAL:HG11	2.56	0.41
2:CCC:151:ARG:NH2	2:CCC:156:PHE:CD2	2.88	0.41
2:CCC:258:ASN:N	2:CCC:258:ASN:OD1	2.54	0.41
3:DDD:843:VAL:HG21	3:DDD:897:HIS:CA	2.50	0.41
3:DDD:850:LYS:HB2	3:DDD:851:PRO:CD	2.51	0.41
5:FFF:218:ARG:HD2	5:FFF:218:ARG:HA	1.57	0.41
2:CCC:39:ILE:O	2:CCC:73:TYR:OH	2.39	0.41
3:DDD:805:GLN:NE2	3:DDD:1348:LYS:HG3	2.35	0.41
3:DDD:615:LYS:N	3:DDD:616:PRO:CD	2.84	0.41
3:DDD:644:MET:CE	3:DDD:740:LEU:HD22	2.51	0.41
1:BBB:49:SER:O	1:BBB:151:GLY:CA	2.69	0.41
2:CCC:539:THR:CB	2:CCC:542:ARG:HG3	2.48	0.40
2:CCC:658:GLN:O	2:CCC:661:VAL:HG22	2.21	0.40
2:CCC:5:TYR:CD1	2:CCC:778:GLU:HB2	2.56	0.40
2:CCC:878:THR:HG22	2:CCC:879:GLY:H	1.86	0.40
3:DDD:1067:ARG:HD3	3:DDD:1071:GLY:O	2.21	0.40
5:FFF:270:GLN:OE1	5:FFF:312:ARG:HD2	2.20	0.40
6:111:30:DG:C8	6:111:31:DT:H72	2.56	0.40
1:BBB:33:ARG:CG	1:BBB:33:ARG:O	2.70	0.40
2:CCC:1063:GLY:O	3:DDD:354:VAL:HG21	2.21	0.40
2:CCC:914:LYS:CG	2:CCC:915:ASP:H	2.02	0.40
3:DDD:1184:ASP:OD1	3:DDD:1184:ASP:N	2.54	0.40
3:DDD:582:ILE:HG23	3:DDD:623:GLN:HB3	2.03	0.40
3:DDD:864:LEU:HD23	3:DDD:864:LEU:HA	1.82	0.40
1:BBB:192:VAL:CG2	1:BBB:198:LEU:HD12	2.51	0.40
2:CCC:249:GLU:O	2:CCC:269:ILE:HD12	2.22	0.40
2:CCC:245:ARG:HD3	2:CCC:337:PHE:CE1	2.56	0.40
3:DDD:973:LEU:HD22	3:DDD:1006:GLY:CA	2.52	0.40
5:FFF:221:SER:HB3	5:FFF:224:THR:OG1	2.22	0.40
7:222:13:DA:H2''	7:222:14:DC:H5'	2.02	0.40
2:CCC:619:ALA:HB2	2:CCC:654:ASP:HB2	2.03	0.40
2:CCC:696:ASP:CB	2:CCC:798:GLN:HG2	2.52	0.40
3:DDD:282:LEU:HD21	5:FFF:125:LEU:CD2	2.51	0.40
3:DDD:823:THR:HG22	3:DDD:879:ALA:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FFF:144:THR:OG1	6:111:39:DA:H8	2.03	0.40
6:111:53:DG:H2''	6:111:54:DA:H5'	2.04	0.40
1:AAA:29:GLU:HB2	1:AAA:30:PRO:HA	2.04	0.40
2:CCC:894:GLN:NE2	3:DDD:76:LYS:HB3	2.36	0.40
3:DDD:504:GLN:HB3	3:DDD:505:ASP:H	1.63	0.40
5:FFF:88:VAL:O	5:FFF:92:ARG:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	228/242 (94%)	211 (92%)	12 (5%)	5 (2%)	6	38
1	BBB	226/242 (93%)	208 (92%)	16 (7%)	2 (1%)	17	56
2	CCC	1338/1342 (100%)	1244 (93%)	81 (6%)	13 (1%)	15	54
3	DDD	1346/1407 (96%)	1246 (93%)	89 (7%)	11 (1%)	19	60
4	EEE	77/90 (86%)	74 (96%)	3 (4%)	0	100	100
5	FFF	275/336 (82%)	253 (92%)	19 (7%)	3 (1%)	14	52
All	All	3490/3659 (95%)	3236 (93%)	220 (6%)	34 (1%)	15	54

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	DDD	174	ASP
3	DDD	519	ASN
3	DDD	947	GLU
3	DDD	1268	ASN
5	FFF	190	ASP
1	AAA	208	ASN

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Mol	Chain	Res	Type
2	CCC	756	TYR
3	DDD	49	PHE
3	DDD	710	ASP
3	DDD	1053	LEU
3	DDD	1132	LYS
1	AAA	162	GLU
1	BBB	8	PHE
1	BBB	232	VAL
2	CCC	986	ALA
2	CCC	1297	ASP
1	AAA	161	SER
1	AAA	210	THR
1	AAA	211	ILE
2	CCC	519	ASN
2	CCC	1103	VAL
3	DDD	758	PRO
3	DDD	854	ALA
2	CCC	163	LYS
2	CCC	507	GLY
2	CCC	1004	ASP
2	CCC	1137	GLU
3	DDD	805	GLN
5	FFF	113	GLY
2	CCC	45	GLY
2	CCC	1186	VAL
2	CCC	43	PRO
2	CCC	112	GLY
5	FFF	295	ILE

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	AAA	198/208 (95%)	192 (97%)	6 (3%)	41	63
1	BBB	196/208 (94%)	188 (96%)	8 (4%)	30	56
2	CCC	1155/1157 (100%)	1134 (98%)	21 (2%)	59	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	DDD	1127/1168 (96%)	1078 (96%)	49 (4%)	29	55
4	EEE	67/74 (90%)	64 (96%)	3 (4%)	27	54
5	FFF	240/292 (82%)	232 (97%)	8 (3%)	38	61
All	All	2983/3107 (96%)	2888 (97%)	95 (3%)	39	62

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	18	GLN
1	AAA	28	LEU
1	AAA	32	GLU
1	AAA	131	CYS
1	AAA	150	ARG
1	AAA	166	ARG
1	BBB	28	LEU
1	BBB	33	ARG
1	BBB	83	LEU
1	BBB	131	CYS
1	BBB	150	ARG
1	BBB	159	ILE
1	BBB	211	ILE
1	BBB	231	PHE
2	CCC	12	ARG
2	CCC	23	ASP
2	CCC	30	ILE
2	CCC	70	TYR
2	CCC	247	ARG
2	CCC	286	GLU
2	CCC	443	ASP
2	CCC	446	ASP
2	CCC	538	LEU
2	CCC	553	THR
2	CCC	554	HIS
2	CCC	561	ILE
2	CCC	571	LEU
2	CCC	653	MET
2	CCC	700	VAL
2	CCC	851	THR
2	CCC	1159	VAL
2	CCC	1207	SER
2	CCC	1223	ARG

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Mol	Chain	Res	Type
2	CCC	1253	LEU
2	CCC	1299	ASN
3	DDD	93	THR
3	DDD	99	ARG
3	DDD	153	ASN
3	DDD	156	ARG
3	DDD	216	LYS
3	DDD	222	LYS
3	DDD	223	LEU
3	DDD	227	PHE
3	DDD	240	THR
3	DDD	256	ASP
3	DDD	321	LYS
3	DDD	384	LYS
3	DDD	398	LYS
3	DDD	399	LYS
3	DDD	417	ARG
3	DDD	505	ASP
3	DDD	536	LEU
3	DDD	538	ARG
3	DDD	550	VAL
3	DDD	551	ARG
3	DDD	570	LYS
3	DDD	572	THR
3	DDD	579	LEU
3	DDD	599	LYS
3	DDD	619	ILE
3	DDD	641	ILE
3	DDD	646	ILE
3	DDD	648	GLU
3	DDD	690	ASN
3	DDD	695	LYS
3	DDD	707	ILE
3	DDD	716	GLN
3	DDD	736	GLN
3	DDD	743	MET
3	DDD	746	LEU
3	DDD	755	ILE
3	DDD	756	GLU
3	DDD	770	LEU
3	DDD	798	ARG
3	DDD	803	VAL

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Mol	Chain	Res	Type
3	DDD	849	LEU
3	DDD	862	THR
3	DDD	1087	ASP
3	DDD	1175	LEU
3	DDD	1180	VAL
3	DDD	1189	MET
3	DDD	1199	PHE
3	DDD	1210	ILE
3	DDD	1227	HIS
4	EEE	11	GLU
4	EEE	43	ASN
4	EEE	45	LYS
5	FFF	107	ARG
5	FFF	218	ARG
5	FFF	219	ILE
5	FFF	229	ASP
5	FFF	231	GLU
5	FFF	242	LYS
5	FFF	271	ARG
5	FFF	325	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	333	1/3 (33%)	1 (100%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	333	16	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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	$\# Z > 2$
11	GTP	DDD	1504	9	26,34,34	1.14	3 (11%)	33,54,54	1.93	7 (21%)

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
11	GTP	DDD	1504	9	-	4/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	DDD	1504	GTP	C6-C5	3.70	1.47	1.41
11	DDD	1504	GTP	C5-C4	2.49	1.47	1.40
11	DDD	1504	GTP	O4'-C1'	2.19	1.44	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	DDD	1504	GTP	C2-N3-C4	4.54	120.54	115.36
11	DDD	1504	GTP	C5-C6-N1	-4.03	117.92	123.43
11	DDD	1504	GTP	C6-N1-C2	3.86	122.06	115.93
11	DDD	1504	GTP	PA-O3A-PB	-3.68	120.19	132.83
11	DDD	1504	GTP	C6-C5-C4	-3.59	117.37	120.80
11	DDD	1504	GTP	C3'-C2'-C1'	3.34	106.00	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	DDD	1504	GTP	N3-C2-N1	-2.92	123.33	127.22

There are no chirality outliers.

All (4) torsion outliers are listed below:

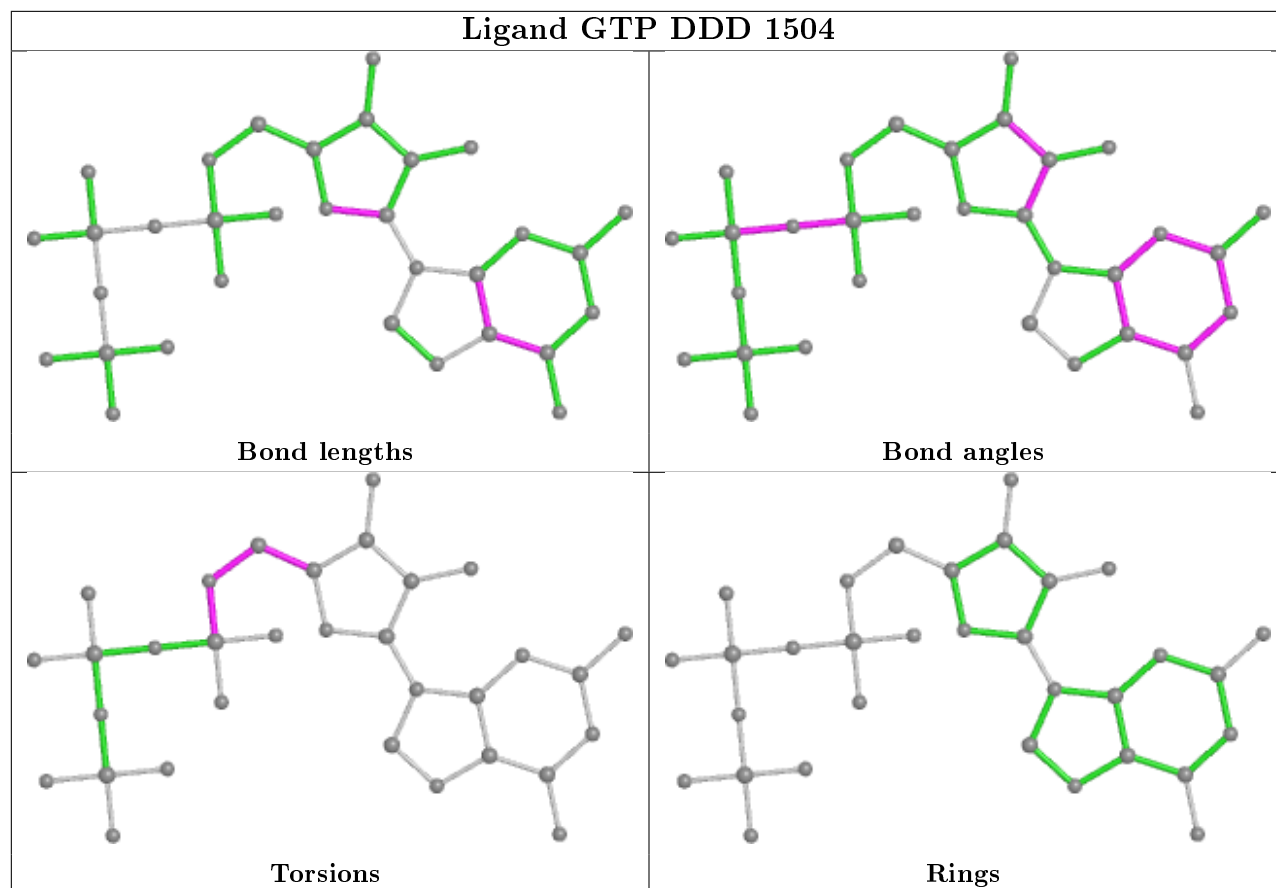
Mol	Chain	Res	Type	Atoms
11	DDD	1504	GTP	C4'-C5'-O5'-PA
11	DDD	1504	GTP	O4'-C4'-C5'-O5'
11	DDD	1504	GTP	C5'-O5'-PA-O3A
11	DDD	1504	GTP	C5'-O5'-PA-O2A

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	DDD	1504	GTP	5	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 ⓘ

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	AAA	230/242 (95%)	-0.02	5 (2%) 62 52	210, 312, 392, 505	0
1	BBB	228/242 (94%)	0.04	11 (4%) 30 26	194, 348, 436, 569	0
2	CCC	1340/1342 (99%)	-0.14	32 (2%) 59 49	113, 282, 477, 654	0
3	DDD	1350/1407 (95%)	0.02	66 (4%) 29 25	134, 303, 497, 689	0
4	EEE	79/90 (87%)	0.01	4 (5%) 28 24	247, 373, 579, 601	0
5	FFF	277/336 (82%)	0.24	21 (7%) 13 12	198, 359, 555, 641	0
6	111	31/50 (62%)	0.18	4 (12%) 3 4	300, 371, 467, 520	0
7	222	35/50 (70%)	0.01	1 (2%) 51 41	250, 350, 491, 543	0
8	333	2/3 (66%)	1.18	0 100 100	326, 326, 326, 340	0
All	All	3572/3762 (94%)	-0.02	144 (4%) 38 31	113, 307, 505, 689	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	164	ASP	6.7
3	DDD	976	THR	6.3
3	DDD	1121	LEU	6.2
2	CCC	1004	ASP	6.2
3	DDD	1110	GLU	6.2
3	DDD	1129	GLY	6.2
6	111	47	DC	5.9
6	111	44	DG	5.7
3	DDD	880	VAL	5.2
3	DDD	847	ASP	5.1
5	FFF	321	GLY	5.0
3	DDD	878	ASP	5.0
1	BBB	166	ARG	4.9
3	DDD	392	THR	4.7
3	DDD	877	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
5	FFF	320	GLN	4.7
3	DDD	853	THR	4.5
3	DDD	1111	ASP	4.5
2	CCC	907	GLY	4.4
3	DDD	1120	THR	4.4
3	DDD	991	THR	4.3
3	DDD	677	GLU	4.3
3	DDD	1030	GLU	4.2
5	FFF	323	ASN	4.2
2	CCC	1003	THR	4.1
2	CCC	906	PHE	4.1
3	DDD	848	VAL	4.1
3	DDD	879	ALA	4.1
6	111	48	DA	4.0
3	DDD	1028	ILE	4.0
3	DDD	856	ILE	3.9
3	DDD	997	VAL	3.9
5	FFF	327	LEU	3.9
3	DDD	977	SER	3.9
4	EEE	2	ALA	3.8
1	BBB	165	GLU	3.8
1	BBB	134	THR	3.7
3	DDD	1109	LEU	3.7
2	CCC	113	THR	3.7
3	DDD	1099	TYR	3.7
3	DDD	854	ALA	3.6
3	DDD	1029	THR	3.6
5	FFF	317	LEU	3.6
3	DDD	992	LYS	3.6
1	BBB	163	GLU	3.5
3	DDD	1078	LEU	3.5
3	DDD	1130	GLY	3.5
3	DDD	975	ILE	3.4
3	DDD	748	ALA	3.4
5	FFF	304	GLN	3.3
5	FFF	111	ASN	3.3
2	CCC	169	LYS	3.3
5	FFF	288	LEU	3.3
1	BBB	210	THR	3.2
3	DDD	1122	ALA	3.2
5	FFF	263	LEU	3.2
2	CCC	239	MET	3.2

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Mol	Chain	Res	Type	RSRZ
3	DDD	980	THR	3.2
3	DDD	864	LEU	3.1
3	DDD	974	VAL	3.1
5	FFF	302	VAL	3.1
1	AAA	134	THR	3.1
3	DDD	732	GLY	3.1
2	CCC	67	GLU	3.1
5	FFF	113	GLY	3.1
4	EEE	38	LEU	3.1
4	EEE	3	ARG	3.1
3	DDD	750	PRO	3.0
3	DDD	1128	SER	3.0
2	CCC	883	LEU	3.0
3	DDD	1080	ILE	3.0
1	AAA	171	LEU	3.0
3	DDD	1107	VAL	3.0
2	CCC	905	ILE	2.9
3	DDD	958	ILE	2.9
1	AAA	172	LEU	2.9
2	CCC	721	GLY	2.9
2	CCC	230	PHE	2.9
5	FFF	314	ARG	2.9
3	DDD	746	LEU	2.8
2	CCC	777	VAL	2.8
1	BBB	133	LEU	2.8
2	CCC	606	LEU	2.8
5	FFF	319	THR	2.7
3	DDD	1027	VAL	2.7
2	CCC	982	GLY	2.7
6	111	43	DT	2.7
3	DDD	855	ASP	2.7
3	DDD	1079	LYS	2.6
3	DDD	978	ARG	2.6
3	DDD	858	VAL	2.6
3	DDD	1115	ILE	2.5
4	EEE	4	VAL	2.5
5	FFF	281	LEU	2.5
2	CCC	1002	LEU	2.5
5	FFF	313	LEU	2.5
5	FFF	322	LEU	2.5
1	BBB	90	VAL	2.5
5	FFF	262	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
3	DDD	995	TYR	2.4
2	CCC	105	TYR	2.4
2	CCC	103	VAL	2.4
3	DDD	1036	ARG	2.4
2	CCC	869	GLY	2.4
1	BBB	108	GLY	2.4
2	CCC	983	GLY	2.4
1	BBB	100	LEU	2.4
2	CCC	740	GLU	2.4
2	CCC	110	PRO	2.3
3	DDD	965	SER	2.3
2	CCC	188	PHE	2.3
3	DDD	1197	ASN	2.3
5	FFF	198	ILE	2.3
2	CCC	117	ILE	2.3
3	DDD	710	ASP	2.3
3	DDD	1119	ASP	2.3
3	DDD	952	VAL	2.3
1	AAA	75	GLN	2.3
2	CCC	909	LYS	2.2
1	BBB	92	VAL	2.2
5	FFF	318	GLN	2.2
2	CCC	722	GLY	2.2
3	DDD	127	LEU	2.2
3	DDD	1050	THR	2.2
7	222	23	DT	2.2
2	CCC	998	LEU	2.2
5	FFF	110	GLY	2.2
3	DDD	951	GLN	2.2
2	CCC	771	VAL	2.2
1	AAA	144	ILE	2.2
3	DDD	1118	GLY	2.1
3	DDD	985	ILE	2.1
3	DDD	1276	GLU	2.1
3	DDD	749	LYS	2.1
3	DDD	993	GLU	2.1
3	DDD	1290	ARG	2.1
2	CCC	990	ASP	2.1
3	DDD	1167	LYS	2.1
2	CCC	720	ARG	2.0
3	DDD	953	LYS	2.0
3	DDD	984	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
5	FFF	329	LEU	2.0
2	CCC	981	ALA	2.0
2	CCC	902	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

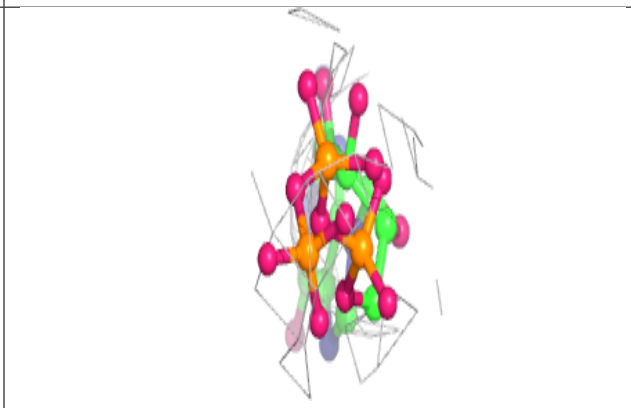
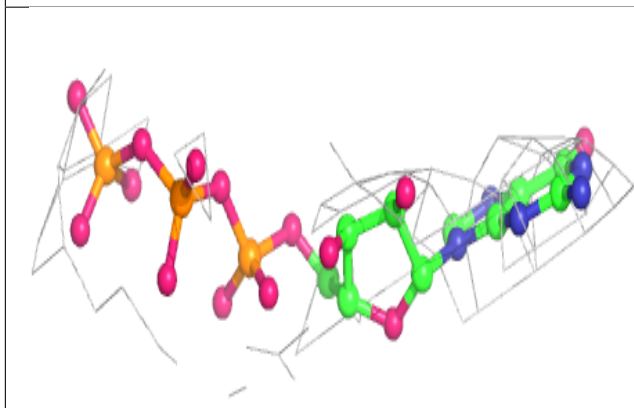
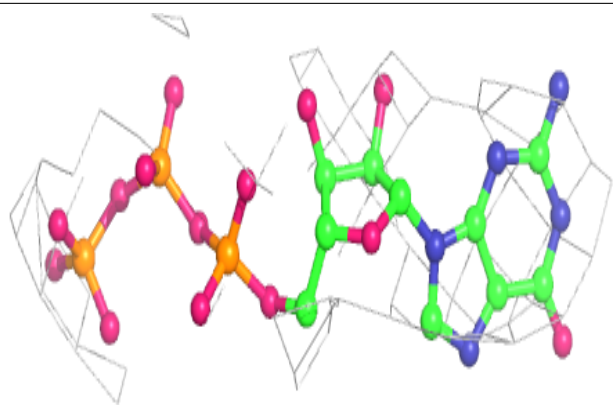
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	GTP	DDD	1504	32/32	0.88	0.37	241,284,349,363	0
9	MG	DDD	1503	1/1	0.94	0.22	122,122,122,122	0
9	MG	CCC	1401	1/1	0.96	0.41	120,120,120,120	0
10	ZN	DDD	1502	1/1	0.97	0.12	314,314,314,314	0
10	ZN	DDD	1501	1/1	0.98	0.03	332,332,332,332	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.

Electron density around GTP DDD 1504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.