Full wwPDB X-ray Structure Validation Report ⓘ

Feb 25, 2024 – 12:54 PM EST

PDB ID	:	5IPL
Title	:	SigmaS-transcription initiation complex with 4-nt nascent RNA
Authors	:	Liu, B.; Zuo, Y.; Steitz, T.A.
Deposited on	:	2016-03-09
Resolution	:	3.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

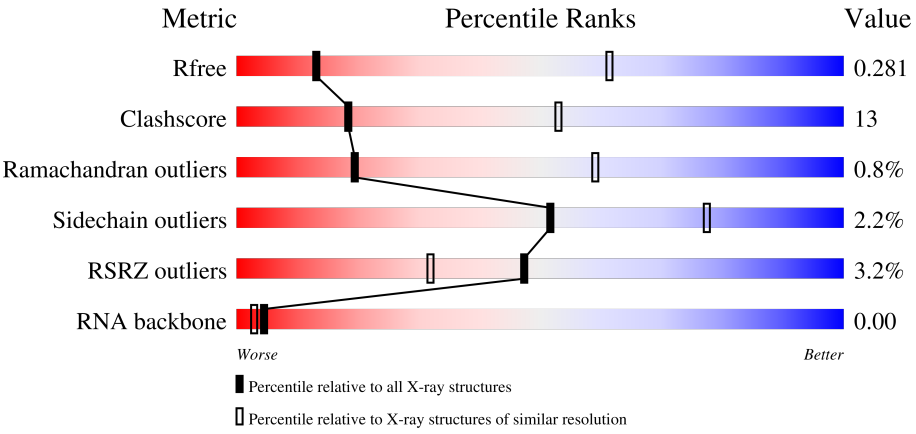
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.60 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)
RNA backbone	3102	1017 (4.20-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	A	242	74% 20% 5%
1	B	242	8% 76% 18% 6%
2	C	1342	2% 75% 23%
3	D	1407	3% 61% 21% 17%

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Mol	Chain	Length	Quality of chain
4	E	90	2% 71% 16% 12%
5	F	336	2% 52% 29% 18%
6	1	50	2% 10% 54% 34%
7	2	50	26% 40% 34%
8	3	4	75% 25%

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	D	1502	-	-	X	-
11	MG	D	1504	-	-	-	X
9	DPO	C	1401	-	X	-	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 27632 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	A	230	Total	C	N	O	S	0	0	0
			1787	1112	317	352	6			
1	B	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
A	-6	ALA	-	expression tag	UNP P0A7Z4
A	-5	HIS	-	expression tag	UNP P0A7Z4
A	-4	HIS	-	expression tag	UNP P0A7Z4
A	-3	HIS	-	expression tag	UNP P0A7Z4
A	-2	HIS	-	expression tag	UNP P0A7Z4
A	-1	HIS	-	expression tag	UNP P0A7Z4
A	0	HIS	-	expression tag	UNP P0A7Z4
B	-6	ALA	-	expression tag	UNP P0A7Z4
B	-5	HIS	-	expression tag	UNP P0A7Z4
B	-4	HIS	-	expression tag	UNP P0A7Z4
B	-3	HIS	-	expression tag	UNP P0A7Z4
B	-2	HIS	-	expression tag	UNP P0A7Z4
B	-1	HIS	-	expression tag	UNP P0A7Z4
B	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	C	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	D	1173	Total	C	N	O	S	0	0	0
			9163	5760	1644	1712	47			

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

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

There are 9 discrepancies between the modelled and reference sequences:

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

- Molecule 6 is a DNA chain called synthetic nontemplate strand DNA (50-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1	33	Total	C	N	O	P	0	0	0
			680	323	124	200	33			

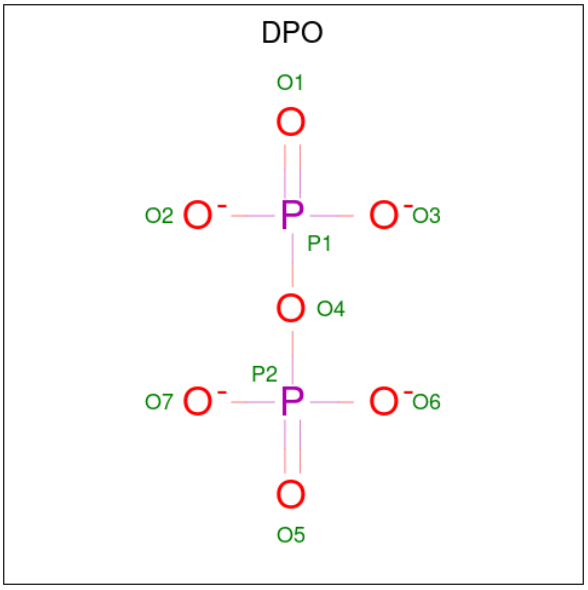
- Molecule 7 is a DNA chain called synthetic template strand DNA (50-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	2	33	Total	C	N	O	P	0	0	0
			675	322	125	196	32			

- Molecule 8 is a RNA chain called nascent RNA 4-mer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	3	4	Total	C	N	O	P	0	0	0
			97	39	17	35	6			

- Molecule 9 is DIPHOSPHATE (three-letter code: DPO) (formula: O_7P_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	O	P	0	0
			9	7	2		

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

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

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

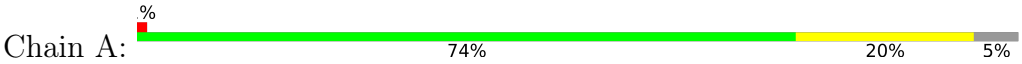
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	2	Total	Mg	0	0
			2	2		

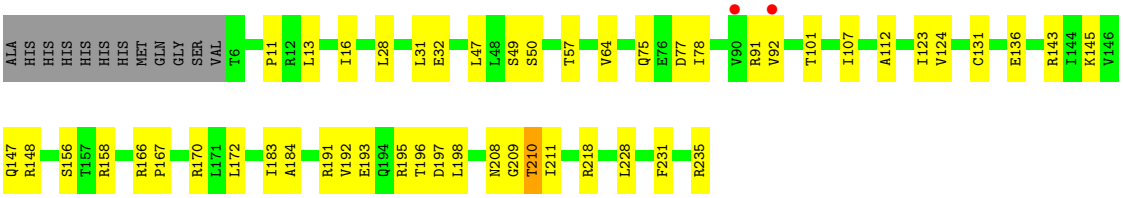
3 Residue-property plots (i)

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

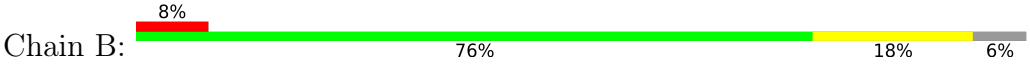
Chain A:

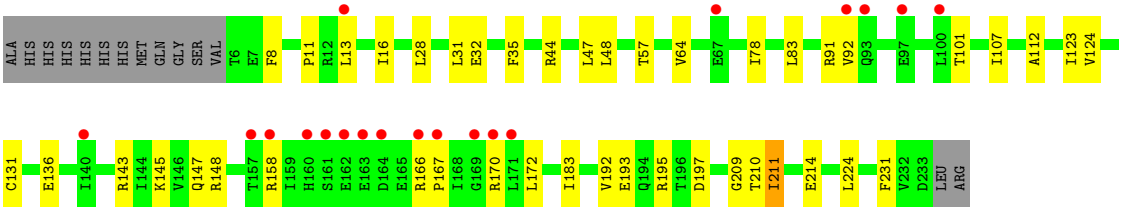




• Molecule 1: DNA-directed RNA polymerase subunit alpha

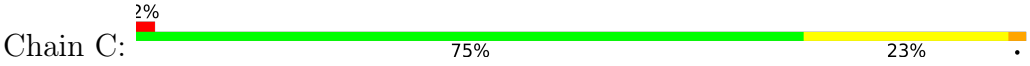
Chain B:

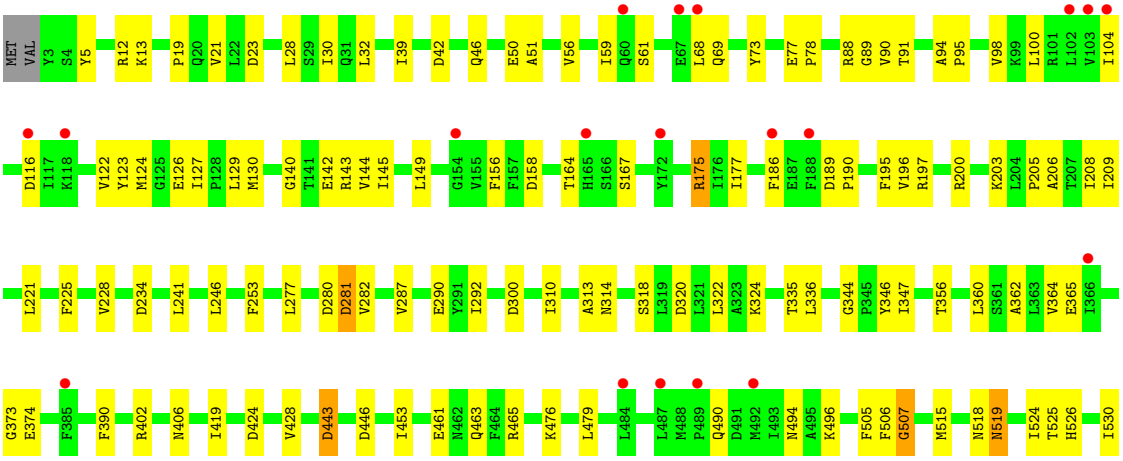


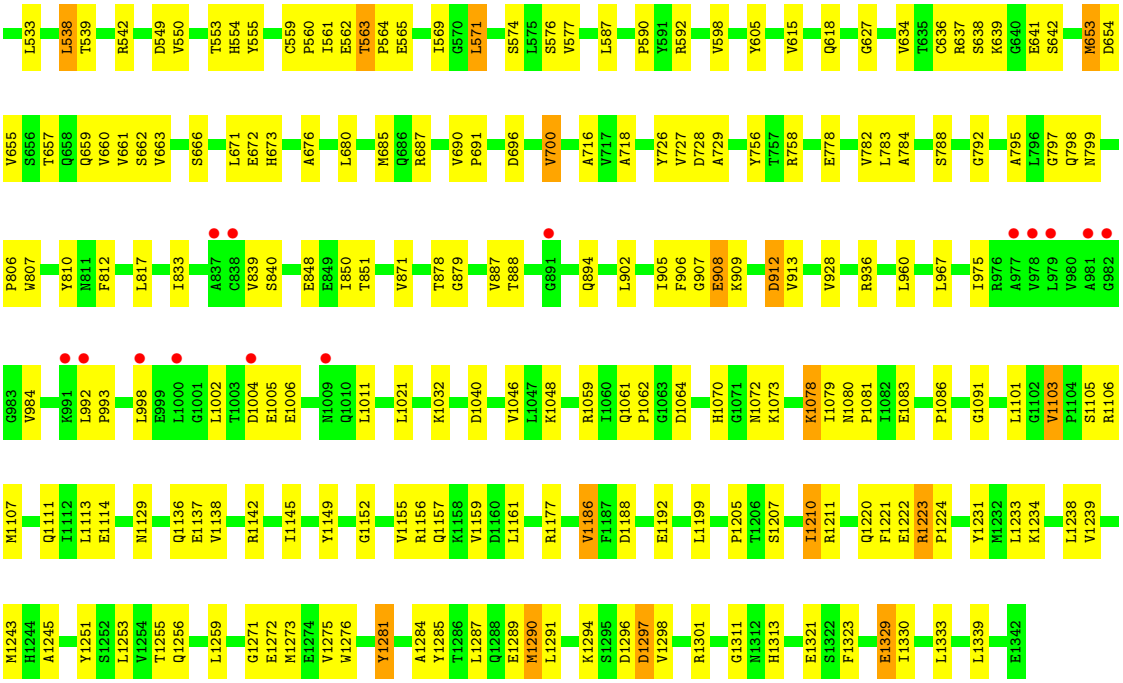


• Molecule 2: DNA-directed RNA polymerase subunit beta

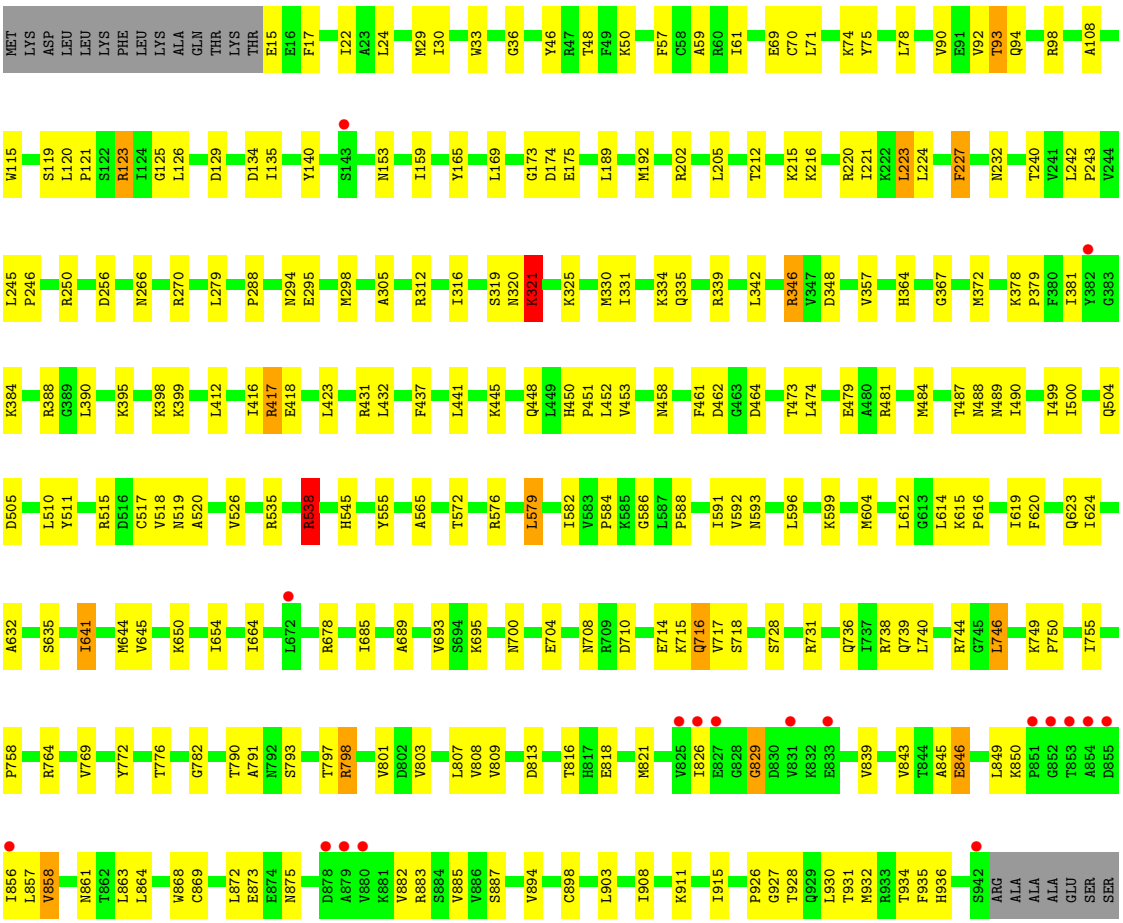
Chain C:

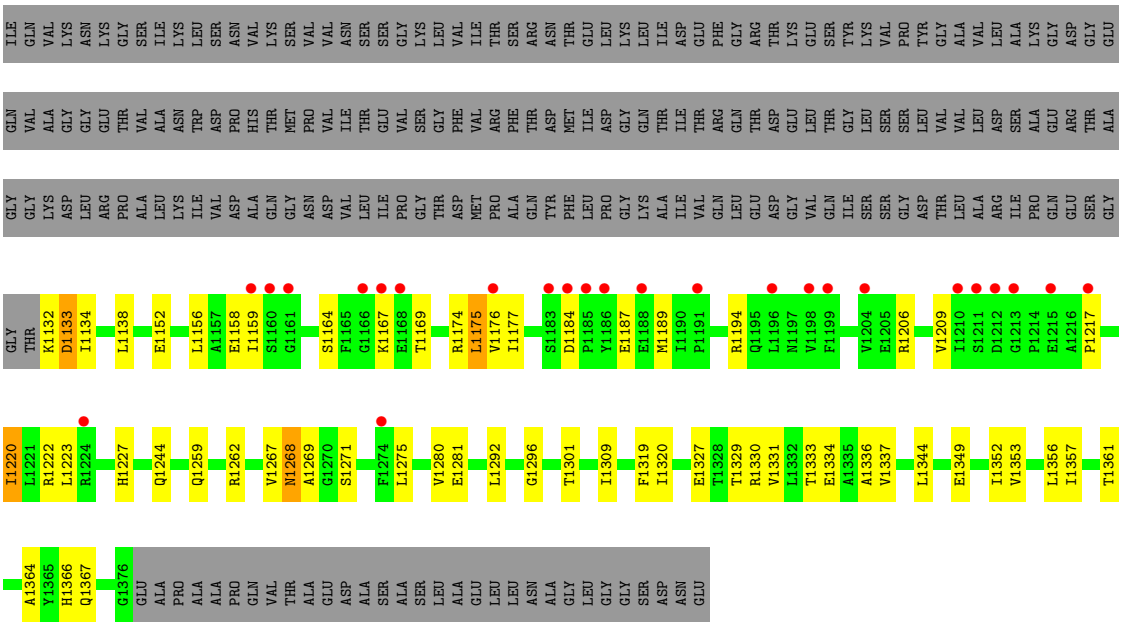




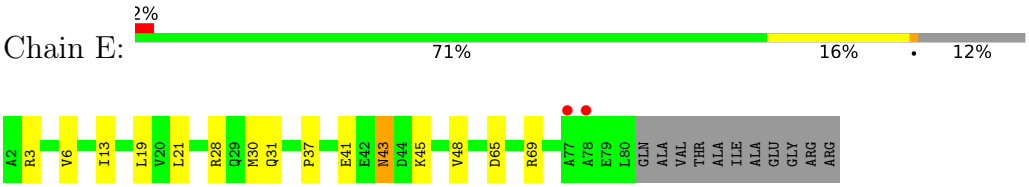


• Molecule 3: DNA-directed RNA polymerase subunit beta'

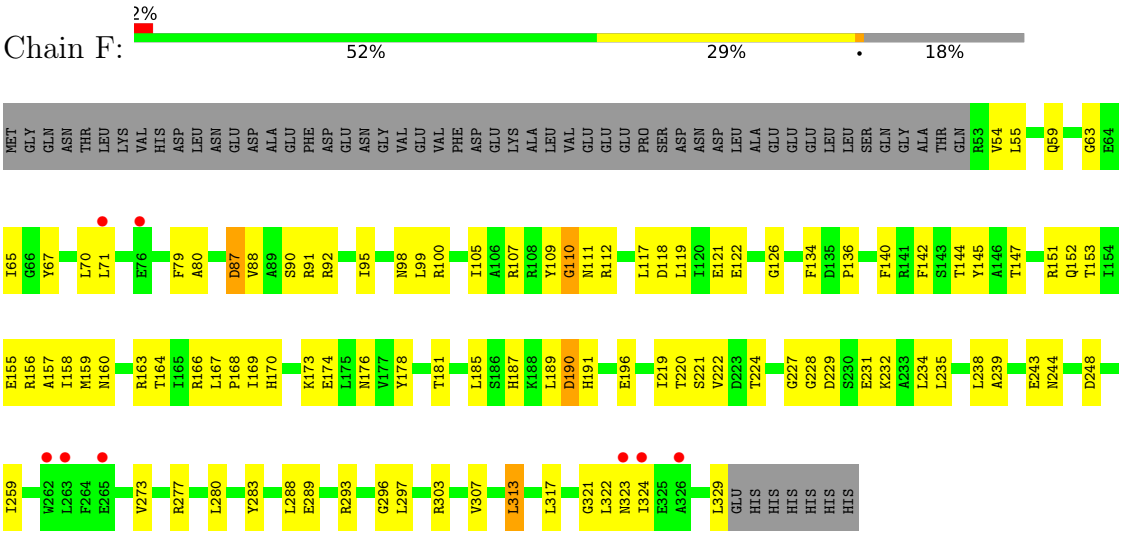




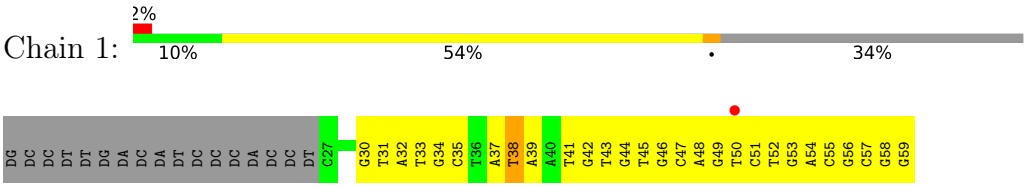
• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 5: RNA polymerase sigma factor RpoS

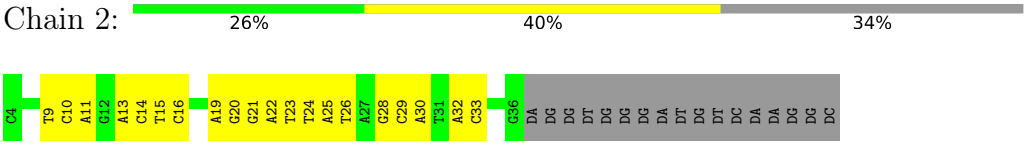


• Molecule 6: synthetic nontemplate strand DNA (50-MER)



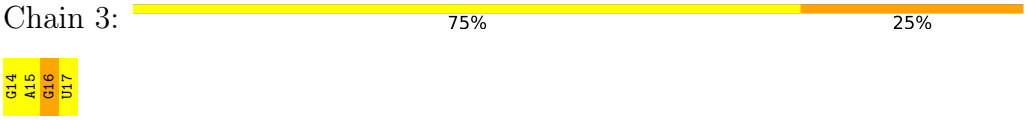
• Molecule 7: synthetic template strand DNA (50-MER)

Chain 2:



• Molecule 8: nascent RNA 4-mer

Chain 3:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	131.71Å 152.67Å 226.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	126.63 – 3.60 49.73 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (126.63-3.60) 99.7 (49.73-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.14 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.247 , 0.293 0.241 , 0.281	Depositor DCC
R_{free} test set	2560 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å^2)	143.0	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 141.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	27632	wwPDB-VP
Average B, all atoms (Å^2)	206.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: DPO, MG, ZN, GTP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.54	0/1809	0.72	0/2450
1	B	0.52	0/1789	0.70	0/2425
2	C	0.64	9/10739 (0.1%)	0.79	4/14489 (0.0%)
3	D	0.59	2/9305 (0.0%)	0.80	6/12556 (0.0%)
4	E	0.50	0/629	0.70	0/847
5	F	0.59	0/2282	0.84	2/3076 (0.1%)
6	1	0.37	0/762	0.65	1/1175 (0.1%)
7	2	0.50	0/757	0.70	0/1167
8	3	0.78	1/71 (1.4%)	0.86	0/106
All	All	0.59	12/28143 (0.0%)	0.78	13/38291 (0.0%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	565	GLU	CD-OE1	11.18	1.38	1.25
3	D	346	ARG	CD-NE	10.32	1.64	1.46
2	C	565	GLU	CD-OE2	8.43	1.34	1.25
2	C	1272	GLU	CD-OE2	8.18	1.34	1.25
2	C	1192	GLU	CB-CG	7.58	1.66	1.52
2	C	1281	TYR	CB-CG	7.25	1.62	1.51
2	C	1192	GLU	CG-CD	-6.77	1.41	1.51
2	C	1329	GLU	CD-OE1	6.68	1.32	1.25
2	C	1329	GLU	CG-CD	5.58	1.60	1.51
2	C	1281	TYR	CG-CD1	5.36	1.46	1.39
8	3	15	A	O3'-P	-5.36	1.54	1.61
3	D	15	GLU	CG-CD	5.04	1.59	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	538	ARG	NE-CZ-NH1	8.24	124.42	120.30
3	D	346	ARG	NE-CZ-NH2	7.10	123.85	120.30
3	D	346	ARG	NE-CZ-NH1	-6.77	116.92	120.30
6	1	38	DT	O5'-P-OP1	-6.66	99.71	105.70
3	D	417	ARG	NE-CZ-NH1	6.39	123.50	120.30
2	C	549	ASP	CB-CG-OD1	5.90	123.61	118.30
2	C	1106	ARG	NE-CZ-NH1	5.63	123.12	120.30
2	C	1290	MET	CG-SD-CE	-5.36	91.62	100.20
5	F	87	ASP	N-CA-C	-5.24	96.86	111.00
3	D	1220	ILE	CB-CA-C	-5.10	101.40	111.60
2	C	175	ARG	NE-CZ-NH1	5.09	122.84	120.30
3	D	538	ARG	NE-CZ-NH2	-5.08	117.76	120.30
5	F	296	GLY	N-CA-C	-5.02	100.55	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	A	1787	0	1813	42	0
1	B	1767	0	1789	34	0
2	C	10570	0	10582	263	0
3	D	9163	0	9357	257	0
4	E	627	0	634	14	0
5	F	2253	0	2298	135	0
6	1	680	0	373	69	0
7	2	675	0	373	44	0
8	3	97	0	45	6	0
9	C	9	0	0	0	0
10	D	2	0	0	2	0
11	D	2	0	0	0	0
All	All	27632	0	27264	728	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 13.

All (728) 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:D:1133:ASP:O	3:D:1244:GLN:NE2	1.66	1.24
5:F:110:GLY:HA2	5:F:119:LEU:HD11	1.33	1.07
5:F:231:GLU:HG3	5:F:232:LYS:H	1.16	1.06
2:C:967:LEU:HD21	2:C:1021:LEU:HD13	1.44	1.00
6:1:50:DT:H3'	6:1:51:DC:H5"	1.47	0.95
3:D:320:ASN:OD1	7:2:22:DA:N6	2.00	0.95
5:F:189:LEU:O	5:F:191:HIS:N	2.02	0.92
2:C:292:ILE:HD12	2:C:322:LEU:HD22	1.54	0.90
2:C:373:GLY:HA3	5:F:54:VAL:HG21	1.52	0.88
6:1:50:DT:H3'	6:1:51:DC:C5'	2.03	0.88
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.56	0.88
2:C:560:PRO:HB2	3:D:776:THR:HG21	1.57	0.86
5:F:163:ARG:CD	5:F:167:LEU:HD12	2.06	0.86
2:C:539:THR:HB	2:C:542:ARG:HG3	1.55	0.85
3:D:1330:ARG:NH2	7:2:9:DT:O3'	2.09	0.85
3:D:173:GLY:O	3:D:175:GLU:N	2.09	0.85
3:D:381:ILE:HD11	3:D:412:LEU:HD13	1.60	0.84
2:C:1273:MET:HG3	7:2:14:DC:H4'	1.57	0.83
3:D:936:HIS:CE1	8:3:17:U:OP1	2.31	0.83
5:F:317:LEU:O	5:F:321:GLY:HA3	1.79	0.83
1:B:13:LEU:HD21	1:B:16:ILE:HD11	1.60	0.82
3:D:346:ARG:NH1	7:2:16:DC:OP1	2.13	0.82
3:D:481:ARG:NH1	4:E:3:ARG:O	2.13	0.81
6:1:47:DC:C2'	6:1:48:DA:H5'	2.10	0.81
3:D:1344:LEU:HD23	3:D:1349:GLU:HB3	1.62	0.81
5:F:231:GLU:CG	5:F:232:LYS:H	1.94	0.81
1:A:13:LEU:HD21	1:A:16:ILE:HD11	1.62	0.81
3:D:320:ASN:O	3:D:321:LYS:HB3	1.80	0.81
3:D:936:HIS:ND1	8:3:17:U:OP1	2.14	0.81
5:F:110:GLY:HA2	5:F:119:LEU:CD1	2.10	0.80
5:F:158:ILE:HG22	5:F:158:ILE:O	1.81	0.80
2:C:241:LEU:CD2	2:C:277:LEU:HD21	2.12	0.80
2:C:373:GLY:HA3	5:F:54:VAL:CG2	2.12	0.79
2:C:1284:ALA:HA	3:D:1357:ILE:HD12	1.63	0.78
2:C:618:GLN:HE21	3:D:769:VAL:HB	1.47	0.78
3:D:294:ASN:ND2	5:F:121:GLU:OE2	2.17	0.77
1:B:83:LEU:HD21	3:D:526:VAL:HB	1.66	0.77
2:C:577:VAL:HG23	2:C:661:VAL:O	1.84	0.77
2:C:205:PRO:O	2:C:208:ILE:HG22	1.85	0.77
3:D:490:ILE:HD11	3:D:614:LEU:CD1	2.15	0.76
2:C:1245:ALA:HB2	3:D:372:MET:HG3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1251:TYR:OH	3:D:348:ASP:OD2	2.01	0.76
2:C:887:VAL:HB	2:C:913:VAL:CG1	2.16	0.75
5:F:227:GLY:N	7:2:20:DG:O6	2.18	0.75
6:1:51:DC:OP1	6:1:51:DC:H2'	1.86	0.75
3:D:59:ALA:HB3	3:D:71:LEU:HD11	1.69	0.74
5:F:122:GLU:OE1	5:F:157:ALA:CB	2.35	0.74
6:1:45:DT:O3'	6:1:46:DG:O4'	2.04	0.74
2:C:562:GLU:HG2	2:C:574:SER:HB2	1.69	0.74
2:C:241:LEU:HD21	2:C:277:LEU:HD21	1.68	0.74
5:F:317:LEU:O	5:F:321:GLY:CA	2.36	0.73
2:C:902:LEU:HD11	5:F:259:ILE:HD11	1.71	0.73
5:F:71:LEU:HD22	5:F:79:PHE:HE2	1.52	0.73
6:1:44:DG:H4'	6:1:45:DT:OP2	1.88	0.73
6:1:47:DC:H2'	6:1:48:DA:H5'	1.71	0.73
2:C:46:GLN:HB2	2:C:51:ALA:HA	1.71	0.73
5:F:231:GLU:HG3	5:F:232:LYS:N	1.99	0.72
2:C:494:ASN:ND2	7:2:25:DA:OP1	2.22	0.72
5:F:71:LEU:CD2	5:F:79:PHE:HE2	2.02	0.72
3:D:395:LYS:HE2	5:F:329:LEU:HD11	1.71	0.72
3:D:856:ILE:HG23	3:D:858:VAL:HG23	1.71	0.72
5:F:122:GLU:OE1	5:F:157:ALA:HB3	1.90	0.72
5:F:144:THR:HG1	6:1:39:DA:H8	1.38	0.72
5:F:190:ASP:OD1	5:F:191:HIS:N	2.22	0.72
5:F:112:ARG:NH1	7:2:23:DT:O2	2.23	0.72
5:F:317:LEU:O	5:F:321:GLY:N	2.23	0.72
3:D:78:LEU:O	5:F:283:TYR:OH	2.06	0.71
3:D:898:CYS:HG	10:D:1502:ZN:ZN	1.03	0.71
5:F:54:VAL:CG1	5:F:59:GLN:OE1	2.38	0.71
7:2:15:DT:H5"	7:2:15:DT:H6	1.56	0.70
3:D:739:GLN:HG3	3:D:744:ARG:HD2	1.72	0.70
2:C:1101:LEU:O	3:D:731:ARG:HG2	1.92	0.69
3:D:134:ASP:HB3	3:D:159:ILE:HD11	1.75	0.69
5:F:119:LEU:CD2	5:F:158:ILE:HD11	2.22	0.69
2:C:525:THR:HG21	2:C:687:ARG:CD	2.22	0.69
2:C:848:GLU:HG2	2:C:888:THR:HG22	1.74	0.69
2:C:142:GLU:OE1	2:C:515:MET:CE	2.41	0.68
3:D:591:ILE:HD11	3:D:604:MET:HA	1.74	0.68
7:2:16:DC:H6	7:2:16:DC:H5"	1.58	0.68
3:D:749:LYS:HB3	3:D:750:PRO:HD2	1.75	0.68
2:C:967:LEU:HD21	2:C:1021:LEU:CD1	2.22	0.68
5:F:169:ILE:HG22	5:F:173:LYS:HD3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:967:LEU:CD2	2:C:1021:LEU:HD13	2.22	0.68
5:F:163:ARG:HD2	5:F:167:LEU:HD12	1.76	0.68
2:C:672:GLU:HG3	2:C:673:HIS:CD2	2.29	0.67
5:F:227:GLY:CA	7:2:19:DA:H2	2.06	0.67
6:1:49:DG:C2'	6:1:50:DT:H5"	2.25	0.67
3:D:388:ARG:HB3	3:D:390:LEU:HD13	1.74	0.67
5:F:119:LEU:HD21	5:F:158:ILE:HD11	1.77	0.67
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.77	0.67
3:D:331:ILE:HD12	3:D:331:ILE:N	2.10	0.67
3:D:582:ILE:HG23	3:D:623:GLN:HB3	1.76	0.67
2:C:1287:LEU:HD23	3:D:1357:ILE:HD11	1.77	0.66
3:D:782:GLY:O	3:D:935:PHE:HB3	1.94	0.66
7:2:22:DA:H2"	7:2:23:DT:O5'	1.96	0.66
6:1:33:DT:H2"	6:1:34:DG:H5'	1.76	0.66
2:C:221:LEU:HD22	2:C:336:LEU:HD11	1.77	0.66
2:C:1105:SER:HB2	3:D:731:ARG:HD2	1.78	0.66
2:C:196:VAL:HG23	2:C:206:ALA:HA	1.77	0.65
2:C:1323:PHE:CE1	3:D:1353:VAL:HG12	2.31	0.65
1:A:156:SER:OG	2:C:1059:ARG:NH1	2.28	0.65
5:F:176:ASN:OD1	7:2:26:DT:H71	1.96	0.65
6:1:52:DT:H2"	6:1:53:DG:C8	2.32	0.65
5:F:227:GLY:O	5:F:229:ASP:N	2.23	0.65
5:F:122:GLU:CD	5:F:157:ALA:HB1	2.16	0.65
2:C:142:GLU:OE1	2:C:515:MET:HE2	1.97	0.65
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.77	0.65
5:F:71:LEU:HD22	5:F:79:PHE:CE2	2.32	0.65
5:F:98:ASN:HA	6:1:41:DT:O2	1.97	0.65
5:F:54:VAL:HG13	5:F:59:GLN:OE1	1.97	0.64
5:F:110:GLY:CA	5:F:119:LEU:HD11	2.19	0.64
3:D:205:LEU:HD23	3:D:205:LEU:O	1.97	0.64
3:D:898:CYS:SG	10:D:1502:ZN:ZN	1.84	0.64
5:F:163:ARG:CD	5:F:167:LEU:CD1	2.75	0.64
3:D:716:GLN:HG3	3:D:717:VAL:N	2.12	0.64
5:F:227:GLY:CA	7:2:19:DA:C2	2.81	0.64
2:C:206:ALA:O	2:C:209:ILE:HG22	1.97	0.63
2:C:1145:ILE:HG22	2:C:1161:LEU:HD11	1.80	0.63
3:D:826:ILE:O	3:D:826:ILE:HG22	1.97	0.63
2:C:156:PHE:CE2	2:C:158:ASP:HB2	2.34	0.63
5:F:155:GLU:O	5:F:159:MET:HG3	1.98	0.63
5:F:227:GLY:HA2	7:2:19:DA:H2	1.63	0.63
4:E:65:ASP:HB3	4:E:69:ARG:HH21	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:782:VAL:HG21	2:C:792:GLY:HA2	1.81	0.63
6:1:45:DT:H2"	6:1:46:DG:N9	2.14	0.63
7:2:21:DG:H2"	7:2:22:DA:OP2	1.97	0.63
2:C:19:PRO:HA	2:C:1156:ARG:HD2	1.80	0.62
3:D:746:LEU:H	3:D:746:LEU:HD12	1.64	0.62
2:C:200:ARG:O	2:C:200:ARG:HG2	2.00	0.62
3:D:242:LEU:HD12	3:D:243:PRO:HD2	1.81	0.62
3:D:319:SER:OG	7:2:22:DA:N6	2.32	0.62
5:F:122:GLU:CD	5:F:157:ALA:CB	2.68	0.62
3:D:615:LYS:HB2	3:D:616:PRO:HD3	1.82	0.62
6:1:46:DG:H2"	6:1:47:DC:O4'	1.99	0.62
1:A:210:THR:HG22	1:A:211:ILE:N	2.13	0.62
6:1:49:DG:H2"	6:1:50:DT:C4'	2.30	0.62
1:A:228:LEU:HD11	1:B:224:LEU:HD23	1.81	0.62
5:F:164:THR:HB	5:F:219:ILE:HD12	1.81	0.62
2:C:356:THR:HG21	2:C:362:ALA:HA	1.82	0.61
2:C:653:MET:HG2	2:C:654:ASP:N	2.13	0.61
5:F:169:ILE:HG22	5:F:173:LYS:CD	2.29	0.61
5:F:317:LEU:CD2	5:F:324:ILE:HD12	2.30	0.61
3:D:319:SER:OG	7:2:22:DA:N1	2.30	0.61
2:C:542:ARG:HD2	6:1:50:DT:OP2	2.00	0.61
2:C:1311:GLY:O	4:E:31:GLN:NE2	2.33	0.61
3:D:1134:ILE:CD1	3:D:1244:GLN:HG3	2.31	0.61
3:D:298:MET:SD	5:F:117:LEU:HB3	2.41	0.60
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.84	0.60
2:C:975:ILE:HD13	2:C:998:LEU:HD21	1.83	0.60
5:F:160:ASN:ND2	5:F:166:ARG:NH1	2.49	0.60
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.83	0.60
5:F:170:HIS:O	5:F:174:GLU:HG2	2.01	0.60
3:D:1267:VAL:O	3:D:1268:ASN:CB	2.50	0.60
2:C:123:TYR:CZ	5:F:190:ASP:O	2.55	0.60
5:F:321:GLY:HA2	5:F:324:ILE:HG22	1.84	0.60
2:C:1271:GLY:O	2:C:1275:VAL:HG23	2.02	0.59
3:D:885:VAL:HG13	3:D:894:VAL:HG11	1.84	0.59
5:F:158:ILE:O	5:F:158:ILE:CG2	2.47	0.59
6:1:49:DG:H2"	6:1:50:DT:C5'	2.31	0.59
2:C:1287:LEU:CD2	3:D:1357:ILE:HD11	2.32	0.59
3:D:423:LEU:HD12	3:D:437:PHE:CD1	2.37	0.59
3:D:452:LEU:HB3	3:D:500:ILE:HG23	1.83	0.59
3:D:572:THR:HG22	3:D:593:ASN:OD1	2.02	0.59
3:D:708:ASN:HD21	3:D:716:GLN:HB3	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:69:GLN:O	2:C:100:LEU:HD12	2.03	0.59
5:F:122:GLU:OE2	5:F:157:ALA:HB1	2.03	0.59
2:C:56:VAL:HG12	2:C:59:ILE:HD11	1.84	0.58
1:B:47:LEU:HD13	1:B:183:ILE:HD12	1.85	0.58
2:C:1129:ASN:OD1	2:C:1177:ARG:NH2	2.36	0.58
3:D:927:GLY:O	3:D:931:THR:OG1	2.19	0.58
3:D:746:LEU:HD12	3:D:746:LEU:N	2.19	0.58
2:C:638:SER:O	2:C:639:LYS:CG	2.52	0.58
3:D:555:TYR:CD2	3:D:565:ALA:HB2	2.38	0.58
5:F:170:HIS:CE1	6:1:32:DA:N7	2.72	0.58
7:2:22:DA:H2"	7:2:23:DT:C5'	2.34	0.58
2:C:200:ARG:O	2:C:200:ARG:CG	2.50	0.57
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.85	0.57
1:B:47:LEU:HD13	1:B:183:ILE:CD1	2.34	0.57
3:D:24:LEU:HD12	3:D:232:ASN:HB3	1.86	0.57
3:D:295:GLU:OE1	5:F:121:GLU:HG3	2.05	0.57
5:F:227:GLY:HA3	7:2:19:DA:C2	2.39	0.57
7:2:19:DA:H2'	7:2:20:DG:O4'	2.05	0.57
2:C:700:VAL:HG21	2:C:1114:GLU:HG2	1.86	0.57
2:C:143:ARG:HH12	2:C:507:GLY:HA2	1.69	0.57
6:1:30:DG:N2	7:2:33:DC:O2	2.37	0.57
2:C:186:PHE:CE2	2:C:196:VAL:HG22	2.40	0.57
2:C:1255:THR:O	2:C:1256:GLN:HB2	2.05	0.57
1:A:47:LEU:HD13	1:A:183:ILE:CD1	2.34	0.57
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.87	0.57
2:C:563:THR:H	2:C:680:LEU:HD11	1.69	0.57
6:1:31:DT:H2"	6:1:32:DA:OP2	2.05	0.57
3:D:689:ALA:O	3:D:693:VAL:HG23	2.05	0.56
3:D:845:ALA:O	3:D:846:GLU:CB	2.50	0.56
2:C:550:VAL:HG21	3:D:776:THR:CG2	2.35	0.56
2:C:1149:TYR:HB3	2:C:1159:VAL:CG1	2.36	0.56
3:D:490:ILE:HD11	3:D:614:LEU:HD13	1.87	0.56
6:1:45:DT:H2"	6:1:46:DG:C4	2.40	0.56
3:D:342:LEU:HG	3:D:1352:ILE:HG23	1.87	0.56
5:F:100:ARG:HB3	6:1:42:DG:H5"	1.87	0.56
6:1:54:DA:H2	7:2:10:DC:O2	1.89	0.56
8:3:16:G:H2'	8:3:17:U:O4'	2.06	0.56
2:C:840:SER:O	2:C:840:SER:OG	2.21	0.56
2:C:902:LEU:CD1	5:F:259:ILE:HD11	2.35	0.56
1:A:47:LEU:HD13	1:A:183:ILE:HD12	1.88	0.56
2:C:122:VAL:HG13	5:F:187:HIS:CE1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1:57:DC:H2"	6:1:58:DG:OP2	2.06	0.56
7:2:13:DA:H2"	7:2:14:DC:H5'	1.86	0.56
2:C:453:ILE:HD12	2:C:587:LEU:HD21	1.87	0.56
3:D:320:ASN:O	3:D:321:LYS:CB	2.50	0.56
2:C:590:PRO:HB2	2:C:655:VAL:HG21	1.87	0.55
2:C:1273:MET:HG3	7:2:14:DC:C4'	2.33	0.55
3:D:1175:LEU:HD12	3:D:1177:ILE:HG12	1.88	0.55
5:F:163:ARG:NE	5:F:167:LEU:HD12	2.21	0.55
5:F:170:HIS:CE1	6:1:31:DT:C5	2.94	0.55
3:D:93:THR:HG22	3:D:94:GLN:H	1.70	0.55
2:C:142:GLU:OE1	2:C:515:MET:HE1	2.06	0.55
2:C:960:LEU:HD11	2:C:1032:LYS:HG3	1.87	0.55
2:C:907:GLY:O	2:C:909:LYS:N	2.40	0.55
5:F:170:HIS:CG	6:1:31:DT:H73	2.42	0.55
5:F:222:VAL:HG12	5:F:235:LEU:HB2	1.88	0.55
2:C:374:GLU:OE2	6:1:43:DT:H72	2.07	0.55
5:F:140:PHE:CG	6:1:37:DA:H2"	2.41	0.55
2:C:1005:GLU:HG2	2:C:1006:GLU:H	1.71	0.55
5:F:164:THR:CB	5:F:219:ILE:HD12	2.37	0.55
5:F:313:LEU:O	5:F:317:LEU:HG	2.07	0.55
6:1:48:DA:H8	6:1:48:DA:OP2	1.90	0.55
3:D:129:ASP:HB2	3:D:220:ARG:NH1	2.23	0.54
1:B:92:VAL:O	1:B:148:ARG:NH2	2.40	0.54
2:C:241:LEU:HD21	2:C:277:LEU:CD2	2.37	0.54
1:B:64:VAL:HG13	1:B:78:ILE:HD13	1.90	0.54
2:C:241:LEU:HD23	2:C:277:LEU:HD21	1.87	0.54
2:C:390:PHE:HA	2:C:419:ILE:CG2	2.38	0.54
3:D:1330:ARG:CZ	7:2:10:DC:C5'	2.86	0.54
5:F:169:ILE:CG2	5:F:173:LYS:HD2	2.38	0.54
5:F:176:ASN:OD1	7:2:26:DT:C7	2.55	0.54
7:2:20:DG:H2"	7:2:21:DG:H5'	1.90	0.54
2:C:28:LEU:HD21	2:C:524:ILE:HG13	1.89	0.54
1:A:92:VAL:O	1:A:148:ARG:NH2	2.41	0.54
1:A:228:LEU:HD21	1:B:224:LEU:HD23	1.90	0.54
2:C:88:ARG:NH1	2:C:1040:ASP:OD1	2.41	0.54
2:C:122:VAL:HG22	2:C:490:GLN:HB3	1.89	0.54
2:C:1276:TRP:CE2	3:D:801:VAL:HG11	2.42	0.54
3:D:319:SER:OG	7:2:22:DA:C6	2.60	0.54
2:C:525:THR:HG21	2:C:687:ARG:HD3	1.89	0.54
3:D:845:ALA:O	3:D:846:GLU:HB3	2.07	0.54
2:C:716:ALA:HB3	2:C:784:ALA:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:48:THR:O	3:D:50:LYS:N	2.36	0.54
3:D:839:VAL:HG13	3:D:882:VAL:HG11	1.90	0.54
5:F:63:GLY:O	5:F:67:TYR:HD2	1.91	0.54
2:C:685:MET:SD	2:C:1073:LYS:HG2	2.47	0.54
3:D:515:ARG:HH22	3:D:718:SER:C	2.12	0.54
3:D:716:GLN:CG	3:D:717:VAL:N	2.71	0.54
5:F:87:ASP:OD2	5:F:90:SER:OG	2.19	0.54
1:A:64:VAL:HG13	1:A:78:ILE:HD13	1.91	0.53
2:C:817:LEU:HD11	2:C:1080:ASN:HB2	1.90	0.53
3:D:108:ALA:HB3	3:D:279:LEU:HD23	1.89	0.53
3:D:816:THR:HG22	3:D:818:GLU:H	1.74	0.53
3:D:339:ARG:CZ	3:D:798:ARG:HH22	2.21	0.53
3:D:1330:ARG:CZ	7:2:10:DC:H5"	2.38	0.53
1:A:191:ARG:HG3	1:A:196:THR:HG22	1.90	0.53
2:C:39:ILE:O	2:C:73:TYR:OH	2.26	0.53
2:C:1339:LEU:HD13	3:D:17:PHE:CE2	2.43	0.53
3:D:813:ASP:OD1	3:D:883:ARG:NH2	2.40	0.53
2:C:533:LEU:HD21	2:C:571:LEU:HD13	1.90	0.53
2:C:496:LYS:HB3	7:2:24:DT:OP1	2.07	0.53
3:D:1271:SER:OG	3:D:1292:LEU:HD21	2.08	0.53
5:F:105:ILE:HG23	5:F:109:TYR:HE2	1.73	0.53
5:F:321:GLY:CA	5:F:324:ILE:HG22	2.38	0.53
5:F:163:ARG:HD3	5:F:167:LEU:CD1	2.38	0.53
2:C:1137:GLU:HG3	2:C:1138:VAL:H	1.73	0.53
2:C:253:PHE:CZ	2:C:287:VAL:HG12	2.43	0.53
2:C:1287:LEU:O	2:C:1291:LEU:HG	2.09	0.53
3:D:664:ILE:HD11	3:D:685:ILE:HD11	1.90	0.53
1:A:50:SER:OG	1:B:35:PHE:HZ	1.91	0.53
1:A:210:THR:O	1:A:211:ILE:C	2.47	0.52
2:C:164:THR:OG1	2:C:167:SER:OG	2.24	0.52
3:D:125:GLY:HA2	3:D:135:ILE:HD11	1.91	0.52
3:D:126:LEU:HG	3:D:223:LEU:CD1	2.39	0.52
1:B:158:ARG:NE	1:B:172:LEU:HD11	2.24	0.52
5:F:277:ARG:HE	5:F:288:LEU:HD21	1.74	0.52
5:F:317:LEU:HD22	5:F:324:ILE:HG21	1.92	0.52
2:C:186:PHE:CD2	2:C:196:VAL:HG22	2.44	0.52
2:C:390:PHE:HA	2:C:419:ILE:HG23	1.92	0.52
2:C:461:GLU:OE2	2:C:465:ARG:NH2	2.42	0.52
2:C:590:PRO:HG3	2:C:605:TYR:CE2	2.44	0.52
3:D:1156:LEU:HD23	3:D:1209:VAL:HA	1.91	0.52
6:1:53:DG:H2"	6:1:54:DA:H5'	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ALA:HB1	1:A:123:ILE:HG21	1.91	0.52
1:B:48:LEU:HD22	3:D:535:ARG:HG3	1.92	0.52
2:C:424:ASP:O	2:C:428:VAL:HG23	2.09	0.52
2:C:443:ASP:OD1	2:C:443:ASP:N	2.41	0.52
3:D:490:ILE:O	3:D:499:ILE:HG22	2.10	0.52
2:C:799:ASN:HA	2:C:1231:TYR:HA	1.92	0.52
3:D:739:GLN:CG	3:D:744:ARG:HD2	2.37	0.52
2:C:61:SER:HB3	2:C:479:LEU:HB3	1.92	0.52
3:D:36:GLY:HA3	3:D:61:ILE:HG23	1.91	0.52
3:D:555:TYR:HA	3:D:565:ALA:HA	1.92	0.52
3:D:843:VAL:HG13	3:D:861:ASN:HA	1.92	0.52
5:F:222:VAL:CG1	5:F:235:LEU:HB2	2.39	0.52
6:1:53:DG:H1'	6:1:54:DA:C5'	2.40	0.52
2:C:806:PRO:HG2	3:D:632:ALA:O	2.09	0.52
5:F:234:LEU:O	5:F:238:LEU:HG	2.10	0.52
1:B:112:ALA:HB1	1:B:123:ILE:HG21	1.91	0.52
2:C:195:PHE:CG	2:C:203:LYS:HD3	2.44	0.52
3:D:1158:GLU:HA	3:D:1223:LEU:HD22	1.91	0.52
3:D:1361:THR:HG23	4:E:21:LEU:HD21	1.91	0.52
2:C:696:ASP:O	2:C:795:ALA:HB1	2.10	0.52
3:D:518:VAL:HG23	3:D:716:GLN:NE2	2.25	0.52
3:D:797:THR:O	3:D:801:VAL:HG23	2.09	0.52
1:A:158:ARG:NE	1:A:172:LEU:HD11	2.25	0.52
2:C:1136:GLN:O	2:C:1137:GLU:HB2	2.10	0.52
3:D:416:ILE:CD1	3:D:441:LEU:HD21	2.40	0.52
2:C:797:GLY:HA3	2:C:1233:LEU:HD23	1.91	0.51
2:C:1199:LEU:HD13	2:C:1205:PRO:O	2.10	0.51
3:D:803:VAL:HG21	3:D:1309:ILE:O	2.10	0.51
6:1:48:DA:H2'	6:1:49:DG:C1'	2.41	0.51
3:D:1280:VAL:HG12	3:D:1281:GLU:N	2.25	0.51
5:F:317:LEU:HD22	5:F:324:ILE:HD12	1.92	0.51
2:C:576:SER:OG	2:C:659:GLN:O	2.27	0.51
2:C:1081:PRO:HB2	2:C:1083:GLU:OE1	2.10	0.51
3:D:488:ASN:HD21	4:E:6:VAL:HG23	1.74	0.51
2:C:550:VAL:HG21	3:D:776:THR:HG22	1.92	0.51
3:D:134:ASP:CB	3:D:159:ILE:HD11	2.39	0.51
3:D:620:PHE:CZ	3:D:624:ILE:HD11	2.45	0.51
2:C:42:ASP:O	2:C:50:GLU:HG2	2.10	0.51
2:C:46:GLN:HB2	2:C:51:ALA:CA	2.41	0.51
1:A:49:SER:HB3	2:C:1083:GLU:OE2	2.11	0.51
2:C:967:LEU:HD21	2:C:1021:LEU:HD22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:70:CYS:SG	3:D:74:LYS:N	2.83	0.51
2:C:936:ARG:HD2	2:C:1046:VAL:O	2.10	0.51
2:C:1313:HIS:HB3	3:D:473:THR:HA	1.91	0.51
1:A:11:PRO:HG2	1:B:231:PHE:CZ	2.46	0.51
1:A:77:ASP:OD1	2:C:729:ALA:HB1	2.11	0.51
1:A:235:ARG:HB3	1:B:214:GLU:OE2	2.11	0.51
2:C:98:VAL:HG21	2:C:124:MET:HE3	1.91	0.51
2:C:1103:VAL:HG22	2:C:1111:GLN:NE2	2.25	0.51
3:D:620:PHE:CE2	3:D:624:ILE:HD11	2.46	0.51
2:C:676:ALA:HA	3:D:772:TYR:OH	2.11	0.51
5:F:110:GLY:CA	5:F:119:LEU:CD1	2.84	0.51
2:C:518:ASN:O	2:C:519:ASN:HB2	2.10	0.50
2:C:1105:SER:CB	3:D:731:ARG:HD2	2.40	0.50
6:1:47:DC:H2"	6:1:48:DA:H5'	1.88	0.50
1:A:166:ARG:HB3	1:A:167:PRO:HD2	1.93	0.50
2:C:104:ILE:HD12	2:C:116:ASP:HB2	1.92	0.50
3:D:30:ILE:HD13	3:D:243:PRO:HD3	1.94	0.50
3:D:818:GLU:HB3	3:D:887:SER:HB2	1.92	0.50
5:F:107:ARG:NH1	6:1:43:DT:OP1	2.44	0.50
3:D:331:ILE:N	3:D:331:ILE:CD1	2.75	0.50
2:C:144:VAL:HB	2:C:526:HIS:CE1	2.46	0.50
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.47	0.50
3:D:1132:LYS:CG	3:D:1133:ASP:H	2.24	0.50
2:C:758:ARG:HG3	2:C:833:ILE:O	2.12	0.50
3:D:555:TYR:CE2	3:D:565:ALA:HB2	2.47	0.50
3:D:934:THR:HB	3:D:1133:ASP:OD2	2.10	0.50
5:F:317:LEU:HD13	5:F:324:ILE:HD13	1.92	0.50
1:B:124:VAL:HG11	1:B:209:GLY:CA	2.42	0.50
2:C:871:VAL:HG11	2:C:928:VAL:HG21	1.93	0.50
1:A:228:LEU:HD11	1:B:224:LEU:CD2	2.41	0.50
2:C:280:ASP:O	2:C:281:ASP:HB3	2.12	0.50
2:C:1285:TYR:HD2	3:D:1361:THR:HG21	1.76	0.50
2:C:1329:GLU:OE1	3:D:330:MET:HB3	2.12	0.50
3:D:334:LYS:HG2	3:D:339:ARG:HD2	1.93	0.50
2:C:1061:GLN:HB2	2:C:1062:PRO:HD2	1.94	0.50
2:C:1289:GLU:HG2	2:C:1294:LYS:HE3	1.94	0.50
5:F:144:THR:OG1	6:1:39:DA:H8	1.95	0.50
5:F:231:GLU:CG	5:F:232:LYS:N	2.66	0.50
6:1:44:DG:H3'	6:1:45:DT:H5"	1.94	0.50
3:D:716:GLN:HG3	3:D:717:VAL:H	1.77	0.49
5:F:70:LEU:HD11	6:1:41:DT:C5	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1301:ARG:NH1	5:F:243:GLU:OE2	2.45	0.49
3:D:1217:PRO:HA	3:D:1220:ILE:HD12	1.93	0.49
1:B:166:ARG:HB3	1:B:167:PRO:HD2	1.94	0.49
7:2:10:DC:H2'	7:2:11:DA:C8	2.47	0.49
1:B:124:VAL:HG11	1:B:209:GLY:HA3	1.94	0.49
2:C:641:GLU:HG2	2:C:642:SER:H	1.77	0.49
2:C:1259:LEU:HD11	5:F:239:ALA:HB2	1.94	0.49
2:C:1157:GLN:O	2:C:1157:GLN:HG3	2.12	0.49
3:D:220:ARG:O	3:D:224:LEU:HG	2.12	0.49
3:D:1330:ARG:NH2	7:2:10:DC:H5'	2.28	0.49
5:F:152:GLN:HG3	5:F:153:THR:N	2.27	0.49
2:C:32:LEU:HD23	2:C:130:MET:SD	2.52	0.49
2:C:1222:GLU:HB2	3:D:635:SER:O	2.12	0.49
1:A:124:VAL:HG11	1:A:209:GLY:CA	2.42	0.49
2:C:1107:MET:HE2	3:D:739:GLN:HB2	1.95	0.49
5:F:151:ARG:HG3	5:F:152:GLN:N	2.28	0.49
2:C:782:VAL:HG21	2:C:792:GLY:CA	2.42	0.49
2:C:905:ILE:HD11	5:F:313:LEU:HD23	1.95	0.49
3:D:803:VAL:CG2	3:D:1309:ILE:O	2.60	0.49
3:D:1159:ILE:HA	3:D:1206:ARG:HG2	1.94	0.49
1:A:124:VAL:HG11	1:A:209:GLY:HA3	1.94	0.49
2:C:241:LEU:CD1	2:C:246:LEU:HD11	2.43	0.49
3:D:71:LEU:HG	3:D:90:VAL:HG21	1.95	0.48
3:D:582:ILE:HG23	3:D:623:GLN:CB	2.41	0.48
3:D:700:ASN:O	3:D:704:GLU:HB2	2.12	0.48
6:1:48:DA:H2'	6:1:49:DG:O4'	2.13	0.48
2:C:1339:LEU:HD13	3:D:17:PHE:CD2	2.48	0.48
5:F:147:THR:O	5:F:151:ARG:HG2	2.12	0.48
5:F:277:ARG:HE	5:F:288:LEU:CD2	2.27	0.48
5:F:289:GLU:O	5:F:293:ARG:HB2	2.13	0.48
6:1:49:DG:H2"	6:1:50:DT:H5"	1.90	0.48
2:C:123:TYR:CE2	5:F:190:ASP:O	2.67	0.48
2:C:564:PRO:O	2:C:569:ILE:HA	2.13	0.48
2:C:634:VAL:HG12	2:C:636:CYS:SG	2.53	0.48
3:D:357:VAL:HG12	3:D:461:PHE:CE2	2.47	0.48
3:D:809:VAL:HB	3:D:911:LYS:HA	1.94	0.48
3:D:1175:LEU:HD12	3:D:1177:ILE:CG1	2.43	0.48
3:D:250:ARG:HD2	3:D:266:ASN:OD1	2.13	0.48
3:D:809:VAL:HG22	3:D:915:ILE:HD11	1.95	0.48
3:D:1167:LYS:HB2	3:D:1174:ARG:HD2	1.94	0.48
5:F:317:LEU:HD21	5:F:324:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1:54:DA:N7	6:1:55:DC:N4	2.62	0.48
1:B:44:ARG:HD2	3:D:538:ARG:NH2	2.29	0.48
2:C:839:VAL:O	2:C:839:VAL:HG13	2.13	0.48
3:D:793:SER:OG	3:D:928:THR:HA	2.13	0.48
3:D:839:VAL:HG12	3:D:839:VAL:O	2.13	0.48
6:1:53:DG:H1'	6:1:54:DA:H5"	1.94	0.48
3:D:57:PHE:O	3:D:98:ARG:NH2	2.46	0.48
1:A:11:PRO:HB3	1:A:31:LEU:HD23	1.95	0.48
1:A:50:SER:HG	1:B:35:PHE:HZ	1.62	0.48
1:B:11:PRO:HB3	1:B:31:LEU:HD23	1.96	0.48
2:C:1152:GLY:CA	2:C:1155:VAL:HG23	2.44	0.48
3:D:245:LEU:HG	3:D:246:PRO:HD2	1.95	0.48
3:D:612:LEU:HB3	3:D:616:PRO:HG2	1.96	0.48
7:2:16:DC:H6	7:2:16:DC:C5'	2.23	0.48
2:C:1323:PHE:CZ	3:D:1353:VAL:HG12	2.49	0.48
5:F:317:LEU:HD22	5:F:324:ILE:CD1	2.44	0.48
2:C:615:VAL:O	2:C:615:VAL:HG13	2.13	0.47
6:1:31:DT:H2"	6:1:32:DA:H5'	1.95	0.47
2:C:992:LEU:HB3	2:C:993:PRO:HD2	1.96	0.47
5:F:145:TYR:CD1	6:1:37:DA:C5	3.03	0.47
1:A:218:ARG:HG3	1:B:231:PHE:O	2.14	0.47
2:C:175:ARG:NE	6:1:50:DT:O4	2.48	0.47
5:F:174:GLU:O	5:F:178:TYR:CD2	2.66	0.47
6:1:34:DG:H2"	6:1:35:DC:C6	2.50	0.47
1:A:50:SER:OG	1:B:35:PHE:CZ	2.67	0.47
6:1:33:DT:C2'	6:1:34:DG:H5'	2.44	0.47
2:C:788:SER:OG	2:C:795:ALA:O	2.21	0.47
2:C:1062:PRO:HD3	2:C:1079:ILE:HD11	1.95	0.47
2:C:1210:ILE:CG2	2:C:1211:ARG:N	2.78	0.47
3:D:120:LEU:HA	3:D:121:PRO:C	2.34	0.47
3:D:202:ARG:HH21	3:D:221:ILE:HG23	1.80	0.47
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.97	0.47
3:D:645:VAL:O	3:D:645:VAL:HG23	2.14	0.47
3:D:807:LEU:HD11	3:D:894:VAL:HG13	1.95	0.47
5:F:219:ILE:CG2	5:F:220:THR:N	2.77	0.47
2:C:145:ILE:HD11	2:C:506:PHE:CD2	2.50	0.47
2:C:660:VAL:HG13	2:C:661:VAL:HG13	1.97	0.47
2:C:1281:TYR:HE2	3:D:431:ARG:O	1.98	0.47
2:C:200:ARG:HD3	6:1:50:DT:O2	2.16	0.46
1:B:158:ARG:HB3	1:B:172:LEU:HD21	1.97	0.46
6:1:49:DG:H2"	6:1:50:DT:H4'	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:127:ILE:O	2:C:127:ILE:HG13	2.14	0.46
2:C:533:LEU:HD23	2:C:538:LEU:O	2.15	0.46
3:D:46:TYR:HH	6:1:31:DT:P	2.39	0.46
3:D:708:ASN:HB2	3:D:714:GLU:HB3	1.97	0.46
2:C:21:VAL:HG21	2:C:592:ARG:CZ	2.46	0.46
3:D:298:MET:HE1	5:F:118:ASP:HA	1.97	0.46
3:D:518:VAL:O	3:D:520:ALA:N	2.49	0.46
2:C:1070:HIS:NE2	2:C:1114:GLU:OE1	2.46	0.46
3:D:926:PRO:O	3:D:930:LEU:HG	2.16	0.46
5:F:65:ILE:HG22	5:F:99:LEU:HD13	1.96	0.46
1:A:145:LYS:HD3	1:A:147:GLN:HE21	1.81	0.46
2:C:360:LEU:O	2:C:364:VAL:HG23	2.16	0.46
2:C:657:THR:HG21	2:C:1188:ASP:HB2	1.98	0.46
3:D:868:TRP:O	3:D:872:LEU:HG	2.16	0.46
3:D:1133:ASP:O	3:D:1134:ILE:HD13	2.15	0.46
2:C:277:LEU:HD12	2:C:282:VAL:HG21	1.98	0.46
1:B:145:LYS:HD3	1:B:147:GLN:HE21	1.80	0.46
2:C:673:HIS:CD2	2:C:1113:LEU:HD13	2.51	0.46
3:D:1327:GLU:O	3:D:1331:VAL:HG23	2.16	0.46
5:F:126:GLY:HA3	5:F:153:THR:HG21	1.98	0.46
6:1:54:DA:C2	7:2:10:DC:O2	2.68	0.46
2:C:277:LEU:CD1	2:C:282:VAL:HG21	2.46	0.45
3:D:474:LEU:HD12	4:E:28:ARG:HD3	1.97	0.45
6:1:34:DG:C2	7:2:30:DA:C2	3.04	0.45
7:2:28:DG:H2"	7:2:29:DC:OP2	2.16	0.45
2:C:205:PRO:O	2:C:208:ILE:CG2	2.61	0.45
3:D:903:LEU:H	3:D:903:LEU:HD12	1.80	0.45
5:F:196:GLU:O	5:F:196:GLU:HG2	2.15	0.45
6:1:32:DA:C2	7:2:32:DA:C2	3.04	0.45
2:C:189:ASP:HB2	2:C:190:PRO:HD2	1.97	0.45
2:C:539:THR:CB	2:C:542:ARG:HG3	2.37	0.45
3:D:22:ILE:HG22	3:D:1336:ALA:HA	1.98	0.45
3:D:22:ILE:HG13	3:D:1319:PHE:CZ	2.51	0.45
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.52	0.45
2:C:539:THR:HB	2:C:542:ARG:CG	2.36	0.45
2:C:562:GLU:HG2	2:C:574:SER:CB	2.44	0.45
2:C:638:SER:O	2:C:639:LYS:HG2	2.16	0.45
2:C:906:PHE:CE2	5:F:317:LEU:HD13	2.52	0.45
2:C:1220:GLN:HG2	2:C:1221:PHE:N	2.31	0.45
3:D:126:LEU:HG	3:D:223:LEU:HD12	1.98	0.45
3:D:736:GLN:O	3:D:740:LEU:HG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:572:THR:CG2	3:D:593:ASN:OD1	2.65	0.45
3:D:1134:ILE:HD13	3:D:1244:GLN:HG3	1.97	0.45
5:F:70:LEU:HD11	6:1:41:DT:C4	2.51	0.45
2:C:563:THR:OG1	2:C:569:ILE:O	2.26	0.45
2:C:598:VAL:HA	2:C:627:GLY:O	2.17	0.45
3:D:288:PRO:HG2	5:F:95:ILE:HG21	1.98	0.45
2:C:671:LEU:HD23	2:C:1186:VAL:CG1	2.46	0.45
2:C:1064:ASP:OD1	2:C:1239:VAL:HG12	2.17	0.45
3:D:140:TYR:OH	3:D:312:ARG:NH1	2.50	0.45
3:D:488:ASN:HD21	4:E:6:VAL:CG2	2.30	0.45
3:D:1175:LEU:O	3:D:1187:GLU:HA	2.17	0.45
6:1:52:DT:H2"	6:1:53:DG:N7	2.31	0.45
6:1:58:DG:H2"	6:1:59:DG:C8	2.52	0.45
3:D:515:ARG:NH2	3:D:717:VAL:HB	2.32	0.45
3:D:790:THR:HG21	3:D:932:MET:CG	2.47	0.45
2:C:848:GLU:CG	2:C:888:THR:HG22	2.45	0.45
2:C:1107:MET:HG2	3:D:740:LEU:HD21	1.98	0.45
3:D:1330:ARG:CZ	7:2:10:DC:H5'	2.47	0.45
2:C:1107:MET:CE	3:D:736:GLN:HA	2.46	0.45
3:D:1169:THR:OG1	3:D:1174:ARG:NH2	2.49	0.45
5:F:227:GLY:C	5:F:229:ASP:H	2.16	0.45
2:C:726:TYR:CE2	2:C:728:ASP:HB2	2.52	0.44
3:D:266:ASN:O	3:D:270:ARG:HG3	2.17	0.44
3:D:458:ASN:ND2	8:3:17:U:O3'	2.51	0.44
5:F:244:ASN:HB3	5:F:248:ASP:HB3	1.99	0.44
2:C:807:TRP:CZ3	2:C:1086:PRO:HG3	2.52	0.44
2:C:1061:GLN:HB2	2:C:1062:PRO:CD	2.48	0.44
3:D:412:LEU:HD11	3:D:416:ILE:HD11	1.98	0.44
3:D:714:GLU:HG2	3:D:715:LYS:N	2.32	0.44
5:F:181:THR:O	5:F:185:LEU:HG	2.18	0.44
8:3:14:GTP:N3	8:3:14:GTP:H2'	2.32	0.44
2:C:1296:ASP:O	2:C:1297:ASP:C	2.56	0.44
3:D:189:LEU:O	3:D:192:MET:HG2	2.18	0.44
3:D:212:THR:HA	3:D:215:LYS:HE3	1.99	0.44
1:A:91:ARG:HE	1:A:210:THR:HG23	1.82	0.44
2:C:59:ILE:HG21	2:C:476:LYS:HE3	1.99	0.44
2:C:149:LEU:HB2	2:C:530:ILE:CG2	2.47	0.44
3:D:464:ASP:OD1	8:3:16:G:H4'	2.17	0.44
3:D:1364:ALA:O	3:D:1367:GLN:HG2	2.18	0.44
5:F:152:GLN:HE22	5:F:156:ARG:HD3	1.82	0.44
1:B:101:THR:HG22	1:B:143:ARG:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:887:VAL:HB	2:C:913:VAL:HG11	1.98	0.44
2:C:1281:TYR:CD2	3:D:484:MET:HE3	2.52	0.44
3:D:325:LYS:HE2	3:D:330:MET:CG	2.48	0.44
4:E:41:GLU:HG3	4:E:43:ASN:H	1.82	0.44
6:1:51:DC:H2"	6:1:52:DT:O5'	2.17	0.44
1:A:101:THR:HG22	1:A:143:ARG:HG2	2.00	0.44
1:B:209:GLY:O	1:B:211:ILE:N	2.50	0.44
2:C:402:ARG:HD2	2:C:406:ASN:HD21	1.82	0.44
5:F:63:GLY:O	5:F:67:TYR:CD2	2.70	0.44
5:F:134:PHE:CD1	5:F:142:PHE:HD1	2.36	0.44
5:F:323:ASN:OD1	5:F:324:ILE:N	2.51	0.44
1:A:75:GLN:HE21	2:C:727:VAL:HG11	1.82	0.44
2:C:89:GLY:HA2	2:C:140:GLY:HA3	2.00	0.44
2:C:718:ALA:HB2	2:C:783:LEU:HD21	2.00	0.44
3:D:140:TYR:CE2	5:F:55:LEU:HD13	2.53	0.44
2:C:292:ILE:HD12	2:C:322:LEU:CD2	2.35	0.43
2:C:1113:LEU:HG	3:D:641:ILE:HD11	1.99	0.43
2:C:1287:LEU:HD23	3:D:1357:ILE:CG1	2.48	0.43
3:D:165:TYR:O	3:D:169:LEU:HB2	2.18	0.43
3:D:615:LYS:N	3:D:616:PRO:CD	2.81	0.43
5:F:80:ALA:HB1	5:F:136:PRO:HG3	2.01	0.43
2:C:144:VAL:HB	2:C:526:HIS:HE1	1.83	0.43
2:C:453:ILE:HD12	2:C:587:LEU:CD2	2.49	0.43
2:C:618:GLN:NE2	3:D:769:VAL:HB	2.24	0.43
2:C:1287:LEU:HD23	3:D:1357:ILE:CD1	2.45	0.43
1:A:158:ARG:HB3	1:A:172:LEU:HD21	2.00	0.43
2:C:310:ILE:HG23	2:C:324:LYS:HE2	2.00	0.43
3:D:755:ILE:HD12	3:D:755:ILE:H	1.82	0.43
3:D:1222:ARG:NH1	3:D:1223:LEU:HD21	2.32	0.43
5:F:231:GLU:HG3	5:F:232:LYS:HG2	1.99	0.43
2:C:690:VAL:HA	2:C:691:PRO:HD3	1.91	0.43
3:D:432:LEU:HD13	3:D:499:ILE:HG21	1.99	0.43
3:D:839:VAL:HG12	3:D:864:LEU:HD12	2.01	0.43
6:1:58:DG:C6	6:1:59:DG:C6	3.07	0.43
2:C:164:THR:HG1	2:C:167:SER:HG	1.58	0.43
2:C:850:ILE:HD11	2:C:1048:LYS:HG3	2.00	0.43
3:D:115:TRP:O	3:D:119:SER:HB3	2.18	0.43
3:D:863:LEU:HD22	3:D:908:ILE:CG1	2.48	0.43
5:F:71:LEU:HD21	5:F:79:PHE:HE2	1.82	0.43
5:F:91:ARG:O	5:F:95:ILE:HG13	2.17	0.43
2:C:641:GLU:HG2	2:C:642:SER:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:887:VAL:HB	2:C:913:VAL:HG13	1.96	0.43
2:C:1073:LYS:HD3	3:D:462:ASP:HB2	2.00	0.43
3:D:490:ILE:HD11	3:D:614:LEU:HD11	2.00	0.43
3:D:555:TYR:HB2	3:D:586:GLY:H	1.83	0.43
3:D:1132:LYS:O	3:D:1133:ASP:HB3	2.19	0.43
3:D:1152:GLU:CG	3:D:1194:ARG:HD3	2.48	0.43
5:F:321:GLY:O	5:F:324:ILE:N	2.52	0.43
6:1:37:DA:H4'	6:1:38:DT:OP1	2.18	0.43
1:A:195:ARG:HH21	1:A:197:ASP:HB3	1.84	0.43
2:C:228:VAL:HB	2:C:335:THR:OG1	2.18	0.43
2:C:615:VAL:HA	2:C:638:SER:HB3	2.00	0.43
3:D:325:LYS:HE2	3:D:330:MET:HG3	2.00	0.43
3:D:576:ARG:HD3	3:D:593:ASN:HA	2.00	0.43
3:D:1292:LEU:O	3:D:1296:GLY:N	2.52	0.43
5:F:80:ALA:CB	5:F:136:PRO:HG3	2.49	0.43
7:2:13:DA:C2'	7:2:14:DC:H5'	2.49	0.43
2:C:300:ASP:OD1	2:C:313:ALA:N	2.52	0.43
2:C:1234:LYS:CE	2:C:1238:LEU:HD21	2.49	0.43
3:D:591:ILE:HG23	3:D:592:VAL:N	2.33	0.43
5:F:164:THR:HB	5:F:219:ILE:CD1	2.49	0.43
2:C:1002:LEU:CD1	2:C:1011:LEU:HD11	2.49	0.43
3:D:29:MET:HG3	3:D:33:TRP:CZ2	2.54	0.43
3:D:1333:THR:O	3:D:1337:VAL:HG23	2.19	0.42
6:1:48:DA:C6	6:1:49:DG:O6	2.72	0.42
2:C:208:ILE:HD11	2:C:365:GLU:HB2	2.00	0.42
2:C:812:PHE:CB	3:D:357:VAL:HG11	2.49	0.42
3:D:644:MET:O	3:D:764:ARG:NH1	2.52	0.42
3:D:849:LEU:HD23	3:D:857:LEU:CD2	2.49	0.42
5:F:88:VAL:O	5:F:92:ARG:HG3	2.19	0.42
5:F:221:SER:HB3	5:F:224:THR:OG1	2.19	0.42
2:C:122:VAL:HG13	5:F:187:HIS:HE1	1.83	0.42
3:D:809:VAL:HG22	3:D:915:ILE:CD1	2.48	0.42
3:D:1280:VAL:CG1	3:D:1281:GLU:N	2.82	0.42
5:F:105:ILE:HG23	5:F:109:TYR:CE2	2.54	0.42
2:C:13:LYS:NZ	2:C:1149:TYR:O	2.52	0.42
2:C:907:GLY:O	2:C:909:LYS:HG3	2.20	0.42
2:C:1281:TYR:HE1	3:D:489:ASN:ND2	2.17	0.42
2:C:1329:GLU:OE1	3:D:330:MET:CB	2.67	0.42
3:D:504:GLN:HE22	3:D:731:ARG:HH21	1.68	0.42
3:D:1267:VAL:O	3:D:1268:ASN:HB2	2.18	0.42
1:A:192:VAL:CG2	1:A:198:LEU:HD12	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:THR:O	1:B:172:LEU:HD12	2.20	0.42
2:C:68:LEU:HD13	2:C:100:LEU:HD21	2.02	0.42
6:1:48:DA:H2'	6:1:49:DG:N9	2.34	0.42
1:A:107:ILE:CG1	1:A:136:GLU:HB3	2.50	0.42
2:C:1004:ASP:OD1	2:C:1004:ASP:N	2.53	0.42
2:C:1298:VAL:O	2:C:1301:ARG:HG2	2.20	0.42
3:D:22:ILE:HD11	3:D:1319:PHE:CE1	2.54	0.42
3:D:75:TYR:HB2	3:D:92:VAL:HG21	2.01	0.42
3:D:123:ARG:HH22	3:D:1334:GLU:HG2	1.84	0.42
3:D:223:LEU:O	3:D:227:PHE:HB2	2.19	0.42
3:D:1320:ILE:HG22	3:D:1352:ILE:HD12	2.02	0.42
5:F:65:ILE:HG22	5:F:99:LEU:CD1	2.49	0.42
5:F:140:PHE:CD1	6:1:37:DA:H2"	2.54	0.42
3:D:791:ALA:HA	7:2:13:DA:H5'	2.02	0.42
3:D:1134:ILE:CD1	3:D:1244:GLN:CG	2.97	0.42
3:D:1184:ASP:OD1	3:D:1184:ASP:N	2.52	0.42
2:C:663:VAL:O	2:C:666:SER:OG	2.32	0.42
2:C:912:ASP:OD1	2:C:912:ASP:N	2.53	0.42
2:C:1284:ALA:N	3:D:479:GLU:OE1	2.52	0.42
3:D:115:TRP:CZ2	3:D:1329:THR:HG22	2.54	0.42
4:E:30:MET:HE1	4:E:37:PRO:HB3	2.02	0.42
5:F:303:ARG:O	5:F:307:VAL:HG23	2.20	0.42
1:A:57:THR:O	1:A:172:LEU:HD12	2.20	0.42
1:B:91:ARG:HE	1:B:210:THR:HG23	1.84	0.42
2:C:561:ILE:O	2:C:561:ILE:HG22	2.20	0.42
2:C:90:VAL:HG12	2:C:91:THR:N	2.34	0.41
2:C:1142:ARG:NH1	2:C:1161:LEU:O	2.53	0.41
3:D:746:LEU:HG	3:D:758:PRO:HB3	2.01	0.41
3:D:1134:ILE:HG22	3:D:1138:LEU:HG	2.02	0.41
3:D:1164:SER:HB2	3:D:1176:VAL:O	2.19	0.41
5:F:122:GLU:OE1	5:F:157:ALA:HB1	2.14	0.41
1:A:91:ARG:HB2	1:A:210:THR:OG1	2.20	0.41
2:C:59:ILE:CG2	2:C:476:LYS:HE3	2.49	0.41
2:C:197:ARG:HD3	2:C:200:ARG:HA	2.01	0.41
2:C:810:TYR:CE1	2:C:1078:LYS:HD2	2.54	0.41
3:D:664:ILE:HG22	3:D:678:ARG:HG3	2.03	0.41
3:D:1259:GLN:OE1	3:D:1262:ARG:NH2	2.53	0.41
4:E:13:ILE:HD12	4:E:19:LEU:CD1	2.50	0.41
5:F:227:GLY:C	5:F:229:ASP:N	2.74	0.41
6:1:49:DG:H2'	6:1:50:DT:H5"	2.00	0.41
1:B:192:VAL:HG12	1:B:193:GLU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:77:GLU:HB2	2:C:78:PRO:HD2	2.02	0.41
3:D:418:GLU:CD	4:E:48:VAL:HG21	2.40	0.41
3:D:619:ILE:O	3:D:623:GLN:HG2	2.20	0.41
5:F:169:ILE:CG2	5:F:173:LYS:CD	2.95	0.41
1:A:192:VAL:HG12	1:A:193:GLU:N	2.34	0.41
3:D:584:PRO:HD3	3:D:620:PHE:CD1	2.55	0.41
1:A:184:ALA:HB2	2:C:1091:GLY:CA	2.49	0.41
2:C:95:PRO:HA	2:C:126:GLU:HG2	2.01	0.41
2:C:1149:TYR:CG	2:C:1159:VAL:HG11	2.55	0.41
5:F:227:GLY:HA2	7:2:19:DA:C2	2.47	0.41
2:C:5:TYR:CD1	2:C:778:GLU:HB2	2.55	0.41
2:C:696:ASP:HB3	2:C:798:GLN:HG2	2.01	0.41
2:C:984:VAL:O	2:C:984:VAL:HG13	2.20	0.41
6:1:53:DG:H1'	6:1:54:DA:H5'	2.03	0.41
7:2:24:DT:H2"	7:2:25:DA:OP2	2.20	0.41
1:B:166:ARG:HD2	1:B:170:ARG:HD3	2.01	0.41
2:C:555:TYR:CD1	2:C:637:ARG:NH2	2.89	0.41
2:C:638:SER:O	2:C:639:LYS:HG3	2.19	0.41
2:C:878:THR:HG22	2:C:879:GLY:N	2.35	0.41
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.40	0.41
3:D:517:CYS:HB3	3:D:545:HIS:HB2	2.01	0.41
3:D:826:ILE:HG23	3:D:829:GLY:O	2.21	0.41
3:D:1268:ASN:HB3	3:D:1301:THR:HB	2.02	0.41
5:F:160:ASN:HD22	5:F:166:ARG:NH1	2.18	0.41
1:A:228:LEU:HA	1:A:231:PHE:CD2	2.56	0.41
3:D:510:LEU:HD23	3:D:579:LEU:HD11	2.03	0.41
3:D:869:CYS:O	3:D:873:GLU:OE1	2.39	0.41
3:D:1133:ASP:O	3:D:1244:GLN:CD	2.46	0.41
4:E:6:VAL:HG12	4:E:6:VAL:O	2.21	0.41
5:F:63:GLY:HA2	6:1:42:DG:C2	2.56	0.41
6:1:49:DG:H2"	6:1:50:DT:OP1	2.20	0.41
2:C:1243:MET:HE2	3:D:445:LYS:HD3	2.03	0.41
3:D:335:GLN:O	3:D:335:GLN:HG3	2.20	0.41
3:D:650:LYS:HE3	3:D:654:ILE:HD12	2.02	0.41
3:D:856:ILE:HG13	3:D:875:ASN:ND2	2.36	0.41
3:D:1269:ALA:HB2	3:D:1275:LEU:HD23	2.02	0.41
5:F:166:ARG:HH12	5:F:168:PRO:HA	1.85	0.41
5:F:273:VAL:O	5:F:277:ARG:HB2	2.20	0.41
6:1:54:DA:C8	6:1:55:DC:C5	3.08	0.41
2:C:225:PHE:CE2	2:C:347:ILE:HB	2.56	0.41
2:C:907:GLY:O	2:C:908:GLU:C	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1155:VAL:HG12	2:C:1157:GLN:O	2.21	0.41
2:C:1223:ARG:HB2	2:C:1224:PRO:HD2	2.01	0.41
2:C:1330:ILE:O	2:C:1333:LEU:HB2	2.20	0.41
3:D:511:TYR:CG	3:D:728:SER:HB3	2.56	0.41
3:D:588:PRO:O	3:D:591:ILE:HG22	2.20	0.41
4:E:13:ILE:HD12	4:E:19:LEU:HD13	2.03	0.41
2:C:1290:MET:HA	2:C:1294:LYS:HB2	2.03	0.40
3:D:450:HIS:HA	3:D:451:PRO:HD3	1.96	0.40
6:1:56:DG:H2"	6:1:57:DC:C6	2.56	0.40
1:A:166:ARG:HD2	1:A:170:ARG:HD3	2.03	0.40
1:B:107:ILE:CG1	1:B:136:GLU:HB3	2.51	0.40
3:D:305:ALA:CB	3:D:316:ILE:HD12	2.51	0.40
6:1:45:DT:H3'	6:1:45:DT:H6	1.86	0.40
7:2:20:DG:C2'	7:2:21:DG:H5'	2.51	0.40
1:B:11:PRO:HB3	1:B:31:LEU:CD2	2.52	0.40
1:B:195:ARG:HH21	1:B:197:ASP:HB3	1.87	0.40
2:C:196:VAL:CG2	2:C:206:ALA:HA	2.48	0.40
2:C:1234:LYS:HE2	2:C:1238:LEU:HD21	2.03	0.40
2:C:1285:TYR:O	2:C:1289:GLU:HB2	2.20	0.40
3:D:596:LEU:HD23	3:D:596:LEU:HA	1.94	0.40
1:A:11:PRO:HB3	1:A:31:LEU:CD2	2.51	0.40
2:C:241:LEU:HD11	2:C:246:LEU:CD1	2.49	0.40
2:C:318:SER:OG	2:C:320:ASP:OD1	2.24	0.40
2:C:894:GLN:NE2	3:D:69:GLU:HG2	2.36	0.40
3:D:378:LYS:N	3:D:379:PRO:HD2	2.36	0.40
4:E:30:MET:CE	4:E:37:PRO:HB3	2.51	0.40
6:1:48:DA:OP2	6:1:48:DA:C8	2.72	0.40
7:2:22:DA:H2"	7:2:23:DT:H5'	2.02	0.40
2:C:1296:ASP:HB3	2:C:1321:GLU:H	1.87	0.40
3:D:364:HIS:HB3	3:D:487:THR:HG23	2.02	0.40
3:D:808:VAL:HG12	3:D:809:VAL:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	228/242 (94%)	216 (95%)	10 (4%)	2 (1%)	17	57
1	B	226/242 (93%)	212 (94%)	13 (6%)	1 (0%)	34	71
2	C	1338/1342 (100%)	1244 (93%)	85 (6%)	9 (1%)	22	61
3	D	1169/1407 (83%)	1095 (94%)	64 (6%)	10 (1%)	17	57
4	E	77/90 (86%)	74 (96%)	3 (4%)	0	100	100
5	F	275/336 (82%)	256 (93%)	13 (5%)	6 (2%)	6	39
All	All	3313/3659 (90%)	3097 (94%)	188 (6%)	28 (1%)	19	59

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	908	GLU
3	D	174	ASP
3	D	519	ASN
3	D	710	ASP
3	D	1268	ASN
5	F	190	ASP
2	C	519	ASN
2	C	756	TYR
3	D	829	GLY
3	D	1133	ASP
5	F	110	GLY
5	F	297	LEU
5	F	322	LEU
1	A	208	ASN
1	B	8	PHE
2	C	1297	ASP
1	A	210	THR
2	C	234	ASP
2	C	1103	VAL
3	D	321	LYS
2	C	281	ASP
3	D	123	ARG
3	D	846	GLU
3	D	858	VAL
5	F	111	ASN
2	C	507	GLY
5	F	228	GLY

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Mol	Chain	Res	Type
2	C	1186	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	198/208 (95%)	195 (98%)	3 (2%)	65 84
1	B	196/208 (94%)	192 (98%)	4 (2%)	55 79
2	C	1155/1157 (100%)	1134 (98%)	21 (2%)	59 81
3	D	980/1168 (84%)	950 (97%)	30 (3%)	40 71
4	E	67/74 (90%)	65 (97%)	2 (3%)	41 71
5	F	240/292 (82%)	238 (99%)	2 (1%)	81 91
All	All	2836/3107 (91%)	2774 (98%)	62 (2%)	52 77

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	32	GLU
1	A	131	CYS
1	B	28	LEU
1	B	32	GLU
1	B	131	CYS
1	B	211	ILE
2	C	12	ARG
2	C	23	ASP
2	C	30	ILE
2	C	177	ILE
2	C	290	GLU
2	C	443	ASP
2	C	446	ASP
2	C	538	LEU
2	C	553	THR
2	C	554	HIS

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Mol	Chain	Res	Type
2	C	563	THR
2	C	571	LEU
2	C	653	MET
2	C	700	VAL
2	C	851	THR
2	C	912	ASP
2	C	1078	LYS
2	C	1207	SER
2	C	1210	ILE
2	C	1223	ARG
2	C	1253	LEU
3	D	93	THR
3	D	153	ASN
3	D	216	LYS
3	D	223	LEU
3	D	227	PHE
3	D	240	THR
3	D	256	ASP
3	D	321	LYS
3	D	384	LYS
3	D	398	LYS
3	D	399	LYS
3	D	417	ARG
3	D	453	VAL
3	D	505	ASP
3	D	538	ARG
3	D	579	LEU
3	D	599	LYS
3	D	641	ILE
3	D	695	LYS
3	D	716	GLN
3	D	738	ARG
3	D	746	LEU
3	D	798	ARG
3	D	821	MET
3	D	850	LYS
3	D	1175	LEU
3	D	1189	MET
3	D	1227	HIS
3	D	1356	LEU
3	D	1366	HIS
4	E	43	ASN

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Mol	Chain	Res	Type
4	E	45	LYS
5	F	280	LEU
5	F	313	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	75	GLN
1	A	132	HIS
1	A	147	GLN
1	B	132	HIS
1	B	147	GLN
2	C	343	HIS
2	C	526	HIS
2	C	618	GLN
2	C	894	GLN
2	C	1220	GLN
2	C	1313	HIS
3	D	153	ASN
3	D	196	GLN
3	D	341	ASN
3	D	458	ASN
3	D	488	ASN
3	D	489	ASN
3	D	504	GLN
3	D	545	HIS
3	D	623	GLN
3	D	690	ASN
3	D	708	ASN
3	D	716	GLN
3	D	736	GLN
3	D	929	GLN
3	D	1218	HIS
3	D	1244	GLN
3	D	1279	GLN
4	E	43	ASN
5	F	152	GLN
5	F	160	ASN
5	F	251	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	3	1/4 (25%)	1 (100%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	3	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	$\#\|Z\| > 2$
9	DPO	C	1401	11	6,8,8	2.59	4 (66%)	13,13,13	2.89	7 (53%)

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
9	DPO	C	1401	11	-	0/6/6/6	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1401	DPO	P2-O5	-4.12	1.37	1.50
9	C	1401	DPO	P1-O2	-3.15	1.42	1.54
9	C	1401	DPO	P1-O3	-2.78	1.44	1.54
9	C	1401	DPO	P2-O6	2.27	1.63	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	1401	DPO	P2-O4-P1	-5.13	115.21	132.83
9	C	1401	DPO	O2-P1-O4	4.47	119.63	104.64
9	C	1401	DPO	O6-P2-O5	3.88	125.86	110.68
9	C	1401	DPO	O4-P1-O1	-3.28	92.99	111.19
9	C	1401	DPO	O7-P2-O5	-3.20	98.14	110.68
9	C	1401	DPO	O7-P2-O6	3.18	119.78	107.64
9	C	1401	DPO	O4-P2-O5	-2.45	97.58	111.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	3	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3	16:G	O3'	17:U	P	3.02

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	230/242 (95%)	-0.10	2 (0%) 84 73	158, 205, 278, 328	0
1	B	228/242 (94%)	0.32	19 (8%) 11 7	161, 241, 296, 359	0
2	C	1340/1342 (99%)	-0.06	33 (2%) 57 41	115, 181, 287, 402	0
3	D	1173/1407 (83%)	0.03	43 (3%) 41 27	124, 189, 286, 340	0
4	E	79/90 (87%)	-0.25	2 (2%) 57 41	166, 227, 324, 373	0
5	F	277/336 (82%)	0.17	8 (2%) 51 35	161, 225, 276, 362	0
6	1	33/50 (66%)	-0.38	1 (3%) 50 34	190, 238, 348, 380	0
7	2	33/50 (66%)	-0.30	0 100 100	129, 239, 314, 386	0
8	3	3/4 (75%)	1.57	0 100 100	128, 128, 146, 150	0
All	All	3396/3763 (90%)	0.00	108 (3%) 47 32	115, 198, 290, 402	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	323	ASN	9.6
3	D	855	ASP	6.5
3	D	853	THR	5.9
3	D	852	GLY	5.8
3	D	1185	PRO	5.6
3	D	1160	SER	5.5
3	D	1166	GLY	5.5
2	C	982	GLY	5.1
3	D	879	ALA	5.0
3	D	1215	GLU	4.9
5	F	324	ILE	4.9
3	D	854	ALA	4.7
3	D	143	SER	4.5
3	D	856	ILE	4.5
2	C	998	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
5	F	262	TRP	4.0
1	B	67	GLU	3.9
3	D	1199	PHE	3.9
1	B	161	SER	3.9
1	B	163	GLU	3.9
2	C	385	PHE	3.6
3	D	1183	SER	3.6
2	C	1000	LEU	3.5
2	C	102	LEU	3.5
2	C	992	LEU	3.5
1	B	167	PRO	3.4
3	D	1196	LEU	3.3
1	B	160	HIS	3.3
1	B	162	GLU	3.3
5	F	326	ALA	3.2
3	D	1161	GLY	3.2
2	C	165	HIS	3.2
5	F	71	LEU	3.2
2	C	68	LEU	3.2
3	D	1198	VAL	3.1
3	D	851	PRO	3.1
1	B	157	THR	3.1
3	D	1191	PRO	3.0
2	C	991	LYS	3.0
3	D	825	VAL	2.9
2	C	103	VAL	2.9
2	C	484	LEU	2.9
2	C	492	MET	2.8
2	C	979	LEU	2.8
3	D	1204	VAL	2.8
1	B	97	GLU	2.8
1	B	170	ARG	2.8
2	C	981	ALA	2.8
5	F	263	LEU	2.8
2	C	67	GLU	2.7
4	E	77	ALA	2.7
4	E	78	ALA	2.7
1	A	90	VAL	2.7
1	B	13	LEU	2.6
3	D	1167	LYS	2.6
2	C	489	PRO	2.6
3	D	1213	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	158	ARG	2.6
1	B	92	VAL	2.6
3	D	1212	ASP	2.5
3	D	1176	VAL	2.5
3	D	1210	ILE	2.5
1	B	171	LEU	2.5
2	C	116	ASP	2.4
3	D	1188	GLU	2.4
1	B	169	GLY	2.4
3	D	1217	PRO	2.4
1	B	164	ASP	2.4
5	F	76	GLU	2.4
2	C	838	CYS	2.4
3	D	382	TYR	2.4
3	D	942	SER	2.4
2	C	891	GLY	2.4
2	C	188	PHE	2.4
1	B	166	ARG	2.3
2	C	366	ILE	2.3
3	D	1168	GLU	2.3
1	B	93	GLN	2.3
3	D	1186	TYR	2.3
2	C	118	LYS	2.3
5	F	265	GLU	2.3
2	C	487	LEU	2.3
3	D	880	VAL	2.3
3	D	833	GLU	2.3
3	D	826	ILE	2.2
2	C	104	ILE	2.2
2	C	60	GLN	2.2
1	A	92	VAL	2.2
2	C	154	GLY	2.2
1	B	140	ILE	2.2
3	D	1224	ARG	2.2
3	D	878	ASP	2.1
3	D	827	GLU	2.1
3	D	1184	ASP	2.1
3	D	1159	ILE	2.1
3	D	672	LEU	2.1
6	1	50	DT	2.1
2	C	186	PHE	2.1
3	D	1274	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	978	VAL	2.1
2	C	977	ALA	2.1
2	C	1004	ASP	2.1
2	C	172	TYR	2.1
2	C	837	ALA	2.0
2	C	1009	ASN	2.0
1	B	100	LEU	2.0
3	D	831	VAL	2.0
3	D	1211	SER	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	MG	D	1504	1/1	0.72	0.46	129,129,129,129	0
9	DPO	C	1401	9/9	0.92	0.42	147,158,172,173	0
11	MG	D	1503	1/1	0.98	0.33	101,101,101,101	0
10	ZN	D	1501	1/1	0.98	0.15	200,200,200,200	0
10	ZN	D	1502	1/1	0.99	0.16	211,211,211,211	0

6.5 Other polymers (i)

There are no such residues in this entry.