



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2020 – 02:09 PM BST

PDB ID : 6UU7
Title : E. coli sigma-S transcription initiation complex with a 6-nt RNA and an NTP ("Old" crystal soaked with UTP, CTP, ddGTP, and dinucleotide ApG 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

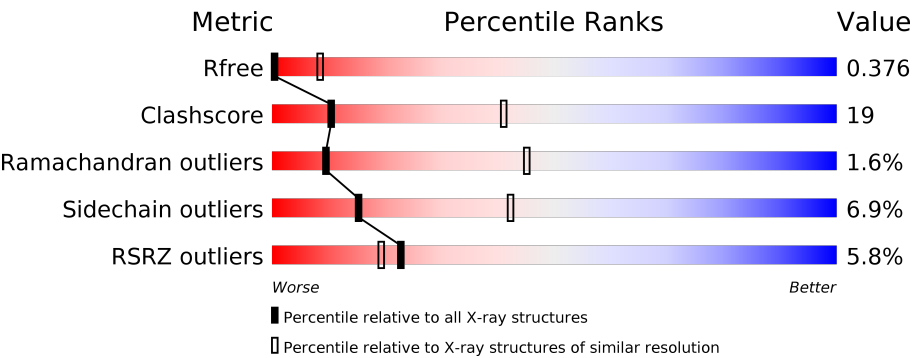
1 Overall quality at a glance i

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.



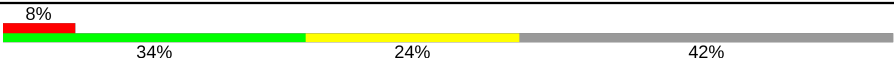

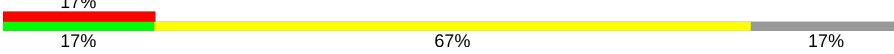
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1043 (5.00-3.80)
Clashscore	141614	1111 (5.00-3.80)
Ramachandran outliers	138981	1059 (5.00-3.80)
Sidechain outliers	138945	1041 (5.00-3.80)
RSRZ outliers	127900	1095 (5.08-3.70)

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>8%</div><div><div></div><div>60%</div><div>31%</div><div>• 5%</div></div></div>
1	BBB	242	<div><div>5%</div><div><div></div><div>61%</div><div>31%</div><div>• 6%</div></div></div>
2	CCC	1342	<div><div>3%</div><div><div></div><div>64%</div><div>32%</div><div>•</div></div></div>
3	DDD	1407	<div><div>7%</div><div><div></div><div>61%</div><div>33%</div><div>• •</div></div></div>
4	EEE	90	<div><div>3%</div><div><div></div><div>59%</div><div>27%</div><div>• 12%</div></div></div>
5	FFF	336	<div><div>5%</div><div><div></div><div>54%</div><div>24%</div><div>• 20%</div></div></div>

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Mol	Chain	Length	Quality of chain
6	111	50	
7	222	50	
8	333	6	

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
11	DG3	DDD	1505	-	-	X	X
9	ZN	DDD	1502	-	-	X	-

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 28934 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 P0A7Z4
AAA	-5	HIS	-	expression tag	UNP P0A7Z4
AAA	-4	HIS	-	expression tag	UNP P0A7Z4
AAA	-3	HIS	-	expression tag	UNP P0A7Z4
AAA	-2	HIS	-	expression tag	UNP P0A7Z4
AAA	-1	HIS	-	expression tag	UNP P0A7Z4
AAA	0	HIS	-	expression tag	UNP P0A7Z4
BBB	-6	ALA	-	expression tag	UNP P0A7Z4
BBB	-5	HIS	-	expression tag	UNP P0A7Z4
BBB	-4	HIS	-	expression tag	UNP P0A7Z4
BBB	-3	HIS	-	expression tag	UNP P0A7Z4
BBB	-2	HIS	-	expression tag	UNP P0A7Z4
BBB	-1	HIS	-	expression tag	UNP P0A7Z4
BBB	0	HIS	-	expression tag	UNP P0A7Z4

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	CCC	1341	Total	C	N	O	S	0	0	0
			10576	6636	1842	2055	43			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	DDD	1362	Total	C	N	O	S	0	0	0
			10568	6633	1887	1998	50			

- 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	270	Total	C	N	O	S	0	0	0
			2205	1383	407	411	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	29	Total	C	N	O	P	0	0	0
			595	283	107	176	29			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	222	32	Total	C	N	O	P	0	0	0
			652	312	117	192	31			

- Molecule 8 is DNA/RNA hybrid called DNA/RNA (5'-R(*AP*GP*UP*CP*U)-D(P*(DDG

))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	333	5	Total	C	N	O	P	0	0	0
			102	47	17	34	4			

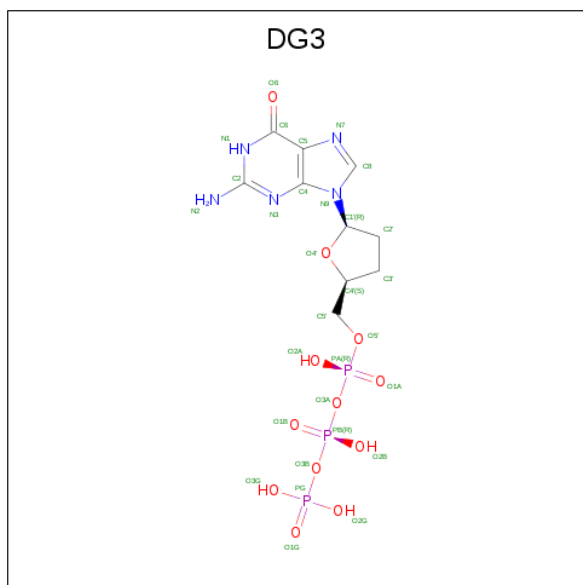
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

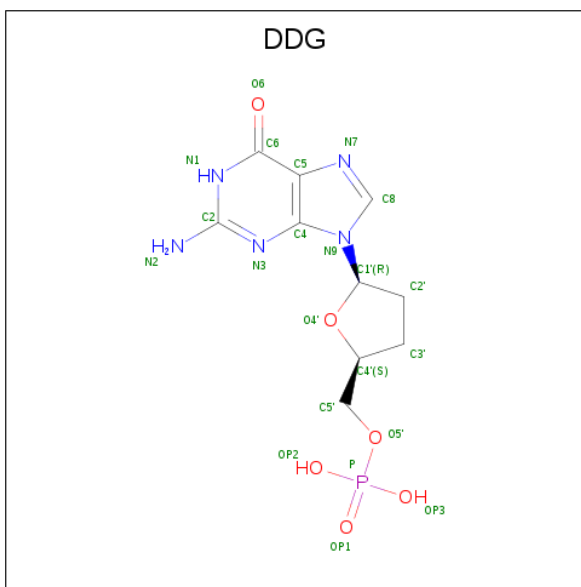
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	DDD	2	Total	Mg	0	0
			2	2		

- Molecule 11 is 2'-3'-DIDEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DG3) (formula: C₁₀H₁₆N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	DDD	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 12 is 2',3'-DIDEOXY-GUANOSINE-5'-MONOPHOSPHATE (three-letter code: DDG) (formula: C₁₀H₁₄N₅O₆P).

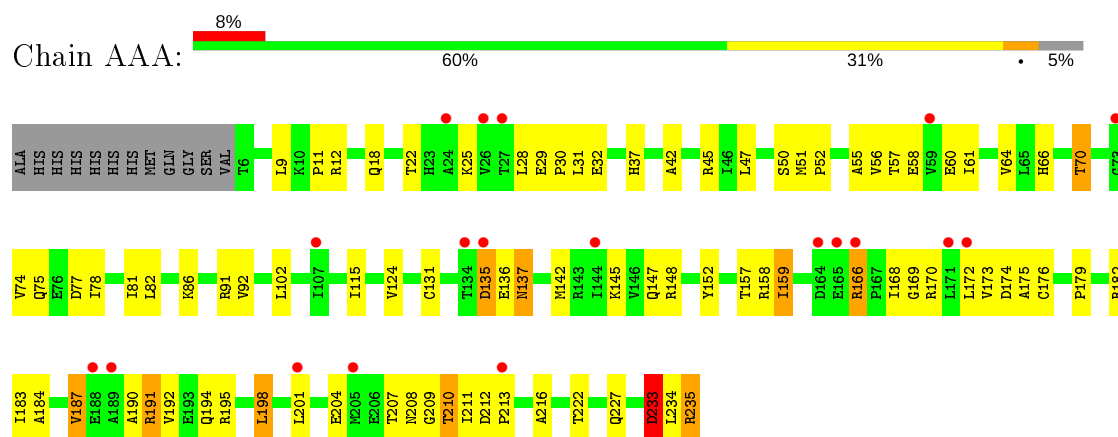


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	333	1	Total	C	N	O	P	0	0
			21	10	5	5	1		

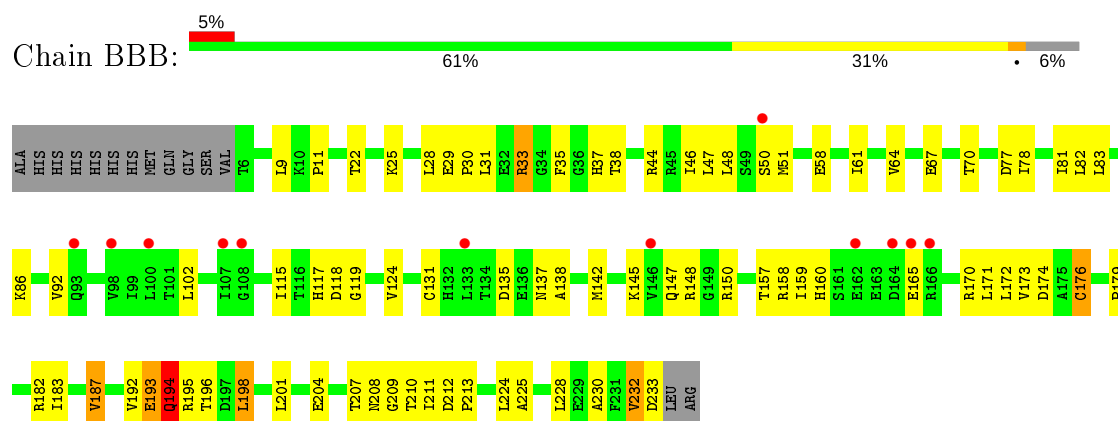
3 Residue-property plots [i](#)

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

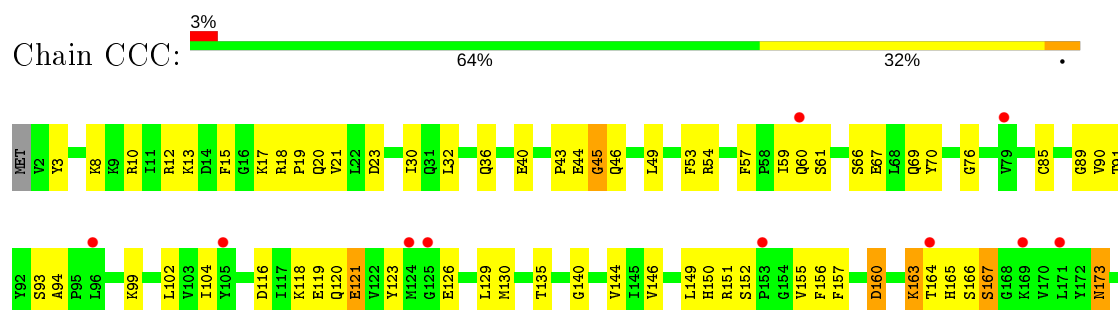
- Molecule 1: DNA-directed RNA polymerase subunit alpha

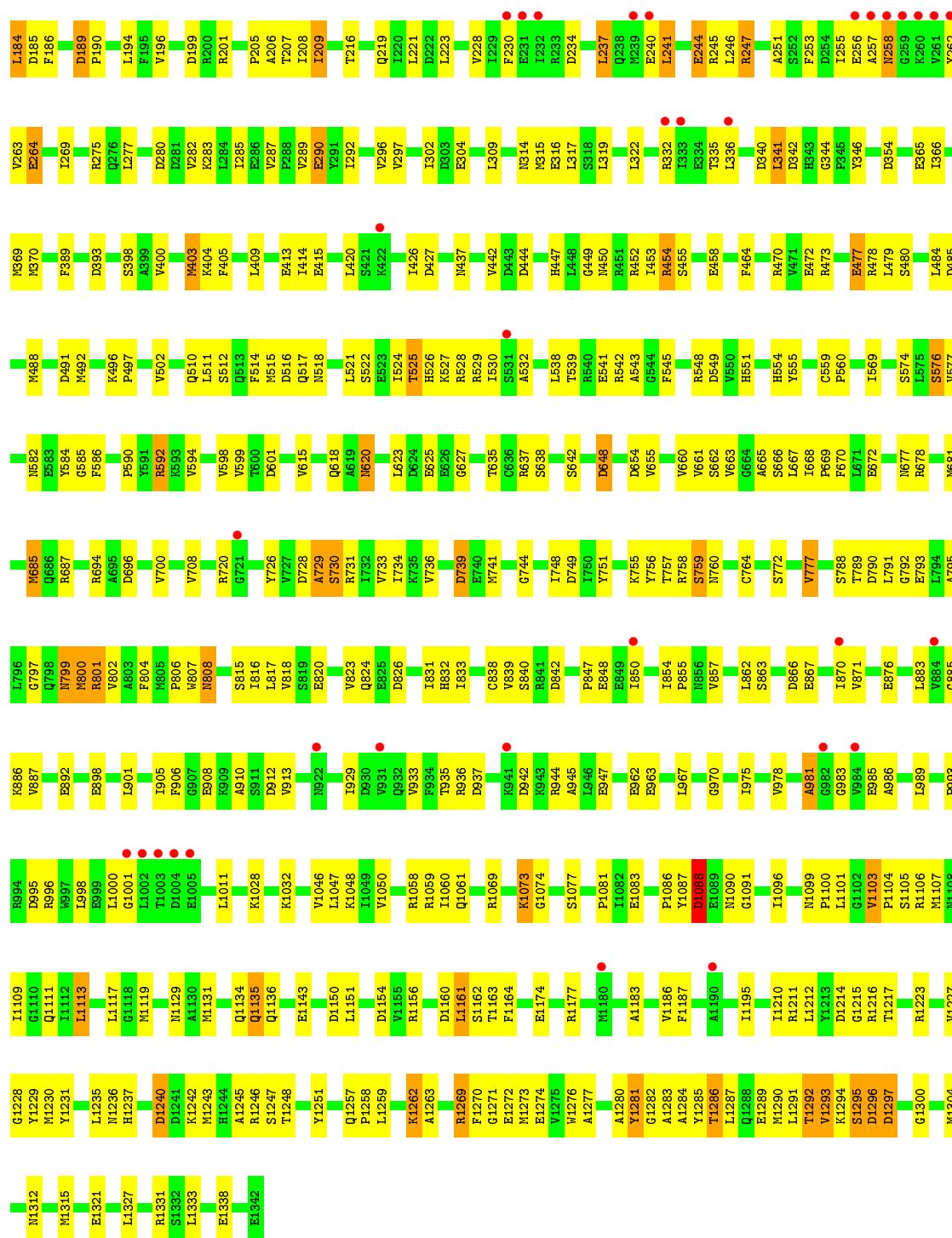


- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 2: DNA-directed RNA polymerase subunit beta

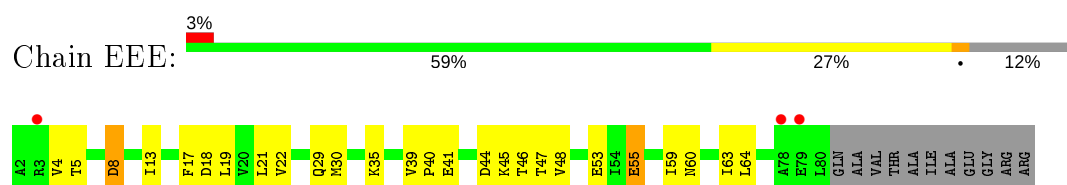




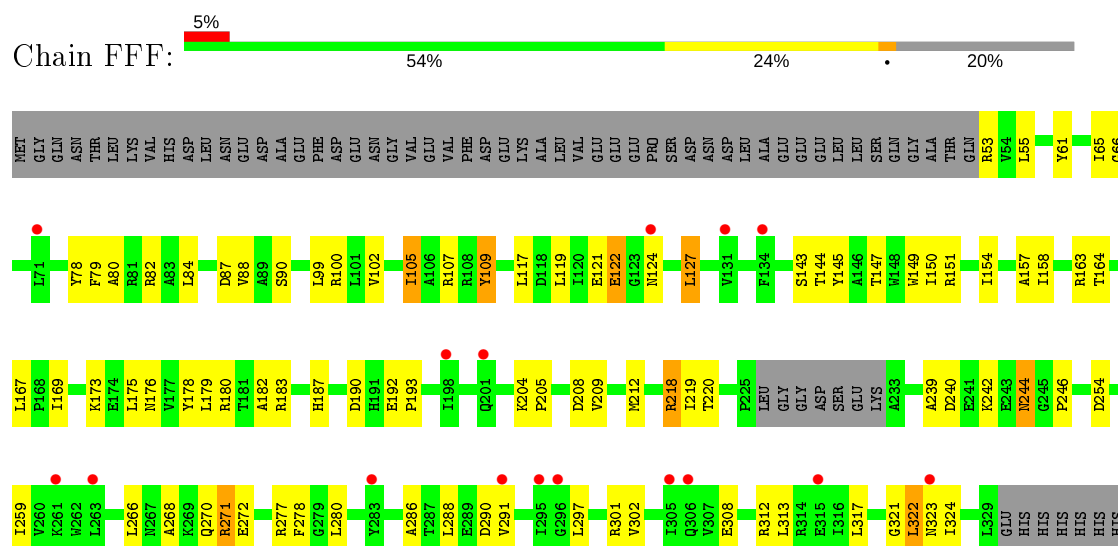
• Molecule 3: DNA-directed RNA polymerase subunit beta'



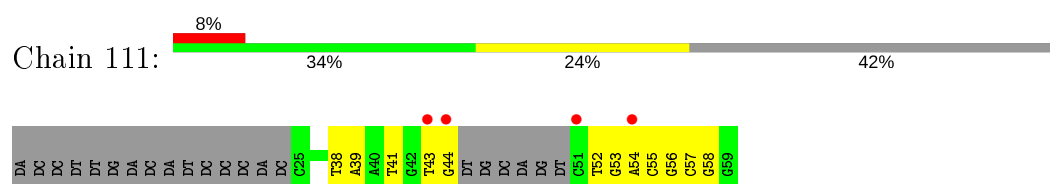




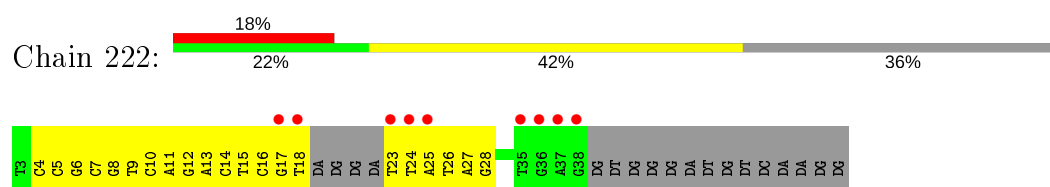
- Molecule 5: RNA polymerase sigma factor RpoS



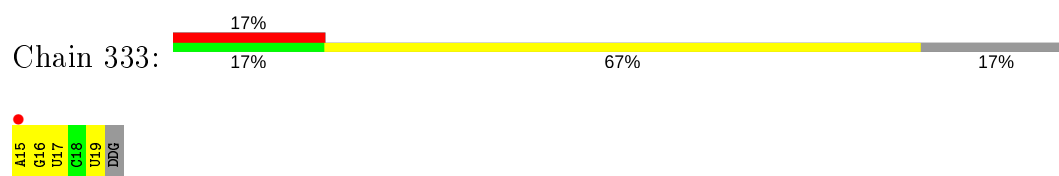
- Molecule 6: Synthetic DNA 50-mer (promoter non-template strand)



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



- Molecule 8: DNA/RNA (5'-R(*AP*GP*UP*CP*U)-D(P*(DDG))-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.94Å 153.77Å 232.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.15 – 4.40 49.15 – 4.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.15-4.40) 99.3 (49.15-4.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 4.45Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.344 , 0.390 0.332 , 0.376	Depositor DCC
R_{free} test set	1464 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	179.5	Xtriage
Anisotropy	0.664	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 229.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.30$, $\langle L^2 \rangle = 0.14$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	28934	wwPDB-VP
Average B, all atoms (Å ²)	304.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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: DG3, ZN, DDG, 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	0.63	0/1809	0.73	0/2450
1	BBB	0.64	0/1789	0.73	0/2425
2	CCC	0.62	0/10745	0.80	3/14499 (0.0%)
3	DDD	0.63	0/10729	0.78	0/14487
4	EEE	0.62	0/629	0.79	0/847
5	FFF	0.64	0/2233	0.63	0/3010
6	111	0.27	0/665	0.66	0/1022
7	222	0.26	0/729	0.62	0/1121
8	333	0.23	0/113	0.54	0/174
All	All	0.62	0/29441	0.76	3/40035 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	CCC	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	CCC	1088	ASP	CB-CA-C	-6.58	97.24	110.40
2	CCC	454	ARG	CB-CA-C	-5.48	99.44	110.40
2	CCC	1048	LYS	CB-CA-C	-5.36	99.69	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	CCC	1282	GLY	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	82	0
1	BBB	1767	0	1789	74	0
2	CCC	10576	0	10591	422	0
3	DDD	10568	0	10781	455	0
4	EEE	627	0	634	17	0
5	FFF	2205	0	2249	116	0
6	111	595	0	329	30	0
7	222	652	0	364	39	0
8	333	102	0	54	5	0
9	DDD	2	0	0	2	0
10	DDD	2	0	0	0	0
11	DDD	30	0	12	11	0
12	333	21	0	12	3	0
All	All	28934	0	28628	1068	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 19.

All (1068) 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:825:VAL:HG11	3:DDD:1242:ARG:NH1	1.51	1.24
3:DDD:572:THR:HG21	3:DDD:589:TYR:OH	1.35	1.19
5:FFF:266:LEU:HB3	5:FFF:312:ARG:HD2	1.29	1.13
5:FFF:266:LEU:HB3	5:FFF:312:ARG:CD	1.81	1.10
3:DDD:825:VAL:CG1	3:DDD:1242:ARG:HH12	1.70	1.04
2:CCC:525:THR:HG21	2:CCC:687:ARG:HD3	1.36	1.04
2:CCC:1281:TYR:OH	3:DDD:434:ILE:O	1.80	1.00
5:FFF:266:LEU:HD22	5:FFF:312:ARG:HB3	1.43	0.99
2:CCC:199:ASP:OD1	6:111:53:DG:N2	1.98	0.96
3:DDD:750:PRO:HA	3:DDD:781:LYS:HG2	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FFF:317:LEU:O	5:FFF:321:GLY:HA3	1.63	0.96
3:DDD:888:CYS:SG	9:DDD:1502:ZN:ZN	1.53	0.96
2:CCC:196:VAL:HG23	2:CCC:206:ALA:HA	1.45	0.96
3:DDD:800:LEU:HD22	3:DDD:1256:ILE:HD13	1.49	0.93
1:AAA:86:LYS:HG2	1:AAA:174:ASP:O	1.68	0.93
3:DDD:836:ARG:HD3	3:DDD:873:GLU:OE2	1.69	0.92
2:CCC:251:ALA:CB	2:CCC:263:VAL:HG11	1.99	0.92
1:BBB:179:PRO:HG3	1:BBB:211:ILE:HD12	1.50	0.91
3:DDD:388:ARG:NH2	3:DDD:414:GLU:OE1	2.02	0.91
2:CCC:32:LEU:HA	2:CCC:130:MET:HE1	1.50	0.91
3:DDD:932:MET:SD	11:DDD:1505:DG3:H2'2	2.11	0.91
5:FFF:317:LEU:O	5:FFF:321:GLY:CA	2.19	0.90
3:DDD:933:ARG:NH1	11:DDD:1505:DG3:O2B	2.04	0.90
1:AAA:227:GLN:OE1	1:BBB:11:PRO:HD3	1.71	0.88
5:FFF:183:ARG:NH2	7:222:26:DT:OP2	2.07	0.88
1:BBB:193:GLU:O	1:BBB:194:GLN:HB2	1.73	0.88
3:DDD:527:LEU:HB2	3:DDD:550:VAL:HG13	1.55	0.88
2:CCC:1073:LYS:NZ	12:333:101:DDG:OP2	2.07	0.88
3:DDD:791:ALA:HB2	7:222:9:DT:H72	1.56	0.88
2:CCC:199:ASP:HA	6:111:53:DG:H22	1.38	0.87
1:AAA:82:LEU:HD22	1:AAA:173:VAL:HG21	1.58	0.85
5:FFF:266:LEU:CD2	5:FFF:312:ARG:HB3	2.06	0.85
2:CCC:1291:LEU:HD11	3:DDD:1351:VAL:HG13	1.59	0.85
2:CCC:681:MET:O	2:CCC:685:MET:HG2	1.76	0.84
2:CCC:726:TYR:HB3	2:CCC:733:VAL:CG2	2.06	0.84
5:FFF:105:ILE:HG21	5:FFF:150:ILE:HG22	1.60	0.84
3:DDD:525:MET:O	3:DDD:548:VAL:HG22	1.78	0.84
2:CCC:804:PHE:O	3:DDD:638:SER:HB2	1.79	0.83
3:DDD:673:VAL:CG1	3:DDD:678:ARG:HB2	2.09	0.83
3:DDD:572:THR:CG2	3:DDD:589:TYR:OH	2.23	0.82
3:DDD:121:PRO:O	3:DDD:122:SER:HB3	1.80	0.82
3:DDD:793:SER:OG	3:DDD:928:THR:OG1	1.95	0.82
1:BBB:124:VAL:HG21	1:BBB:210:THR:HG22	1.59	0.82
3:DDD:888:CYS:HG	9:DDD:1502:ZN:ZN	0.86	0.82
3:DDD:800:LEU:HD23	3:DDD:1309:ILE:HD11	1.60	0.81
3:DDD:644:MET:O	3:DDD:764:ARG:NH1	2.12	0.81
2:CCC:555:TYR:CD1	2:CCC:637:ARG:NH2	2.49	0.81
1:BBB:67:GLU:HB3	1:BBB:171:LEU:HD22	1.63	0.80
2:CCC:790:ASP:O	2:CCC:792:GLY:N	2.14	0.80
3:DDD:26:SER:OG	3:DDD:28:ASP:OD1	1.99	0.80
2:CCC:1295:SER:OG	3:DDD:346:ARG:O	1.99	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FFF:288:LEU:HD22	5:FFF:302:VAL:HG11	1.64	0.80
3:DDD:528:THR:O	3:DDD:528:THR:OG1	1.99	0.79
1:AAA:227:GLN:OE1	1:BBB:11:PRO:CD	2.30	0.79
2:CCC:255:ILE:HD12	2:CCC:263:VAL:HG21	1.64	0.79
2:CCC:901:LEU:HD13	5:FFF:278:PHE:CE2	2.17	0.79
1:AAA:11:PRO:O	1:BBB:230:ALA:HB2	1.83	0.79
5:FFF:317:LEU:O	5:FFF:321:GLY:N	2.15	0.79
3:DDD:739:GLN:HG2	3:DDD:744:ARG:HG3	1.65	0.78
3:DDD:895:CYS:SG	3:DDD:898:CYS:HB2	2.22	0.78
1:AAA:11:PRO:O	1:BBB:230:ALA:CB	2.31	0.78
2:CCC:199:ASP:HA	6:111:53:DG:N2	1.99	0.78
3:DDD:820:ILE:HG12	3:DDD:1227:HIS:CD2	2.19	0.78
2:CCC:237:LEU:HD12	2:CCC:289:VAL:HA	1.65	0.78
2:CCC:165:HIS:CE1	2:CCC:190:PRO:HG3	2.18	0.78
3:DDD:475:GLU:O	3:DDD:479:GLU:HG2	1.84	0.77
2:CCC:1333:LEU:O	3:DDD:113:HIS:CE1	2.38	0.77
2:CCC:1281:TYR:OH	3:DDD:431:ARG:O	2.02	0.77
3:DDD:816:THR:HG22	3:DDD:818:GLU:H	1.48	0.77
2:CCC:1269:ARG:N	7:222:12:DG:OP1	2.17	0.76
5:FFF:163:ARG:HD3	5:FFF:167:LEU:HD12	1.67	0.76
3:DDD:22:ILE:HD11	3:DDD:1319:PHE:CE1	2.20	0.76
5:FFF:313:LEU:O	5:FFF:317:LEU:HG	1.86	0.76
2:CCC:186:PHE:CE1	2:CCC:196:VAL:HG22	2.19	0.76
3:DDD:839:VAL:HG13	3:DDD:882:VAL:HG11	1.67	0.75
1:AAA:56:VAL:O	1:AAA:175:ALA:HB2	1.86	0.75
2:CCC:525:THR:HG21	2:CCC:687:ARG:CD	2.14	0.75
3:DDD:525:MET:O	3:DDD:548:VAL:CG2	2.33	0.75
3:DDD:1029:THR:HG23	3:DDD:1121:LEU:HG	1.69	0.74
2:CCC:1077:SER:HA	3:DDD:356:THR:CG2	2.16	0.74
5:FFF:266:LEU:HD22	5:FFF:312:ARG:CB	2.17	0.74
2:CCC:94:ALA:HB2	2:CCC:129:LEU:HD11	1.68	0.74
2:CCC:898:GLU:HG3	5:FFF:259:ILE:CD1	2.17	0.74
2:CCC:560:PRO:HB2	3:DDD:776:THR:HG21	1.69	0.74
1:AAA:9:LEU:HD21	1:AAA:198:LEU:HD11	1.67	0.74
2:CCC:855:PRO:HB3	2:CCC:910:ALA:HB1	1.70	0.74
3:DDD:572:THR:OG1	3:DDD:576:ARG:HD2	1.88	0.74
2:CCC:3:TYR:O	2:CCC:8:LYS:HE3	1.88	0.73
2:CCC:510:GLN:HG3	8:333:16:G:H5'	1.70	0.73
3:DDD:698:MET:O	3:DDD:702:GLN:HB3	1.88	0.73
2:CCC:10:ARG:NH2	2:CCC:790:ASP:OD1	2.21	0.72
5:FFF:105:ILE:HG21	5:FFF:150:ILE:CG2	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:555:TYR:CE1	2:CCC:637:ARG:NH2	2.57	0.72
2:CCC:648:ASP:N	2:CCC:648:ASP:OD1	2.21	0.72
3:DDD:930:LEU:HD11	3:DDD:1246:VAL:CG2	2.18	0.72
2:CCC:251:ALA:HB2	2:CCC:263:VAL:HG11	1.68	0.72
3:DDD:1133:ASP:OD2	3:DDD:1134:ILE:N	2.23	0.72
3:DDD:820:ILE:CG1	3:DDD:1227:HIS:CD2	2.73	0.72
2:CCC:1088:ASP:HB3	2:CCC:1090:ASN:H	1.54	0.72
3:DDD:703:THR:OG1	3:DDD:704:GLU:N	2.22	0.72
1:BBB:9:LEU:HD21	1:BBB:198:LEU:HD11	1.71	0.72
5:FFF:144:THR:HG21	6:111:39:DA:OP2	1.90	0.71
2:CCC:244:GLU:HG2	2:CCC:245:ARG:N	2.06	0.71
2:CCC:700:VAL:O	2:CCC:1069:ARG:NH2	2.18	0.71
3:DDD:895:CYS:SG	3:DDD:898:CYS:CB	2.77	0.71
3:DDD:836:ARG:CD	3:DDD:873:GLU:OE2	2.36	0.71
5:FFF:164:THR:HB	5:FFF:219:ILE:HD12	1.71	0.71
3:DDD:291:ILE:HD11	5:FFF:99:LEU:HD21	1.73	0.71
2:CCC:32:LEU:HD23	2:CCC:130:MET:CE	2.21	0.70
2:CCC:18:ARG:NH2	2:CCC:620:ASN:O	2.24	0.70
3:DDD:312:ARG:O	3:DDD:312:ARG:HG2	1.91	0.70
3:DDD:552:ILE:CG2	3:DDD:580:TRP:CD1	2.74	0.70
3:DDD:820:ILE:CG1	3:DDD:1227:HIS:HD2	2.03	0.70
3:DDD:572:THR:HG21	3:DDD:589:TYR:CZ	2.27	0.70
3:DDD:931:THR:O	3:DDD:935:PHE:CD2	2.45	0.70
5:FFF:182:ALA:HB1	5:FFF:193:PRO:HG3	1.72	0.70
1:BBB:47:LEU:HA	1:BBB:51:MET:HG2	1.74	0.70
2:CCC:163:LYS:HG2	2:CCC:164:THR:N	2.06	0.70
1:BBB:82:LEU:HD22	1:BBB:173:VAL:HG21	1.72	0.69
2:CCC:93:SER:OG	2:CCC:126:GLU:OE1	2.10	0.69
2:CCC:221:LEU:HD11	2:CCC:314:ASN:HB2	1.74	0.69
3:DDD:134:ASP:CG	3:DDD:159:ILE:HD11	2.13	0.69
3:DDD:800:LEU:HD22	3:DDD:1256:ILE:CD1	2.22	0.69
3:DDD:173:GLY:O	3:DDD:175:GLU:N	2.25	0.69
2:CCC:230:PHE:CD1	2:CCC:292:ILE:HD11	2.28	0.69
5:FFF:266:LEU:HB3	5:FFF:312:ARG:HD3	1.70	0.69
2:CCC:342:ASP:O	2:CCC:437:ASN:CG	2.30	0.69
3:DDD:519:ASN:OD1	3:DDD:520:ALA:N	2.21	0.69
1:BBB:176:CYS:HB3	3:DDD:535:ARG:HH22	1.58	0.69
1:BBB:193:GLU:O	1:BBB:194:GLN:CB	2.41	0.69
2:CCC:1333:LEU:O	3:DDD:113:HIS:HE1	1.75	0.69
3:DDD:510:LEU:HD11	3:DDD:624:ILE:HG23	1.75	0.69
2:CCC:1237:HIS:HB3	2:CCC:1242:LYS:NZ	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:958:ILE:HG23	3:DDD:982:LEU:HD11	1.75	0.68
5:FFF:266:LEU:CB	5:FFF:312:ARG:HD2	2.18	0.68
3:DDD:458:ASN:HD21	11:DDD:1505:DG3:H3'1	1.57	0.68
1:AAA:82:LEU:HB3	1:AAA:173:VAL:HG11	1.75	0.68
1:AAA:182:ARG:NH1	2:CCC:1090:ASN:O	2.27	0.68
2:CCC:1106:ARG:HH12	11:DDD:1505:DG3:PG	2.16	0.68
3:DDD:958:ILE:HG23	3:DDD:982:LEU:CD1	2.24	0.68
6:111:58:DG:C2	7:222:6:DG:C2	2.82	0.68
1:AAA:86:LYS:NZ	2:CCC:826:ASP:OD2	2.27	0.68
1:BBB:83:LEU:HG	3:DDD:526:VAL:CG1	2.24	0.68
5:FFF:288:LEU:CD2	5:FFF:302:VAL:HG11	2.23	0.68
1:AAA:158:ARG:HD2	1:AAA:172:LEU:HD21	1.76	0.67
1:BBB:83:LEU:HG	3:DDD:526:VAL:HG11	1.76	0.67
6:111:55:DC:H42	7:222:8:DG:H1	1.42	0.67
5:FFF:107:ARG:HB2	6:111:44:DG:OP1	1.95	0.67
3:DDD:820:ILE:HG13	3:DDD:1227:HIS:HD2	1.60	0.67
2:CCC:1106:ARG:NH1	11:DDD:1505:DG3:PG	2.68	0.67
3:DDD:320:ASN:O	3:DDD:321:LYS:CB	2.43	0.67
3:DDD:58:CYS:SG	3:DDD:60:ARG:HB3	2.35	0.67
1:AAA:184:ALA:HB2	2:CCC:1091:GLY:HA3	1.76	0.67
1:BBB:176:CYS:HB3	3:DDD:535:ARG:NH2	2.10	0.67
2:CCC:1284:ALA:HA	3:DDD:1357:ILE:HD12	1.76	0.67
3:DDD:792:ASN:N	3:DDD:792:ASN:OD1	2.26	0.67
3:DDD:320:ASN:O	3:DDD:321:LYS:HB2	1.95	0.66
2:CCC:696:ASP:O	2:CCC:795:ALA:HB1	1.96	0.66
3:DDD:933:ARG:CZ	11:DDD:1505:DG3:O2B	2.43	0.66
2:CCC:906:PHE:HZ	5:FFF:324:ILE:HG12	1.60	0.66
2:CCC:201:ARG:HB2	2:CCC:369:MET:CE	2.26	0.66
3:DDD:378:LYS:N	3:DDD:379:PRO:HD2	2.10	0.66
3:DDD:525:MET:N	3:DDD:548:VAL:HG23	2.10	0.66
2:CCC:1287:LEU:HD23	3:DDD:1357:ILE:HD11	1.78	0.66
2:CCC:257:ALA:HB3	2:CCC:262:TYR:CE2	2.31	0.66
2:CCC:263:VAL:HG13	2:CCC:269:ILE:HD11	1.78	0.66
2:CCC:223:LEU:HD13	2:CCC:426:ILE:HD13	1.76	0.66
1:AAA:211:ILE:CG2	1:AAA:216:ALA:HB2	2.25	0.65
5:FFF:266:LEU:CB	5:FFF:312:ARG:CD	2.70	0.65
3:DDD:1023:HIS:O	3:DDD:1024:THR:HB	1.95	0.65
1:AAA:45:ARG:NH2	1:BBB:37:HIS:HB2	2.12	0.65
1:AAA:58:GLU:OE1	1:AAA:170:ARG:NE	2.30	0.64
3:DDD:552:ILE:HG21	3:DDD:580:TRP:CD1	2.32	0.64
6:111:52:DT:H2"	6:111:53:DG:C8	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:263:VAL:CG1	2:CCC:269:ILE:HD11	2.28	0.64
3:DDD:1134:ILE:HG23	3:DDD:1138:LEU:HG	1.79	0.64
3:DDD:114:ILE:HG12	3:DDD:311:ARG:HD2	1.78	0.64
2:CCC:541:GLU:HG3	2:CCC:542:ARG:N	2.12	0.64
3:DDD:97:VAL:HG12	3:DDD:101:ARG:HG3	1.80	0.64
5:FFF:61:TYR:CZ	5:FFF:65:ILE:HD11	2.33	0.64
2:CCC:1304:MET:CE	3:DDD:472:LEU:HD13	2.27	0.64
5:FFF:192:GLU:HG3	5:FFF:193:PRO:HD2	1.80	0.64
3:DDD:458:ASN:OD1	3:DDD:933:ARG:NH2	2.31	0.64
3:DDD:572:THR:HG21	3:DDD:589:TYR:HH	1.56	0.64
3:DDD:1161:GLY:HA3	3:DDD:1179:PRO:HA	1.80	0.63
3:DDD:839:VAL:HG12	3:DDD:839:VAL:O	1.97	0.63
3:DDD:555:TYR:O	3:DDD:586:GLY:HA2	1.98	0.63
2:CCC:19:PRO:HA	2:CCC:1156:ARG:HD2	1.80	0.63
2:CCC:1077:SER:HA	3:DDD:356:THR:HG23	1.79	0.63
3:DDD:609:TYR:HA	3:DDD:617:THR:HG21	1.81	0.63
4:EEE:8:ASP:OD1	4:EEE:8:ASP:N	2.30	0.63
5:FFF:119:LEU:HD21	5:FFF:158:ILE:HD11	1.80	0.63
1:BBB:22:THR:OG1	1:BBB:207:THR:O	2.10	0.63
1:AAA:158:ARG:HB3	1:AAA:172:LEU:HD21	1.80	0.63
1:AAA:37:HIS:NE2	1:AAA:187:VAL:HG21	2.13	0.63
2:CCC:1259:LEU:HD11	5:FFF:239:ALA:HB2	1.81	0.63
2:CCC:262:TYR:OH	2:CCC:280:ASP:OD2	2.16	0.63
2:CCC:201:ARG:HB2	2:CCC:369:MET:HE2	1.80	0.63
3:DDD:800:LEU:HD23	3:DDD:1309:ILE:CD1	2.28	0.63
3:DDD:850:LYS:HB2	3:DDD:851:PRO:HD2	1.79	0.63
2:CCC:199:ASP:CA	6:111:53:DG:N2	2.61	0.63
2:CCC:389:PHE:HB3	2:CCC:420:LEU:HD12	1.81	0.63
1:BBB:30:PRO:HB2	1:BBB:198:LEU:HD12	1.80	0.62
2:CCC:414:ILE:HG13	2:CCC:415:GLU:N	2.14	0.62
3:DDD:97:VAL:HG11	3:DDD:101:ARG:HE	1.64	0.62
3:DDD:48:THR:O	3:DDD:50:LYS:N	2.30	0.62
3:DDD:975:ILE:HD12	3:DDD:997:VAL:HG11	1.80	0.62
5:FFF:143:SER:CB	6:111:41:DT:H72	2.29	0.62
5:FFF:266:LEU:HD22	5:FFF:312:ARG:HD3	1.81	0.62
1:BBB:86:LYS:CE	1:BBB:173:VAL:HG12	2.29	0.62
2:CCC:43:PRO:O	2:CCC:54:ARG:NH1	2.31	0.62
3:DDD:139:LEU:HD22	3:DDD:300:GLN:HE22	1.63	0.62
2:CCC:241:LEU:HD13	2:CCC:285:ILE:HD12	1.82	0.62
2:CCC:184:LEU:HG	2:CCC:389:PHE:CE2	2.35	0.62
3:DDD:825:VAL:HG11	3:DDD:1242:ARG:HH12	0.73	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:807:LEU:CD2	3:DDD:1255:VAL:HG13	2.29	0.62
3:DDD:975:ILE:CD1	3:DDD:997:VAL:HG11	2.30	0.62
3:DDD:1338:ALA:HB3	3:DDD:1340:LYS:HG3	1.81	0.62
2:CCC:577:VAL:HG23	2:CCC:661:VAL:O	1.99	0.62
3:DDD:886:VAL:HG21	3:DDD:1230:THR:HG21	1.81	0.62
2:CCC:447:HIS:CD2	2:CCC:449:GLY:H	2.18	0.62
1:BBB:44:ARG:HH12	3:DDD:538:ARG:HB3	1.65	0.62
1:BBB:86:LYS:HE2	1:BBB:174:ASP:H	1.65	0.61
2:CCC:157:PHE:O	2:CCC:442:VAL:HG13	2.00	0.61
2:CCC:548:ARG:HD3	2:CCC:569:ILE:O	2.00	0.61
2:CCC:804:PHE:O	3:DDD:638:SER:CB	2.48	0.61
2:CCC:663:VAL:O	2:CCC:666:SER:OG	2.17	0.61
3:DDD:1029:THR:CG2	3:DDD:1121:LEU:HG	2.29	0.61
1:AAA:60:GLU:HG3	1:AAA:169:GLY:O	2.00	0.61
2:CCC:1270:PHE:CE1	2:CCC:1290:MET:CE	2.84	0.61
3:DDD:334:LYS:O	3:DDD:339:ARG:HB2	2.00	0.61
3:DDD:552:ILE:CG2	3:DDD:580:TRP:NE1	2.63	0.61
2:CCC:118:LYS:HD3	2:CCC:488:MET:HG2	1.82	0.61
2:CCC:151:ARG:HD3	6:111:54:DA:H61	1.64	0.61
2:CCC:49:LEU:CD2	2:CCC:464:PHE:CE2	2.84	0.61
1:BBB:25:LYS:HG2	1:BBB:204:GLU:HG2	1.83	0.61
3:DDD:849:LEU:HD11	3:DDD:853:THR:HA	1.83	0.61
5:FFF:268:ALA:HA	5:FFF:271:ARG:HG2	1.82	0.61
2:CCC:524:ILE:O	2:CCC:528:ARG:HG2	2.00	0.61
4:EEE:30:MET:HG2	4:EEE:35:LYS:O	2.01	0.61
1:BBB:33:ARG:NH1	2:CCC:1081:PRO:HB3	2.16	0.61
2:CCC:1129:ASN:HA	2:CCC:1177:ARG:HG3	1.81	0.61
3:DDD:609:TYR:HA	3:DDD:617:THR:CG2	2.31	0.60
3:DDD:791:ALA:HB2	7:222:9:DT:C7	2.30	0.60
2:CCC:3:TYR:O	2:CCC:8:LYS:CE	2.49	0.60
5:FFF:144:THR:HG22	6:111:39:DA:H8	1.66	0.60
2:CCC:340:ASP:HB3	2:CCC:341:LEU:HG	1.83	0.60
3:DDD:1257:VAL:HG22	3:DDD:1260:MET:CE	2.32	0.60
5:FFF:266:LEU:HD22	5:FFF:312:ARG:CD	2.30	0.60
2:CCC:289:VAL:HG12	2:CCC:319:LEU:HD23	1.82	0.60
2:CCC:898:GLU:HG3	5:FFF:259:ILE:HD11	1.82	0.60
1:BBB:48:LEU:HD22	3:DDD:535:ARG:HG3	1.83	0.60
5:FFF:271:ARG:HG3	5:FFF:272:GLU:N	2.16	0.60
1:BBB:37:HIS:NE2	1:BBB:187:VAL:HG21	2.16	0.60
2:CCC:1103:VAL:HB	2:CCC:1104:PRO:CD	2.32	0.60
2:CCC:302:ILE:HG22	2:CCC:309:LEU:HD23	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:559:CYS:HB2	2:CCC:662:SER:HB3	1.84	0.60
2:CCC:685:MET:HE2	2:CCC:1235:LEU:HD11	1.83	0.60
3:DDD:514:THR:OG1	3:DDD:595:ALA:HA	2.02	0.60
1:AAA:22:THR:OG1	1:AAA:207:THR:O	2.15	0.60
3:DDD:43:THR:OG1	3:DDD:44:ILE:N	2.34	0.60
1:AAA:30:PRO:HB2	1:AAA:198:LEU:HD12	1.84	0.60
1:AAA:55:ALA:HB1	1:AAA:175:ALA:HB1	1.83	0.60
2:CCC:514:PHE:HZ	7:222:16:DC:H4'	1.66	0.59
1:BBB:124:VAL:HG21	1:BBB:210:THR:CG2	2.31	0.59
3:DDD:797:THR:O	3:DDD:801:VAL:HG23	2.03	0.59
3:DDD:1134:ILE:HD11	3:DDD:1244:GLN:HG3	1.85	0.59
3:DDD:1282:TYR:CE1	3:DDD:1286:LYS:HD2	2.38	0.59
4:EEE:29:GLN:HB3	4:EEE:35:LYS:HG3	1.84	0.59
2:CCC:734:ILE:HD11	2:CCC:777:VAL:HG23	1.85	0.59
3:DDD:458:ASN:ND2	11:DDD:1505:DG3:H3'1	2.17	0.59
2:CCC:642:SER:CB	3:DDD:770:LEU:HD21	2.33	0.59
1:BBB:208:ASN:OD1	1:BBB:209:GLY:N	2.35	0.59
2:CCC:292:ILE:CG2	2:CCC:322:LEU:HD11	2.33	0.59
2:CCC:297:VAL:HG13	2:CCC:317:LEU:HG	1.84	0.59
2:CCC:1101:LEU:HD22	3:DDD:731:ARG:HB2	1.85	0.59
3:DDD:825:VAL:CG1	3:DDD:1242:ARG:NH1	2.45	0.59
3:DDD:385:LEU:CD2	3:DDD:411:ILE:HD13	2.31	0.59
4:EEE:53:GLU:HB3	4:EEE:59:ILE:HG12	1.84	0.59
3:DDD:1000:GLY:HA2	3:DDD:1028:ILE:HD12	1.83	0.58
2:CCC:549:ASP:CG	3:DDD:750:PRO:HG3	2.24	0.58
2:CCC:244:GLU:HG2	2:CCC:245:ARG:H	1.66	0.58
3:DDD:1003:LEU:HD23	3:DDD:1018:ALA:HB2	1.86	0.58
3:DDD:22:ILE:CD1	3:DDD:1319:PHE:CE1	2.86	0.58
3:DDD:673:VAL:HG11	3:DDD:678:ARG:HB2	1.83	0.58
2:CCC:1077:SER:HA	3:DDD:356:THR:HG21	1.84	0.58
2:CCC:1210:ILE:HD12	2:CCC:1227:VAL:HB	1.84	0.58
3:DDD:552:ILE:HG23	3:DDD:580:TRP:CD1	2.38	0.58
5:FFF:61:TYR:CE2	5:FFF:65:ILE:HD11	2.39	0.58
2:CCC:292:ILE:HB	2:CCC:322:LEU:HD11	1.86	0.58
2:CCC:1161:LEU:HD12	2:CCC:1164:PHE:CD2	2.39	0.58
3:DDD:245:LEU:HD12	3:DDD:246:PRO:HD2	1.84	0.58
1:AAA:86:LYS:CG	1:AAA:174:ASP:O	2.50	0.58
3:DDD:362:ARG:N	3:DDD:365:GLN:OE1	2.27	0.58
5:FFF:144:THR:HG22	6:111:39:DA:C8	2.38	0.58
2:CCC:1287:LEU:HD23	3:DDD:1357:ILE:CD1	2.33	0.58
3:DDD:519:ASN:HA	3:DDD:523:GLU:CD	2.24	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:211:ILE:HG21	1:AAA:216:ALA:HB2	1.85	0.58
1:BBB:58:GLU:OE1	1:BBB:170:ARG:NE	2.32	0.58
1:AAA:166:ARG:NH2	2:CCC:863:SER:OG	2.37	0.58
3:DDD:1257:VAL:HG22	3:DDD:1260:MET:HE3	1.85	0.58
3:DDD:1309:ILE:HG22	3:DDD:1310:THR:N	2.19	0.58
2:CCC:1304:MET:HE1	3:DDD:472:LEU:HD13	1.85	0.58
2:CCC:1161:LEU:HD12	2:CCC:1164:PHE:CE2	2.39	0.57
2:CCC:582:ASN:OD1	2:CCC:586:PHE:N	2.36	0.57
3:DDD:572:THR:OG1	3:DDD:576:ARG:CD	2.52	0.57
3:DDD:750:PRO:HB3	3:DDD:781:LYS:HB2	1.85	0.57
3:DDD:68:TYR:CD2	3:DDD:78:LEU:HD23	2.38	0.57
2:CCC:599:VAL:HG21	2:CCC:623:LEU:HD21	1.86	0.57
2:CCC:1186:VAL:HG12	2:CCC:1187:PHE:CD2	2.38	0.57
2:CCC:150:HIS:CE1	2:CCC:454:ARG:HG3	2.39	0.57
2:CCC:1106:ARG:NH1	11:DDD:1505:DG3:O2G	2.35	0.57
3:DDD:836:ARG:HD2	3:DDD:873:GLU:CD	2.25	0.57
3:DDD:1110:GLU:O	3:DDD:1113:VAL:HG23	2.03	0.57
3:DDD:385:LEU:HD23	3:DDD:411:ILE:HD13	1.86	0.57
5:FFF:78:TYR:OH	5:FFF:82:ARG:NH1	2.38	0.57
2:CCC:1105:SER:HB3	3:DDD:731:ARG:HG3	1.87	0.57
2:CCC:993:PRO:HG2	2:CCC:996:ARG:CZ	2.34	0.57
3:DDD:574:VAL:O	3:DDD:578:ILE:HG13	2.05	0.57
1:BBB:83:LEU:HD21	3:DDD:526:VAL:HB	1.86	0.57
2:CCC:1312:ASN:O	2:CCC:1312:ASN:OD1	2.21	0.57
2:CCC:528:ARG:HD2	2:CCC:663:VAL:HG21	1.87	0.57
3:DDD:1156:LEU:HB3	3:DDD:1207:GLY:HA2	1.85	0.57
5:FFF:244:ASN:N	5:FFF:244:ASN:OD1	2.37	0.57
1:BBB:86:LYS:HG2	1:BBB:174:ASP:O	2.04	0.57
2:CCC:369:MET:HG3	2:CCC:370:MET:N	2.19	0.57
2:CCC:516:ASP:O	2:CCC:522:SER:OG	2.16	0.57
2:CCC:726:TYR:HB3	2:CCC:733:VAL:HG22	1.85	0.57
2:CCC:734:ILE:CG2	2:CCC:749:ASP:HB2	2.34	0.57
3:DDD:1134:ILE:CD1	3:DDD:1244:GLN:HG3	2.35	0.57
2:CCC:342:ASP:O	2:CCC:437:ASN:ND2	2.37	0.57
2:CCC:36:GLN:O	2:CCC:40:GLU:HB2	2.05	0.57
1:BBB:135:ASP:OD1	1:BBB:138:ALA:HB2	2.04	0.57
3:DDD:803:VAL:CG2	3:DDD:1313:SER:OG	2.53	0.57
3:DDD:343:LEU:HD11	3:DDD:1324:SER:HB2	1.86	0.57
3:DDD:883:ARG:HG2	3:DDD:898:CYS:HA	1.87	0.57
3:DDD:176:PHE:O	3:DDD:176:PHE:CD2	2.58	0.56
3:DDD:609:TYR:CA	3:DDD:617:THR:HG21	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:1245:ALA:HB2	3:DDD:372:MET:HG3	1.86	0.56
2:CCC:898:GLU:HG3	5:FFF:259:ILE:HD13	1.85	0.56
2:CCC:560:PRO:O	3:DDD:780:ARG:NH2	2.38	0.56
2:CCC:661:VAL:HG13	2:CCC:665:ALA:HB3	1.86	0.56
2:CCC:736:VAL:HB	2:CCC:741:MET:HE2	1.88	0.56
1:AAA:145:LYS:HD3	1:AAA:147:GLN:HE21	1.71	0.56
2:CCC:12:ARG:NH2	2:CCC:793:GLU:OE1	2.36	0.56
3:DDD:1042:ASP:OD1	3:DDD:1043:GLY:N	2.38	0.56
3:DDD:849:LEU:HA	3:DDD:857:LEU:HB3	1.86	0.56
2:CCC:726:TYR:HB3	2:CCC:733:VAL:HG23	1.86	0.56
3:DDD:1275:LEU:HG	3:DDD:1276:GLU:H	1.71	0.56
3:DDD:800:LEU:CD2	3:DDD:1309:ILE:HD11	2.34	0.56
1:AAA:135:ASP:OD1	1:AAA:137:ASN:N	2.37	0.56
3:DDD:367:GLY:HA3	3:DDD:448:GLN:HB2	1.87	0.56
3:DDD:750:PRO:CA	3:DDD:781:LYS:HG2	2.29	0.56
6:111:58:DG:N2	7:222:6:DG:N3	2.54	0.56
1:AAA:50:SER:HG	1:BBB:35:PHE:HZ	1.54	0.56
2:CCC:666:SER:HA	2:CCC:1186:VAL:HG21	1.87	0.56
2:CCC:1294:LYS:HB3	3:DDD:347:VAL:HG13	1.86	0.56
1:BBB:86:LYS:HE2	1:BBB:173:VAL:HG12	1.88	0.56
2:CCC:1270:PHE:N	3:DDD:345:LYS:O	2.32	0.56
4:EEE:29:GLN:HE22	4:EEE:64:LEU:HD22	1.70	0.56
2:CCC:748:ILE:HD11	2:CCC:970:GLY:HA3	1.87	0.55
3:DDD:112:ALA:H	3:DDD:300:GLN:HE21	1.53	0.55
3:DDD:707:ILE:HD12	3:DDD:716:GLN:HE21	1.71	0.55
3:DDD:750:PRO:HA	3:DDD:781:LYS:CG	2.29	0.55
2:CCC:532:ALA:HB1	2:CCC:538:LEU:HD12	1.89	0.55
1:AAA:135:ASP:OD1	1:AAA:136:GLU:N	2.39	0.55
3:DDD:279:LEU:HD13	3:DDD:295:GLU:HB3	1.87	0.55
3:DDD:555:TYR:O	3:DDD:586:GLY:CA	2.54	0.55
3:DDD:488:ASN:OD1	4:EEE:5:THR:HG23	2.06	0.55
3:DDD:620:PHE:O	3:DDD:624:ILE:HG13	2.06	0.55
2:CCC:344:GLY:HA3	2:CCC:346:TYR:CZ	2.42	0.55
3:DDD:923:ILE:HD12	3:DDD:1256:ILE:HD12	1.89	0.55
3:DDD:68:TYR:C	3:DDD:92:VAL:HG13	2.27	0.55
3:DDD:950:ILE:HD13	3:DDD:995:TYR:HB3	1.89	0.55
6:111:58:DG:C2	7:222:6:DG:N2	2.75	0.55
2:CCC:1269:ARG:HD3	7:222:11:DA:H5'	1.89	0.55
3:DDD:820:ILE:HG13	3:DDD:1227:HIS:CD2	2.40	0.55
3:DDD:807:LEU:HD11	3:DDD:894:VAL:HG13	1.89	0.55
5:FFF:82:ARG:HG2	5:FFF:87:ASP:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:45:ARG:NH1	2:CCC:1216:ARG:HA	2.21	0.55
2:CCC:1283:ALA:HB1	2:CCC:1286:THR:OG1	2.07	0.55
3:DDD:111:THR:HG21	3:DDD:303:VAL:HG11	1.88	0.55
3:DDD:820:ILE:HG12	3:DDD:1227:HIS:CG	2.42	0.55
3:DDD:335:GLN:O	3:DDD:336:GLY:O	2.24	0.55
3:DDD:936:HIS:CE1	3:DDD:937:ILE:HG13	2.42	0.55
5:FFF:163:ARG:NH2	7:222:26:DT:O4	2.40	0.55
2:CCC:582:ASN:ND2	2:CCC:586:PHE:HB2	2.21	0.55
2:CCC:685:MET:HE2	2:CCC:1235:LEU:CD1	2.37	0.55
3:DDD:929:GLN:O	3:DDD:933:ARG:HB2	2.06	0.55
2:CCC:731:ARG:NH2	2:CCC:962:GLU:OE1	2.40	0.55
2:CCC:739:ASP:N	2:CCC:739:ASP:OD1	2.40	0.55
1:AAA:45:ARG:HH12	2:CCC:1216:ARG:HA	1.70	0.54
2:CCC:263:VAL:HG22	2:CCC:269:ILE:HD12	1.89	0.54
3:DDD:427:PRO:HG2	3:DDD:429:LEU:HD21	1.87	0.54
1:BBB:145:LYS:HD3	1:BBB:147:GLN:HE21	1.71	0.54
2:CCC:290:GLU:HG2	2:CCC:290:GLU:O	2.06	0.54
2:CCC:1160:ASP:O	2:CCC:1161:LEU:C	2.46	0.54
5:FFF:53:ARG:O	5:FFF:55:LEU:HG	2.07	0.54
2:CCC:514:PHE:HZ	7:222:16:DC:C4'	2.20	0.54
2:CCC:555:TYR:OH	2:CCC:654:ASP:OD2	2.18	0.54
1:AAA:124:VAL:HG21	1:AAA:210:THR:H	1.71	0.54
1:AAA:31:LEU:CD1	1:AAA:201:LEU:HB2	2.37	0.54
1:BBB:82:LEU:HD22	1:BBB:173:VAL:CG2	2.38	0.54
2:CCC:1210:ILE:HG22	2:CCC:1211:ARG:N	2.22	0.54
3:DDD:51:PRO:HB3	3:DDD:57:PHE:O	2.07	0.54
3:DDD:709:ARG:O	3:DDD:709:ARG:CG	2.56	0.54
2:CCC:199:ASP:C	6:111:53:DG:H21	2.11	0.54
3:DDD:134:ASP:CB	3:DDD:159:ILE:HD11	2.37	0.54
3:DDD:295:GLU:CD	5:FFF:121:GLU:HG2	2.27	0.54
3:DDD:476:ALA:HA	3:DDD:479:GLU:HG3	1.89	0.54
2:CCC:905:ILE:HD13	5:FFF:313:LEU:CD2	2.38	0.54
2:CCC:253:PHE:CE1	2:CCC:287:VAL:HG12	2.43	0.54
2:CCC:369:MET:CG	2:CCC:370:MET:N	2.70	0.54
2:CCC:118:LYS:NZ	2:CCC:485:ASP:O	2.31	0.54
2:CCC:496:LYS:HB3	7:222:24:DT:OP1	2.08	0.54
2:CCC:734:ILE:HD11	2:CCC:777:VAL:CG2	2.38	0.54
2:CCC:524:ILE:HD12	2:CCC:708:VAL:HG13	1.89	0.54
2:CCC:807:TRP:CH2	2:CCC:1086:PRO:HD3	2.43	0.54
5:FFF:297:LEU:HD22	5:FFF:301:ARG:HG2	1.89	0.54
8:333:19:U:O5'	8:333:19:U:H6	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:1270:PHE:CE1	2:CCC:1290:MET:HE1	2.43	0.53
7:222:10:DC:O2	12:333:101:DDG:N2	2.40	0.53
2:CCC:1274:GLU:HG2	3:DDD:424:ASN:ND2	2.23	0.53
3:DDD:812:ASP:N	3:DDD:812:ASP:OD1	2.40	0.53
5:FFF:122:GLU:HG2	5:FFF:157:ALA:HB2	1.88	0.53
1:AAA:209:GLY:O	1:AAA:210:THR:C	2.46	0.53
5:FFF:102:VAL:HG11	5:FFF:124:ASN:OD1	2.08	0.53
1:BBB:86:LYS:CE	1:BBB:174:ASP:HB2	2.38	0.53
3:DDD:974:VAL:HG11	3:DDD:1028:ILE:HD13	1.91	0.53
3:DDD:1029:THR:HG22	3:DDD:1121:LEU:HD11	1.90	0.53
3:DDD:1163:VAL:HG13	3:DDD:1176:VAL:O	2.07	0.53
3:DDD:803:VAL:HG23	3:DDD:1313:SER:OG	2.09	0.53
3:DDD:97:VAL:HG11	3:DDD:101:ARG:NE	2.23	0.53
1:BBB:225:ALA:HA	1:BBB:228:LEU:HD12	1.91	0.53
2:CCC:240:GLU:HA	2:CCC:283:LYS:O	2.09	0.53
2:CCC:661:VAL:HG12	2:CCC:662:SER:O	2.08	0.53
3:DDD:1133:ASP:CG	3:DDD:1134:ILE:H	2.11	0.53
3:DDD:16:GLU:OE2	3:DDD:1369:ARG:NH2	2.42	0.53
3:DDD:686:TRP:CD2	3:DDD:758:PRO:HG3	2.43	0.53
3:DDD:965:SER:CB	3:DDD:975:ILE:HA	2.37	0.53
3:DDD:886:VAL:HG21	3:DDD:1230:THR:CG2	2.39	0.53
2:CCC:199:ASP:OD1	6:111:53:DG:C2	2.61	0.53
3:DDD:97:VAL:CG1	3:DDD:101:ARG:HG3	2.39	0.53
3:DDD:525:MET:H	3:DDD:548:VAL:HG23	1.73	0.53
3:DDD:63:GLY:O	3:DDD:98:ARG:HD2	2.09	0.53
1:AAA:25:LYS:HG2	1:AAA:204:GLU:HG2	1.90	0.53
2:CCC:807:TRP:HZ3	2:CCC:1086:PRO:HG3	1.73	0.53
3:DDD:118:LYS:NZ	3:DDD:136:GLU:OE2	2.41	0.53
3:DDD:795:TYR:CZ	3:DDD:799:ARG:HD3	2.44	0.53
5:FFF:266:LEU:CB	5:FFF:312:ARG:HD3	2.37	0.53
1:AAA:29:GLU:HB2	1:AAA:30:PRO:HA	1.91	0.53
1:BBB:165:GLU:O	1:BBB:165:GLU:HG3	2.09	0.53
3:DDD:930:LEU:HD11	3:DDD:1246:VAL:HG21	1.89	0.53
3:DDD:1249:ASN:OD1	3:DDD:1250:ASP:N	2.41	0.53
3:DDD:836:ARG:CD	3:DDD:873:GLU:CD	2.77	0.53
5:FFF:220:THR:HG22	7:222:18:DT:H2'	1.91	0.53
7:222:14:DC:O5'	7:222:14:DC:H6	1.91	0.52
1:AAA:47:LEU:HD13	1:AAA:183:ILE:HD12	1.92	0.52
3:DDD:101:ARG:O	3:DDD:246:PRO:HG3	2.09	0.52
3:DDD:278:ARG:HB3	3:DDD:295:GLU:OE2	2.09	0.52
3:DDD:807:LEU:HD23	3:DDD:1255:VAL:HG13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:809:VAL:CG2	3:DDD:915:ILE:HD11	2.39	0.52
2:CCC:820:GLU:O	2:CCC:824:GLN:HG3	2.10	0.52
1:AAA:32:GLU:OE2	1:BBB:150:ARG:NH2	2.42	0.52
2:CCC:842:ASP:HB3	2:CCC:1047:LEU:HD21	1.92	0.52
3:DDD:1292:LEU:O	3:DDD:1296:GLY:N	2.36	0.52
4:EEE:18:ASP:O	4:EEE:22:VAL:HG23	2.10	0.52
2:CCC:277:LEU:HD12	2:CCC:282:VAL:HG21	1.92	0.52
2:CCC:444:ASP:O	2:CCC:450:ASN:ND2	2.41	0.52
3:DDD:396:ALA:HB2	5:FFF:323:ASN:HA	1.92	0.52
5:FFF:218:ARG:HB2	7:222:23:DT:O4	2.09	0.52
2:CCC:477:GLU:HG3	2:CCC:478:ARG:N	2.24	0.52
3:DDD:1155:ILE:HG22	3:DDD:1210:ILE:HD12	1.92	0.52
3:DDD:198:CYS:SG	3:DDD:224:LEU:HB3	2.50	0.52
3:DDD:97:VAL:CG1	3:DDD:101:ARG:HE	2.23	0.52
6:111:38:DT:H2"	6:111:39:DA:C8	2.44	0.52
1:BBB:192:VAL:O	1:BBB:194:GLN:N	2.43	0.52
1:BBB:29:GLU:HB2	1:BBB:30:PRO:HA	1.90	0.52
2:CCC:1103:VAL:HB	2:CCC:1104:PRO:HD3	1.91	0.52
3:DDD:115:TRP:CZ2	3:DDD:1329:THR:HG22	2.45	0.52
5:FFF:240:ASP:OD1	5:FFF:242:LYS:HG2	2.10	0.52
1:AAA:124:VAL:HG11	1:AAA:209:GLY:CA	2.40	0.52
1:BBB:86:LYS:HE3	1:BBB:173:VAL:HG12	1.91	0.52
2:CCC:720:ARG:HD2	2:CCC:736:VAL:HG21	1.91	0.52
3:DDD:622:ASP:HB3	3:DDD:626:TYR:HE2	1.75	0.52
3:DDD:709:ARG:O	3:DDD:710:ASP:C	2.46	0.52
2:CCC:700:VAL:HG13	2:CCC:1117:LEU:HD23	1.92	0.51
3:DDD:333:GLY:O	3:DDD:336:GLY:N	2.35	0.51
2:CCC:590:PRO:HB2	2:CCC:655:VAL:HG21	1.91	0.51
1:AAA:152:TYR:CE2	2:CCC:824:GLN:HA	2.45	0.51
3:DDD:209:ASN:HB2	3:DDD:214:ARG:HG3	1.92	0.51
1:BBB:176:CYS:CB	3:DDD:535:ARG:HH22	2.23	0.51
3:DDD:517:CYS:HB3	3:DDD:545:HIS:HB2	1.91	0.51
3:DDD:974:VAL:CG1	3:DDD:1028:ILE:HD13	2.40	0.51
1:AAA:42:ALA:HA	1:BBB:38:THR:HG23	1.93	0.51
1:BBB:86:LYS:HE2	1:BBB:174:ASP:N	2.25	0.51
2:CCC:13:LYS:NZ	2:CCC:1151:LEU:HB3	2.26	0.51
2:CCC:661:VAL:CG1	2:CCC:665:ALA:HB3	2.40	0.51
3:DDD:396:ALA:HB2	5:FFF:323:ASN:CB	2.40	0.51
3:DDD:464:ASP:OD1	3:DDD:464:ASP:N	2.43	0.51
2:CCC:1214:ASP:OD2	2:CCC:1217:THR:HG23	2.10	0.51
3:DDD:1270:GLY:HA2	3:DDD:1298:VAL:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FFF:66:GLY:HA2	5:FFF:100:ARG:NH2	2.25	0.51
3:DDD:279:LEU:O	3:DDD:283:LEU:HG	2.10	0.51
2:CCC:672:GLU:HG2	2:CCC:1187:PHE:HA	1.92	0.51
3:DDD:888:CYS:CB	3:DDD:898:CYS:SG	2.98	0.51
5:FFF:317:LEU:CD1	5:FFF:324:ILE:HD13	2.41	0.51
7:222:5:DC:H2'	7:222:6:DG:OP2	2.10	0.51
3:DDD:1064:SER:HA	3:DDD:1067:ARG:HB3	1.93	0.51
3:DDD:1146:GLU:OE2	3:DDD:1309:ILE:CG2	2.59	0.51
2:CCC:1284:ALA:HA	3:DDD:1357:ILE:CD1	2.40	0.51
2:CCC:1101:LEU:HD13	3:DDD:504:GLN:HG3	1.91	0.51
3:DDD:707:ILE:HD12	3:DDD:716:GLN:NE2	2.26	0.51
2:CCC:1292:THR:CG2	2:CCC:1293:VAL:N	2.74	0.51
2:CCC:302:ILE:CG2	2:CCC:309:LEU:HD23	2.40	0.51
3:DDD:487:THR:O	3:DDD:490:ILE:HG13	2.11	0.50
3:DDD:885:VAL:O	3:DDD:1258:ARG:HD2	2.11	0.50
2:CCC:1111:GLN:HB2	2:CCC:1230:MET:HE1	1.92	0.50
2:CCC:555:TYR:CE1	2:CCC:637:ARG:CZ	2.95	0.50
2:CCC:799:ASN:HA	2:CCC:1231:TYR:HA	1.92	0.50
3:DDD:97:VAL:CG1	3:DDD:101:ARG:NE	2.74	0.50
2:CCC:1291:LEU:CD1	3:DDD:1351:VAL:HG13	2.35	0.50
3:DDD:295:GLU:OE1	5:FFF:121:GLU:HG2	2.10	0.50
3:DDD:530:PRO:HD3	3:DDD:552:ILE:CD1	2.40	0.50
2:CCC:89:GLY:HA2	2:CCC:140:GLY:HA3	1.94	0.50
3:DDD:423:LEU:HB3	3:DDD:466:MET:HE1	1.92	0.50
1:BBB:64:VAL:HG13	1:BBB:78:ILE:HD13	1.94	0.50
2:CCC:1099:ASN:ND2	3:DDD:504:GLN:HE21	2.09	0.50
2:CCC:1327:LEU:O	2:CCC:1331:ARG:HG3	2.12	0.50
3:DDD:1052:GLU:HG2	3:DDD:1053:LEU:H	1.75	0.50
3:DDD:261:ALA:HA	5:FFF:220:THR:O	2.12	0.50
8:333:15:A:H2'	8:333:16:G:H8	1.77	0.50
2:CCC:1312:ASN:C	2:CCC:1312:ASN:OD1	2.50	0.50
2:CCC:155:VAL:CG2	2:CCC:405:PHE:CD2	2.94	0.50
2:CCC:366:ILE:O	2:CCC:369:MET:HG2	2.10	0.50
2:CCC:871:VAL:CG2	2:CCC:883:LEU:HA	2.42	0.50
3:DDD:1368:ASP:O	3:DDD:1371:ARG:HG2	2.11	0.50
1:AAA:55:ALA:CB	1:AAA:175:ALA:HB1	2.41	0.50
1:BBB:29:GLU:CB	1:BBB:30:PRO:HA	2.42	0.50
2:CCC:66:SER:HB2	2:CCC:479:LEU:HD22	1.93	0.50
3:DDD:68:TYR:CE1	3:DDD:93:THR:HA	2.47	0.50
1:AAA:179:PRO:HG3	1:AAA:211:ILE:CD1	2.42	0.50
2:CCC:292:ILE:HG21	2:CCC:322:LEU:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:421:VAL:CG1	3:DDD:468:VAL:HG13	2.42	0.50
3:DDD:1263:LYS:CG	3:DDD:1307:LEU:HD11	2.42	0.50
2:CCC:1281:TYR:CE1	3:DDD:431:ARG:HG3	2.47	0.50
7:222:14:DC:H2'	7:222:15:DT:C6	2.47	0.49
1:BBB:92:VAL:O	1:BBB:148:ARG:NH2	2.45	0.49
2:CCC:478:ARG:NH1	2:CCC:491:ASP:O	2.45	0.49
3:DDD:850:LYS:HB2	3:DDD:851:PRO:CD	2.41	0.49
3:DDD:364:HIS:CD2	4:EEE:4:VAL:HG13	2.46	0.49
2:CCC:521:LEU:HD13	2:CCC:667:LEU:HD11	1.94	0.49
3:DDD:234:PRO:O	3:DDD:237:MET:HG3	2.12	0.49
3:DDD:295:GLU:OE2	5:FFF:121:GLU:HG2	2.12	0.49
3:DDD:378:LYS:N	3:DDD:379:PRO:CD	2.76	0.49
1:BBB:182:ARG:HG3	3:DDD:534:GLU:OE2	2.12	0.49
3:DDD:478:LEU:HG	4:EEE:47:THR:HG23	1.94	0.49
3:DDD:1082:ASP:OD1	3:DDD:1084:GLN:N	2.45	0.49
2:CCC:1273:MET:SD	3:DDD:428:THR:O	2.71	0.49
2:CCC:1161:LEU:O	2:CCC:1163:THR:N	2.45	0.49
2:CCC:555:TYR:CD1	2:CCC:637:ARG:CZ	2.96	0.49
3:DDD:121:PRO:O	3:DDD:122:SER:CB	2.53	0.49
3:DDD:925:GLU:HB3	3:DDD:926:PRO:HD3	1.94	0.49
3:DDD:943:ARG:HG2	3:DDD:944:ALA:N	2.28	0.49
5:FFF:277:ARG:HB2	5:FFF:291:VAL:HG21	1.93	0.49
2:CCC:1269:ARG:HB2	7:222:12:DG:P	2.53	0.49
5:FFF:180:ARG:NH2	7:222:27:DA:O5'	2.45	0.49
1:AAA:86:LYS:HE2	1:AAA:174:ASP:N	2.28	0.49
3:DDD:1133:ASP:CG	3:DDD:1134:ILE:N	2.66	0.49
3:DDD:425:ARG:HH22	11:DDD:1505:DG3:C4'	2.25	0.49
5:FFF:80:ALA:O	5:FFF:84:LEU:HG	2.13	0.49
5:FFF:163:ARG:NH2	7:222:25:DA:N1	2.61	0.49
2:CCC:32:LEU:HD23	2:CCC:130:MET:HE1	1.92	0.49
1:AAA:70:THR:HG21	2:CCC:755:LYS:HG3	1.93	0.49
5:FFF:169:ILE:O	5:FFF:173:LYS:HG2	2.12	0.49
2:CCC:797:GLY:O	2:CCC:1231:TYR:OH	2.31	0.49
2:CCC:850:ILE:O	2:CCC:850:ILE:HG22	2.13	0.49
3:DDD:1060:VAL:HG22	3:DDD:1106:ILE:HG12	1.94	0.49
1:AAA:152:TYR:CZ	2:CCC:824:GLN:HA	2.48	0.49
1:BBB:157:THR:HG22	1:BBB:157:THR:O	2.13	0.49
2:CCC:244:GLU:O	2:CCC:245:ARG:C	2.51	0.49
2:CCC:297:VAL:HG22	2:CCC:315:MET:O	2.13	0.49
2:CCC:369:MET:HG2	2:CCC:370:MET:HG2	1.95	0.49
2:CCC:447:HIS:HD2	2:CCC:449:GLY:H	1.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:551:HIS:H	2:CCC:554:HIS:CE1	2.30	0.49
5:FFF:208:ASP:O	5:FFF:212:MET:HG2	2.12	0.49
5:FFF:317:LEU:HD13	5:FFF:324:ILE:HD13	1.94	0.49
2:CCC:1285:TYR:CD2	3:DDD:1361:THR:HG21	2.48	0.49
2:CCC:216:THR:HG23	2:CCC:219:GLN:OE1	2.12	0.49
2:CCC:344:GLY:HA3	2:CCC:346:TYR:CE2	2.47	0.49
2:CCC:49:LEU:HD22	2:CCC:464:PHE:CE2	2.48	0.49
3:DDD:1238:GLN:O	3:DDD:1242:ARG:HB2	2.12	0.49
1:AAA:92:VAL:O	1:AAA:148:ARG:NH2	2.46	0.48
1:AAA:86:LYS:HE2	1:AAA:174:ASP:H	1.78	0.48
1:AAA:174:ASP:OD2	2:CCC:1059:ARG:NH2	2.46	0.48
2:CCC:257:ALA:O	2:CCC:258:ASN:HB3	2.13	0.48
2:CCC:263:VAL:HG12	2:CCC:264:GLU:O	2.13	0.48
2:CCC:799:ASN:C	2:CCC:800:MET:HG2	2.33	0.48
3:DDD:1041:ILE:CG2	3:DDD:1044:GLN:HG3	2.43	0.48
3:DDD:151:MET:SD	3:DDD:151:MET:N	2.86	0.48
3:DDD:584:PRO:HD3	3:DDD:620:PHE:CD1	2.48	0.48
1:AAA:86:LYS:CE	1:AAA:174:ASP:HB2	2.43	0.48
2:CCC:61:SER:HG	2:CCC:480:SER:HG	1.61	0.48
3:DDD:1079:LYS:HE3	3:DDD:1087:ASP:OD1	2.13	0.48
3:DDD:1308:GLY:O	3:DDD:1310:THR:N	2.47	0.48
3:DDD:382:TYR:OH	3:DDD:398:LYS:HG2	2.14	0.48
3:DDD:1146:GLU:OE2	3:DDD:1309:ILE:HG22	2.13	0.48
2:CCC:1251:TYR:HE2	5:FFF:246:PRO:HD3	1.78	0.48
2:CCC:660:VAL:HG21	3:DDD:769:VAL:HG12	1.95	0.48
8:333:16:G:H2'	8:333:17:U:C6	2.49	0.48
3:DDD:1111:ASP:OD1	3:DDD:1112:GLY:N	2.46	0.48
3:DDD:1029:THR:CG2	3:DDD:1121:LEU:HD11	2.43	0.48
7:222:9:DT:H2'	7:222:10:DC:C6	2.48	0.48
7:222:27:DA:H2''	7:222:28:DG:C8	2.48	0.48
2:CCC:479:LEU:HD21	2:CCC:492:MET:HE1	1.96	0.48
2:CCC:49:LEU:HD23	2:CCC:464:PHE:CD2	2.49	0.48
2:CCC:521:LEU:HD13	2:CCC:667:LEU:CD1	2.44	0.48
3:DDD:1029:THR:CG2	3:DDD:1121:LEU:CG	2.90	0.48
3:DDD:848:VAL:O	3:DDD:848:VAL:HG12	2.13	0.48
2:CCC:199:ASP:CA	6:111:53:DG:H22	2.14	0.48
1:AAA:190:ALA:O	1:AAA:192:VAL:N	2.47	0.48
2:CCC:20:GLN:O	2:CCC:20:GLN:HG3	2.14	0.48
6:111:53:DG:H2''	6:111:54:DA:OP1	2.14	0.48
1:AAA:52:PRO:O	1:AAA:211:ILE:HD11	2.12	0.48
2:CCC:453:ILE:HD11	2:CCC:530:ILE:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:803:VAL:HG21	3:DDD:1309:ILE:HA	1.95	0.48
5:FFF:178:TYR:CE1	5:FFF:209:VAL:HG22	2.49	0.48
2:CCC:823:VAL:HG22	2:CCC:1060:ILE:CG2	2.44	0.48
2:CCC:228:VAL:HG22	2:CCC:245:ARG:NH1	2.28	0.48
2:CCC:569:ILE:O	2:CCC:569:ILE:HG23	2.13	0.48
3:DDD:645:VAL:O	3:DDD:645:VAL:HG23	2.14	0.48
1:AAA:102:LEU:HB2	1:AAA:115:ILE:HG12	1.96	0.47
2:CCC:1001:GLY:HA2	2:CCC:1011:LEU:CD2	2.44	0.47
3:DDD:1163:VAL:HG11	3:DDD:1175:LEU:HD11	1.95	0.47
3:DDD:115:TRP:O	3:DDD:119:SER:HB3	2.14	0.47
1:AAA:211:ILE:HG22	1:AAA:216:ALA:HB2	1.94	0.47
2:CCC:119:GLU:O	2:CCC:119:GLU:HG3	2.13	0.47
2:CCC:194:LEU:HA	2:CCC:194:LEU:HD12	1.78	0.47
3:DDD:807:LEU:HD22	3:DDD:1255:VAL:HG13	1.96	0.47
3:DDD:418:GLU:OE1	4:EEE:48:VAL:HG21	2.14	0.47
5:FFF:266:LEU:CD2	5:FFF:312:ARG:HD3	2.44	0.47
2:CCC:1081:PRO:CB	2:CCC:1083:GLU:OE2	2.61	0.47
5:FFF:192:GLU:CG	5:FFF:193:PRO:HD2	2.43	0.47
1:AAA:124:VAL:HG11	1:AAA:209:GLY:HA2	1.95	0.47
2:CCC:1083:GLU:H	2:CCC:1083:GLU:CD	2.17	0.47
2:CCC:1269:ARG:HH21	2:CCC:1271:GLY:HA2	1.80	0.47
2:CCC:594:VAL:HG22	2:CCC:599:VAL:HG22	1.95	0.47
3:DDD:108:ALA:HB3	3:DDD:279:LEU:HD23	1.96	0.47
3:DDD:44:ILE:HG22	3:DDD:51:PRO:HA	1.95	0.47
3:DDD:739:GLN:HG2	3:DDD:744:ARG:HA	1.97	0.47
4:EEE:17:PHE:O	4:EEE:21:LEU:HG	2.14	0.47
2:CCC:870:ILE:HD12	2:CCC:1050:VAL:HG11	1.97	0.47
2:CCC:173:ASN:C	2:CCC:173:ASN:OD1	2.52	0.47
2:CCC:296:VAL:HB	2:CCC:336:LEU:HD12	1.95	0.47
2:CCC:854:ILE:HD11	2:CCC:885:GLY:HA3	1.95	0.47
3:DDD:1168:GLU:OE2	3:DDD:1173:ARG:NH1	2.48	0.47
3:DDD:965:SER:HB2	3:DDD:975:ILE:HA	1.97	0.47
5:FFF:182:ALA:CB	5:FFF:193:PRO:HG3	2.43	0.47
2:CCC:452:ARG:NH1	2:CCC:458:GLU:OE2	2.42	0.47
2:CCC:840:SER:HB3	2:CCC:850:ILE:HD11	1.97	0.47
3:DDD:347:VAL:HG12	3:DDD:348:ASP:O	2.15	0.47
3:DDD:809:VAL:HG22	3:DDD:915:ILE:HD11	1.96	0.47
2:CCC:1088:ASP:HB3	2:CCC:1090:ASN:N	2.25	0.47
2:CCC:1214:ASP:C	2:CCC:1214:ASP:OD1	2.49	0.47
2:CCC:263:VAL:HG22	2:CCC:269:ILE:CD1	2.44	0.47
2:CCC:545:PHE:CE1	3:DDD:788:LEU:HD12	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FFF:183:ARG:O	5:FFF:187:HIS:ND1	2.48	0.47
6:111:58:DG:N2	7:222:6:DG:C2	2.82	0.47
1:AAA:29:GLU:CB	1:AAA:30:PRO:HA	2.43	0.47
2:CCC:1117:LEU:HD13	2:CCC:1195:ILE:HG12	1.96	0.47
3:DDD:1029:THR:HG22	3:DDD:1121:LEU:CD1	2.45	0.47
3:DDD:120:LEU:HA	3:DDD:121:PRO:C	2.34	0.47
1:BBB:64:VAL:CG1	1:BBB:78:ILE:HD13	2.45	0.47
2:CCC:201:ARG:HB2	2:CCC:369:MET:HE1	1.96	0.47
3:DDD:820:ILE:HG12	3:DDD:1227:HIS:CB	2.45	0.47
2:CCC:1291:LEU:HD13	3:DDD:1351:VAL:O	2.14	0.47
2:CCC:1101:LEU:O	3:DDD:731:ARG:HG2	2.14	0.47
3:DDD:795:TYR:CE2	3:DDD:799:ARG:NE	2.83	0.47
3:DDD:863:LEU:HD22	3:DDD:908:ILE:HG13	1.96	0.47
1:AAA:12:ARG:HA	1:BBB:230:ALA:HB1	1.95	0.47
3:DDD:1174:ARG:O	3:DDD:1176:VAL:HG23	2.15	0.47
3:DDD:857:LEU:HG	3:DDD:858:VAL:HG23	1.97	0.47
1:BBB:31:LEU:CD1	1:BBB:201:LEU:HB2	2.45	0.47
2:CCC:839:VAL:HG13	2:CCC:1046:VAL:HG13	1.97	0.47
2:CCC:473:ARG:O	2:CCC:477:GLU:HB3	2.15	0.47
3:DDD:518:VAL:O	3:DDD:520:ALA:N	2.49	0.47
3:DDD:525:MET:O	3:DDD:548:VAL:HG23	2.13	0.47
3:DDD:528:THR:HG23	3:DDD:532:GLU:OE1	2.15	0.47
3:DDD:622:ASP:HB3	3:DDD:626:TYR:CE2	2.49	0.47
2:CCC:677:ASN:OD1	3:DDD:779:ALA:HB1	2.14	0.47
2:CCC:1119:MET:HB2	2:CCC:1228:GLY:HA2	1.96	0.46
2:CCC:660:VAL:HG21	3:DDD:769:VAL:CG1	2.45	0.46
3:DDD:114:ILE:HG23	3:DDD:115:TRP:N	2.28	0.46
3:DDD:377:PHE:O	3:DDD:381:ILE:HG13	2.15	0.46
3:DDD:525:MET:C	3:DDD:548:VAL:CG2	2.83	0.46
5:FFF:270:GLN:NE2	5:FFF:308:GLU:OE2	2.48	0.46
1:BBB:47:LEU:HD13	1:BBB:183:ILE:HD12	1.97	0.46
2:CCC:44:GLU:HG3	2:CCC:45:GLY:H	1.80	0.46
2:CCC:720:ARG:HB2	2:CCC:749:ASP:OD2	2.16	0.46
3:DDD:889:ASP:OD1	3:DDD:1290:ARG:NH2	2.49	0.46
2:CCC:1290:MET:SD	3:DDD:347:VAL:HG11	2.55	0.46
3:DDD:500:ILE:HG22	3:DDD:500:ILE:O	2.15	0.46
5:FFF:144:THR:O	5:FFF:147:THR:OG1	2.33	0.46
1:BBB:46:ILE:HD11	1:BBB:224:LEU:HD13	1.98	0.46
2:CCC:1214:ASP:OD1	2:CCC:1215:GLY:N	2.48	0.46
2:CCC:155:VAL:HG23	2:CCC:405:PHE:CD2	2.50	0.46
1:AAA:70:THR:OG1	2:CCC:729:ALA:O	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:848:GLU:OE1	2:CCC:886:LYS:HD3	2.16	0.46
6:111:55:DC:N4	7:222:8:DG:H1	2.09	0.46
2:CCC:150:HIS:CE1	2:CCC:452:ARG:HD3	2.51	0.46
5:FFF:266:LEU:HD22	5:FFF:312:ARG:CG	2.44	0.46
1:AAA:11:PRO:O	1:BBB:230:ALA:HB1	2.10	0.46
2:CCC:1107:MET:HE3	3:DDD:739:GLN:HB2	1.97	0.46
2:CCC:1109:ILE:HG22	2:CCC:1113:LEU:HD12	1.98	0.46
2:CCC:206:ALA:O	2:CCC:209:ILE:HG22	2.16	0.46
2:CCC:615:VAL:HA	2:CCC:638:SER:HB3	1.98	0.46
3:DDD:747:MET:SD	3:DDD:759:ILE:HD12	2.55	0.46
5:FFF:176:ASN:OD1	7:222:26:DT:H73	2.16	0.46
2:CCC:887:VAL:HB	2:CCC:913:VAL:HG12	1.97	0.46
3:DDD:582:ILE:HG23	3:DDD:623:GLN:HB3	1.97	0.46
3:DDD:58:CYS:SG	3:DDD:61:ILE:N	2.89	0.46
3:DDD:665:GLN:O	3:DDD:668:PHE:HB3	2.16	0.46
6:111:56:DG:H1	7:222:7:DC:H42	1.64	0.46
2:CCC:818:VAL:HG12	2:CCC:1096:ILE:HG12	1.97	0.46
2:CCC:538:LEU:HD23	2:CCC:542:ARG:NH2	2.30	0.46
2:CCC:720:ARG:HD3	2:CCC:736:VAL:HG11	1.98	0.46
3:DDD:1212:ASP:N	3:DDD:1212:ASP:OD1	2.46	0.46
3:DDD:1330:ARG:NH2	7:222:5:DC:O3'	2.49	0.46
3:DDD:490:ILE:HG12	3:DDD:500:ILE:HD12	1.98	0.46
3:DDD:832:LYS:HG3	3:DDD:1242:ARG:HD3	1.97	0.46
3:DDD:925:GLU:OE1	3:DDD:926:PRO:N	2.48	0.46
5:FFF:122:GLU:HG2	5:FFF:157:ALA:CB	2.46	0.46
1:BBB:50:SER:HA	1:BBB:150:ARG:HD2	1.97	0.46
5:FFF:105:ILE:HG23	5:FFF:109:TYR:CE1	2.51	0.46
2:CCC:1296:ASP:CB	2:CCC:1321:GLU:H	2.29	0.46
2:CCC:207:THR:CG2	2:CCC:354:ASP:HB2	2.45	0.46
2:CCC:871:VAL:HG23	2:CCC:883:LEU:O	2.16	0.46
2:CCC:1291:LEU:HA	3:DDD:345:LYS:HD2	1.98	0.46
5:FFF:204:LYS:HB3	5:FFF:205:PRO:CD	2.47	0.46
2:CCC:1286:THR:HG23	3:DDD:476:ALA:HB1	1.97	0.45
2:CCC:1338:GLU:OE2	3:DDD:21:LYS:HE2	2.16	0.45
2:CCC:277:LEU:CD1	2:CCC:282:VAL:HG21	2.46	0.45
2:CCC:32:LEU:HD23	2:CCC:130:MET:HE3	1.97	0.45
2:CCC:543:ALA:HB3	2:CCC:548:ARG:HH21	1.81	0.45
2:CCC:93:SER:OG	2:CCC:126:GLU:HB3	2.15	0.45
1:AAA:135:ASP:OD1	1:AAA:135:ASP:C	2.55	0.45
2:CCC:1028:LYS:O	2:CCC:1032:LYS:HG2	2.15	0.45
2:CCC:292:ILE:CB	2:CCC:322:LEU:HD11	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:807:TRP:CZ3	2:CCC:1086:PRO:HG3	2.51	0.45
3:DDD:1037:PHE:CZ	3:DDD:1059:LEU:CD1	3.00	0.45
2:CCC:1276:TRP:CH2	3:DDD:798:ARG:HG3	2.51	0.45
7:222:16:DC:H2'	7:222:17:DG:C8	2.52	0.45
1:AAA:179:PRO:HG3	1:AAA:211:ILE:HD12	1.99	0.45
1:AAA:195:ARG:HD2	1:AAA:198:LEU:HD23	1.97	0.45
1:AAA:45:ARG:NE	1:BBB:38:THR:OG1	2.32	0.45
2:CCC:150:HIS:HE1	2:CCC:452:ARG:HH11	1.64	0.45
2:CCC:871:VAL:HG23	2:CCC:883:LEU:HA	1.99	0.45
2:CCC:1247:SER:HB3	3:DDD:375:GLU:O	2.15	0.45
3:DDD:795:TYR:CE2	3:DDD:799:ARG:CZ	2.99	0.45
2:CCC:205:PRO:O	2:CCC:208:ILE:HG22	2.17	0.45
3:DDD:423:LEU:HB3	3:DDD:466:MET:CE	2.45	0.45
5:FFF:79:PHE:O	5:FFF:90:SER:OG	2.30	0.45
2:CCC:292:ILE:HG21	2:CCC:322:LEU:HD21	1.99	0.45
3:DDD:1156:LEU:HD23	3:DDD:1209:VAL:HA	1.99	0.45
4:EEE:60:ASN:HB3	4:EEE:63:ILE:HD12	1.99	0.45
7:222:13:DA:H2'	7:222:14:DC:C6	2.51	0.45
2:CCC:1061:GLN:NE2	2:CCC:1240:ASP:OD1	2.49	0.45
2:CCC:61:SER:OG	2:CCC:480:SER:OG	2.29	0.45
3:DDD:248:ASP:OD1	3:DDD:248:ASP:N	2.49	0.45
3:DDD:930:LEU:CD1	3:DDD:1246:VAL:HG21	2.47	0.45
2:CCC:32:LEU:CD2	2:CCC:130:MET:CE	2.94	0.45
2:CCC:53:PHE:HB3	2:CCC:70:TYR:CD2	2.52	0.45
3:DDD:1364:ALA:O	3:DDD:1367:GLN:HG2	2.16	0.45
3:DDD:490:ILE:HA	3:DDD:500:ILE:HD12	1.97	0.45
2:CCC:1304:MET:HE3	3:DDD:472:LEU:HD13	1.99	0.45
3:DDD:622:ASP:O	3:DDD:626:TYR:CD2	2.70	0.45
3:DDD:664:ILE:HG21	3:DDD:681:LYS:HD3	1.99	0.45
2:CCC:905:ILE:HD13	5:FFF:313:LEU:HD21	1.99	0.45
2:CCC:978:VAL:O	2:CCC:981:ALA:HB3	2.17	0.45
3:DDD:1029:THR:CG2	3:DDD:1121:LEU:CD1	2.95	0.45
3:DDD:579:LEU:HB3	3:DDD:592:VAL:HG21	1.99	0.45
3:DDD:849:LEU:CD1	3:DDD:853:THR:HA	2.47	0.45
3:DDD:886:VAL:CG1	3:DDD:1226:VAL:CG1	2.95	0.45
7:222:7:DC:H5''	7:222:7:DC:H6	1.81	0.45
2:CCC:1099:ASN:OD1	2:CCC:1100:PRO:HD2	2.17	0.45
2:CCC:57:PHE:CE1	2:CCC:59:ILE:HD12	2.52	0.45
3:DDD:174:ASP:OD1	3:DDD:174:ASP:N	2.50	0.45
3:DDD:492:SER:HB2	3:DDD:499:ILE:CD1	2.47	0.45
5:FFF:268:ALA:O	5:FFF:272:GLU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:670:PHE:CD2	2:CCC:1113:LEU:HB3	2.52	0.44
2:CCC:736:VAL:O	2:CCC:741:MET:HE3	2.17	0.44
3:DDD:161:THR:N	3:DDD:164:GLN:HB2	2.32	0.44
3:DDD:785:ASP:HB3	3:DDD:935:PHE:CE2	2.51	0.44
5:FFF:317:LEU:CD2	5:FFF:324:ILE:HD13	2.47	0.44
1:AAA:57:THR:HG23	1:AAA:158:ARG:CZ	2.48	0.44
2:CCC:1081:PRO:HB2	2:CCC:1083:GLU:OE2	2.17	0.44
2:CCC:1293:VAL:HG12	2:CCC:1300:GLY:C	2.38	0.44
2:CCC:993:PRO:HG2	2:CCC:996:ARG:NH1	2.33	0.44
1:AAA:212:ASP:OD1	1:AAA:213:PRO:HD2	2.18	0.44
1:AAA:75:GLN:O	2:CCC:729:ALA:HB2	2.17	0.44
1:BBB:67:GLU:CB	1:BBB:171:LEU:HD22	2.42	0.44
2:CCC:1296:ASP:HB3	2:CCC:1321:GLU:H	1.81	0.44
2:CCC:598:VAL:HG13	2:CCC:627:GLY:HA2	1.98	0.44
3:DDD:667:GLN:O	3:DDD:670:SER:OG	2.22	0.44
3:DDD:750:PRO:O	3:DDD:781:LYS:HE3	2.17	0.44
4:EEE:13:ILE:HD12	4:EEE:19:LEU:HA	1.99	0.44
6:111:57:DC:H2''	6:111:58:DG:H5'	1.98	0.44
2:CCC:297:VAL:HG13	2:CCC:317:LEU:CG	2.48	0.44
1:AAA:66:HIS:CE1	2:CCC:929:ILE:HG13	2.52	0.44
3:DDD:332:LYS:O	3:DDD:333:GLY:O	2.36	0.44
3:DDD:519:ASN:HA	3:DDD:523:GLU:OE2	2.17	0.44
3:DDD:58:CYS:SG	3:DDD:60:ARG:N	2.91	0.44
4:EEE:8:ASP:HB2	4:EEE:55:GLU:CG	2.47	0.44
1:AAA:159:ILE:O	1:AAA:159:ILE:HG23	2.17	0.44
1:AAA:64:VAL:CG1	1:AAA:78:ILE:HD13	2.48	0.44
2:CCC:165:HIS:HB3	2:CCC:167:SER:HB3	2.00	0.44
2:CCC:751:TYR:N	2:CCC:751:TYR:CD2	2.86	0.44
3:DDD:703:THR:O	3:DDD:704:GLU:C	2.56	0.44
2:CCC:887:VAL:HB	2:CCC:913:VAL:CG1	2.46	0.44
2:CCC:90:VAL:HG12	2:CCC:91:THR:N	2.32	0.44
3:DDD:572:THR:HB	3:DDD:593:ASN:OD1	2.18	0.44
7:222:4:DC:C5	7:222:5:DC:N4	2.86	0.44
1:BBB:82:LEU:HB3	1:BBB:173:VAL:HG11	1.99	0.44
2:CCC:1131:MET:HG2	2:CCC:1136:GLN:OE1	2.18	0.44
2:CCC:135:THR:HG22	2:CCC:527:LYS:HE2	2.00	0.44
2:CCC:808:ASN:N	2:CCC:808:ASN:HD22	2.15	0.44
3:DDD:572:THR:OG1	3:DDD:573:THR:N	2.51	0.44
1:AAA:86:LYS:CE	1:AAA:173:VAL:HG12	2.48	0.44
2:CCC:832:HIS:CD2	2:CCC:1058:ARG:HD2	2.53	0.44
2:CCC:1269:ARG:NE	7:222:11:DA:OP1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:244:GLU:O	2:CCC:247:ARG:HB2	2.17	0.44
2:CCC:244:GLU:CG	2:CCC:245:ARG:N	2.79	0.44
2:CCC:32:LEU:CD2	2:CCC:130:MET:HE3	2.48	0.44
2:CCC:847:PRO:HB3	2:CCC:1047:LEU:HD11	1.98	0.44
3:DDD:1041:ILE:HG21	3:DDD:1044:GLN:HG3	2.00	0.44
3:DDD:119:SER:O	3:DDD:122:SER:N	2.51	0.44
3:DDD:364:HIS:HB3	3:DDD:487:THR:CG2	2.48	0.44
3:DDD:45:ASN:HB2	3:DDD:52:GLU:OE1	2.18	0.44
3:DDD:62:PHE:CD1	3:DDD:247:PRO:HD3	2.53	0.44
2:CCC:1251:TYR:HE2	5:FFF:246:PRO:CD	2.31	0.44
7:222:15:DT:H2'	7:222:16:DC:C6	2.53	0.44
1:AAA:91:ARG:HG3	1:AAA:210:THR:HA	1.99	0.44
3:DDD:517:CYS:SG	3:DDD:518:VAL:N	2.91	0.44
3:DDD:846:GLU:HG3	3:DDD:881:LYS:HD3	1.98	0.44
1:AAA:64:VAL:HG13	1:AAA:78:ILE:HD13	1.99	0.43
2:CCC:1237:HIS:HB3	2:CCC:1242:LYS:CE	2.48	0.43
2:CCC:201:ARG:CB	2:CCC:369:MET:HE2	2.45	0.43
2:CCC:720:ARG:HB3	2:CCC:736:VAL:HG13	1.99	0.43
3:DDD:1106:ILE:O	3:DDD:1106:ILE:HG22	2.17	0.43
2:CCC:1284:ALA:HB3	3:DDD:1361:THR:HB	1.99	0.43
3:DDD:305:ALA:CB	3:DDD:316:ILE:HD12	2.47	0.43
3:DDD:823:THR:HB	3:DDD:824:PRO:HD2	2.00	0.43
5:FFF:145:TYR:CZ	5:FFF:149:TRP:NE1	2.83	0.43
2:CCC:199:ASP:C	6:111:53:DG:N2	2.72	0.43
2:CCC:1160:ASP:O	2:CCC:1161:LEU:O	2.36	0.43
2:CCC:189:ASP:OD1	2:CCC:190:PRO:N	2.52	0.43
2:CCC:764:CYS:SG	2:CCC:833:ILE:HD11	2.58	0.43
2:CCC:76:GLY:O	2:CCC:94:ALA:HB1	2.17	0.43
3:DDD:384:LYS:NZ	4:EEE:45:LYS:NZ	2.66	0.43
3:DDD:733:SER:H	3:DDD:736:GLN:HG3	1.83	0.43
3:DDD:948:SER:OG	3:DDD:1019:ASN:ND2	2.52	0.43
4:EEE:39:VAL:HG13	4:EEE:40:PRO:HD2	2.00	0.43
1:AAA:179:PRO:HG3	1:AAA:211:ILE:HG13	2.00	0.43
2:CCC:102:LEU:HD23	2:CCC:118:LYS:HD2	1.99	0.43
2:CCC:144:VAL:HB	2:CCC:526:HIS:CE1	2.53	0.43
2:CCC:512:SER:OG	2:CCC:512:SER:O	2.30	0.43
2:CCC:734:ILE:HG22	2:CCC:749:ASP:HB2	2.00	0.43
2:CCC:963:GLU:O	2:CCC:967:LEU:HB2	2.18	0.43
3:DDD:1357:ILE:HG13	3:DDD:1357:ILE:H	1.51	0.43
3:DDD:325:LYS:HE2	3:DDD:330:MET:CG	2.48	0.43
3:DDD:949:SER:HB3	3:DDD:1019:ASN:HD22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:160:ASP:HB3	2:CCC:163:LYS:HD3	1.99	0.43
3:DDD:502:PRO:HB3	3:DDD:506:VAL:CG1	2.48	0.43
3:DDD:960:LEU:HB3	3:DDD:963:VAL:HG11	2.00	0.43
5:FFF:109:TYR:CD2	5:FFF:109:TYR:N	2.84	0.43
1:AAA:195:ARG:HD2	1:AAA:198:LEU:CD2	2.48	0.43
3:DDD:709:ARG:O	3:DDD:709:ARG:HG3	2.18	0.43
3:DDD:731:ARG:HA	3:DDD:731:ARG:HD3	1.75	0.43
3:DDD:71:LEU:HB2	3:DDD:90:VAL:HG21	2.00	0.43
4:EEE:41:GLU:O	4:EEE:44:ASP:HB2	2.18	0.43
2:CCC:60:GLN:HG2	2:CCC:67:GLU:CB	2.49	0.43
2:CCC:801:ARG:HG3	2:CCC:1229:TYR:CE1	2.54	0.43
3:DDD:294:ASN:HB2	5:FFF:61:TYR:CD1	2.54	0.43
11:DDD:1505:DG3:C8	12:333:101:DDG:H2"	2.48	0.43
2:CCC:409:LEU:HD13	2:CCC:427:ASP:HB3	2.01	0.43
2:CCC:496:LYS:N	2:CCC:497:PRO:CD	2.81	0.43
2:CCC:726:TYR:CZ	2:CCC:728:ASP:HB2	2.54	0.43
3:DDD:161:THR:H	3:DDD:164:GLN:HB2	1.83	0.43
3:DDD:427:PRO:CG	3:DDD:429:LEU:HD21	2.49	0.43
3:DDD:835:LEU:HD13	3:DDD:878:ASP:O	2.19	0.43
1:AAA:233:ASP:O	1:AAA:235:ARG:N	2.50	0.43
2:CCC:104:ILE:HD13	2:CCC:484:LEU:HB3	2.00	0.43
2:CCC:1315:MET:HB2	3:DDD:473:THR:HG21	2.01	0.43
2:CCC:403:MET:HB3	2:CCC:403:MET:HE2	1.80	0.43
3:DDD:859:PRO:HG2	3:DDD:862:THR:HG21	2.01	0.43
5:FFF:119:LEU:HD22	5:FFF:154:ILE:HG23	2.00	0.43
5:FFF:163:ARG:CD	5:FFF:167:LEU:HD12	2.45	0.43
5:FFF:87:ASP:OD1	5:FFF:88:VAL:N	2.51	0.43
2:CCC:806:PRO:HB3	3:DDD:505:ASP:OD2	2.18	0.43
5:FFF:117:LEU:HD23	5:FFF:117:LEU:HA	1.90	0.43
5:FFF:175:LEU:O	5:FFF:179:LEU:HG	2.18	0.43
2:CCC:1129:ASN:CA	2:CCC:1177:ARG:HG3	2.49	0.43
2:CCC:801:ARG:HG3	2:CCC:1229:TYR:CZ	2.53	0.43
2:CCC:15:PHE:O	2:CCC:17:LYS:HE3	2.18	0.43
2:CCC:49:LEU:HD23	2:CCC:464:PHE:CE2	2.53	0.43
2:CCC:599:VAL:HG21	2:CCC:623:LEU:CD2	2.48	0.43
3:DDD:1262:ARG:CZ	3:DDD:1316:THR:HG22	2.49	0.43
3:DDD:205:LEU:HD22	3:DDD:214:ARG:HG2	2.01	0.43
2:CCC:196:VAL:CG2	2:CCC:206:ALA:HA	2.32	0.42
2:CCC:208:ILE:HD11	2:CCC:365:GLU:HB3	2.01	0.42
2:CCC:582:ASN:HD21	2:CCC:586:PHE:HB2	1.84	0.42
2:CCC:838:CYS:SG	2:CCC:886:LYS:HE2	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:1165:PHE:HZ	3:DDD:1196:LEU:HD12	1.84	0.42
3:DDD:290:ILE:HD12	3:DDD:290:ILE:H	1.83	0.42
3:DDD:784:ALA:O	3:DDD:788:LEU:HG	2.19	0.42
5:FFF:321:GLY:O	5:FFF:324:ILE:N	2.52	0.42
5:FFF:107:ARG:HD2	6:111:43:DT:H4'	2.01	0.42
3:DDD:1196:LEU:HD22	3:DDD:1210:ILE:HG22	2.01	0.42
3:DDD:599:LYS:H	3:DDD:599:LYS:HG3	1.52	0.42
3:DDD:925:GLU:HB3	3:DDD:926:PRO:CD	2.49	0.42
1:AAA:78:ILE:HA	1:AAA:81:ILE:HD12	2.01	0.42
2:CCC:1134:GLN:O	2:CCC:1136:GLN:N	2.51	0.42
1:AAA:74:VAL:O	2:CCC:729:ALA:CB	2.67	0.42
2:CCC:985:GLU:HB2	2:CCC:989:LEU:HG	2.00	0.42
3:DDD:519:ASN:HA	3:DDD:523:GLU:CG	2.50	0.42
3:DDD:58:CYS:SG	3:DDD:61:ILE:HG13	2.60	0.42
3:DDD:810:THR:OG1	3:DDD:893:GLY:HA3	2.18	0.42
3:DDD:816:THR:HG22	3:DDD:818:GLU:N	2.25	0.42
1:BBB:212:ASP:OD1	1:BBB:213:PRO:HD2	2.20	0.42
1:BBB:78:ILE:HA	1:BBB:81:ILE:HD12	2.01	0.42
2:CCC:1087:TYR:HD2	2:CCC:1091:GLY:HA2	1.83	0.42
2:CCC:1262:LYS:HG2	2:CCC:1263:ALA:N	2.35	0.42
3:DDD:1186:TYR:CZ	3:DDD:1188:GLU:OE2	2.72	0.42
3:DDD:809:VAL:CG2	3:DDD:915:ILE:CD1	2.97	0.42
2:CCC:898:GLU:OE2	5:FFF:259:ILE:HD13	2.19	0.42
2:CCC:816:ILE:HD11	2:CCC:1074:GLY:HA3	2.00	0.42
2:CCC:1273:MET:HB3	3:DDD:428:THR:HB	2.02	0.42
2:CCC:21:VAL:HG21	2:CCC:592:ARG:CZ	2.50	0.42
3:DDD:805:GLN:HG2	3:DDD:806:ASP:N	2.33	0.42
5:FFF:119:LEU:CD2	5:FFF:158:ILE:HD11	2.47	0.42
1:AAA:30:PRO:HB2	1:AAA:198:LEU:CD1	2.48	0.42
1:AAA:61:ILE:HG12	1:AAA:142:MET:HB3	2.02	0.42
2:CCC:668:ILE:HG12	2:CCC:1069:ARG:O	2.20	0.42
2:CCC:944:ARG:O	2:CCC:947:GLU:HG2	2.20	0.42
5:FFF:266:LEU:CD1	5:FFF:312:ARG:HB3	2.49	0.42
5:FFF:143:SER:HB2	6:111:41:DT:H72	2.02	0.42
2:CCC:12:ARG:HD3	2:CCC:1183:ALA:HB2	2.01	0.42
3:DDD:608:CYS:SG	3:DDD:612:LEU:HD12	2.59	0.42
5:FFF:220:THR:HG22	7:222:18:DT:C2	2.54	0.42
2:CCC:1212:LEU:HD23	2:CCC:1212:LEU:HA	1.84	0.42
2:CCC:1246:ARG:NH2	2:CCC:1258:PRO:HB3	2.35	0.42
3:DDD:809:VAL:HG22	3:DDD:915:ILE:CD1	2.50	0.42
1:BBB:102:LEU:HB2	1:BBB:115:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:157:THR:CG2	1:BBB:157:THR:O	2.68	0.42
2:CCC:1286:THR:O	2:CCC:1289:GLU:HB2	2.20	0.42
2:CCC:216:THR:N	2:CCC:219:GLN:OE1	2.38	0.42
2:CCC:400:VAL:HG13	2:CCC:584:TYR:HB3	2.01	0.42
2:CCC:1243:MET:SD	3:DDD:445:LYS:HG2	2.60	0.42
3:DDD:570:LYS:HE3	3:DDD:589:TYR:HB3	2.01	0.42
3:DDD:958:ILE:HG23	3:DDD:982:LEU:HD13	2.02	0.42
3:DDD:1061:VAL:O	3:DDD:1104:LYS:N	2.42	0.42
3:DDD:113:HIS:CD2	3:DDD:115:TRP:HB2	2.55	0.42
5:FFF:143:SER:HB3	6:111:41:DT:C7	2.49	0.42
1:AAA:32:GLU:CD	1:BBB:150:ARG:HH21	2.23	0.41
2:CCC:1274:GLU:HG2	3:DDD:424:ASN:HD21	1.85	0.41
2:CCC:582:ASN:OD1	2:CCC:585:GLY:N	2.51	0.41
3:DDD:1169:THR:OG1	3:DDD:1174:ARG:NH2	2.52	0.41
3:DDD:211:GLU:HG2	3:DDD:212:THR:HG23	2.02	0.41
3:DDD:697:MET:SD	3:DDD:741:ALA:HB3	2.60	0.41
2:CCC:1000:LEU:O	2:CCC:1011:LEU:HD21	2.20	0.41
2:CCC:149:LEU:HB2	2:CCC:530:ILE:CG2	2.50	0.41
2:CCC:936:ARG:CG	2:CCC:937:ASP:N	2.82	0.41
3:DDD:886:VAL:HG12	3:DDD:1226:VAL:CG1	2.50	0.41
3:DDD:438:GLU:HA	3:DDD:439:PRO:HD3	1.90	0.41
3:DDD:664:ILE:HD13	3:DDD:681:LYS:HG2	2.01	0.41
3:DDD:679:TYR:HE1	3:DDD:754:ILE:O	2.04	0.41
3:DDD:994:SER:O	3:DDD:995:TYR:CG	2.73	0.41
5:FFF:317:LEU:HD22	5:FFF:324:ILE:HD13	2.02	0.41
2:CCC:576:SER:OG	2:CCC:577:VAL:N	2.53	0.41
3:DDD:916:GLY:HA2	3:DDD:1255:VAL:HG11	2.02	0.41
2:CCC:800:MET:O	2:CCC:1229:TYR:HA	2.21	0.41
2:CCC:135:THR:HG21	2:CCC:515:MET:CE	2.50	0.41
3:DDD:608:CYS:SG	3:DDD:617:THR:HG22	2.61	0.41
3:DDD:935:PHE:HZ	3:DDD:1135:THR:OG1	2.03	0.41
2:CCC:898:GLU:OE2	5:FFF:280:LEU:HD22	2.20	0.41
1:BBB:195:ARG:HD2	1:BBB:198:LEU:CD2	2.50	0.41
2:CCC:1280:ALA:HB1	3:DDD:918:ILE:HG12	2.03	0.41
2:CCC:160:ASP:N	2:CCC:160:ASP:OD1	2.53	0.41
2:CCC:257:ALA:HB3	2:CCC:262:TYR:HE2	1.85	0.41
2:CCC:759:SER:OG	2:CCC:760:ASN:N	2.51	0.41
2:CCC:975:ILE:HG23	2:CCC:1011:LEU:CD1	2.50	0.41
3:DDD:680:ASN:HB3	3:DDD:1023:HIS:CE1	2.56	0.41
3:DDD:1047:THR:HB	3:DDD:1062:LEU:HD11	2.02	0.41
3:DDD:130:MET:SD	3:DDD:157:GLN:HB3	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:703:THR:C	3:DDD:705:THR:N	2.73	0.41
3:DDD:820:ILE:HG23	3:DDD:1227:HIS:HB3	2.00	0.41
3:DDD:822:MET:HE1	3:DDD:882:VAL:HG21	2.03	0.41
8:333:15:A:H8	8:333:15:A:HO5'	1.62	0.41
1:BBB:158:ARG:HD2	1:BBB:172:LEU:HD21	2.03	0.41
1:BBB:160:HIS:C	1:BBB:160:HIS:CD2	2.94	0.41
2:CCC:123:TYR:CE1	5:FFF:190:ASP:O	2.73	0.41
2:CCC:237:LEU:HD11	2:CCC:292:ILE:HD12	2.02	0.41
3:DDD:703:THR:O	3:DDD:705:THR:N	2.54	0.41
5:FFF:119:LEU:HD21	5:FFF:158:ILE:CD1	2.47	0.41
1:AAA:222:THR:OG1	1:BBB:233:ASP:HB3	2.20	0.41
1:BBB:232:VAL:HB	1:BBB:233:ASP:H	1.64	0.41
2:CCC:1272:GLU:OE1	3:DDD:339:ARG:HD3	2.21	0.41
2:CCC:146:VAL:O	2:CCC:511:LEU:HD13	2.20	0.41
2:CCC:152:SER:O	2:CCC:156:PHE:CZ	2.73	0.41
2:CCC:155:VAL:HG12	2:CCC:156:PHE:N	2.36	0.41
3:DDD:803:VAL:HG22	3:DDD:1313:SER:OG	2.21	0.41
3:DDD:932:MET:SD	11:DDD:1505:DG3:C4	3.09	0.41
1:BBB:196:THR:HG21	3:DDD:370:LYS:NZ	2.35	0.41
3:DDD:432:LEU:HD12	3:DDD:499:ILE:CD1	2.50	0.41
5:FFF:109:TYR:HD1	5:FFF:154:ILE:HG21	1.86	0.41
2:CCC:1257:GLN:NE2	3:DDD:341:ASN:O	2.54	0.41
2:CCC:453:ILE:CD1	2:CCC:530:ILE:HD13	2.51	0.41
2:CCC:857:VAL:HG11	2:CCC:862:LEU:HD21	2.02	0.41
2:CCC:906:PHE:C	2:CCC:908:GLU:H	2.24	0.41
3:DDD:1054:THR:OG1	3:DDD:1055:GLY:N	2.54	0.41
3:DDD:111:THR:HG21	3:DDD:303:VAL:CG1	2.51	0.41
2:CCC:1277:ALA:HB3	3:DDD:434:ILE:CD1	2.51	0.41
3:DDD:442:ILE:HD13	3:DDD:448:GLN:OE1	2.20	0.41
3:DDD:615:LYS:N	3:DDD:616:PRO:CD	2.84	0.41
2:CCC:1107:MET:CE	3:DDD:739:GLN:HB2	2.50	0.41
3:DDD:872:LEU:CD2	3:DDD:877:VAL:HG21	2.50	0.41
1:AAA:47:LEU:HA	1:AAA:51:MET:HG2	2.02	0.41
1:BBB:61:ILE:HG12	1:BBB:142:MET:HB3	2.02	0.41
3:DDD:1082:ASP:C	3:DDD:1082:ASP:OD1	2.60	0.41
1:BBB:83:LEU:HD11	3:DDD:526:VAL:O	2.20	0.41
5:FFF:286:ALA:HB1	5:FFF:290:ASP:HB2	2.02	0.41
5:FFF:266:LEU:HD13	5:FFF:312:ARG:CB	2.51	0.41
2:CCC:1119:MET:SD	2:CCC:1210:ILE:HD11	2.61	0.41
2:CCC:1285:TYR:CE2	3:DDD:1361:THR:HG21	2.56	0.41
3:DDD:783:LEU:HD12	3:DDD:783:LEU:HA	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:111:38:DT:C2'	6:111:39:DA:C8	3.03	0.41
2:CCC:1262:LYS:HE3	7:222:14:DC:OP1	2.21	0.41
3:DDD:128:LEU:HD21	3:DDD:189:LEU:HD23	2.03	0.41
3:DDD:360:TYR:OH	3:DDD:448:GLN:OE1	2.31	0.41
3:DDD:510:LEU:O	3:DDD:514:THR:HG23	2.20	0.41
3:DDD:780:ARG:HE	3:DDD:780:ARG:HB2	1.60	0.41
3:DDD:802:ASP:OD1	3:DDD:1348:LYS:HE3	2.21	0.41
3:DDD:291:ILE:HG23	5:FFF:121:GLU:OE2	2.21	0.41
2:CCC:1296:ASP:O	2:CCC:1297:ASP:C	2.59	0.40
2:CCC:251:ALA:CB	2:CCC:263:VAL:CG1	2.85	0.40
2:CCC:518:ASN:OD1	2:CCC:1236:ASN:ND2	2.54	0.40
5:FFF:266:LEU:HD13	5:FFF:312:ARG:HB3	2.03	0.40
5:FFF:143:SER:HB3	6:111:41:DT:H72	2.00	0.40
2:CCC:43:PRO:O	2:CCC:54:ARG:NH2	2.54	0.40
2:CCC:515:MET:HG2	2:CCC:517:GLN:HG3	2.03	0.40
2:CCC:807:TRP:CZ3	2:CCC:1086:PRO:HD3	2.56	0.40
2:CCC:823:VAL:HG22	2:CCC:1060:ILE:HG22	2.03	0.40
2:CCC:933:VAL:HG11	2:CCC:945:ALA:HB2	2.03	0.40
3:DDD:1370:MET:O	3:DDD:1373:ARG:HB2	2.22	0.40
3:DDD:625:MET:HG2	3:DDD:629:PHE:CE2	2.56	0.40
5:FFF:176:ASN:ND2	7:222:26:DT:H2'	2.36	0.40
3:DDD:1199:PHE:CD1	3:DDD:1200:GLU:N	2.90	0.40
3:DDD:644:MET:HB2	3:DDD:764:ARG:HD2	2.02	0.40
3:DDD:746:LEU:HD23	3:DDD:758:PRO:HB3	2.03	0.40
2:CCC:905:ILE:CD1	5:FFF:313:LEU:CD2	2.99	0.40
2:CCC:99:LYS:HG2	2:CCC:121:GLU:HG3	2.02	0.40
3:DDD:659:ALA:O	3:DDD:663:GLU:HG3	2.21	0.40
3:DDD:742:GLY:O	3:DDD:762:ASN:HB3	2.22	0.40
3:DDD:805:GLN:CG	3:DDD:806:ASP:N	2.84	0.40
5:FFF:61:TYR:CE2	5:FFF:65:ILE:CD1	3.04	0.40
7:222:7:DC:C2'	7:222:8:DG:H5'	2.52	0.40
2:CCC:549:ASP:OD2	3:DDD:750:PRO:CG	2.69	0.40
5:FFF:127:LEU:HA	5:FFF:127:LEU:HD23	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	228/242 (94%)	209 (92%)	14 (6%)	5 (2%)	6	38
1	BBB	226/242 (93%)	207 (92%)	13 (6%)	6 (3%)	5	34
2	CCC	1339/1342 (100%)	1239 (92%)	73 (6%)	27 (2%)	7	40
3	DDD	1360/1407 (97%)	1251 (92%)	92 (7%)	17 (1%)	12	48
4	EEE	77/90 (86%)	73 (95%)	4 (5%)	0	100	100
5	FFF	266/336 (79%)	247 (93%)	18 (7%)	1 (0%)	34	72
All	All	3496/3659 (96%)	3226 (92%)	214 (6%)	56 (2%)	9	45

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	117	HIS
1	BBB	193	GLU
1	BBB	194	GLN
2	CCC	46	GLN
2	CCC	247	ARG
2	CCC	791	LEU
2	CCC	892	GLU
2	CCC	1162	SER
2	CCC	1281	TYR
3	DDD	53	ARG
3	DDD	174	ASP
3	DDD	336	GLY
3	DDD	519	ASN
1	AAA	168	ILE
1	AAA	234	LEU
1	BBB	119	GLY
2	CCC	258	ASN
2	CCC	625	GLU
2	CCC	730	SER
2	CCC	756	TYR

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Mol	Chain	Res	Type
2	CCC	1161	LEU
3	DDD	122	SER
3	DDD	321	LYS
3	DDD	1309	ILE
1	AAA	191	ARG
1	BBB	232	VAL
2	CCC	867	GLU
2	CCC	981	ALA
2	CCC	1103	VAL
2	CCC	1135	GLN
3	DDD	1053	LEU
3	DDD	1200	GLU
1	AAA	210	THR
1	AAA	233	ASP
2	CCC	45	GLY
2	CCC	163	LYS
2	CCC	234	ASP
2	CCC	455	SER
2	CCC	669	PRO
2	CCC	1297	ASP
3	DDD	1024	THR
5	FFF	322	LEU
2	CCC	341	LEU
2	CCC	729	ALA
2	CCC	986	ALA
3	DDD	854	ALA
3	DDD	946	ALA
3	DDD	1091	PRO
3	DDD	1170	LYS
1	BBB	118	ASP
2	CCC	246	LEU
3	DDD	986	ASP
3	DDD	829	GLY
3	DDD	1103	GLY
2	CCC	983	GLY
2	CCC	744	GLY

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%)	180 (91%)	18 (9%)	9	32
1	BBB	196/208 (94%)	185 (94%)	11 (6%)	21	48
2	CCC	1156/1157 (100%)	1065 (92%)	91 (8%)	12	38
3	DDD	1135/1168 (97%)	1061 (94%)	74 (6%)	17	44
4	EEE	67/74 (90%)	64 (96%)	3 (4%)	27	54
5	FFF	235/292 (80%)	225 (96%)	10 (4%)	29	55
All	All	2987/3107 (96%)	2780 (93%)	207 (7%)	15	42

All (207) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	18	GLN
1	AAA	28	LEU
1	AAA	70	THR
1	AAA	77	ASP
1	AAA	131	CYS
1	AAA	135	ASP
1	AAA	137	ASN
1	AAA	157	THR
1	AAA	159	ILE
1	AAA	166	ARG
1	AAA	176	CYS
1	AAA	187	VAL
1	AAA	191	ARG
1	AAA	194	GLN
1	AAA	198	LEU
1	AAA	208	ASN
1	AAA	233	ASP
1	AAA	235	ARG
1	BBB	28	LEU
1	BBB	33	ARG
1	BBB	70	THR
1	BBB	77	ASP
1	BBB	131	CYS
1	BBB	137	ASN
1	BBB	159	ILE
1	BBB	176	CYS
1	BBB	187	VAL

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Mol	Chain	Res	Type
1	BBB	194	GLN
1	BBB	198	LEU
2	CCC	23	ASP
2	CCC	30	ILE
2	CCC	69	GLN
2	CCC	85	CYS
2	CCC	116	ASP
2	CCC	120	GLN
2	CCC	121	GLU
2	CCC	160	ASP
2	CCC	166	SER
2	CCC	167	SER
2	CCC	173	ASN
2	CCC	184	LEU
2	CCC	185	ASP
2	CCC	189	ASP
2	CCC	209	ILE
2	CCC	237	LEU
2	CCC	241	LEU
2	CCC	244	GLU
2	CCC	256	GLU
2	CCC	264	GLU
2	CCC	275	ARG
2	CCC	290	GLU
2	CCC	304	GLU
2	CCC	316	GLU
2	CCC	332	ARG
2	CCC	335	THR
2	CCC	393	ASP
2	CCC	398	SER
2	CCC	403	MET
2	CCC	404	LYS
2	CCC	413	GLU
2	CCC	470	ARG
2	CCC	472	GLU
2	CCC	477	GLU
2	CCC	502	VAL
2	CCC	525	THR
2	CCC	529	ARG
2	CCC	539	THR
2	CCC	574	SER
2	CCC	576	SER

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Mol	Chain	Res	Type
2	CCC	592	ARG
2	CCC	601	ASP
2	CCC	618	GLN
2	CCC	620	ASN
2	CCC	635	THR
2	CCC	648	ASP
2	CCC	678	ARG
2	CCC	685	MET
2	CCC	694	ARG
2	CCC	730	SER
2	CCC	739	ASP
2	CCC	757	THR
2	CCC	758	ARG
2	CCC	759	SER
2	CCC	772	SER
2	CCC	777	VAL
2	CCC	788	SER
2	CCC	789	THR
2	CCC	799	ASN
2	CCC	800	MET
2	CCC	801	ARG
2	CCC	802	VAL
2	CCC	808	ASN
2	CCC	815	SER
2	CCC	817	LEU
2	CCC	831	ILE
2	CCC	866	ASP
2	CCC	876	GLU
2	CCC	912	ASP
2	CCC	935	THR
2	CCC	942	ASP
2	CCC	995	ASP
2	CCC	998	LEU
2	CCC	1073	LYS
2	CCC	1088	ASP
2	CCC	1113	LEU
2	CCC	1135	GLN
2	CCC	1143	GLU
2	CCC	1150	ASP
2	CCC	1154	ASP
2	CCC	1174	GLU
2	CCC	1223	ARG

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Mol	Chain	Res	Type
2	CCC	1240	ASP
2	CCC	1248	THR
2	CCC	1262	LYS
2	CCC	1269	ARG
2	CCC	1286	THR
2	CCC	1292	THR
2	CCC	1293	VAL
2	CCC	1295	SER
2	CCC	1296	ASP
3	DDD	34	SER
3	DDD	52	GLU
3	DDD	60	ARG
3	DDD	67	ASP
3	DDD	70	CYS
3	DDD	143	SER
3	DDD	167	ASP
3	DDD	176	PHE
3	DDD	210	SER
3	DDD	211	GLU
3	DDD	223	LEU
3	DDD	237	MET
3	DDD	256	ASP
3	DDD	319	SER
3	DDD	339	ARG
3	DDD	345	LYS
3	DDD	443	GLU
3	DDD	460	ASP
3	DDD	464	ASP
3	DDD	479	GLU
3	DDD	492	SER
3	DDD	499	ILE
3	DDD	503	SER
3	DDD	543	SER
3	DDD	550	VAL
3	DDD	551	ARG
3	DDD	579	LEU
3	DDD	590	SER
3	DDD	591	ILE
3	DDD	599	LYS
3	DDD	604	MET
3	DDD	610	ARG
3	DDD	619	ILE

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Mol	Chain	Res	Type
3	DDD	627	THR
3	DDD	704	GLU
3	DDD	705	THR
3	DDD	715	LYS
3	DDD	717	VAL
3	DDD	731	ARG
3	DDD	736	GLN
3	DDD	747	MET
3	DDD	751	ASP
3	DDD	769	VAL
3	DDD	786	THR
3	DDD	790	THR
3	DDD	792	ASN
3	DDD	812	ASP
3	DDD	830	ASP
3	DDD	835	LEU
3	DDD	846	GLU
3	DDD	849	LEU
3	DDD	862	THR
3	DDD	864	LEU
3	DDD	889	ASP
3	DDD	911	LYS
3	DDD	932	MET
3	DDD	957	SER
3	DDD	961	SER
3	DDD	969	SER
3	DDD	970	SER
3	DDD	1021	ASP
3	DDD	1025	MET
3	DDD	1032	SER
3	DDD	1051	ASP
3	DDD	1058	SER
3	DDD	1064	SER
3	DDD	1073	ASP
3	DDD	1187	GLU
3	DDD	1200	GLU
3	DDD	1283	SER
3	DDD	1303	SER
3	DDD	1309	ILE
3	DDD	1330	ARG
3	DDD	1345	ARG
4	EEE	8	ASP

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Mol	Chain	Res	Type
4	EEE	46	THR
4	EEE	55	GLU
5	FFF	105	ILE
5	FFF	109	TYR
5	FFF	122	GLU
5	FFF	127	LEU
5	FFF	151	ARG
5	FFF	218	ARG
5	FFF	244	ASN
5	FFF	254	ASP
5	FFF	271	ARG
5	FFF	322	LEU

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	DG3	DDD	1505	10	25,32,32	1.10	1 (4%)	28,50,50	2.28	4 (14%)
12	DDG	333	101	-	17,23,24	1.38	2 (11%)	15,33,36	2.62	7 (46%)

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	DG3	DDD	1505	10	-	2/18/31/31	0/3/3/3
12	DDG	333	101	-	-	0/3/18/19	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	333	101	DDG	C6-C5	4.60	1.49	1.41
11	DDD	1505	DG3	C6-N1	3.99	1.40	1.33
12	333	101	DDG	C5-C4	2.56	1.47	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	DDD	1505	DG3	C5-C6-N1	-8.74	111.47	123.43
11	DDD	1505	DG3	C6-N1-C2	5.87	125.25	115.93
12	333	101	DDG	C2-N3-C4	4.64	120.66	115.36
12	333	101	DDG	C5-C6-N1	-4.29	117.56	123.43
12	333	101	DDG	C6-N1-C2	3.63	121.70	115.93
12	333	101	DDG	C3'-C2'-C1'	3.27	106.56	102.78
12	333	101	DDG	C4-C5-N7	-3.17	106.09	109.40
12	333	101	DDG	C6-C5-C4	-3.01	117.93	120.80
11	DDD	1505	DG3	C2-N3-C4	-2.83	112.13	115.36
11	DDD	1505	DG3	N3-C2-N1	-2.72	123.59	127.22
12	333	101	DDG	N3-C2-N1	-2.46	123.94	127.22

There are no chirality outliers.

All (2) torsion outliers are listed below:

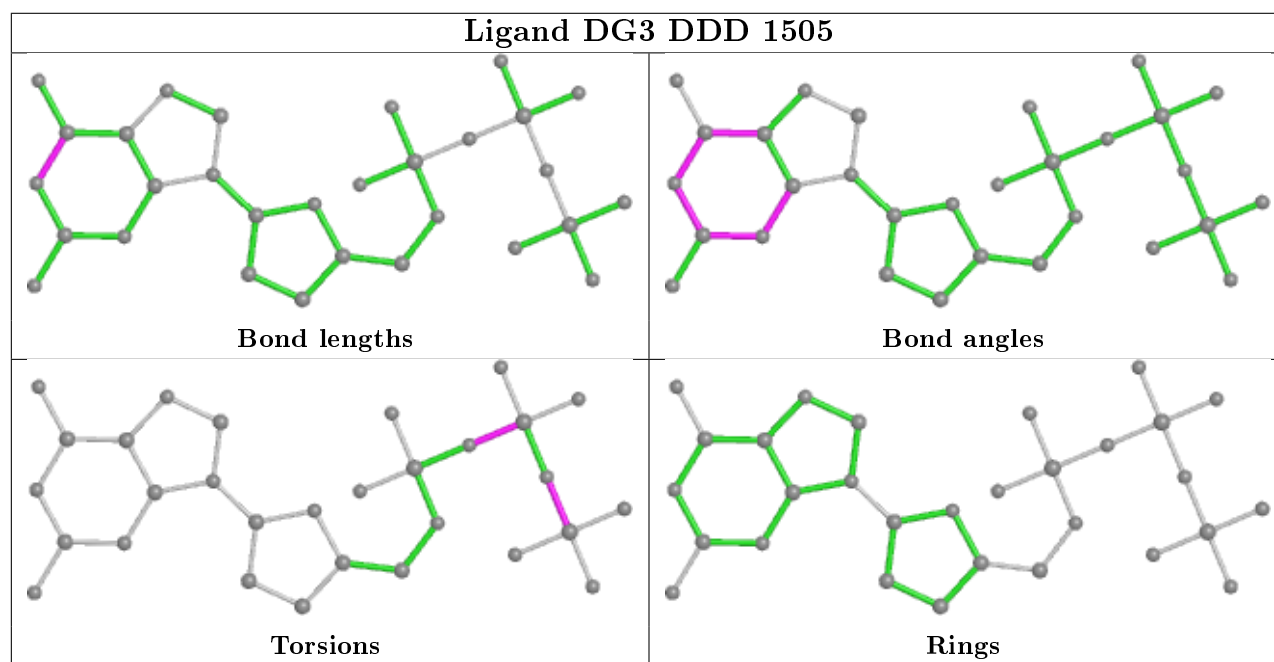
Mol	Chain	Res	Type	Atoms
11	DDD	1505	DG3	PB-O3B-PG-O3G
11	DDD	1505	DG3	PA-O3A-PB-O1B

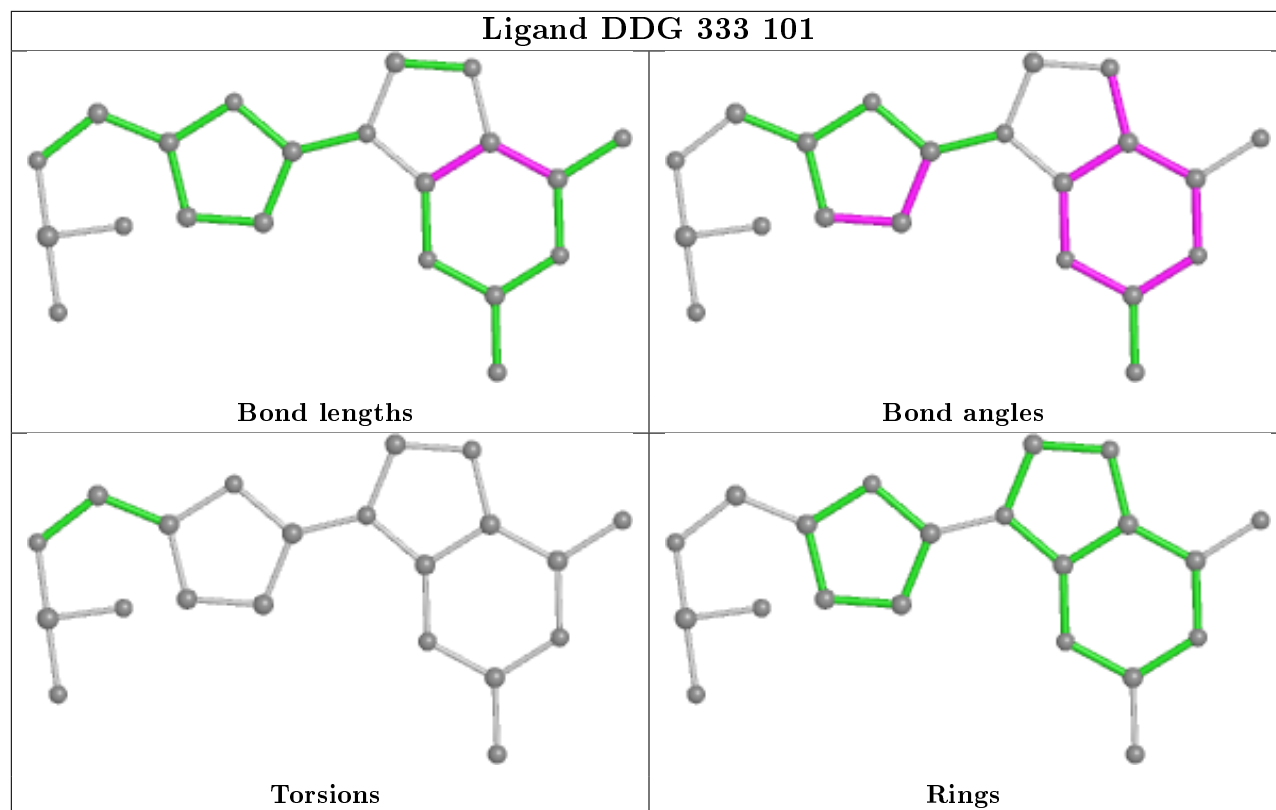
There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	DDD	1505	DG3	11	0
12	333	101	DDG	3	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%)	0.36	19 (8%)	11 10	235, 332, 394, 420	0
1	BBB	228/242 (94%)	0.17	12 (5%)	26 23	219, 299, 405, 493	0
2	CCC	1341/1342 (99%)	0.00	43 (3%)	47 37	135, 265, 411, 503	0
3	DDD	1362/1407 (96%)	0.17	99 (7%)	15 12	138, 283, 458, 547	0
4	EEE	79/90 (87%)	0.07	3 (3%)	40 32	208, 315, 468, 542	0
5	FFF	270/336 (80%)	0.33	16 (5%)	22 19	263, 376, 482, 500	0
6	111	29/50 (58%)	0.42	4 (13%)	2 3	304, 372, 557, 600	0
7	222	32/50 (64%)	1.08	9 (28%)	0 1	256, 367, 577, 639	0
8	333	5/6 (83%)	0.99	1 (20%)	1 1	340, 354, 386, 388	0
All	All	3576/3765 (94%)	0.14	206 (5%)	23 19	135, 295, 457, 639	0

All (206) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	DDD	748	ALA	11.2
3	DDD	1059	LEU	6.9
7	222	36	DG	6.5
2	CCC	1004	ASP	6.4
2	CCC	1001	GLY	6.3
3	DDD	1066	GLU	6.3
3	DDD	1111	ASP	6.2
3	DDD	1110	GLU	6.0
3	DDD	750	PRO	5.7
2	CCC	259	GLY	5.5
3	DDD	1099	TYR	5.3
3	DDD	943	ARG	5.3
3	DDD	1121	LEU	5.2
2	CCC	230	PHE	5.2
5	FFF	323	ASN	5.1

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Mol	Chain	Res	Type	RSRZ
3	DDD	732	GLY	5.0
3	DDD	1129	GLY	4.9
2	CCC	1002	LEU	4.9
3	DDD	854	ALA	4.9
3	DDD	941	ALA	4.9
3	DDD	1030	GLU	4.9
2	CCC	169	LYS	4.7
3	DDD	1029	THR	4.7
3	DDD	856	ILE	4.7
3	DDD	940	ALA	4.6
1	BBB	166	ARG	4.6
1	BBB	165	GLU	4.6
3	DDD	1122	ALA	4.5
3	DDD	1098	GLN	4.5
2	CCC	1005	GLU	4.5
1	AAA	134	THR	4.4
3	DDD	752	GLY	4.4
1	AAA	171	LEU	4.4
3	DDD	965	SER	4.4
1	BBB	50	SER	4.3
3	DDD	1065	ALA	4.3
3	DDD	1203	ARG	4.3
3	DDD	997	VAL	4.3
5	FFF	295	ILE	4.3
4	EEE	78	ALA	4.3
3	DDD	853	THR	4.3
3	DDD	880	VAL	4.3
2	CCC	164	THR	4.2
2	CCC	240	GLU	4.2
3	DDD	1130	GLY	4.1
3	DDD	1266	ILE	4.1
6	111	54	DA	4.0
1	AAA	59	VAL	4.0
4	EEE	3	ARG	3.9
1	BBB	108	GLY	3.9
3	DDD	1118	GLY	3.9
2	CCC	231	GLU	3.9
7	222	35	DT	3.8
2	CCC	257	ALA	3.7
3	DDD	1271	SER	3.7
2	CCC	850	ILE	3.7
1	AAA	201	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
7	222	38	DG	3.6
5	FFF	263	LEU	3.6
3	DDD	232	ASN	3.6
3	DDD	966	VAL	3.6
6	111	44	DG	3.5
3	DDD	855	ASP	3.5
1	AAA	164	ASP	3.5
1	BBB	162	GLU	3.5
2	CCC	1003	THR	3.5
3	DDD	586	GLY	3.4
3	DDD	746	LEU	3.4
7	222	37	DA	3.4
3	DDD	749	LYS	3.4
3	DDD	1028	ILE	3.4
2	CCC	124	MET	3.4
1	BBB	133	LEU	3.4
2	CCC	870	ILE	3.4
4	EEE	79	GLU	3.3
3	DDD	1035	VAL	3.3
2	CCC	333	ILE	3.3
1	AAA	144	ILE	3.3
1	AAA	213	PRO	3.3
3	DDD	1087	ASP	3.3
7	222	23	DT	3.2
5	FFF	131	VAL	3.2
1	AAA	107	ILE	3.2
5	FFF	315	GLU	3.2
5	FFF	201	GLN	3.2
7	222	24	DT	3.2
3	DDD	1272	SER	3.2
2	CCC	984	VAL	3.2
5	FFF	71	LEU	3.1
3	DDD	1187	GLU	3.1
3	DDD	978	ARG	3.1
1	AAA	205	MET	3.1
1	BBB	93	GLN	3.0
3	DDD	992	LYS	3.0
3	DDD	1054	THR	3.0
3	DDD	958	ILE	3.0
3	DDD	1128	SER	3.0
3	DDD	1112	GLY	2.9
1	BBB	164	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
2	CCC	261	VAL	2.9
2	CCC	239	MET	2.9
3	DDD	731	ARG	2.9
3	DDD	989	GLY	2.9
3	DDD	1078	LEU	2.8
5	FFF	261	LYS	2.8
3	DDD	945	ALA	2.8
3	DDD	730	ALA	2.8
2	CCC	982	GLY	2.8
3	DDD	969	SER	2.8
1	AAA	188	GLU	2.7
1	AAA	135	ASP	2.7
6	111	51	DC	2.7
3	DDD	1058	SER	2.7
3	DDD	1198	VAL	2.7
3	DDD	585	LYS	2.7
3	DDD	942	SER	2.7
1	AAA	24	ALA	2.7
3	DDD	848	VAL	2.7
3	DDD	743	MET	2.7
3	DDD	976	THR	2.7
2	CCC	256	GLU	2.6
3	DDD	1196	LEU	2.6
3	DDD	1276	GLU	2.6
3	DDD	1115	ILE	2.6
3	DDD	1037	PHE	2.6
3	DDD	993	GLU	2.6
7	222	17	DG	2.6
2	CCC	721	GLY	2.6
3	DDD	1077	ALA	2.6
3	DDD	127	LEU	2.6
2	CCC	96	LEU	2.6
2	CCC	332	ARG	2.6
3	DDD	1038	THR	2.6
3	DDD	176	PHE	2.5
3	DDD	1113	VAL	2.5
3	DDD	1036	ARG	2.5
3	DDD	1007	ASP	2.5
7	222	25	DA	2.5
7	222	18	DT	2.5
2	CCC	105	TYR	2.5
2	CCC	260	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	CCC	941	LYS	2.4
1	AAA	172	LEU	2.4
6	111	43	DT	2.4
3	DDD	1063	ASP	2.4
3	DDD	1079	LYS	2.4
3	DDD	1003	LEU	2.4
8	333	15	A	2.4
2	CCC	531	SER	2.4
3	DDD	1267	VAL	2.4
5	FFF	306	GLN	2.4
3	DDD	392	THR	2.4
2	CCC	1190	ALA	2.4
3	DDD	1158	GLU	2.4
3	DDD	996	LYS	2.4
3	DDD	1131	THR	2.4
2	CCC	1180	MET	2.3
1	BBB	98	VAL	2.3
3	DDD	844	THR	2.3
5	FFF	283	TYR	2.3
1	AAA	26	VAL	2.3
3	DDD	970	SER	2.3
3	DDD	1107	VAL	2.3
5	FFF	134	PHE	2.3
2	CCC	125	GLY	2.3
2	CCC	60	GLN	2.3
2	CCC	232	ILE	2.3
3	DDD	1159	ILE	2.3
1	AAA	165	GLU	2.3
2	CCC	336	LEU	2.3
3	DDD	747	MET	2.3
1	BBB	146	VAL	2.3
2	CCC	922	ASN	2.3
3	DDD	1051	ASP	2.3
3	DDD	986	ASP	2.3
5	FFF	296	GLY	2.3
5	FFF	124	ASN	2.3
2	CCC	262	TYR	2.2
5	FFF	198	ILE	2.2
3	DDD	1090	ILE	2.2
3	DDD	1268	ASN	2.2
1	AAA	27	THR	2.2
2	CCC	422	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	CCC	258	ASN	2.2
3	DDD	112	ALA	2.2
3	DDD	666	GLU	2.2
2	CCC	931	VAL	2.2
1	AAA	73	GLY	2.2
2	CCC	79	VAL	2.2
2	CCC	153	PRO	2.1
3	DDD	24	LEU	2.1
5	FFF	291	VAL	2.1
5	FFF	305	ILE	2.1
2	CCC	884	VAL	2.1
2	CCC	171	LEU	2.1
1	AAA	189	ALA	2.1
1	BBB	107	ILE	2.1
3	DDD	1274	PHE	2.1
1	AAA	166	ARG	2.1
3	DDD	949	SER	2.0
1	BBB	100	LEU	2.0
3	DDD	1270	GLY	2.0
3	DDD	670	SER	2.0
3	DDD	951	GLN	2.0
3	DDD	1005	LYS	2.0
3	DDD	1027	VAL	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](#)

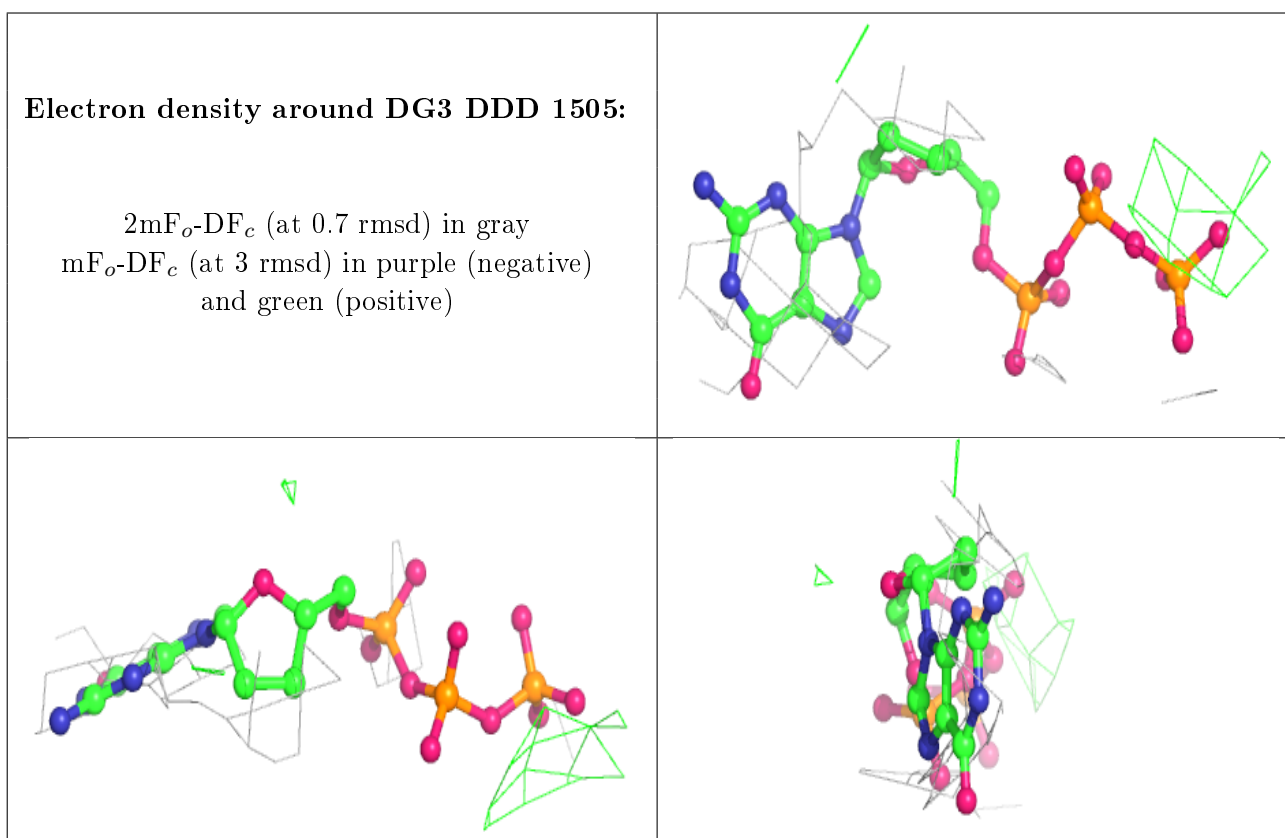
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

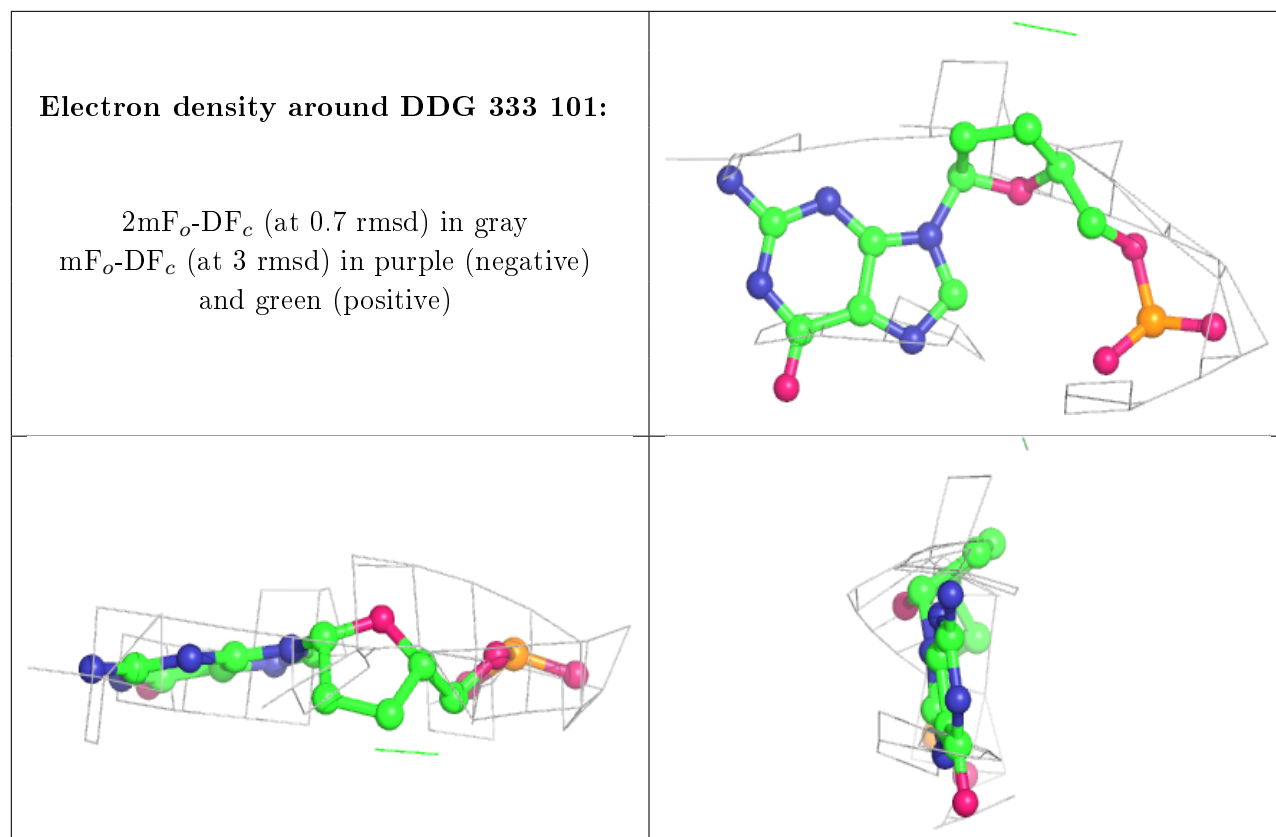
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	ZN	DDD	1501	1/1	0.73	0.05	406,406,406,406	0
11	DG3	DDD	1505	30/30	0.74	0.48	310,341,366,385	0
12	DDG	333	101	21/22	0.81	0.43	294,315,317,318	0
10	MG	DDD	1503	1/1	0.88	0.36	149,149,149,149	0
9	ZN	DDD	1502	1/1	0.93	0.13	348,348,348,348	0
10	MG	DDD	1504	1/1	0.99	0.31	113,113,113,113	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.