



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2020 – 02:08 PM BST

PDB ID : 6UUC
Title : E. coli sigma-S transcription initiation complex with a 3-nt RNA and a mismatching ATP ("Fresh" crystal soaked with ATP for 2 hours)
Authors : Zuo, Y.; De, S.; Steitz, T.A.
Deposited on : 2019-10-30
Resolution : 4.10 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

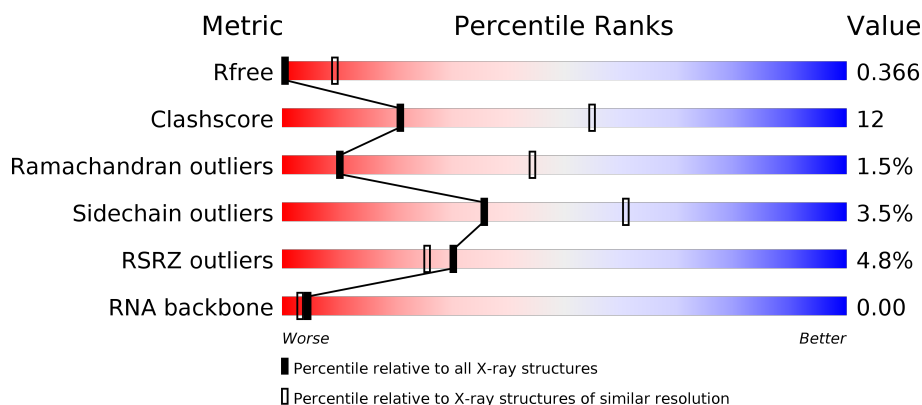
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 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.






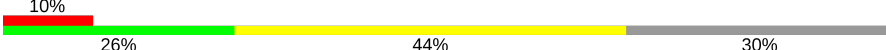
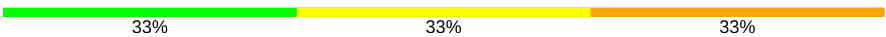
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1193 (4.50-3.70)
Clashscore	141614	1003 (4.44-3.76)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)
RSRZ outliers	127900	1034 (4.50-3.70)
RNA backbone	3102	1049 (5.04-3.00)

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>5%</div> <div> <div></div> <div>73%</div> <div>20%</div> <div>• 5%</div> </div> </div>
1	BBB	242	<div> <div>8%</div> <div> <div></div> <div>72%</div> <div>21%</div> <div>• 6%</div> </div> </div>
2	CCC	1342	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>20%</div> <div>•</div> </div> </div>
3	DDD	1407	<div> <div>5%</div> <div> <div></div> <div>72%</div> <div>22%</div> <div>• •</div> </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 28970 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	32	Total	C	N	O	P	0	0	0
			660	313	122	193	32			

- 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			

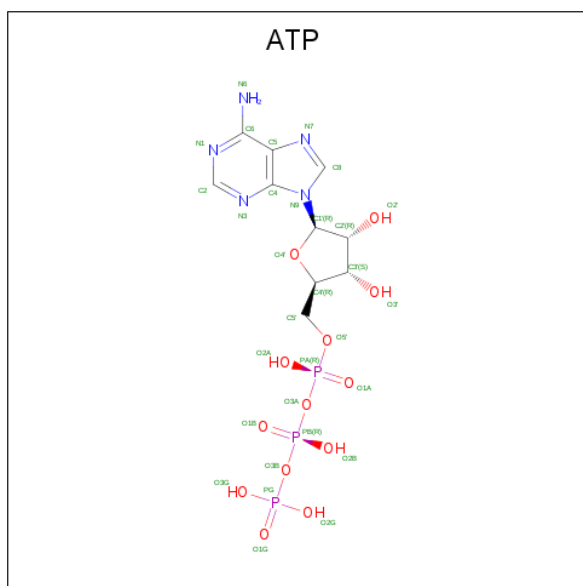
- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- Molecule 11 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$).

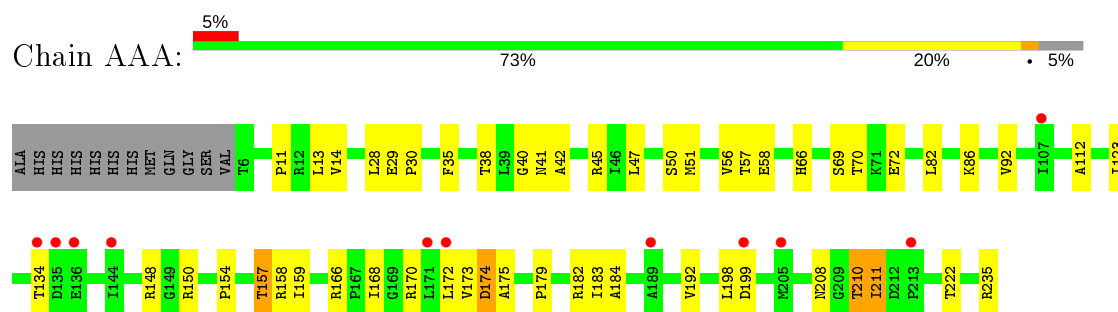


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	DDD	1	Total 31	C 10	N 5	O 13	P 3	0	0

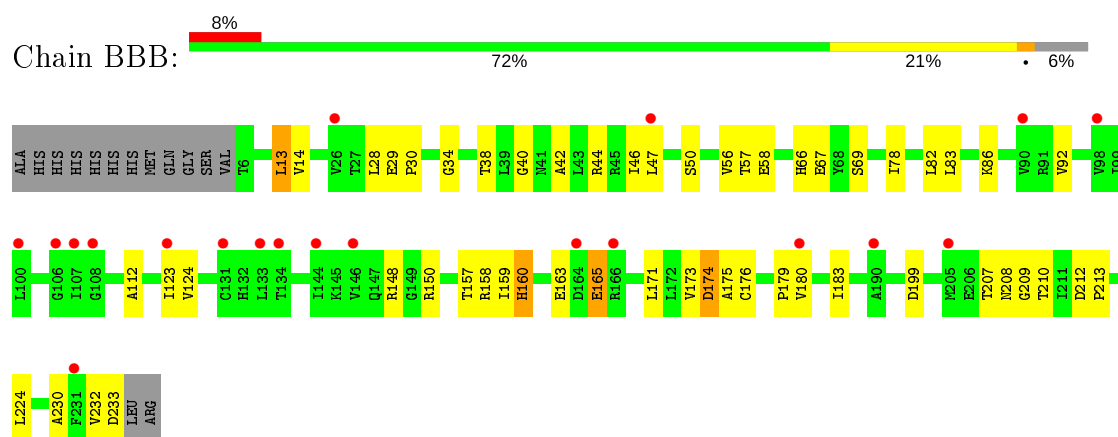
3 Residue-property plots [i](#)

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.

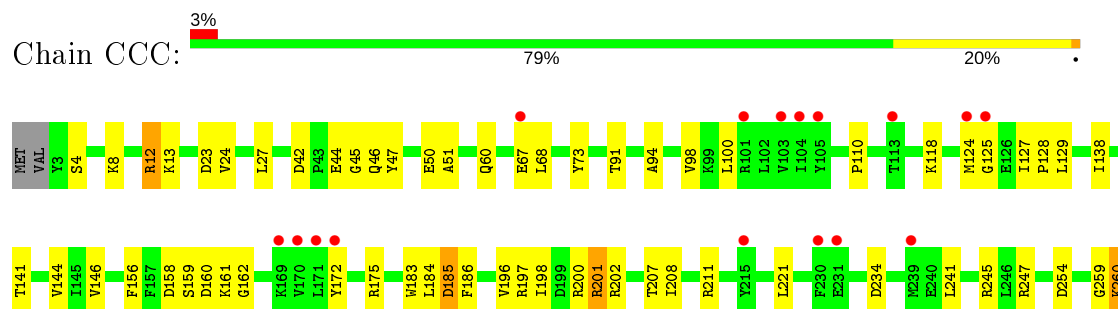
- Molecule 1: DNA-directed RNA polymerase subunit alpha

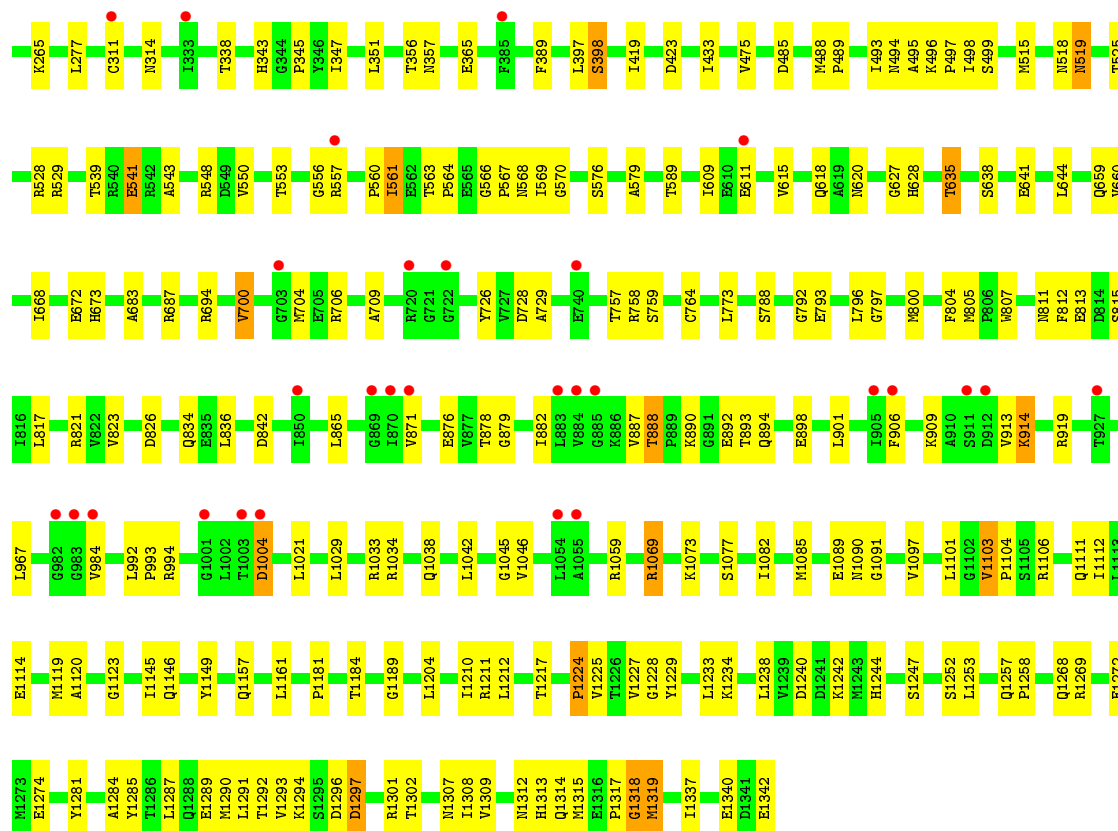


- Molecule 1: DNA-directed RNA polymerase subunit alpha

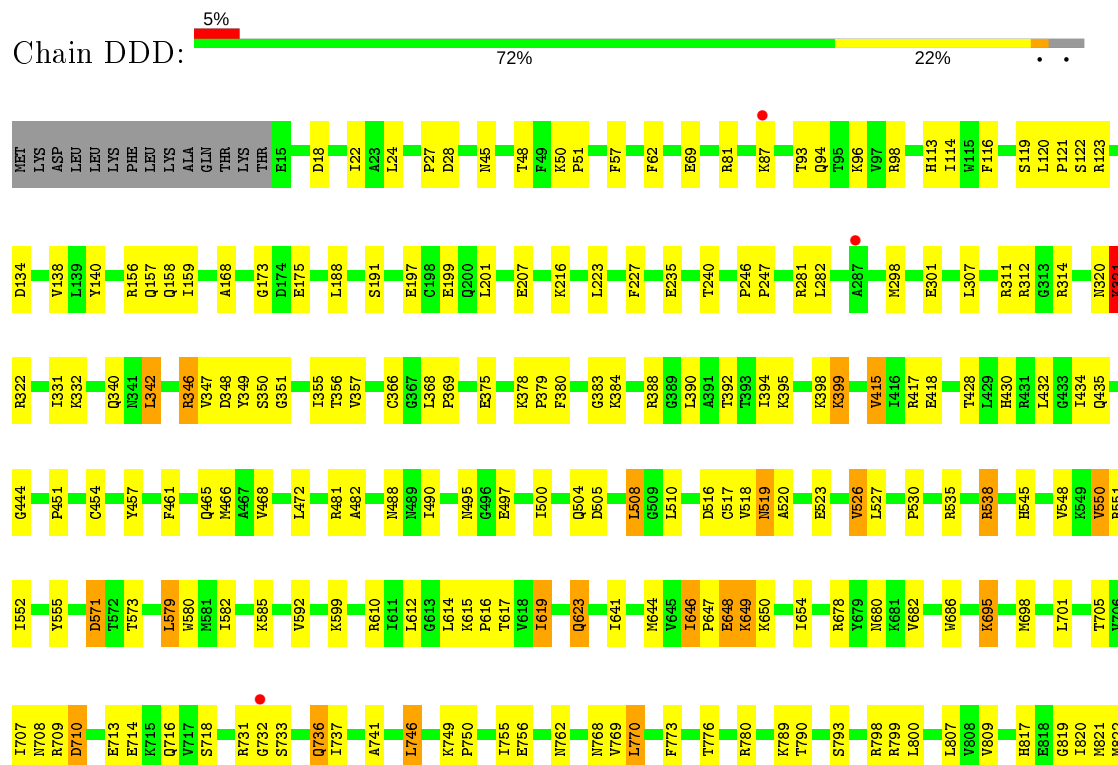


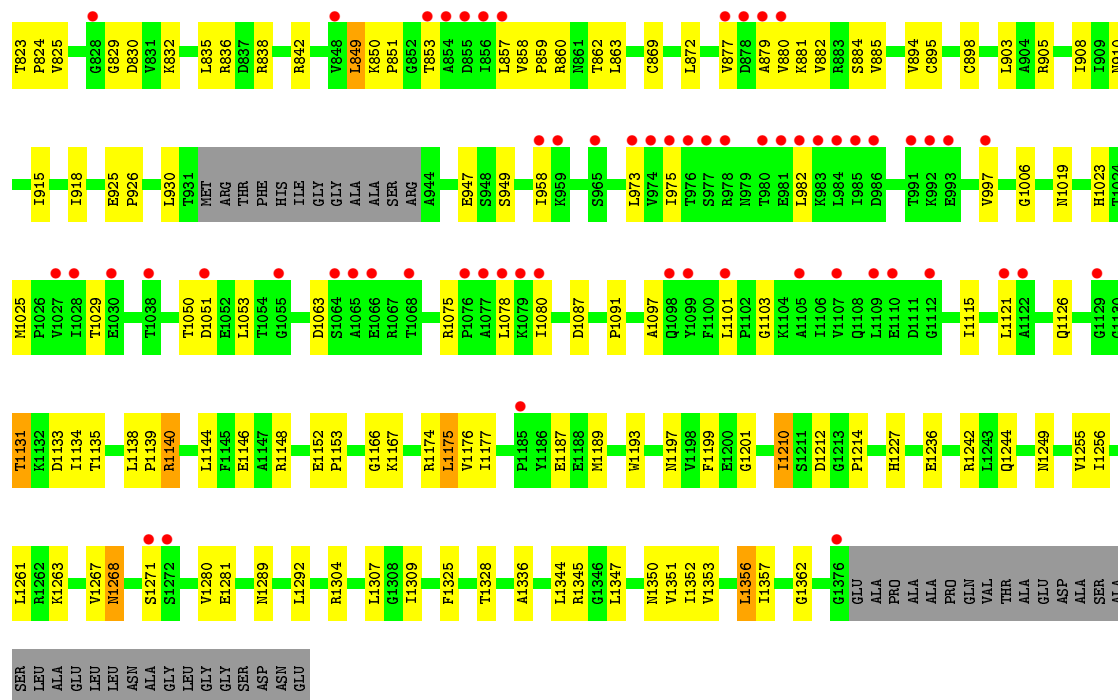
- Molecule 2: DNA-directed RNA polymerase subunit beta





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

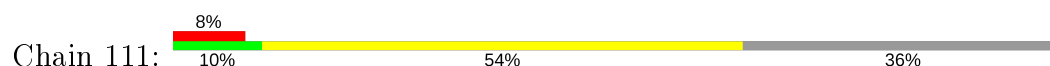




- Molecule 4: DNA-directed RNA polymerase subunit omega

- 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: 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	133.10Å 154.92Å 231.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.30 – 4.10 49.32 – 4.10	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.30-4.10) 98.4 (49.32-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 4.14Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.322 , 0.380 0.310 , 0.366	Depositor DCC
R_{free} test set	1809 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	187.4	Xtriage
Anisotropy	0.618	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 276.5	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	0.91	EDS
Total number of atoms	28970	wwPDB-VP
Average B, all atoms (Å ²)	329.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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, ATP

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	0.70	0/2450
1	BBB	0.65	0/1789	0.70	0/2425
2	CCC	0.62	0/10739	0.71	0/14489
3	DDD	0.63	0/10636	0.71	0/14362
4	EEE	0.63	0/629	0.71	0/847
5	FFF	0.65	0/2282	0.63	0/3076
6	111	0.29	0/739	0.62	0/1137
7	222	0.26	0/803	0.62	0/1238
8	333	0.55	0/50	0.68	0/76
All	All	0.62	0/29476	0.70	0/40100

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	1787	0	1813	54	0
1	BBB	1767	0	1789	69	0
2	CCC	10570	0	10582	223	0
3	DDD	10478	0	10691	287	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	EEE	627	0	634	8	0
5	FFF	2253	0	2298	83	1
6	111	660	0	362	58	0
7	222	716	0	396	45	0
8	333	77	0	34	9	0
9	CCC	1	0	0	0	0
9	DDD	1	0	0	0	0
10	DDD	2	0	0	2	0
11	DDD	31	0	12	5	0
All	All	28970	0	28611	698	1

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 12.

All (698) 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:898:CYS:SG	10:DDD:1502:ZN:ZN	1.18	1.31
3:DDD:320:ASN:OD1	7:222:22:DA:N6	1.70	1.23
1:BBB:179:PRO:O	1:BBB:207:THR:OG1	1.57	1.22
2:CCC:496:LYS:HD3	7:222:24:DT:OP1	1.42	1.19
6:111:50:DT:H3'	6:111:51:DC:H5''	1.25	1.14
3:DDD:731:ARG:NH1	11:DDD:1504:ATP:O3G	1.85	1.09
3:DDD:646:ILE:CG2	3:DDD:647:PRO:HD2	1.80	1.09
1:AAA:82:LEU:HD22	1:AAA:173:VAL:HG21	1.18	1.09
3:DDD:821:MET:HE3	3:DDD:879:ALA:HB1	1.30	1.06
6:111:50:DT:H3'	6:111:51:DC:C5'	1.86	1.04
2:CCC:1073:LYS:NZ	8:333:16:G:OP1	1.89	1.04
1:BBB:82:LEU:HD22	1:BBB:173:VAL:CG2	1.87	1.04
2:CCC:563:THR:OG1	2:CCC:569:ILE:O	1.75	1.04
3:DDD:646:ILE:HG22	3:DDD:647:PRO:HD2	1.06	1.04
1:BBB:82:LEU:HD22	1:BBB:173:VAL:HG21	1.41	1.01
2:CCC:175:ARG:NE	6:111:50:DT:O4	1.95	0.99
1:BBB:67:GLU:HB3	1:BBB:171:LEU:HD22	1.44	0.98
1:BBB:212:ASP:OD1	1:BBB:213:PRO:HD2	1.62	0.97
3:DDD:527:LEU:HB2	3:DDD:550:VAL:CG1	1.94	0.97
1:AAA:82:LEU:HD22	1:AAA:173:VAL:CG2	1.94	0.96
3:DDD:821:MET:HA	3:DDD:880:VAL:O	1.66	0.96
3:DDD:898:CYS:HG	10:DDD:1502:ZN:ZN	0.74	0.96
3:DDD:821:MET:CE	3:DDD:879:ALA:HB1	1.93	0.96
2:CCC:560:PRO:O	3:DDD:780:ARG:NH2	2.01	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:817:HIS:HB3	3:DDD:860:ARG:NH2	1.83	0.93
3:DDD:646:ILE:HG22	3:DDD:647:PRO:CD	1.97	0.93
5:FFF:273:VAL:HG13	5:FFF:291:VAL:HG11	1.51	0.93
3:DDD:527:LEU:HB2	3:DDD:550:VAL:HG12	1.46	0.92
2:CCC:1284:ALA:HA	3:DDD:1357:ILE:HD12	1.51	0.92
5:FFF:227:GLY:N	7:222:20:DG:O6	2.03	0.91
1:AAA:45:ARG:NE	1:BBB:38:THR:OG1	2.01	0.91
1:BBB:212:ASP:CG	1:BBB:213:PRO:HD2	1.92	0.90
2:CCC:888:THR:O	2:CCC:914:LYS:N	2.04	0.89
2:CCC:901:LEU:HD13	5:FFF:278:PHE:CE2	2.08	0.88
2:CCC:200:ARG:HD3	6:111:50:DT:O2	1.71	0.88
2:CCC:200:ARG:HD3	6:111:50:DT:C2	2.10	0.87
3:DDD:822:MET:CE	3:DDD:882:VAL:HG11	2.05	0.87
3:DDD:646:ILE:HG23	3:DDD:741:ALA:O	1.75	0.87
5:FFF:218:ARG:HA	5:FFF:218:ARG:NE	1.89	0.85
3:DDD:822:MET:HE1	3:DDD:882:VAL:HG21	1.57	0.85
7:222:30:DA:H2'	7:222:31:DT:H72	1.57	0.85
2:CCC:1073:LYS:HZ3	8:333:16:G:P	1.99	0.85
2:CCC:1287:LEU:HD23	3:DDD:1357:ILE:HD11	1.58	0.84
1:BBB:56:VAL:O	1:BBB:175:ALA:HB2	1.78	0.84
1:AAA:56:VAL:O	1:AAA:175:ALA:HB2	1.77	0.83
1:BBB:179:PRO:C	1:BBB:207:THR:OG1	2.18	0.82
1:AAA:235:ARG:HB2	1:BBB:13:LEU:HD23	1.62	0.81
3:DDD:822:MET:HE2	3:DDD:882:VAL:HG11	1.63	0.81
2:CCC:564:PRO:HB3	8:333:14:GTP:O2A	1.82	0.79
3:DDD:518:VAL:HG23	3:DDD:716:GLN:NE2	1.97	0.78
2:CCC:564:PRO:HB3	8:333:14:GTP:PA	2.24	0.78
2:CCC:1342:GLU:HA	3:DDD:18:ASP:HB2	1.66	0.77
7:222:30:DA:C2'	7:222:31:DT:H72	2.14	0.77
6:111:32:DA:C2	7:222:32:DA:C4	2.73	0.77
3:DDD:555:TYR:CD1	3:DDD:585:LYS:HD2	2.19	0.77
3:DDD:832:LYS:HG3	3:DDD:1242:ARG:HD3	1.67	0.77
1:AAA:92:VAL:O	1:AAA:148:ARG:NH2	2.18	0.77
1:BBB:92:VAL:O	1:BBB:148:ARG:NH2	2.18	0.77
5:FFF:242:LYS:HG3	5:FFF:243:GLU:H	1.50	0.76
6:111:47:DC:C2'	6:111:48:DA:H5'	2.15	0.76
3:DDD:1140:ARG:NH1	3:DDD:1144:LEU:HD11	2.01	0.76
7:222:30:DA:H2''	7:222:31:DT:C6	2.21	0.76
2:CCC:1281:TYR:OH	3:DDD:434:ILE:O	2.01	0.76
1:BBB:124:VAL:HG21	1:BBB:210:THR:HG22	1.68	0.75
3:DDD:615:LYS:HB2	3:DDD:616:PRO:HD3	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:67:GLU:N	1:BBB:171:LEU:HD21	2.03	0.74
3:DDD:555:TYR:CE1	3:DDD:585:LYS:HD2	2.23	0.73
6:111:51:DC:OP1	6:111:51:DC:H2'	1.87	0.73
3:DDD:378:LYS:H	3:DDD:379:PRO:HD2	1.54	0.73
3:DDD:821:MET:CE	3:DDD:879:ALA:CB	2.65	0.72
7:222:30:DA:H2''	7:222:31:DT:C7	2.19	0.72
3:DDD:378:LYS:N	3:DDD:379:PRO:HD2	2.05	0.72
1:AAA:158:ARG:HB3	1:AAA:172:LEU:HD21	1.72	0.71
2:CCC:496:LYS:HB3	7:222:24:DT:OP1	1.89	0.71
2:CCC:560:PRO:HB2	3:DDD:776:THR:HG21	1.71	0.71
4:EEE:25:ARG:NH2	4:EEE:68:GLU:OE1	2.22	0.71
2:CCC:901:LEU:HD11	5:FFF:310:LEU:HD21	1.73	0.71
1:AAA:57:THR:HG23	1:AAA:158:ARG:CZ	2.20	0.71
3:DDD:822:MET:CE	3:DDD:882:VAL:HG21	2.20	0.70
1:BBB:212:ASP:OD1	1:BBB:213:PRO:CD	2.36	0.70
2:CCC:1234:LYS:HE2	2:CCC:1238:LEU:HD21	1.74	0.70
2:CCC:1103:VAL:HB	2:CCC:1104:PRO:HD3	1.74	0.70
3:DDD:320:ASN:OD1	7:222:22:DA:C6	2.44	0.70
7:222:31:DT:H1'	7:222:32:DA:H5'	1.73	0.70
1:BBB:46:ILE:HD11	1:BBB:224:LEU:HD13	1.74	0.70
3:DDD:134:ASP:HB3	3:DDD:159:ILE:HD11	1.74	0.70
5:FFF:241:GLU:HG3	5:FFF:242:LYS:H	1.56	0.69
7:222:5:DC:H1'	7:222:6:DG:H5'	1.74	0.69
1:BBB:66:HIS:C	1:BBB:171:LEU:HD21	2.13	0.69
1:AAA:222:THR:OG1	1:BBB:233:ASP:OD2	2.11	0.69
5:FFF:242:LYS:HG3	5:FFF:243:GLU:N	2.07	0.69
3:DDD:680:ASN:HD21	3:DDD:1023:HIS:CD2	2.10	0.69
3:DDD:817:HIS:HB3	3:DDD:860:ARG:HH21	1.58	0.68
3:DDD:832:LYS:CG	3:DDD:1242:ARG:HD3	2.23	0.68
5:FFF:98:ASN:HA	6:111:41:DT:O2	1.94	0.68
3:DDD:504:GLN:HE22	3:DDD:731:ARG:NH2	1.91	0.68
5:FFF:241:GLU:HG3	5:FFF:242:LYS:N	2.07	0.68
2:CCC:528:ARG:NH2	2:CCC:576:SER:O	2.27	0.68
1:BBB:57:THR:HG23	1:BBB:158:ARG:NH2	2.09	0.68
3:DDD:1140:ARG:HH12	3:DDD:1144:LEU:HD11	1.60	0.67
2:CCC:118:LYS:NZ	2:CCC:485:ASP:O	2.28	0.67
3:DDD:822:MET:HE2	3:DDD:882:VAL:CG1	2.24	0.67
2:CCC:548:ARG:HB3	2:CCC:570:GLY:HA3	1.77	0.67
6:111:32:DA:C2	7:222:32:DA:N3	2.63	0.67
2:CCC:1029:LEU:HG	2:CCC:1033:ARG:HD3	1.77	0.67
5:FFF:98:ASN:OD1	6:111:41:DT:N3	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:67:GLU:CB	1:BBB:171:LEU:HD22	2.23	0.66
3:DDD:140:TYR:OH	3:DDD:312:ARG:HD2	1.95	0.66
5:FFF:170:HIS:CG	6:111:31:DT:H73	2.31	0.66
7:222:15:DT:H5"	7:222:15:DT:H6	1.61	0.65
3:DDD:905:ARG:NH1	3:DDD:910:ASN:OD1	2.29	0.65
1:AAA:11:PRO:HG2	1:BBB:230:ALA:HB2	1.77	0.65
3:DDD:1152:GLU:O	3:DDD:1214:PRO:HD2	1.96	0.65
7:222:30:DA:C2'	7:222:31:DT:C7	2.74	0.65
1:AAA:82:LEU:CD2	1:AAA:173:VAL:HG21	2.12	0.65
5:FFF:141:ARG:NH2	6:111:40:DA:OP2	2.27	0.65
3:DDD:1075:ARG:NH2	3:DDD:1193:TRP:CE3	2.64	0.65
2:CCC:576:SER:OG	2:CCC:659:GLN:O	2.15	0.64
1:BBB:212:ASP:CG	1:BBB:213:PRO:CD	2.65	0.64
1:BBB:180:VAL:HA	1:BBB:207:THR:CB	2.28	0.64
7:222:32:DA:H2"	7:222:33:DC:C5	2.33	0.64
6:111:32:DA:C2	7:222:32:DA:C2	2.85	0.64
2:CCC:887:VAL:HB	2:CCC:913:VAL:HG12	1.80	0.64
2:CCC:560:PRO:CB	3:DDD:776:THR:HG21	2.27	0.64
7:222:30:DA:H2"	7:222:31:DT:C5	2.33	0.64
6:111:47:DC:H2'	6:111:48:DA:H5'	1.79	0.63
3:DDD:490:ILE:HD11	3:DDD:614:LEU:HD13	1.79	0.63
5:FFF:262:TRP:HE1	5:FFF:320:GLN:HE22	1.45	0.63
3:DDD:481:ARG:NH1	4:EEE:3:ARG:O	2.31	0.63
2:CCC:550:VAL:HG21	3:DDD:776:THR:HG22	1.80	0.63
2:CCC:700:VAL:HG21	2:CCC:1114:GLU:HG3	1.80	0.63
3:DDD:821:MET:HE1	3:DDD:879:ALA:CB	2.29	0.63
2:CCC:496:LYS:CD	7:222:24:DT:OP1	2.34	0.63
6:111:49:DG:H2"	6:111:50:DT:C4'	2.29	0.63
1:AAA:11:PRO:HG2	1:BBB:230:ALA:CB	2.28	0.63
2:CCC:259:GLY:O	2:CCC:260:LYS:HB2	1.98	0.63
2:CCC:494:ASN:ND2	7:222:25:DA:OP1	2.32	0.63
6:111:46:DG:H2"	6:111:47:DC:O4'	1.99	0.62
1:AAA:57:THR:HG23	1:AAA:158:ARG:NH2	2.14	0.62
2:CCC:46:GLN:HB2	2:CCC:51:ALA:HA	1.79	0.62
2:CCC:672:GLU:HG3	2:CCC:673:HIS:CD2	2.33	0.62
3:DDD:378:LYS:N	3:DDD:379:PRO:CD	2.63	0.62
2:CCC:186:PHE:CD1	2:CCC:196:VAL:HG22	2.34	0.62
6:111:52:DT:H2"	6:111:53:DG:C8	2.34	0.62
2:CCC:906:PHE:HZ	5:FFF:323:ASN:OD1	1.80	0.62
2:CCC:992:LEU:HB3	2:CCC:993:PRO:HD2	1.82	0.62
5:FFF:176:ASN:OD1	7:222:26:DT:H71	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:1318:GLY:O	2:CCC:1319:MET:HB2	1.99	0.62
5:FFF:227:GLY:O	5:FFF:229:ASP:N	2.32	0.62
1:BBB:82:LEU:HD13	1:BBB:173:VAL:HG22	1.82	0.62
2:CCC:1145:ILE:HG22	2:CCC:1161:LEU:HD11	1.82	0.61
3:DDD:1140:ARG:HH12	3:DDD:1236:GLU:HG3	1.64	0.61
3:DDD:614:LEU:O	3:DDD:617:THR:OG1	2.17	0.61
3:DDD:395:LYS:HD3	5:FFF:329:LEU:HD13	1.80	0.61
3:DDD:819:GLY:H	3:DDD:881:LYS:HE2	1.64	0.61
3:DDD:678:ARG:NH1	3:DDD:756:GLU:OE1	2.33	0.61
1:BBB:163:GLU:O	1:BBB:163:GLU:HG3	1.98	0.61
3:DDD:527:LEU:HB2	3:DDD:550:VAL:HG13	1.78	0.61
1:AAA:29:GLU:HB2	1:AAA:30:PRO:HA	1.83	0.61
3:DDD:809:VAL:CG2	3:DDD:915:ILE:HD11	2.31	0.61
3:DDD:649:LYS:HD3	3:DDD:649:LYS:H	1.66	0.61
5:FFF:263:LEU:HD11	5:FFF:280:LEU:HD23	1.83	0.61
7:222:19:DA:H2'	7:222:20:DG:O4'	2.02	0.60
2:CCC:1123:GLY:HA3	2:CCC:1204:LEU:HD11	1.84	0.60
7:222:16:DC:H6	7:222:16:DC:H5"	1.66	0.60
1:BBB:180:VAL:HA	1:BBB:207:THR:HB	1.82	0.59
2:CCC:898:GLU:HG2	5:FFF:256:LYS:HG2	1.84	0.59
2:CCC:27:LEU:O	2:CCC:528:ARG:NH1	2.34	0.59
1:AAA:45:ARG:NH2	1:BBB:34:GLY:O	2.27	0.59
3:DDD:552:ILE:HG21	3:DDD:580:TRP:CD1	2.37	0.59
2:CCC:550:VAL:HG21	3:DDD:776:THR:CG2	2.32	0.59
1:BBB:29:GLU:HB2	1:BBB:30:PRO:HA	1.83	0.59
2:CCC:1073:LYS:NZ	8:333:16:G:P	2.68	0.59
2:CCC:221:LEU:HD11	2:CCC:314:ASN:HB2	1.84	0.59
2:CCC:1308:ILE:HG23	3:DDD:380:PHE:CE1	2.38	0.58
2:CCC:1294:LYS:HD3	3:DDD:347:VAL:HG13	1.84	0.58
3:DDD:518:VAL:HG23	3:DDD:716:GLN:HE22	1.67	0.58
2:CCC:539:THR:O	2:CCC:543:ALA:N	2.35	0.58
5:FFF:207:ASP:O	5:FFF:211:ARG:HB2	2.03	0.58
3:DDD:1263:LYS:HB2	3:DDD:1307:LEU:HD11	1.85	0.58
3:DDD:819:GLY:H	3:DDD:881:LYS:CE	2.16	0.58
3:DDD:949:SER:HB3	3:DDD:1019:ASN:HD22	1.68	0.58
3:DDD:22:ILE:HG22	3:DDD:1336:ALA:HA	1.85	0.58
3:DDD:682:VAL:HG11	3:DDD:756:GLU:HG3	1.84	0.58
7:222:32:DA:H2"	7:222:33:DC:C6	2.38	0.58
3:DDD:863:LEU:HD22	3:DDD:908:ILE:HG13	1.84	0.58
2:CCC:397:LEU:O	2:CCC:398:SER:OG	2.13	0.58
1:AAA:184:ALA:HB2	2:CCC:1091:GLY:HA3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:890:LYS:HE3	2:CCC:893:THR:HG21	1.86	0.58
7:222:23:DT:H1'	7:222:24:DT:H5'	1.86	0.58
2:CCC:12:ARG:HG3	2:CCC:1181:PRO:HB2	1.85	0.58
5:FFF:207:ASP:O	5:FFF:211:ARG:N	2.36	0.58
3:DDD:93:THR:HG22	3:DDD:94:GLN:H	1.68	0.58
1:AAA:154:PRO:HG2	1:AAA:157:THR:HB	1.85	0.57
3:DDD:849:LEU:HD11	3:DDD:853:THR:HA	1.86	0.57
3:DDD:122:SER:O	3:DDD:123:ARG:HB2	2.04	0.57
3:DDD:1267:VAL:O	3:DDD:1268:ASN:CB	2.53	0.57
3:DDD:332:LYS:HA	3:DDD:1328:THR:HG21	1.85	0.57
3:DDD:582:ILE:HG23	3:DDD:623:GLN:CB	2.34	0.57
5:FFF:262:TRP:HE1	5:FFF:320:GLN:NE2	2.02	0.57
3:DDD:1080:ILE:HB	3:DDD:1097:ALA:HB3	1.85	0.57
3:DDD:895:CYS:SG	3:DDD:898:CYS:SG	3.01	0.57
1:AAA:35:PHE:HZ	1:BBB:50:SER:HG	1.45	0.57
2:CCC:1301:ARG:HG3	2:CCC:1302:THR:N	2.20	0.57
2:CCC:564:PRO:HG2	2:CCC:568:ASN:O	2.05	0.57
11:DDD:1504:ATP:O4'	8:333:16:G:O3'	2.20	0.57
3:DDD:517:CYS:HB3	3:DDD:545:HIS:HB2	1.86	0.57
3:DDD:555:TYR:CE1	3:DDD:585:LYS:CD	2.87	0.57
5:FFF:263:LEU:HD11	5:FFF:280:LEU:CD2	2.35	0.57
1:AAA:38:THR:HG21	1:BBB:46:ILE:HD11	1.86	0.57
3:DDD:235:GLU:OE2	3:DDD:235:GLU:N	2.38	0.57
5:FFF:271:ARG:O	5:FFF:271:ARG:HG2	2.04	0.57
2:CCC:1287:LEU:HD23	3:DDD:1357:ILE:CD1	2.31	0.56
7:222:20:DG:H2''	7:222:21:DG:H5'	1.87	0.56
2:CCC:821:ARG:HH11	2:CCC:1082:ILE:HD13	1.70	0.56
5:FFF:72:THR:HG22	5:FFF:73:ALA:H	1.70	0.56
3:DDD:1063:ASP:HB3	3:DDD:1103:GLY:HA3	1.87	0.56
3:DDD:713:GLU:HG2	3:DDD:714:GLU:N	2.21	0.56
2:CCC:207:THR:HG21	2:CCC:351:LEU:HG	1.88	0.56
1:BBB:67:GLU:N	1:BBB:171:LEU:CD2	2.69	0.56
3:DDD:173:GLY:O	3:DDD:175:GLU:N	2.36	0.56
6:111:49:DG:H4'	6:111:50:DT:OP1	2.06	0.56
3:DDD:1197:ASN:N	3:DDD:1210:ILE:O	2.38	0.56
2:CCC:1042:LEU:HD13	2:CCC:1046:VAL:HG12	1.87	0.56
2:CCC:1284:ALA:CA	3:DDD:1357:ILE:HD12	2.32	0.56
3:DDD:301:GLU:HG3	3:DDD:312:ARG:NH2	2.20	0.56
3:DDD:555:TYR:CD1	3:DDD:585:LYS:CD	2.89	0.55
2:CCC:1120:ALA:HA	2:CCC:1204:LEU:HD12	1.88	0.55
2:CCC:1296:ASP:O	2:CCC:1297:ASP:C	2.44	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FFF:170:HIS:CE1	6:111:32:DA:N7	2.74	0.55
2:CCC:1268:GLN:HE21	3:DDD:351:GLY:HA2	1.71	0.55
2:CCC:635:THR:HG22	2:CCC:644:LEU:HD23	1.89	0.55
3:DDD:518:VAL:O	3:DDD:519:ASN:C	2.44	0.55
3:DDD:925:GLU:HB3	3:DDD:926:PRO:HD3	1.88	0.55
1:AAA:82:LEU:HD13	1:AAA:173:VAL:HG22	1.88	0.55
1:BBB:82:LEU:CD2	1:BBB:173:VAL:HG21	2.25	0.55
3:DDD:301:GLU:HG3	3:DDD:312:ARG:HH22	1.70	0.55
3:DDD:695:LYS:HA	3:DDD:695:LYS:CE	2.36	0.55
1:AAA:158:ARG:HD2	1:AAA:172:LEU:HD21	1.88	0.55
6:111:33:DT:H2''	6:111:34:DG:H5'	1.88	0.55
2:CCC:1290:MET:HG2	2:CCC:1294:LYS:HD2	1.89	0.55
11:DDD:1504:ATP:H4'	11:DDD:1504:ATP:O1A	2.07	0.55
2:CCC:638:SER:O	2:CCC:641:GLU:N	2.39	0.54
2:CCC:901:LEU:HD13	5:FFF:278:PHE:CZ	2.42	0.54
3:DDD:351:GLY:O	3:DDD:468:VAL:N	2.25	0.54
1:BBB:83:LEU:HD11	3:DDD:526:VAL:O	2.07	0.54
3:DDD:705:THR:O	3:DDD:705:THR:HG22	2.07	0.54
3:DDD:1167:LYS:HB2	3:DDD:1174:ARG:HD2	1.89	0.54
3:DDD:24:LEU:HD21	3:DDD:116:PHE:CZ	2.42	0.54
3:DDD:527:LEU:HD12	3:DDD:550:VAL:HG13	1.88	0.54
1:AAA:134:THR:HB	2:CCC:773:LEU:HD22	1.88	0.54
1:AAA:199:ASP:OD1	1:AAA:199:ASP:N	2.41	0.54
2:CCC:525:THR:HG21	2:CCC:687:ARG:CD	2.38	0.54
1:BBB:82:LEU:HB3	1:BBB:173:VAL:CG1	2.37	0.54
2:CCC:882:ILE:HG12	2:CCC:919:ARG:HB3	1.90	0.54
3:DDD:378:LYS:H	3:DDD:379:PRO:CD	2.20	0.54
3:DDD:342:LEU:HD21	3:DDD:1352:ILE:HG23	1.89	0.54
1:BBB:83:LEU:HD21	3:DDD:526:VAL:CG2	2.38	0.54
3:DDD:134:ASP:CB	3:DDD:159:ILE:HD11	2.37	0.54
1:BBB:180:VAL:HA	1:BBB:207:THR:OG1	2.07	0.54
2:CCC:200:ARG:HD3	6:111:50:DT:N3	2.23	0.54
2:CCC:797:GLY:HA3	2:CCC:1233:LEU:HD23	1.88	0.54
2:CCC:198:ILE:O	2:CCC:201:ARG:HG3	2.08	0.54
2:CCC:68:LEU:HD12	2:CCC:475:VAL:CG1	2.38	0.54
5:FFF:277:ARG:CD	5:FFF:306:GLN:HE21	2.21	0.54
2:CCC:1212:LEU:HD21	2:CCC:1227:VAL:HG21	1.90	0.53
1:BBB:199:ASP:OD1	1:BBB:199:ASP:N	2.41	0.53
2:CCC:4:SER:O	2:CCC:8:LYS:HG3	2.08	0.53
2:CCC:68:LEU:HD12	2:CCC:475:VAL:HG13	1.90	0.53
3:DDD:799:ARG:HB3	3:DDD:1309:ILE:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:211:ARG:NH1	2:CCC:357:ASN:O	2.42	0.53
5:FFF:144:THR:HG23	6:111:39:DA:N7	2.23	0.53
3:DDD:508:LEU:HD12	3:DDD:508:LEU:O	2.09	0.53
5:FFF:235:LEU:O	5:FFF:235:LEU:HD12	2.08	0.53
2:CCC:241:LEU:HD23	2:CCC:277:LEU:HD21	1.90	0.53
2:CCC:668:ILE:HD11	2:CCC:683:ALA:HB2	1.91	0.53
2:CCC:519:ASN:HD21	2:CCC:796:LEU:HD22	1.74	0.53
1:BBB:176:CYS:HB3	3:DDD:535:ARG:NH2	2.24	0.53
2:CCC:576:SER:HB3	2:CCC:579:ALA:HB2	1.90	0.53
3:DDD:695:LYS:HE3	3:DDD:695:LYS:HA	1.89	0.53
7:222:21:DG:H2"	7:222:22:DA:OP2	2.07	0.53
1:AAA:174:ASP:OD2	2:CCC:826:ASP:OD2	2.27	0.53
2:CCC:804:PHE:O	2:CCC:1225:VAL:HG13	2.09	0.53
3:DDD:490:ILE:HD11	3:DDD:614:LEU:CD1	2.38	0.53
2:CCC:1314:GLN:HA	4:EEE:28:ARG:NH2	2.24	0.53
3:DDD:836:ARG:HG3	3:DDD:869:CYS:HB3	1.90	0.52
2:CCC:1210:ILE:HD12	2:CCC:1227:VAL:HB	1.90	0.52
2:CCC:389:PHE:O	2:CCC:419:ILE:HG23	2.10	0.52
3:DDD:680:ASN:ND2	3:DDD:1023:HIS:CD2	2.76	0.52
2:CCC:1258:PRO:HG2	3:DDD:346:ARG:HB2	1.91	0.52
5:FFF:262:TRP:HB3	5:FFF:313:LEU:HD11	1.89	0.52
1:AAA:210:THR:HG22	1:AAA:211:ILE:N	2.25	0.52
3:DDD:1267:VAL:O	3:DDD:1268:ASN:HB2	2.09	0.52
2:CCC:1101:LEU:HD12	3:DDD:504:GLN:HG3	1.91	0.52
2:CCC:200:ARG:CD	6:111:50:DT:C2	2.90	0.52
2:CCC:709:ALA:HB3	2:CCC:792:GLY:O	2.09	0.52
1:AAA:134:THR:CB	2:CCC:773:LEU:HD22	2.40	0.52
2:CCC:94:ALA:HB2	2:CCC:129:LEU:HD11	1.92	0.52
3:DDD:680:ASN:HD21	3:DDD:1023:HIS:CG	2.28	0.52
3:DDD:807:LEU:HD22	3:DDD:1255:VAL:HG13	1.92	0.52
2:CCC:1269:ARG:HA	3:DDD:346:ARG:HA	1.92	0.52
2:CCC:823:VAL:HG12	2:CCC:1059:ARG:NH2	2.25	0.52
3:DDD:731:ARG:NH1	11:DDD:1504:ATP:PG	2.83	0.52
3:DDD:709:ARG:O	3:DDD:710:ASP:CB	2.58	0.51
2:CCC:1119:MET:HB2	2:CCC:1228:GLY:HA2	1.93	0.51
3:DDD:451:PRO:HA	3:DDD:454:CYS:SG	2.51	0.51
3:DDD:582:ILE:HG23	3:DDD:623:GLN:HB2	1.91	0.51
2:CCC:185:ASP:HB2	2:CCC:197:ARG:HG3	1.93	0.51
3:DDD:1140:ARG:NH1	3:DDD:1236:GLU:HG3	2.25	0.51
2:CCC:660:VAL:HG11	3:DDD:769:VAL:CG1	2.40	0.51
2:CCC:1101:LEU:CD1	3:DDD:504:GLN:HG3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:1347:LEU:HD22	3:DDD:1357:ILE:HG23	1.92	0.51
3:DDD:915:ILE:O	3:DDD:918:ILE:N	2.44	0.51
6:111:48:DA:H2'	6:111:49:DG:C1'	2.41	0.51
4:EEE:29:GLN:HB3	4:EEE:35:LYS:HG3	1.93	0.51
3:DDD:156:ARG:HH22	3:DDD:191:SER:HB2	1.76	0.51
6:111:31:DT:H2''	6:111:32:DA:OP2	2.11	0.50
3:DDD:119:SER:HA	3:DDD:311:ARG:HH21	1.74	0.50
3:DDD:62:PHE:CD1	3:DDD:247:PRO:HD3	2.46	0.50
2:CCC:525:THR:HG21	2:CCC:687:ARG:HD3	1.93	0.50
3:DDD:510:LEU:CD2	3:DDD:579:LEU:HD21	2.42	0.50
3:DDD:850:LYS:HB2	3:DDD:851:PRO:HD2	1.92	0.50
5:FFF:292:GLY:HA2	5:FFF:297:LEU:H	1.75	0.50
2:CCC:73:TYR:HB2	2:CCC:98:VAL:HG22	1.94	0.50
3:DDD:1152:GLU:N	3:DDD:1153:PRO:HD3	2.26	0.50
3:DDD:686:TRP:HB3	3:DDD:746:LEU:HD21	1.92	0.50
3:DDD:708:ASN:ND2	3:DDD:714:GLU:O	2.44	0.50
2:CCC:728:ASP:OD1	2:CCC:729:ALA:N	2.44	0.50
1:BBB:83:LEU:HD21	3:DDD:526:VAL:HG21	1.93	0.50
1:BBB:165:GLU:O	1:BBB:165:GLU:HG3	2.11	0.50
2:CCC:842:ASP:N	2:CCC:1045:GLY:O	2.45	0.50
3:DDD:592:VAL:HG22	3:DDD:592:VAL:O	2.11	0.50
3:DDD:282:LEU:HD21	5:FFF:125:LEU:HD21	1.94	0.50
2:CCC:1257:GLN:HB3	2:CCC:1296:ASP:OD1	2.11	0.50
2:CCC:495:ALA:HB2	5:FFF:187:HIS:CE1	2.47	0.50
3:DDD:800:LEU:HD22	3:DDD:1256:ILE:HG12	1.93	0.50
3:DDD:157:GLN:HG2	3:DDD:188:LEU:HD21	1.92	0.50
2:CCC:1247:SER:HB3	3:DDD:375:GLU:O	2.11	0.50
3:DDD:518:VAL:O	3:DDD:520:ALA:N	2.44	0.50
3:DDD:807:LEU:HD11	3:DDD:894:VAL:HG13	1.94	0.50
1:AAA:35:PHE:HZ	1:BBB:50:SER:CB	2.24	0.50
5:FFF:100:ARG:HB3	6:111:42:DG:H5''	1.94	0.50
1:BBB:86:LYS:HZ1	1:BBB:174:ASP:CG	2.13	0.50
3:DDD:331:ILE:O	3:DDD:331:ILE:HG22	2.12	0.50
6:111:47:DC:H2''	6:111:48:DA:H5'	1.91	0.49
6:111:50:DT:C3'	6:111:51:DC:C5'	2.76	0.49
1:AAA:35:PHE:CZ	1:BBB:50:SER:OG	2.50	0.49
3:DDD:1212:ASP:OD1	3:DDD:1212:ASP:N	2.45	0.49
3:DDD:1261:LEU:HB3	3:DDD:1304:ARG:HD3	1.93	0.49
3:DDD:321:LYS:O	3:DDD:321:LYS:HD2	2.11	0.49
5:FFF:63:GLY:HA2	6:111:42:DG:N2	2.27	0.49
2:CCC:160:ASP:O	2:CCC:162:GLY:N	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:120:LEU:HA	3:DDD:121:PRO:C	2.33	0.49
6:111:48:DA:OP2	6:111:48:DA:H8	1.94	0.49
3:DDD:682:VAL:HG11	3:DDD:756:GLU:CG	2.42	0.49
2:CCC:564:PRO:CB	8:333:14:GTP:PA	3.00	0.49
5:FFF:63:GLY:HA2	6:111:42:DG:C2	2.48	0.49
3:DDD:822:MET:HE1	3:DDD:842:ARG:HD3	1.94	0.49
2:CCC:200:ARG:CD	6:111:50:DT:N3	2.76	0.49
5:FFF:105:ILE:HG21	5:FFF:150:ILE:HG22	1.93	0.49
5:FFF:152:GLN:HE21	5:FFF:156:ARG:HH11	1.60	0.49
2:CCC:1257:GLN:HB2	2:CCC:1258:PRO:HD2	1.94	0.49
6:111:37:DA:H4'	6:111:38:DT:OP1	2.13	0.49
1:AAA:70:THR:OG1	2:CCC:729:ALA:HB3	2.12	0.49
1:AAA:58:GLU:OE1	1:AAA:170:ARG:HD3	2.13	0.48
2:CCC:1318:GLY:O	2:CCC:1319:MET:CB	2.62	0.48
3:DDD:930:LEU:HB3	3:DDD:1134:ILE:HG13	1.94	0.48
7:222:22:DA:H2''	7:222:23:DT:H5'	1.95	0.48
2:CCC:1247:SER:O	3:DDD:348:ASP:HB3	2.13	0.48
3:DDD:1080:ILE:HD12	3:DDD:1115:ILE:HD11	1.96	0.48
3:DDD:1256:ILE:HD12	3:DDD:1256:ILE:N	2.29	0.48
3:DDD:134:ASP:O	3:DDD:138:VAL:HG23	2.13	0.48
3:DDD:519:ASN:O	3:DDD:520:ALA:HB3	2.13	0.48
3:DDD:686:TRP:CB	3:DDD:746:LEU:HD21	2.43	0.48
3:DDD:872:LEU:HD22	3:DDD:877:VAL:HG21	1.95	0.48
5:FFF:72:THR:HG22	5:FFF:73:ALA:N	2.28	0.48
2:CCC:1253:LEU:HB3	5:FFF:235:LEU:CD1	2.44	0.48
2:CCC:208:ILE:HD11	2:CCC:365:GLU:HB2	1.96	0.48
2:CCC:1313:HIS:CE1	3:DDD:380:PHE:HE1	2.31	0.48
5:FFF:267:ASN:HB2	5:FFF:270:GLN:HB2	1.96	0.48
2:CCC:1342:GLU:HA	3:DDD:18:ASP:CB	2.42	0.48
3:DDD:1075:ARG:CZ	3:DDD:1193:TRP:CE3	2.96	0.48
3:DDD:552:ILE:CG2	3:DDD:580:TRP:CD1	2.97	0.48
3:DDD:623:GLN:HA	3:DDD:623:GLN:HE21	1.78	0.48
3:DDD:770:LEU:O	3:DDD:773:PHE:N	2.46	0.48
3:DDD:649:LYS:N	3:DDD:649:LYS:HD3	2.29	0.48
5:FFF:59:GLN:HG2	6:111:43:DT:H3	1.79	0.48
1:BBB:46:ILE:CD1	1:BBB:224:LEU:HD13	2.43	0.48
2:CCC:984:VAL:O	2:CCC:984:VAL:HG13	2.12	0.48
3:DDD:582:ILE:HG23	3:DDD:623:GLN:HB3	1.95	0.48
5:FFF:227:GLY:HA3	7:222:19:DA:H2	1.77	0.48
2:CCC:1313:HIS:CE1	3:DDD:380:PHE:CE1	3.02	0.48
2:CCC:564:PRO:CB	8:333:14:GTP:O1A	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:1106:ARG:NH1	11:DDD:1504:ATP:O1G	2.46	0.47
3:DDD:495:ASN:O	3:DDD:497:GLU:N	2.37	0.47
1:AAA:38:THR:HG23	1:BBB:42:ALA:O	2.13	0.47
1:BBB:78:ILE:HG21	1:BBB:171:LEU:HD11	1.96	0.47
2:CCC:807:TRP:CD1	2:CCC:817:LEU:HD22	2.49	0.47
3:DDD:1138:LEU:N	3:DDD:1139:PRO:CD	2.77	0.47
3:DDD:368:LEU:HD12	3:DDD:369:PRO:HD2	1.97	0.47
3:DDD:1166:GLY:HA3	3:DDD:1176:VAL:HG23	1.95	0.47
3:DDD:349:TYR:CE1	3:DDD:472:LEU:HD11	2.48	0.47
3:DDD:430:HIS:CD2	3:DDD:432:LEU:HB2	2.49	0.47
1:AAA:174:ASP:OD1	1:AAA:174:ASP:N	2.47	0.47
1:AAA:47:LEU:HD13	1:AAA:183:ILE:CD1	2.45	0.47
1:AAA:50:SER:O	1:AAA:150:ARG:HD2	2.13	0.47
1:AAA:72:GLU:OE2	2:CCC:726:TYR:OH	2.21	0.47
3:DDD:320:ASN:O	3:DDD:322:ARG:N	2.47	0.47
2:CCC:1184:THR:HG23	2:CCC:1189:GLY:HA3	1.96	0.47
2:CCC:834:GLN:HE21	2:CCC:836:LEU:HD21	1.79	0.47
3:DDD:1133:ASP:O	3:DDD:1244:GLN:NE2	2.47	0.47
3:DDD:1148:ARG:HG2	6:111:55:DC:OP1	2.15	0.47
1:BBB:47:LEU:HD13	1:BBB:183:ILE:HD12	1.95	0.47
2:CCC:548:ARG:CB	2:CCC:570:GLY:HA3	2.42	0.47
2:CCC:1077:SER:HA	3:DDD:356:THR:OG1	2.15	0.47
1:AAA:179:PRO:HG3	1:AAA:211:ILE:HG13	1.97	0.47
5:FFF:182:ALA:HA	5:FFF:193:PRO:HG3	1.97	0.47
7:222:30:DA:C2'	7:222:31:DT:C5	2.98	0.47
1:AAA:82:LEU:HB3	1:AAA:173:VAL:HG11	1.96	0.47
1:BBB:47:LEU:HD13	1:BBB:183:ILE:CD1	2.44	0.47
2:CCC:1004:ASP:OD1	2:CCC:1004:ASP:N	2.47	0.47
2:CCC:91:THR:HG21	2:CCC:128:PRO:HG3	1.97	0.47
3:DDD:736:GLN:HE21	3:DDD:736:GLN:HA	1.80	0.47
3:DDD:500:ILE:HG22	3:DDD:500:ILE:O	2.14	0.47
1:BBB:176:CYS:SG	3:DDD:535:ARG:NH2	2.88	0.47
1:BBB:29:GLU:CB	1:BBB:30:PRO:HA	2.45	0.47
3:DDD:832:LYS:HG2	3:DDD:1242:ARG:CD	2.44	0.47
1:AAA:45:ARG:HE	1:BBB:38:THR:HG1	1.52	0.46
1:AAA:47:LEU:HD13	1:AAA:183:ILE:HD12	1.96	0.46
2:CCC:488:MET:HB3	2:CCC:489:PRO:HD2	1.96	0.46
2:CCC:518:ASN:O	2:CCC:519:ASN:HB2	2.15	0.46
2:CCC:557:ARG:NH1	2:CCC:611:GLU:OE1	2.48	0.46
5:FFF:287:THR:O	5:FFF:291:VAL:HG23	2.15	0.46
1:BBB:160:HIS:CD2	1:BBB:160:HIS:C	2.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:566:GLY:O	2:CCC:568:ASN:N	2.48	0.46
2:CCC:615:VAL:HA	2:CCC:638:SER:HB3	1.97	0.46
5:FFF:170:HIS:CE1	6:111:31:DT:C5	3.03	0.46
3:DDD:1347:LEU:HD22	3:DDD:1357:ILE:CG2	2.45	0.46
3:DDD:399:LYS:NZ	5:FFF:329:LEU:HD21	2.31	0.46
5:FFF:211:ARG:HA	5:FFF:211:ARG:HD3	1.66	0.46
2:CCC:156:PHE:CE2	2:CCC:158:ASP:HB2	2.51	0.46
2:CCC:185:ASP:OD1	2:CCC:185:ASP:N	2.48	0.46
2:CCC:878:THR:HG22	2:CCC:879:GLY:N	2.30	0.46
3:DDD:1050:THR:HG22	3:DDD:1051:ASP:N	2.31	0.46
7:222:27:DA:H2"	7:222:28:DG:C8	2.50	0.46
2:CCC:1034:ARG:O	2:CCC:1038:GLN:N	2.43	0.46
3:DDD:57:PHE:O	3:DDD:98:ARG:NH2	2.48	0.46
5:FFF:222:VAL:HG12	5:FFF:235:LEU:HB2	1.97	0.46
3:DDD:435:GLN:HB2	3:DDD:457:TYR:OH	2.16	0.46
5:FFF:227:GLY:O	5:FFF:228:GLY:C	2.54	0.46
6:111:30:DG:N2	7:222:34:DG:C2	2.83	0.46
2:CCC:1242:LYS:HD2	3:DDD:465:GLN:NE2	2.31	0.46
3:DDD:93:THR:HG22	3:DDD:94:GLN:N	2.31	0.46
5:FFF:122:GLU:CD	5:FFF:157:ALA:HB1	2.36	0.46
2:CCC:44:GLU:O	2:CCC:46:GLN:N	2.49	0.46
3:DDD:380:PHE:HB3	3:DDD:415:VAL:HG11	1.97	0.46
3:DDD:709:ARG:HB3	3:DDD:710:ASP:H	1.63	0.45
2:CCC:138:ILE:O	2:CCC:141:THR:OG1	2.31	0.45
2:CCC:560:PRO:HB2	3:DDD:776:THR:CG2	2.43	0.45
3:DDD:749:LYS:HB3	3:DDD:750:PRO:HD2	1.98	0.45
3:DDD:820:ILE:O	3:DDD:882:VAL:N	2.47	0.45
3:DDD:197:GLU:O	3:DDD:201:LEU:HG	2.17	0.45
3:DDD:504:GLN:HE22	3:DDD:731:ARG:HH21	1.65	0.45
3:DDD:519:ASN:HA	3:DDD:523:GLU:HB2	1.98	0.45
5:FFF:218:ARG:HA	5:FFF:218:ARG:HE	1.75	0.45
2:CCC:1294:LYS:HB3	3:DDD:347:VAL:HG13	1.97	0.45
2:CCC:42:ASP:O	2:CCC:50:GLU:HG2	2.16	0.45
3:DDD:793:SER:HB2	3:DDD:1138:LEU:HD12	1.98	0.45
1:AAA:47:LEU:HA	1:AAA:51:MET:HG2	1.99	0.45
3:DDD:1025:MET:HB2	3:DDD:1126:GLN:HE21	1.81	0.45
3:DDD:223:LEU:O	3:DDD:227:PHE:HB2	2.17	0.45
2:CCC:1274:GLU:HA	3:DDD:428:THR:HG21	1.98	0.45
1:AAA:192:VAL:CG2	1:AAA:198:LEU:HD12	2.46	0.45
1:AAA:42:ALA:HA	1:BBB:38:THR:HG23	1.99	0.45
2:CCC:967:LEU:HD21	2:CCC:1021:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:800:MET:O	2:CCC:1229:TYR:HA	2.17	0.45
3:DDD:1350:ASN:HA	3:DDD:1353:VAL:HG22	1.99	0.45
2:CCC:541:GLU:OE2	6:111:51:DC:C4	2.70	0.45
1:AAA:35:PHE:HZ	1:BBB:50:SER:HB3	1.81	0.45
3:DDD:701:LEU:O	3:DDD:718:SER:CB	2.65	0.45
5:FFF:292:GLY:HA2	5:FFF:297:LEU:N	2.32	0.45
2:CCC:125:GLY:HA2	2:CCC:499:SER:HB2	1.98	0.45
3:DDD:369:PRO:HB3	3:DDD:444:GLY:O	2.17	0.45
3:DDD:822:MET:HE3	3:DDD:882:VAL:HG11	1.92	0.45
5:FFF:144:THR:O	5:FFF:147:THR:OG1	2.34	0.45
5:FFF:162:THR:HG23	5:FFF:163:ARG:HG3	1.99	0.45
3:DDD:736:GLN:CA	3:DDD:736:GLN:HE21	2.30	0.45
7:222:10:DC:H2'	7:222:11:DA:C8	2.52	0.44
1:BBB:50:SER:O	1:BBB:150:ARG:HD2	2.17	0.44
2:CCC:1085:MET:HE1	2:CCC:1097:VAL:HG23	1.99	0.44
3:DDD:355:ILE:HG21	3:DDD:466:MET:HG3	2.00	0.44
3:DDD:619:ILE:O	3:DDD:623:GLN:HG2	2.17	0.44
6:111:51:DC:H2''	6:111:52:DT:O5'	2.16	0.44
6:111:32:DA:H2	7:222:32:DA:C4	2.34	0.44
2:CCC:1307:ASN:HB3	2:CCC:1312:ASN:O	2.16	0.44
2:CCC:197:ARG:HD3	2:CCC:200:ARG:HG3	1.99	0.44
2:CCC:347:ILE:HD11	2:CCC:433:ILE:HD11	2.00	0.44
3:DDD:930:LEU:HD12	3:DDD:1134:ILE:HD11	1.99	0.44
2:CCC:1242:LYS:HD2	3:DDD:465:GLN:HE22	1.82	0.44
2:CCC:894:GLN:NE2	3:DDD:69:GLU:OE2	2.50	0.44
3:DDD:746:LEU:H	3:DDD:746:LEU:HD12	1.82	0.44
1:BBB:82:LEU:HD22	1:BBB:173:VAL:HG22	1.88	0.44
2:CCC:706:ARG:HA	2:CCC:793:GLU:HA	1.99	0.44
3:DDD:789:LYS:HG3	3:DDD:1135:THR:HG23	2.00	0.44
3:DDD:357:VAL:HG12	3:DDD:461:PHE:CE2	2.53	0.44
3:DDD:809:VAL:HG22	3:DDD:915:ILE:HD11	1.98	0.44
5:FFF:158:ILE:O	5:FFF:162:THR:HB	2.18	0.44
2:CCC:1291:LEU:HD11	3:DDD:1351:VAL:HG13	2.00	0.44
2:CCC:811:ASN:HA	2:CCC:815:SER:O	2.18	0.44
3:DDD:1280:VAL:HG12	3:DDD:1281:GLU:N	2.32	0.44
3:DDD:45:ASN:HB3	3:DDD:48:THR:OG1	2.18	0.44
3:DDD:517:CYS:SG	3:DDD:518:VAL:N	2.90	0.44
3:DDD:903:LEU:HD21	3:DDD:1249:ASN:HD22	1.81	0.44
3:DDD:713:GLU:HG2	3:DDD:714:GLU:H	1.83	0.44
3:DDD:825:VAL:HG12	3:DDD:832:LYS:HB3	1.98	0.44
6:111:53:DG:H1'	6:111:54:DA:H5'	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:1252:SER:OG	2:CCC:1257:GLN:N	2.51	0.44
2:CCC:338:THR:HG23	2:CCC:345:PRO:HG3	1.99	0.44
2:CCC:60:GLN:HA	2:CCC:67:GLU:HA	1.98	0.44
3:DDD:884:SER:OG	3:DDD:885:VAL:N	2.51	0.44
4:EEE:39:VAL:HG13	4:EEE:40:PRO:HD2	2.00	0.44
2:CCC:311:CYS:SG	2:CCC:311:CYS:O	2.76	0.44
3:DDD:320:ASN:O	3:DDD:321:LYS:HG3	2.18	0.44
3:DDD:733:SER:O	3:DDD:737:ILE:HG13	2.18	0.44
3:DDD:755:ILE:H	3:DDD:755:ILE:HD12	1.83	0.44
3:DDD:682:VAL:HG21	3:DDD:756:GLU:OE2	2.18	0.44
5:FFF:159:MET:HG2	7:222:26:DT:C2	2.53	0.44
1:AAA:182:ARG:NH1	2:CCC:1090:ASN:O	2.50	0.44
2:CCC:13:LYS:NZ	2:CCC:1149:TYR:O	2.51	0.44
2:CCC:146:VAL:HG13	2:CCC:529:ARG:O	2.18	0.44
2:CCC:800:MET:HE2	2:CCC:800:MET:HB3	1.92	0.44
3:DDD:114:ILE:HD11	3:DDD:311:ARG:HB3	2.00	0.44
3:DDD:346:ARG:H	3:DDD:346:ARG:HG2	1.66	0.44
2:CCC:813:GLU:O	3:DDD:461:PHE:O	2.36	0.44
3:DDD:518:VAL:N	3:DDD:716:GLN:HE22	2.15	0.44
1:AAA:112:ALA:HB1	1:AAA:123:ILE:HG21	1.99	0.43
2:CCC:347:ILE:HD11	2:CCC:433:ILE:CD1	2.48	0.43
2:CCC:24:VAL:HG11	2:CCC:704:MET:SD	2.58	0.43
3:DDD:1289:ASN:HA	3:DDD:1292:LEU:HD12	2.00	0.43
3:DDD:695:LYS:CA	3:DDD:695:LYS:HE3	2.48	0.43
7:222:31:DT:C2	7:222:32:DA:C8	3.06	0.43
3:DDD:819:GLY:N	3:DDD:881:LYS:HE2	2.29	0.43
7:222:25:DA:H2"	7:222:26:DT:H5"	1.99	0.43
2:CCC:821:ARG:NH1	2:CCC:1082:ILE:HD13	2.33	0.43
2:CCC:887:VAL:HB	2:CCC:913:VAL:CG1	2.47	0.43
1:BBB:78:ILE:HG21	1:BBB:171:LEU:CD1	2.49	0.43
2:CCC:1210:ILE:HG22	2:CCC:1211:ARG:N	2.34	0.43
2:CCC:397:LEU:O	2:CCC:398:SER:CB	2.66	0.43
2:CCC:556:GLY:HA3	2:CCC:589:THR:HG21	2.00	0.43
3:DDD:1356:LEU:HD22	3:DDD:1362:GLY:HA3	2.01	0.43
5:FFF:170:HIS:NE2	6:111:31:DT:C6	2.86	0.43
1:BBB:57:THR:HG23	1:BBB:158:ARG:CZ	2.48	0.43
3:DDD:366:CYS:O	3:DDD:366:CYS:SG	2.77	0.43
6:111:49:DG:H2"	6:111:50:DT:O4'	2.18	0.43
2:CCC:1285:TYR:O	2:CCC:1289:GLU:N	2.44	0.43
2:CCC:807:TRP:CD1	2:CCC:817:LEU:CD2	3.02	0.43
3:DDD:820:ILE:HD12	3:DDD:884:SER:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FFF:298:THR:HG21	5:FFF:301:ARG:HD3	2.00	0.43
1:AAA:66:HIS:CE1	1:AAA:69:SER:HB3	2.54	0.43
2:CCC:124:MET:HB2	2:CCC:498:ILE:HD12	2.00	0.43
3:DDD:958:ILE:HG23	3:DDD:982:LEU:HD11	2.01	0.43
2:CCC:127:ILE:O	2:CCC:127:ILE:HG13	2.18	0.43
2:CCC:259:GLY:O	2:CCC:260:LYS:CB	2.66	0.43
3:DDD:530:PRO:HD3	3:DDD:552:ILE:CD1	2.48	0.43
1:BBB:66:HIS:CE1	1:BBB:69:SER:HB3	2.54	0.43
2:CCC:159:SER:HB3	2:CCC:172:TYR:HA	2.01	0.43
3:DDD:1175:LEU:HD12	3:DDD:1177:ILE:CG1	2.49	0.43
5:FFF:204:LYS:HB3	5:FFF:205:PRO:CD	2.49	0.43
1:AAA:56:VAL:O	1:AAA:175:ALA:CB	2.59	0.42
3:DDD:1078:LEU:HG	3:DDD:1101:LEU:HD11	2.01	0.42
3:DDD:1029:THR:HG22	3:DDD:1121:LEU:HD11	2.01	0.42
3:DDD:832:LYS:CG	3:DDD:1242:ARG:CD	2.95	0.42
4:EEE:5:THR:HG22	4:EEE:7:GLN:H	1.83	0.42
5:FFF:176:ASN:OD1	7:222:26:DT:C7	2.67	0.42
2:CCC:183:TRP:HZ3	6:111:50:DT:C4	2.36	0.42
1:BBB:86:LYS:HG2	1:BBB:174:ASP:O	2.19	0.42
3:DDD:973:LEU:CD2	3:DDD:1006:GLY:HA2	2.49	0.42
3:DDD:1025:MET:CB	3:DDD:1126:GLN:HE21	2.32	0.42
3:DDD:612:LEU:HB3	3:DDD:616:PRO:HG2	2.01	0.42
5:FFF:162:THR:HG23	5:FFF:163:ARG:N	2.34	0.42
2:CCC:906:PHE:CZ	5:FFF:323:ASN:OD1	2.68	0.42
6:111:53:DG:H1'	6:111:54:DA:C5'	2.49	0.42
3:DDD:482:ALA:O	3:DDD:488:ASN:ND2	2.51	0.42
3:DDD:571:ASP:N	3:DDD:571:ASP:OD1	2.53	0.42
3:DDD:1087:ASP:N	3:DDD:1087:ASP:OD1	2.52	0.42
3:DDD:1271:SER:OG	3:DDD:1292:LEU:HD21	2.18	0.42
3:DDD:168:ALA:O	3:DDD:173:GLY:N	2.52	0.42
3:DDD:355:ILE:HG21	3:DDD:466:MET:CG	2.49	0.42
3:DDD:519:ASN:HA	3:DDD:523:GLU:CG	2.49	0.42
2:CCC:1315:MET:HG3	2:CCC:1317:PRO:HD3	2.02	0.42
2:CCC:865:LEU:HD23	2:CCC:871:VAL:HG23	1.99	0.42
3:DDD:394:ILE:N	5:FFF:254:ASP:OD2	2.53	0.42
3:DDD:650:LYS:HE3	3:DDD:654:ILE:HD12	2.02	0.42
5:FFF:155:GLU:O	5:FFF:159:MET:HG3	2.20	0.42
2:CCC:564:PRO:HB2	8:333:14:GTP:O1A	2.20	0.42
2:CCC:100:LEU:HD22	2:CCC:493:ILE:HD11	2.01	0.42
2:CCC:98:VAL:HB	2:CCC:124:MET:HE2	2.00	0.42
3:DDD:516:ASP:HB3	3:DDD:573:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:799:ARG:HD2	3:DDD:1146:GLU:OE2	2.19	0.42
5:FFF:318:GLN:HA	5:FFF:323:ASN:HB2	2.01	0.42
2:CCC:245:ARG:C	2:CCC:247:ARG:H	2.23	0.42
2:CCC:46:GLN:HB2	2:CCC:51:ALA:CA	2.48	0.42
3:DDD:1256:ILE:H	3:DDD:1256:ILE:HD12	1.85	0.42
2:CCC:1309:VAL:O	3:DDD:383:GLY:HA2	2.20	0.42
5:FFF:204:LYS:HB3	5:FFF:205:PRO:HD2	2.00	0.42
3:DDD:1131:THR:O	3:DDD:1131:THR:OG1	2.31	0.42
5:FFF:175:LEU:HD13	5:FFF:212:MET:O	2.20	0.42
6:111:48:DA:H2'	6:111:49:DG:O4'	2.19	0.42
2:CCC:1146:GLN:HB2	2:CCC:1161:LEU:HD12	2.02	0.42
2:CCC:1119:MET:HE2	2:CCC:1204:LEU:HB3	2.00	0.42
2:CCC:254:ASP:HB2	2:CCC:265:LYS:HE3	2.01	0.42
2:CCC:241:LEU:CD2	2:CCC:277:LEU:HD21	2.50	0.42
2:CCC:620:ASN:ND2	3:DDD:768:ASN:HB2	2.35	0.42
2:CCC:1337:ILE:HG23	2:CCC:1337:ILE:O	2.20	0.42
2:CCC:175:ARG:HD3	2:CCC:183:TRP:CZ3	2.55	0.42
2:CCC:557:ARG:HH12	2:CCC:611:GLU:CD	2.23	0.42
3:DDD:27:PRO:HB3	3:DDD:240:THR:OG1	2.19	0.42
3:DDD:975:ILE:CD1	3:DDD:997:VAL:HG11	2.49	0.42
3:DDD:615:LYS:HE2	4:EEE:5:THR:OG1	2.20	0.42
1:BBB:86:LYS:CE	1:BBB:174:ASP:HB2	2.50	0.41
1:AAA:11:PRO:CG	1:BBB:230:ALA:HB2	2.48	0.41
3:DDD:388:ARG:HB3	3:DDD:390:LEU:HD13	2.01	0.41
5:FFF:170:HIS:CG	6:111:31:DT:C7	3.02	0.41
5:FFF:178:TYR:CE2	5:FFF:212:MET:HG3	2.54	0.41
1:AAA:41:ASN:ND2	2:CCC:1217:THR:O	2.52	0.41
2:CCC:561:ILE:H	2:CCC:561:ILE:HG13	1.76	0.41
3:DDD:863:LEU:HD22	3:DDD:908:ILE:CG1	2.50	0.41
6:111:32:DA:N3	7:222:32:DA:C2	2.88	0.41
2:CCC:635:THR:HG22	2:CCC:644:LEU:CD2	2.50	0.41
2:CCC:901:LEU:HD11	5:FFF:310:LEU:CD2	2.47	0.41
4:EEE:59:ILE:HG23	4:EEE:64:LEU:HD11	2.02	0.41
7:222:20:DG:C2'	7:222:21:DG:H5'	2.50	0.41
1:AAA:159:ILE:HD11	2:CCC:876:GLU:OE1	2.20	0.41
3:DDD:113:HIS:CE1	3:DDD:307:LEU:HD13	2.55	0.41
1:BBB:44:ARG:HH12	3:DDD:538:ARG:HG2	1.85	0.41
1:BBB:57:THR:HG22	1:BBB:58:GLU:HG3	2.02	0.41
2:CCC:1292:THR:HB	2:CCC:1297:ASP:HB2	2.01	0.41
5:FFF:147:THR:O	5:FFF:151:ARG:HG2	2.20	0.41
1:AAA:86:LYS:HG2	1:AAA:174:ASP:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:1269:ARG:HH22	3:DDD:340:GLN:HA	1.86	0.41
3:DDD:392:THR:HG21	5:FFF:320:GLN:O	2.21	0.41
3:DDD:48:THR:O	3:DDD:50:LYS:N	2.54	0.41
6:111:34:DG:H2"	6:111:35:DC:C6	2.55	0.41
6:111:48:DA:C6	6:111:49:DG:O6	2.74	0.41
6:111:56:DG:O6	7:222:6:DG:C6	2.74	0.41
2:CCC:208:ILE:HG13	2:CCC:356:THR:HG21	2.02	0.41
2:CCC:618:GLN:HE21	3:DDD:769:VAL:HG23	1.85	0.41
3:DDD:51:PRO:HB3	3:DDD:57:PHE:O	2.21	0.41
3:DDD:850:LYS:HB2	3:DDD:851:PRO:CD	2.50	0.41
6:111:53:DG:H2"	6:111:54:DA:H5'	2.03	0.41
6:111:58:DG:C6	6:111:59:DG:C6	3.09	0.41
1:AAA:158:ARG:HD2	1:AAA:172:LEU:HD11	2.02	0.41
1:AAA:57:THR:HG22	1:AAA:58:GLU:HG3	2.02	0.41
2:CCC:1274:GLU:OE1	2:CCC:1274:GLU:N	2.52	0.41
3:DDD:793:SER:HB2	3:DDD:1138:LEU:CD1	2.50	0.41
3:DDD:417:ARG:C	3:DDD:418:GLU:HG2	2.40	0.41
2:CCC:901:LEU:CD1	5:FFF:278:PHE:CE2	2.94	0.41
6:111:58:DG:H2"	6:111:59:DG:C8	2.55	0.41
1:BBB:112:ALA:HB1	1:BBB:123:ILE:HG21	2.03	0.41
1:BBB:171:LEU:HA	1:BBB:171:LEU:HD23	1.89	0.41
2:CCC:1157:GLN:O	2:CCC:1157:GLN:HG3	2.21	0.41
2:CCC:127:ILE:CG1	2:CCC:127:ILE:O	2.68	0.41
2:CCC:635:THR:CG2	2:CCC:644:LEU:HD23	2.50	0.41
2:CCC:700:VAL:O	2:CCC:1069:ARG:NH2	2.54	0.41
3:DDD:858:VAL:HA	3:DDD:859:PRO:HD3	1.94	0.41
3:DDD:648:GLU:HG3	3:DDD:648:GLU:H	1.68	0.41
5:FFF:265:GLU:OE2	5:FFF:316:ILE:HG12	2.21	0.41
5:FFF:79:PHE:O	5:FFF:90:SER:OG	2.33	0.41
6:111:28:DA:C2	7:222:36:DG:N2	2.89	0.41
5:FFF:141:ARG:HB2	6:111:39:DA:OP2	2.21	0.41
2:CCC:660:VAL:HG11	3:DDD:769:VAL:HG13	2.02	0.41
3:DDD:646:ILE:HD13	3:DDD:762:ASN:HD21	1.86	0.41
3:DDD:732:GLY:HA2	3:DDD:736:GLN:HG3	2.02	0.41
5:FFF:265:GLU:HG2	5:FFF:265:GLU:O	2.21	0.41
6:111:52:DT:H2"	6:111:53:DG:N7	2.35	0.40
1:AAA:35:PHE:CE1	1:BBB:46:ILE:HG12	2.55	0.40
7:222:30:DA:C2'	7:222:31:DT:C6	2.99	0.40
3:DDD:87:LYS:NZ	7:222:36:DG:OP1	2.48	0.40
3:DDD:1175:LEU:O	3:DDD:1187:GLU:HA	2.21	0.40
3:DDD:246:PRO:HA	3:DDD:247:PRO:HD3	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:350:SER:HA	3:DDD:468:VAL:O	2.21	0.40
2:CCC:1111:GLN:HG3	2:CCC:1112:ILE:HD13	2.04	0.40
2:CCC:1292:THR:OG1	2:CCC:1293:VAL:N	2.54	0.40
2:CCC:144:VAL:HG23	2:CCC:515:MET:HB2	2.03	0.40
3:DDD:823:THR:HB	3:DDD:824:PRO:HD2	2.03	0.40
1:BBB:157:THR:O	1:BBB:157:THR:HG22	2.21	0.40
2:CCC:1244:HIS:HD2	2:CCC:1268:GLN:NE2	2.19	0.40
2:CCC:496:LYS:N	2:CCC:497:PRO:CD	2.85	0.40
2:CCC:635:THR:CG2	2:CCC:644:LEU:CD2	3.00	0.40
2:CCC:758:ARG:HG2	2:CCC:759:SER:O	2.21	0.40
1:BBB:82:LEU:HB3	1:BBB:173:VAL:HG11	2.03	0.40
2:CCC:805:MET:HG2	2:CCC:1225:VAL:HG11	2.04	0.40
2:CCC:184:LEU:HB2	2:CCC:389:PHE:CE1	2.56	0.40
3:DDD:1078:LEU:HD12	3:DDD:1121:LEU:HB3	2.03	0.40
3:DDD:822:MET:CE	3:DDD:882:VAL:CG2	2.97	0.40
5:FFF:218:ARG:HG3	7:222:23:DT:H72	2.04	0.40
5:FFF:225:PRO:HB3	5:FFF:230:SER:HA	2.02	0.40
5:FFF:277:ARG:HD3	5:FFF:306:GLN:HE21	1.87	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FFF:67:TYR:O	5:FFF:299:ARG:NH2[3_644]	2.02	0.18

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%)	203 (89%)	19 (8%)	6 (3%)	5	34
1	BBB	226/242 (93%)	205 (91%)	16 (7%)	5 (2%)	6	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	CCC	1338/1342 (100%)	1198 (90%)	120 (9%)	20 (2%)	10	44
3	DDD	1346/1407 (96%)	1206 (90%)	124 (9%)	16 (1%)	13	48
4	EEE	77/90 (86%)	70 (91%)	7 (9%)	0	100	100
5	FFF	275/336 (82%)	249 (90%)	20 (7%)	6 (2%)	6	37
All	All	3490/3659 (95%)	3131 (90%)	306 (9%)	53 (2%)	10	44

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	CCC	161	LYS
2	CCC	1319	MET
3	DDD	519	ASN
3	DDD	710	ASP
3	DDD	1268	ASN
1	AAA	168	ILE
2	CCC	45	GLY
2	CCC	260	LYS
2	CCC	398	SER
2	CCC	1004	ASP
2	CCC	1297	ASP
2	CCC	1318	GLY
3	DDD	207	GLU
3	DDD	1053	LEU
3	DDD	1131	THR
3	DDD	1201	GLY
5	FFF	113	GLY
5	FFF	228	GLY
1	AAA	208	ASN
1	BBB	209	GLY
1	BBB	232	VAL
2	CCC	201	ARG
2	CCC	234	ASP
2	CCC	812	PHE
2	CCC	909	LYS
2	CCC	1103	VAL
3	DDD	321	LYS
3	DDD	342	LEU
3	DDD	947	GLU
3	DDD	1344	LEU
5	FFF	230	SER
2	CCC	567	PRO

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Mol	Chain	Res	Type
1	AAA	210	THR
1	BBB	208	ASN
2	CCC	110	PRO
2	CCC	519	ASN
3	DDD	81	ARG
3	DDD	96	LYS
3	DDD	1325	PHE
1	AAA	211	ILE
2	CCC	343	HIS
2	CCC	892	GLU
2	CCC	1224	PRO
3	DDD	829	GLY
1	BBB	14	VAL
5	FFF	227	GLY
1	AAA	14	VAL
1	BBB	40	GLY
3	DDD	1091	PRO
5	FFF	282	GLY
1	AAA	40	GLY
2	CCC	627	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%)	193 (98%)	5 (2%)	47	68
1	BBB	196/208 (94%)	190 (97%)	6 (3%)	40	63
2	CCC	1155/1157 (100%)	1129 (98%)	26 (2%)	50	70
3	DDD	1127/1168 (96%)	1074 (95%)	53 (5%)	26	53
4	EEE	67/74 (90%)	65 (97%)	2 (3%)	41	64
5	FFF	240/292 (82%)	229 (95%)	11 (5%)	27	54
All	All	2983/3107 (96%)	2880 (96%)	103 (4%)	36	61

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	13	LEU
1	AAA	28	LEU
1	AAA	157	THR
1	AAA	166	ARG
1	AAA	174	ASP
1	BBB	13	LEU
1	BBB	28	LEU
1	BBB	159	ILE
1	BBB	160	HIS
1	BBB	165	GLU
1	BBB	174	ASP
2	CCC	12	ARG
2	CCC	23	ASP
2	CCC	47	TYR
2	CCC	185	ASP
2	CCC	202	ARG
2	CCC	423	ASP
2	CCC	541	GLU
2	CCC	553	THR
2	CCC	561	ILE
2	CCC	609	ILE
2	CCC	628	HIS
2	CCC	635	THR
2	CCC	694	ARG
2	CCC	700	VAL
2	CCC	757	THR
2	CCC	764	CYS
2	CCC	788	SER
2	CCC	888	THR
2	CCC	914	LYS
2	CCC	994	ARG
2	CCC	1069	ARG
2	CCC	1089	GLU
2	CCC	1224	PRO
2	CCC	1240	ASP
2	CCC	1272	GLU
2	CCC	1340	GLU
3	DDD	28	ASP
3	DDD	158	GLN
3	DDD	199	GLU
3	DDD	216	LYS
3	DDD	281	ARG

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Mol	Chain	Res	Type
3	DDD	298	MET
3	DDD	314	ARG
3	DDD	321	LYS
3	DDD	346	ARG
3	DDD	384	LYS
3	DDD	398	LYS
3	DDD	399	LYS
3	DDD	415	VAL
3	DDD	505	ASP
3	DDD	508	LEU
3	DDD	526	VAL
3	DDD	538	ARG
3	DDD	548	VAL
3	DDD	550	VAL
3	DDD	551	ARG
3	DDD	571	ASP
3	DDD	579	LEU
3	DDD	599	LYS
3	DDD	610	ARG
3	DDD	619	ILE
3	DDD	623	GLN
3	DDD	641	ILE
3	DDD	644	MET
3	DDD	646	ILE
3	DDD	648	GLU
3	DDD	649	LYS
3	DDD	695	LYS
3	DDD	698	MET
3	DDD	707	ILE
3	DDD	736	GLN
3	DDD	746	LEU
3	DDD	770	LEU
3	DDD	790	THR
3	DDD	798	ARG
3	DDD	830	ASP
3	DDD	835	LEU
3	DDD	838	ARG
3	DDD	849	LEU
3	DDD	857	LEU
3	DDD	862	THR
3	DDD	1140	ARG
3	DDD	1175	LEU

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Mol	Chain	Res	Type
3	DDD	1189	MET
3	DDD	1199	PHE
3	DDD	1210	ILE
3	DDD	1227	HIS
3	DDD	1345	ARG
3	DDD	1356	LEU
4	EEE	5	THR
4	EEE	43	ASN
5	FFF	54	VAL
5	FFF	156	ARG
5	FFF	183	ARG
5	FFF	203	ASP
5	FFF	211	ARG
5	FFF	217	GLU
5	FFF	218	ARG
5	FFF	220	THR
5	FFF	243	GLU
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

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	ATP	DDD	1504	-	26,33,33	0.65	0	31,52,52	0.75	1 (3%)

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	ATP	DDD	1504	-	-	4/18/38/38	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	DDD	1504	ATP	C5-C6-N6	2.36	123.94	120.35

There are no chirality outliers.

All (4) torsion outliers are listed below:

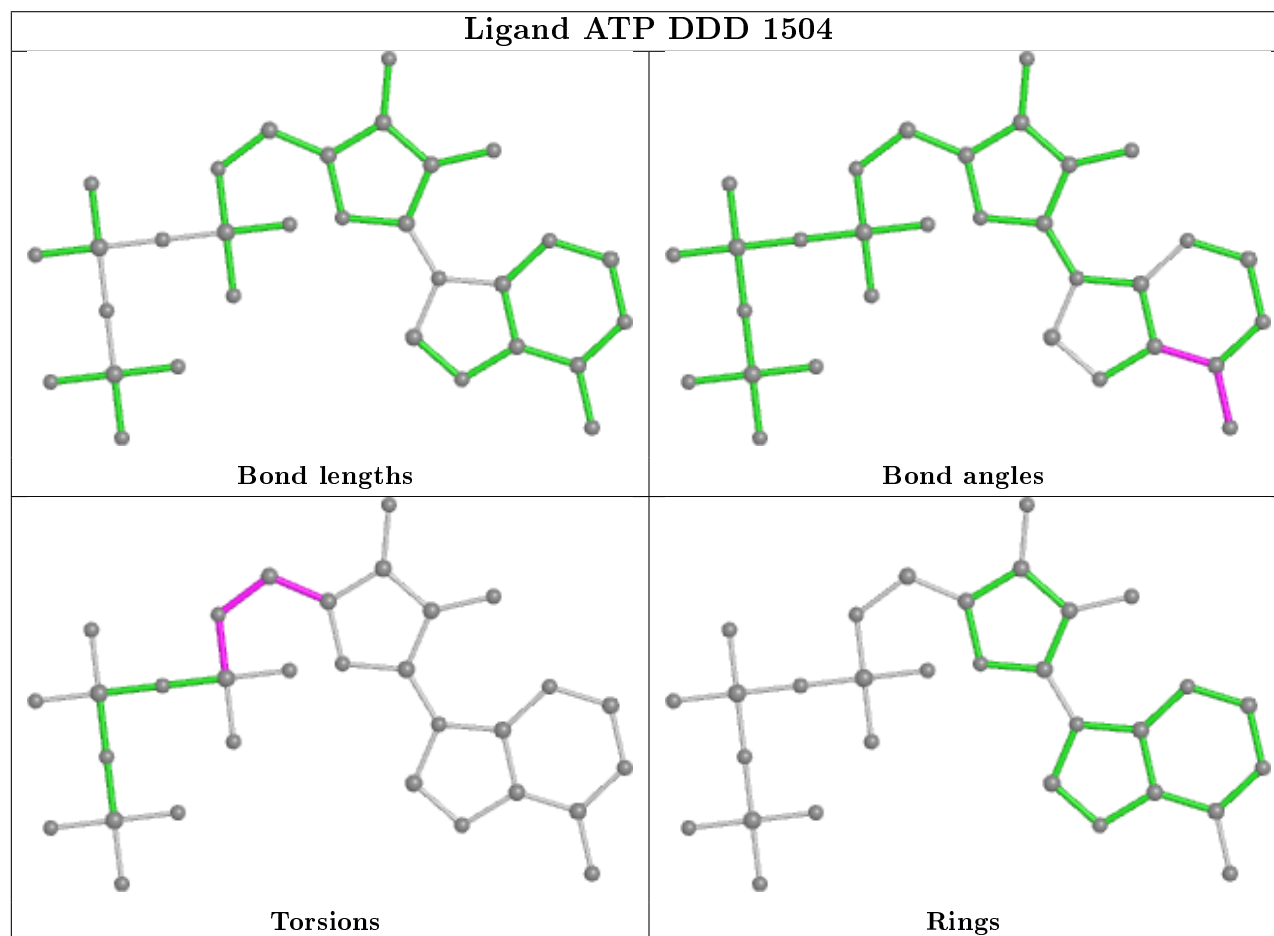
Mol	Chain	Res	Type	Atoms
11	DDD	1504	ATP	C5'-O5'-PA-O3A
11	DDD	1504	ATP	C4'-C5'-O5'-PA
11	DDD	1504	ATP	O4'-C4'-C5'-O5'
11	DDD	1504	ATP	C5'-O5'-PA-O2A

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	DDD	1504	ATP	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	AAA	230/242 (95%)	0.11	11 (4%)	30	26	259, 364, 475, 549	0
1	BBB	228/242 (94%)	0.26	20 (8%)	10	9	267, 362, 499, 567	0
2	CCC	1340/1342 (99%)	-0.12	45 (3%)	45	36	152, 285, 475, 622	0
3	DDD	1350/1407 (95%)	-0.04	64 (4%)	31	26	127, 304, 470, 530	0
4	EEE	79/90 (87%)	-0.12	0	100	100	262, 364, 522, 550	0
5	FFF	277/336 (82%)	0.23	21 (7%)	13	12	220, 344, 556, 634	0
6	111	32/50 (64%)	-0.02	4 (12%)	3	5	318, 362, 528, 568	0
7	222	35/50 (70%)	0.31	5 (14%)	2	3	227, 368, 608, 651	0
8	333	2/3 (66%)	0.33	0	100	100	351, 351, 351, 369	0
All	All	3573/3762 (94%)	-0.02	170 (4%)	30	26	127, 315, 493, 651	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	DDD	1078	LEU	7.7
5	FFF	310	LEU	7.5
3	DDD	878	ASP	6.2
3	DDD	1055	GLY	5.9
1	BBB	133	LEU	5.8
3	DDD	1066	GLU	5.7
3	DDD	976	THR	5.7
3	DDD	732	GLY	5.6
3	DDD	997	VAL	5.4
2	CCC	885	GLY	5.4
3	DDD	1121	LEU	5.2
1	BBB	108	GLY	5.2
5	FFF	301	ARG	5.1
3	DDD	993	GLU	5.1
2	CCC	982	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
3	DDD	983	LYS	4.9
3	DDD	982	LEU	4.9
3	DDD	879	ALA	4.7
3	DDD	992	LYS	4.7
3	DDD	1098	GLN	4.6
5	FFF	263	LEU	4.6
1	AAA	213	PRO	4.6
2	CCC	1003	THR	4.6
3	DDD	980	THR	4.5
5	FFF	305	ILE	4.4
3	DDD	1030	GLU	4.2
1	BBB	107	ILE	4.2
3	DDD	1065	ALA	4.2
1	BBB	90	VAL	4.1
3	DDD	877	VAL	4.1
2	CCC	113	THR	4.0
6	111	46	DG	3.9
5	FFF	312	ARG	3.9
7	222	22	DA	3.9
1	BBB	106	GLY	3.9
7	222	23	DT	3.9
5	FFF	302	VAL	3.7
2	CCC	906	PHE	3.7
2	CCC	169	LYS	3.7
3	DDD	1101	LEU	3.7
7	222	21	DG	3.7
3	DDD	1079	LYS	3.6
2	CCC	230	PHE	3.6
1	BBB	205	MET	3.6
6	111	44	DG	3.5
3	DDD	1376	GLY	3.5
2	CCC	905	ILE	3.5
1	AAA	135	ASP	3.5
5	FFF	306	GLN	3.5
3	DDD	287	ALA	3.4
6	111	47	DC	3.4
3	DDD	978	ARG	3.4
1	BBB	98	VAL	3.4
2	CCC	1055	ALA	3.3
5	FFF	315	GLU	3.3
2	CCC	1001	GLY	3.3
1	BBB	26	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
3	DDD	1099	TYR	3.3
1	AAA	134	THR	3.2
1	AAA	171	LEU	3.2
1	BBB	134	THR	3.2
3	DDD	973	LEU	3.2
5	FFF	198	ILE	3.2
1	AAA	144	ILE	3.1
5	FFF	131	VAL	3.1
5	FFF	273	VAL	3.1
1	BBB	131	CYS	3.1
2	CCC	870	ILE	3.1
2	CCC	883	LEU	3.1
2	CCC	231	GLU	3.0
3	DDD	1068	THR	3.0
1	BBB	146	VAL	3.0
2	CCC	1004	ASP	3.0
3	DDD	977	SER	3.0
5	FFF	298	THR	3.0
3	DDD	1271	SER	3.0
2	CCC	983	GLY	3.0
1	AAA	199	ASP	2.9
1	BBB	144	ILE	2.9
2	CCC	869	GLY	2.9
3	DDD	1077	ALA	2.9
5	FFF	291	VAL	2.9
2	CCC	850	ILE	2.9
3	DDD	981	GLU	2.8
2	CCC	884	VAL	2.8
3	DDD	974	VAL	2.8
2	CCC	170	VAL	2.8
3	DDD	1109	LEU	2.8
5	FFF	311	ARG	2.8
1	AAA	189	ALA	2.8
3	DDD	848	VAL	2.8
2	CCC	103	VAL	2.7
2	CCC	124	MET	2.7
2	CCC	125	GLY	2.7
5	FFF	94	MET	2.7
1	AAA	136	GLU	2.7
2	CCC	611	GLU	2.7
2	CCC	911	SER	2.7
1	BBB	180	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
3	DDD	1122	ALA	2.7
3	DDD	1064	SER	2.7
3	DDD	1112	GLY	2.7
2	CCC	171	LEU	2.6
1	BBB	190	ALA	2.6
3	DDD	975	ILE	2.6
1	BBB	100	LEU	2.6
2	CCC	172	TYR	2.6
3	DDD	857	LEU	2.6
6	111	48	DA	2.6
1	BBB	231	PHE	2.5
1	BBB	164	ASP	2.5
5	FFF	98	ASN	2.5
3	DDD	984	LEU	2.5
1	AAA	107	ILE	2.5
2	CCC	385	PHE	2.5
2	CCC	311	CYS	2.5
2	CCC	105	TYR	2.5
2	CCC	912	ASP	2.5
2	CCC	101	ARG	2.4
2	CCC	703	GLY	2.4
2	CCC	927	THR	2.4
3	DDD	1038	THR	2.4
7	222	18	DT	2.4
3	DDD	958	ILE	2.4
2	CCC	215	TYR	2.4
3	DDD	1110	GLU	2.4
2	CCC	239	MET	2.4
3	DDD	986	ASP	2.4
1	BBB	123	ILE	2.4
3	DDD	1272	SER	2.3
2	CCC	557	ARG	2.3
2	CCC	740	GLU	2.3
7	222	20	DG	2.3
3	DDD	1028	ILE	2.3
1	AAA	172	LEU	2.3
2	CCC	720	ARG	2.3
3	DDD	965	SER	2.3
2	CCC	871	VAL	2.3
3	DDD	1080	ILE	2.3
1	BBB	166	ARG	2.3
3	DDD	1076	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
3	DDD	855	ASP	2.2
2	CCC	333	ILE	2.2
2	CCC	722	GLY	2.2
5	FFF	308	GLU	2.2
3	DDD	880	VAL	2.2
5	FFF	202	LEU	2.2
1	BBB	47	LEU	2.2
3	DDD	1107	VAL	2.1
3	DDD	828	GLY	2.1
2	CCC	104	ILE	2.1
3	DDD	87	LYS	2.1
5	FFF	313	LEU	2.1
3	DDD	1185	PRO	2.1
2	CCC	984	VAL	2.1
3	DDD	985	ILE	2.1
3	DDD	991	THR	2.1
5	FFF	309	GLY	2.1
3	DDD	1027	VAL	2.1
2	CCC	1054	LEU	2.1
3	DDD	1129	GLY	2.1
3	DDD	959	LYS	2.1
3	DDD	854	ALA	2.1
3	DDD	856	ILE	2.1
2	CCC	67	GLU	2.0
3	DDD	1051	ASP	2.0
3	DDD	1105	ALA	2.0
3	DDD	853	THR	2.0
1	AAA	205	MET	2.0
5	FFF	71	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

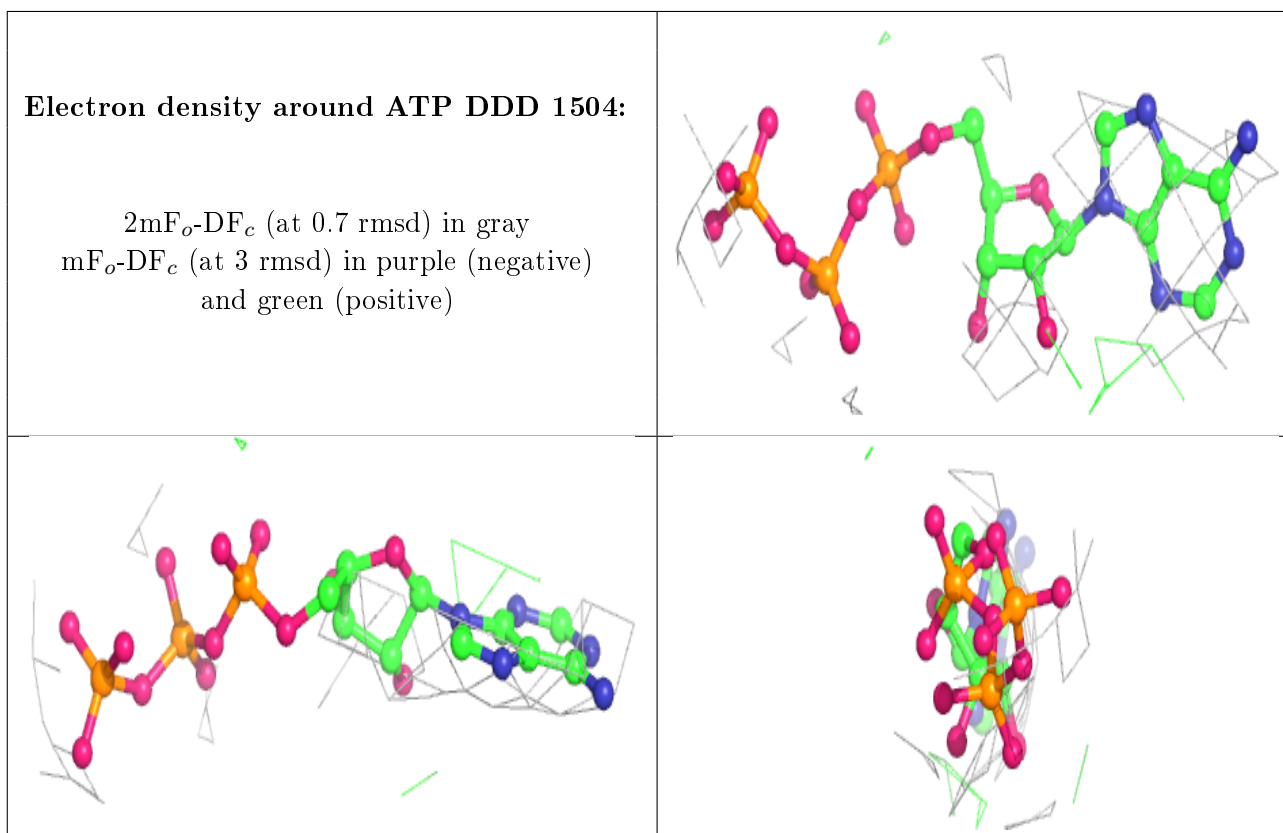
There are no monosaccharides in this entry.

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
10	ZN	DDD	1501	1/1	0.83	0.11	407,407,407,407	0
11	ATP	DDD	1504	31/31	0.88	0.41	220,293,348,403	0
10	ZN	DDD	1502	1/1	0.94	0.17	280,280,280,280	0
9	MG	DDD	1503	1/1	0.96	0.15	119,119,119,119	0
9	MG	CCC	1401	1/1	0.98	0.33	146,146,146,146	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.