Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 01:16 PM EDT

PDB ID	:	6P71
Title	:	X-ray crystal structure of a bacterial reiterative transcription complex of pyrBI promoter
Authors	:	Shin, Y.; Murakami, K.S.
Deposited on	:	2019-06-04
Resolution	:	2.92 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 (i) 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 (i)) were used in the production of this report:

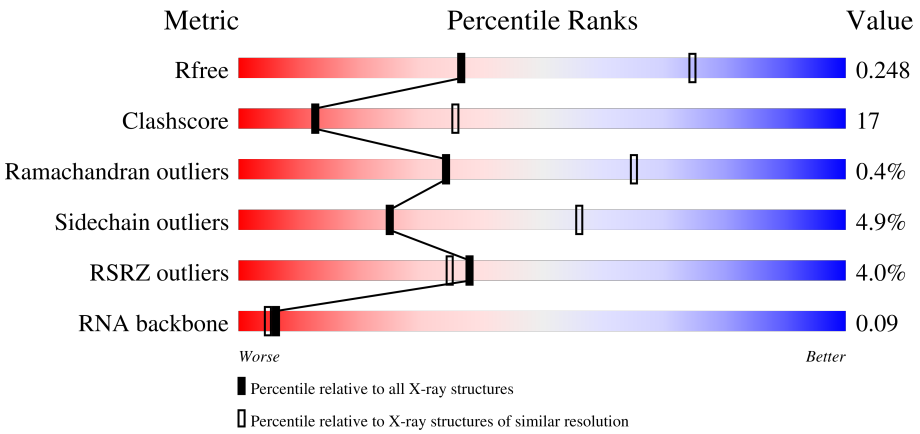
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.92 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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)
RNA backbone	3102	1001 (3.18-2.66)

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	315	46% 23% • 28%
1	B	315	44% 25% • 30%
2	C	1119	6% 65% 32% • •
3	D	1524	4% 68% 28% • •

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Mol	Chain	Length	Quality of chain
4	E	99	3% 78% 16% 5%
5	F	423	3% 56% 25% 18%
6	G	21	24% 43% 5% 29%
7	H	27	26% 33% 41%
8	I	4	50% 50%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 28417 atoms, of which 11 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
			Total	C	N	O	S			
1	A	226	1782	1138	310	332	2	0	0	0
1	B	222	1750	1118	304	326	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	1111	8747	5536	1560	1627	24	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	1500	11820	7489	2083	2212	36	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	94	761	486	132	139	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	346	2796	1764	508	520	4	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	46	THR	ALA	conflict	UNP Q72L95

- Molecule 6 is a DNA chain called DNA (5'-D(P*CP*TP*CP*CP*CP*GP*GP*CP*AP*AP*AP*TP*TP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
6	G	15	304	145	53	91	15	0	0	0

- Molecule 7 is a DNA chain called DNA (5'-D(*TP*AP*TP*AP*AP*TP*CP*GP*AP*GP*CP*CP*GP*GP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
7	H	16	329	157	65	92	15	0	0	0

- Molecule 8 is a RNA chain called RNA (5'-R(P*AP*AP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
8	I	4	84	38	14	28	4	0	0	0

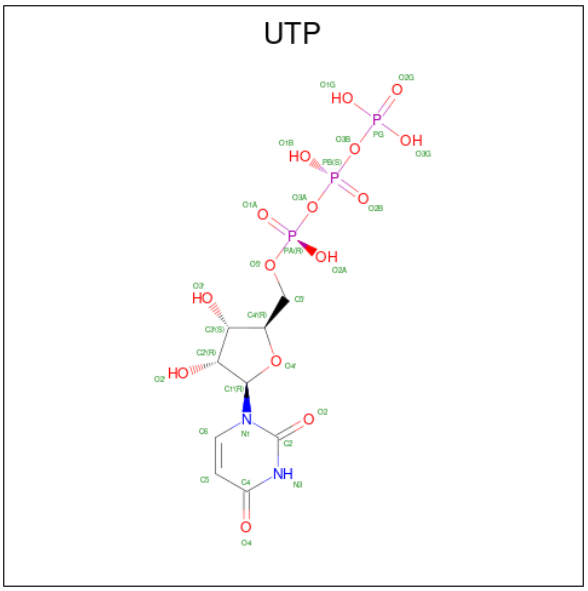
- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- Molecule 11 is URIDINE 5'-TRIPHOSPHATE (three-letter code: UTP) (formula: $C_9H_{15}N_2O_{15}P_3$).



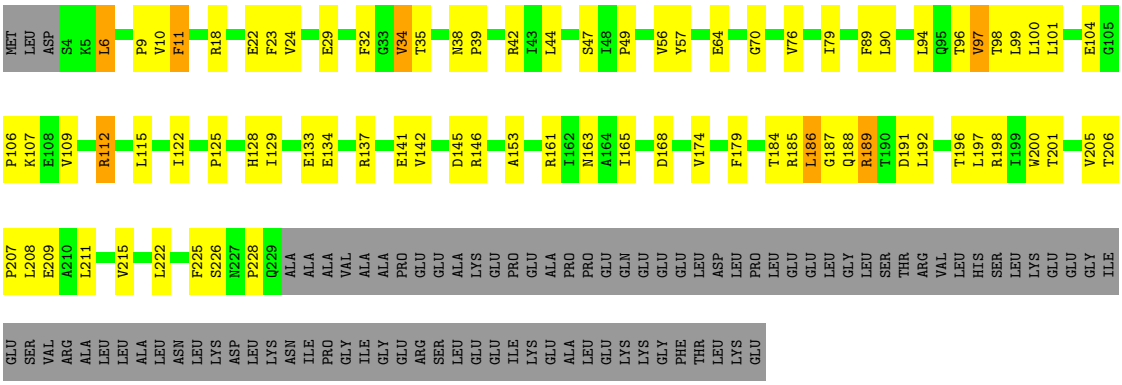
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
11	D	1	40	9	11	2	15	3	0	0

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.

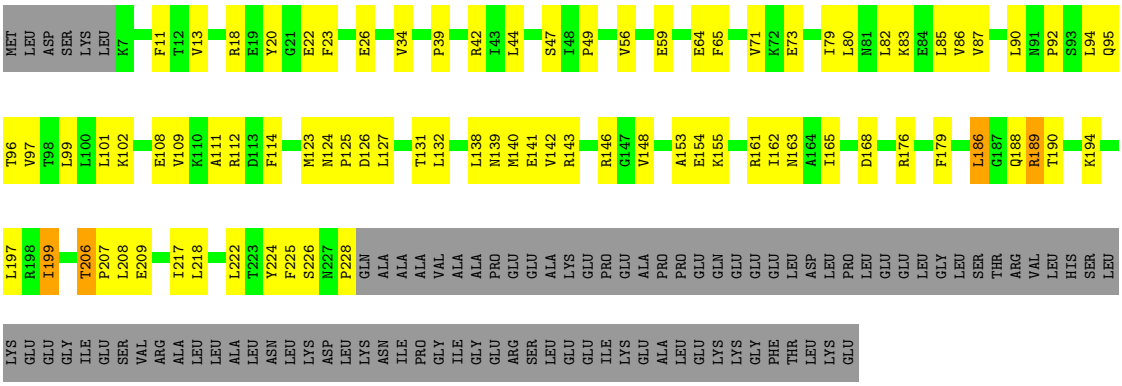
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A: 46% 23% • 28%



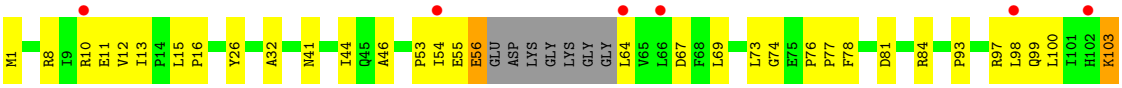
• Molecule 1: DNA-directed RNA polymerase subunit alpha

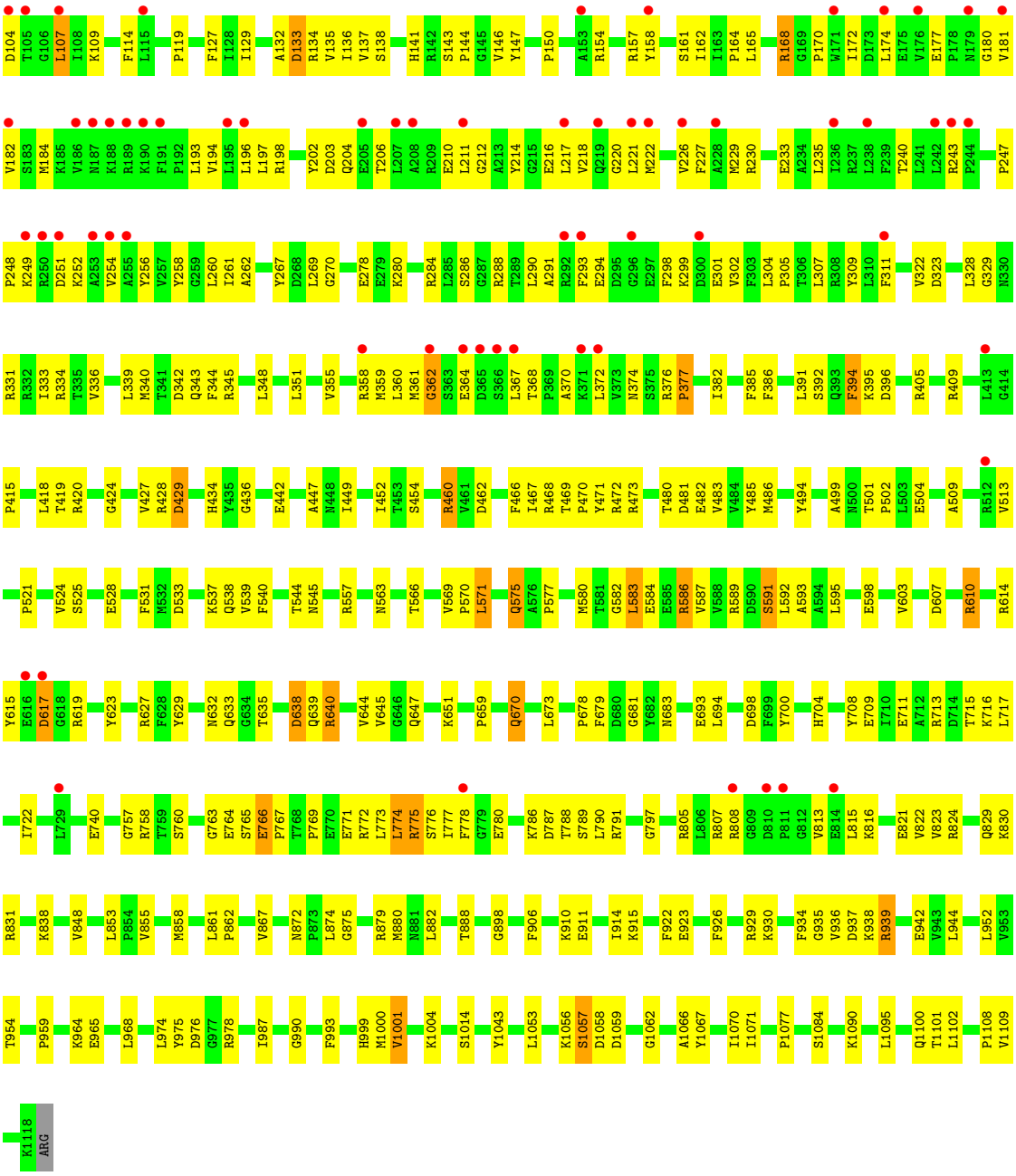
Chain B: 44% 25% • 30%



• Molecule 2: DNA-directed RNA polymerase subunit beta

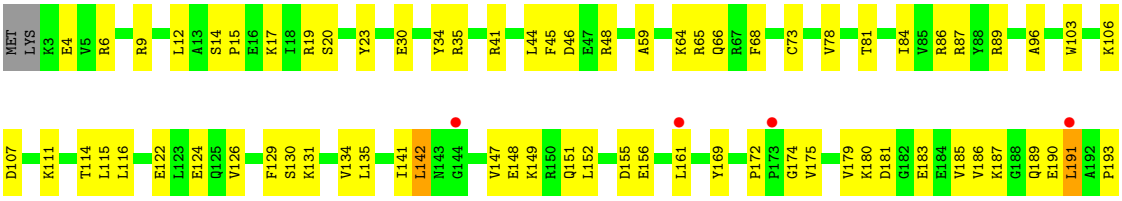
Chain C: 6% 65% 32% • •

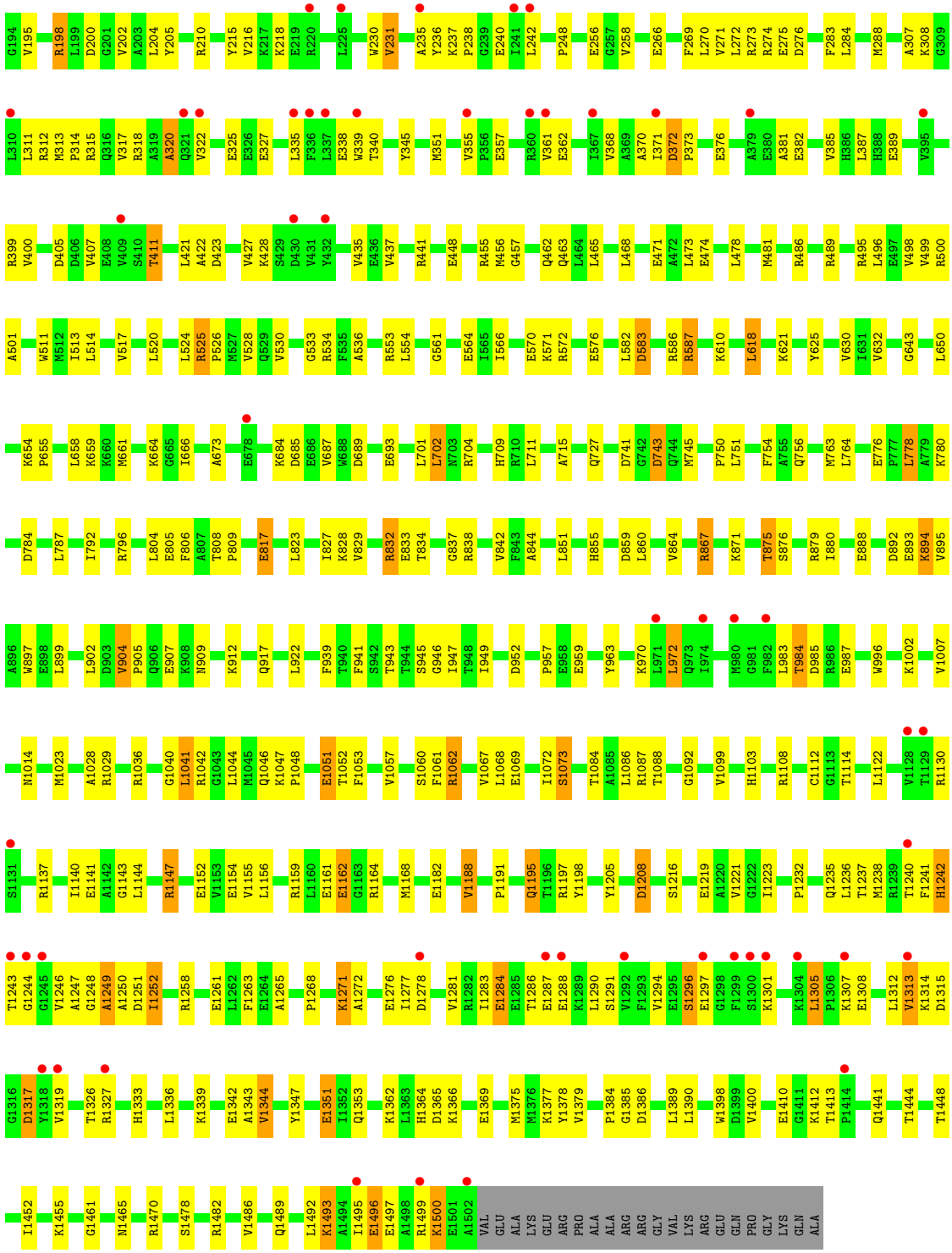




- Molecule 3: DNA-directed RNA polymerase subunit beta'

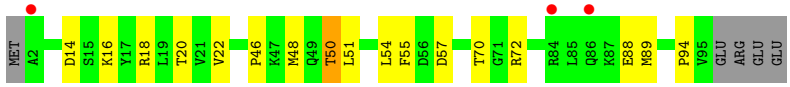
Chain D:





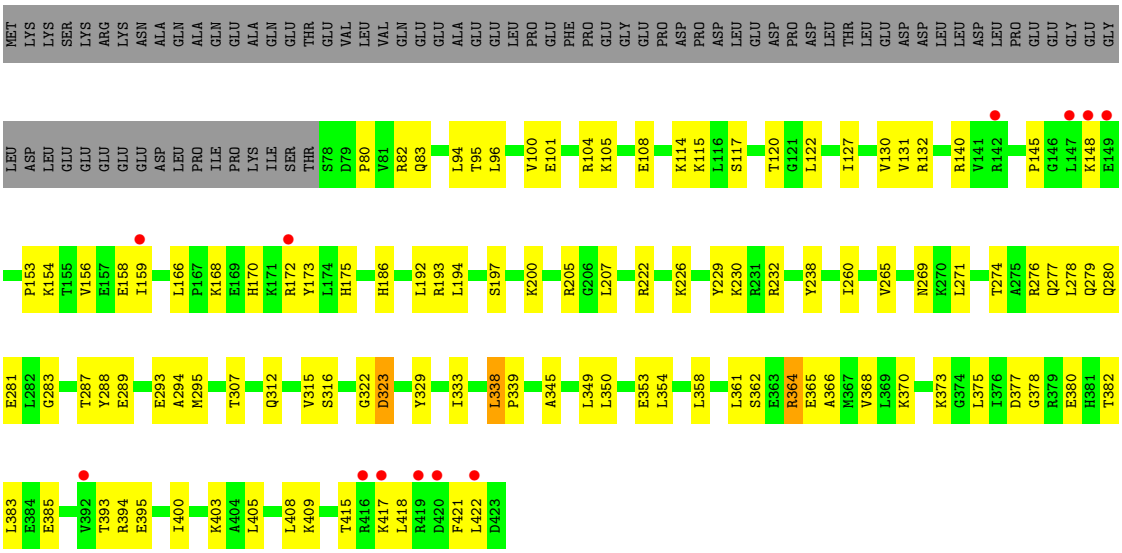
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:



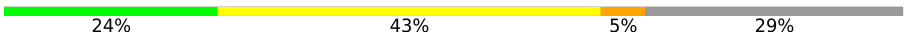
• Molecule 5: RNA polymerase sigma factor SigA

Chain F:



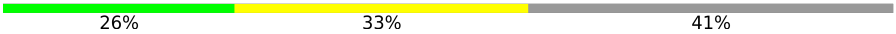
• Molecule 6: DNA (5'-D(P*CP*TP*CP*CP*CP*GP*GP*CP*AP*AP*AP*TP*TP*GP*T)-3')

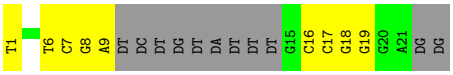
Chain G:



• Molecule 7: DNA (5'-D(*TP*AP*TP*AP*AP*TP*CP*GP*AP*GP*CP*CP*GP*GP*GP*A)-3')

Chain H:





• Molecule 8: RNA (5'-R(P*AP*AP*UP*U)-3')

Chain I:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	187.51Å 100.66Å 296.30Å 90.00° 98.32° 90.00°	Depositor
Resolution (Å)	48.97 – 2.92 48.97 – 2.92	Depositor EDS
% Data completeness (in resolution range)	98.1 (48.97-2.92) 98.1 (48.97-2.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.14_3260)	Depositor
R, R_{free}	0.211 , 0.248 0.211 , 0.248	Depositor DCC
R_{free} test set	1885 reflections (1.62%)	wwPDB-VP
Wilson B-factor (Å^2)	75.8	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 50.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	28417	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: UTP, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.59	1/1814 (0.1%)	0.84	1/2466 (0.0%)
1	B	0.60	0/1782	0.83	1/2424 (0.0%)
2	C	0.58	1/8914 (0.0%)	0.81	7/12060 (0.1%)
3	D	0.62	1/12028 (0.0%)	0.85	11/16265 (0.1%)
4	E	0.54	0/775	0.85	1/1045 (0.1%)
5	F	0.53	0/2841	0.79	2/3824 (0.1%)
6	G	1.15	1/339 (0.3%)	1.03	1/520 (0.2%)
7	H	1.02	0/369	0.98	0/566
8	I	1.46	2/93 (2.2%)	1.07	0/142
All	All	0.62	6/28955 (0.0%)	0.84	24/39312 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	1	A	O3'-P	-7.61	1.52	1.61
8	I	2	U	O3'-P	-6.57	1.53	1.61
6	G	17	DT	O3'-P	-6.42	1.53	1.61
3	D	73	CYS	CB-SG	-6.37	1.71	1.82
2	C	394	PHE	CB-CG	-5.97	1.41	1.51
1	A	200	TRP	CB-CG	-5.16	1.41	1.50

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1455	LYS	CD-CE-NZ	8.13	130.39	111.70
3	D	583	ASP	CB-CG-OD2	-7.16	111.85	118.30
3	D	1344	VAL	CG1-CB-CG2	-7.14	99.47	110.90
3	D	1235	GLN	CA-CB-CG	-6.58	98.92	113.40
3	D	1086	LEU	CA-CB-CG	6.53	130.33	115.30
2	C	944	LEU	CB-CG-CD2	-5.91	100.96	111.00
3	D	1147	ARG	NE-CZ-NH2	-5.69	117.45	120.30
2	C	351	LEU	CA-CB-CG	5.61	128.20	115.30
2	C	107	LEU	CA-CB-CG	5.58	128.13	115.30
2	C	571	LEU	CB-CG-CD2	-5.57	101.54	111.00
5	F	94	LEU	CB-CG-CD2	-5.56	101.55	111.00
3	D	115	LEU	CA-CB-CG	5.53	128.02	115.30
6	G	16	DA	O4'-C4'-C3'	-5.50	102.30	104.50
3	D	702	LEU	CB-CG-CD2	-5.47	101.69	111.00
3	D	743	ASP	CB-CG-OD1	5.45	123.21	118.30
5	F	338	LEU	CB-CG-CD2	-5.42	101.78	111.00
3	D	1041	LEU	CB-CG-CD2	-5.42	101.79	111.00
1	B	186	LEU	CA-CB-CG	5.40	127.72	115.30
3	D	583	ASP	CB-CG-OD1	5.34	123.10	118.30
1	A	42	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	C	974	LEU	CB-CG-CD2	-5.20	102.16	111.00
2	C	780	GLU	N-CA-C	-5.14	97.12	111.00
4	E	20	THR	CA-CB-CG2	-5.06	105.32	112.40
2	C	774	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	583	ASP	Mainchain

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	1782	0	1834	71	0
1	B	1750	0	1797	79	0
2	C	8747	0	8837	340	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	11820	0	12038	403	2
4	E	761	0	778	20	0
5	F	2796	0	2865	100	0
6	G	304	0	170	29	0
7	H	329	0	182	13	0
8	I	84	0	42	16	0
9	D	2	0	0	0	0
10	D	2	0	0	0	0
11	D	29	11	11	1	0
All	All	28406	11	28554	951	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (951) 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)
6:G:17:DT:H3	8:I:1:A:N6	1.07	1.49
6:G:18:DT:H3	8:I:0:A:N6	1.25	1.32
6:G:17:DT:O2	8:I:1:A:N1	1.78	1.15
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.34	1.09
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.47	0.96
3:D:1493:LYS:HA	3:D:1493:LYS:HE3	1.46	0.95
2:C:221:LEU:HD11	2:C:307:LEU:HD21	1.47	0.95
6:G:18:DT:O2	8:I:0:A:N1	2.00	0.94
5:F:168:LYS:HG3	5:F:172:ARG:HH21	1.33	0.93
2:C:617:ASP:OD2	2:C:619:ARG:NE	2.01	0.93
3:D:41:ARG:HA	3:D:46:ASP:OD2	1.69	0.92
3:D:566:ILE:HD11	5:F:192:LEU:HD21	1.48	0.92
3:D:664:LYS:NZ	3:D:693:GLU:OE1	2.03	0.92
2:C:109:LYS:HG2	2:C:368:THR:HG22	1.48	0.92
5:F:193:ARG:HB3	7:H:7:DC:H5"	1.51	0.92
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.52	0.91
2:C:55:GLU:O	2:C:56:GLU:HB3	1.71	0.91
2:C:615:TYR:HH	2:C:623:TYR:HH	1.13	0.90
3:D:1154:GLU:HG2	3:D:1159:ARG:HA	1.54	0.90
5:F:338:LEU:HD23	5:F:339:PRO:HD2	1.54	0.89
2:C:212:GLY:HA2	2:C:218:VAL:HG21	1.54	0.89
3:D:96:ALA:HB3	3:D:554:LEU:HD23	1.54	0.88
6:G:17:DT:C2	8:I:1:A:N1	2.40	0.88
2:C:853:LEU:HB2	2:C:858:MET:CE	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:THR:HG22	1:B:209:GLU:H	1.37	0.88
2:C:32:ALA:HB2	2:C:73:LEU:HD12	1.56	0.88
3:D:1143:GLY:O	3:D:1147:ARG:HD2	1.74	0.88
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.06	0.87
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.56	0.87
2:C:229:MET:HB2	2:C:233:GLU:HB2	1.55	0.86
3:D:65:ARG:HB2	3:D:65:ARG:HH11	1.39	0.85
2:C:394:PHE:HE2	2:C:632:ASN:HB3	1.40	0.85
2:C:168:ARG:NH1	2:C:345:ARG:HD3	1.92	0.85
3:D:322:VAL:HG22	3:D:335:LEU:CD2	2.08	0.84
8:I:0:A:O2'	8:I:1:A:O5'	1.96	0.84
2:C:1070:ILE:HG21	3:D:655:PRO:HB2	1.60	0.83
2:C:358:ARG:HB3	2:C:372:LEU:HD12	1.60	0.83
3:D:1486:VAL:HG21	4:E:22:VAL:HG13	1.60	0.83
2:C:146:VAL:HG22	2:C:162:ILE:HG12	1.60	0.83
2:C:333:ILE:HD11	2:C:467:ILE:HD11	1.61	0.83
1:A:188:GLN:HG2	1:A:189:ARG:HG2	1.59	0.82
3:D:1496:GLU:OE1	3:D:1500:LYS:NZ	2.13	0.82
2:C:521:PRO:HB3	3:D:1068:LEU:HD21	1.61	0.81
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.62	0.81
6:G:18:DT:H2'	6:G:19:DG:C8	2.16	0.81
2:C:294:GLU:HB3	2:C:299:LYS:HD2	1.63	0.80
3:D:566:ILE:HD11	5:F:192:LEU:CD2	2.11	0.80
3:D:658:LEU:HD23	3:D:661:MET:HE3	1.62	0.80
3:D:963:TYR:CE2	3:D:1002:LYS:HD3	2.16	0.80
2:C:16:PRO:HB3	2:C:460:ARG:NH1	1.97	0.79
2:C:286:SER:OG	2:C:301:GLU:OE2	1.99	0.79
2:C:374:ASN:OD1	5:F:276:ARG:HD2	1.81	0.79
3:D:1486:VAL:CG2	4:E:22:VAL:HG13	2.12	0.79
1:B:49:PRO:HA	1:B:148:VAL:HG12	1.66	0.78
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.65	0.78
2:C:615:TYR:OH	2:C:623:TYR:OH	1.97	0.78
2:C:358:ARG:HB3	2:C:372:LEU:CD1	2.14	0.78
3:D:14:SER:HB3	3:D:511:TRP:CE2	2.19	0.78
2:C:180:GLY:O	2:C:220:GLY:HA3	1.85	0.77
2:C:766:GLU:CB	2:C:767:PRO:HD2	2.15	0.77
3:D:65:ARG:HB2	3:D:65:ARG:NH1	1.99	0.77
3:D:114:THR:HG21	3:D:498:VAL:HG21	1.66	0.77
2:C:470:PRO:HD3	2:C:485:TYR:CE2	2.20	0.77
2:C:524:VAL:HG13	2:C:528:GLU:HB2	1.67	0.77
3:D:1283:ILE:HG13	3:D:1315:ASP:OD2	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:400:ILE:HG22	5:F:403:LYS:HE2	1.66	0.77
6:G:18:DT:H2"	6:G:19:DG:H5'	1.66	0.77
1:A:153:ALA:N	1:A:168:ASP:OD1	2.14	0.76
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.19	0.76
1:A:56:VAL:HG22	1:A:142:VAL:HG12	1.66	0.76
2:C:504:GLU:HG2	2:C:509:ALA:HB2	1.67	0.76
3:D:437:VAL:HG11	5:F:175:HIS:CD2	2.20	0.76
2:C:769:PRO:HG3	3:D:65:ARG:NH2	2.01	0.76
3:D:1084:THR:HG23	3:D:1238:MET:HA	1.67	0.76
2:C:607:ASP:HB2	2:C:610:ARG:NH1	2.00	0.75
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.68	0.75
3:D:1084:THR:O	3:D:1088:THR:HG23	1.87	0.75
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.69	0.74
3:D:314:PRO:HB2	3:D:317:VAL:HG12	1.69	0.74
1:B:80:LEU:HB3	3:D:867:ARG:NH2	2.03	0.74
5:F:168:LYS:HG3	5:F:172:ARG:NH2	2.02	0.74
2:C:470:PRO:HD3	2:C:485:TYR:HE2	1.53	0.74
3:D:904:VAL:HG22	3:D:905:PRO:HD2	1.70	0.73
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.21	0.73
2:C:164:PRO:HA	2:C:269:LEU:HD12	1.69	0.73
2:C:204:GLN:NE2	2:C:222:MET:SD	2.61	0.73
2:C:617:ASP:HB2	2:C:619:ARG:HG2	1.70	0.73
3:D:1283:ILE:HG13	3:D:1315:ASP:CG	2.09	0.73
3:D:204:LEU:HD22	3:D:441:ARG:CZ	2.19	0.73
3:D:658:LEU:HD23	3:D:661:MET:CE	2.19	0.72
3:D:1047:LYS:HG2	3:D:1053:PHE:CE1	2.24	0.72
5:F:405:LEU:O	5:F:409:LYS:HG3	1.89	0.72
2:C:168:ARG:HH11	2:C:345:ARG:HD3	1.51	0.72
2:C:170:PRO:HD2	2:C:267:TYR:CE1	2.24	0.72
3:D:180:LYS:NZ	3:D:357:GLU:OE1	2.20	0.72
2:C:136:ILE:HB	2:C:336:VAL:HG13	1.72	0.72
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.71	0.72
6:G:11:DG:H2'	6:G:12:DG:H5"	1.72	0.72
1:B:138:LEU:HD21	1:B:140:MET:HE3	1.71	0.71
3:D:500:ARG:NH1	3:D:1390:LEU:HD21	2.05	0.71
2:C:772:ARG:NH2	5:F:380:GLU:OE1	2.23	0.71
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.72	0.71
1:A:201:THR:HG21	1:A:205:VAL:O	1.90	0.71
3:D:959:GLU:HB3	3:D:963:TYR:CE1	2.26	0.71
2:C:394:PHE:CE2	2:C:632:ASN:HB3	2.24	0.71
3:D:1493:LYS:NZ	3:D:1496:GLU:HG3	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:130:VAL:HG21	5:F:159:ILE:HG21	1.73	0.70
3:D:1495:ILE:HG12	4:E:88:GLU:CG	2.21	0.70
3:D:1263:PHE:HD2	3:D:1375:MET:CE	2.05	0.70
2:C:181:VAL:HG23	2:C:220:GLY:O	1.91	0.70
5:F:289:GLU:O	5:F:293:GLU:HG3	1.92	0.70
3:D:704:ARG:HB2	3:D:745:MET:HG2	1.74	0.70
2:C:915:LYS:NZ	3:D:952:ASP:OD2	2.25	0.69
2:C:132:ALA:HB1	2:C:394:PHE:HE1	1.57	0.69
5:F:393:THR:HG22	5:F:395:GLU:H	1.56	0.69
2:C:937:ASP:OD1	2:C:939:ARG:HG2	1.92	0.69
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.74	0.69
2:C:165:LEU:HD11	2:C:270:GLY:HA2	1.72	0.69
3:D:959:GLU:HB3	3:D:963:TYR:HE1	1.57	0.69
2:C:344:PHE:HD2	2:C:382:ILE:HD11	1.58	0.69
6:G:12:DG:H5”	6:G:12:DG:H8	1.58	0.69
3:D:322:VAL:HG22	3:D:335:LEU:HD21	1.73	0.69
3:D:949:ILE:HD11	3:D:1023:MET:HE1	1.73	0.69
1:A:99:LEU:HB2	1:A:142:VAL:HG23	1.75	0.69
3:D:45:PHE:O	3:D:86:ARG:NH2	2.26	0.69
1:B:80:LEU:HD22	3:D:844:ALA:HA	1.75	0.68
3:D:1386:ASP:CG	3:D:1413:THR:HG22	2.13	0.68
5:F:115:LYS:HD3	5:F:173:TYR:CZ	2.28	0.68
2:C:41:ASN:OD1	2:C:46:ALA:HA	1.93	0.68
5:F:166:LEU:HD13	5:F:170:HIS:HB3	1.75	0.68
1:B:143:ARG:HG2	1:B:143:ARG:HH11	1.59	0.68
3:D:258:VAL:HG12	3:D:273:ARG:O	1.93	0.68
3:D:501:ALA:HB1	3:D:1452:ILE:HG22	1.75	0.68
2:C:74:GLY:HA3	2:C:93:PRO:HG2	1.75	0.68
2:C:376:ARG:NH1	5:F:279:GLN:OE1	2.26	0.68
3:D:270:LEU:HD23	3:D:271:VAL:N	2.09	0.68
3:D:1364:HIS:ND1	3:D:1366:LYS:HB2	2.09	0.68
2:C:12:VAL:HG11	2:C:472:ARG:HD3	1.77	0.67
3:D:1087:ARG:CB	3:D:1237:THR:HG21	2.24	0.67
2:C:460:ARG:HD2	2:C:485:TYR:CZ	2.29	0.67
3:D:44:LEU:HB3	3:D:525:ARG:NH2	2.10	0.67
3:D:1140:ILE:HG22	3:D:1144:LEU:HD12	1.76	0.67
1:A:97:VAL:HG13	1:A:98:THR:N	2.10	0.67
2:C:11:GLU:OE2	2:C:537:LYS:HE2	1.95	0.67
3:D:661:MET:HE3	3:D:673:ALA:HB1	1.77	0.67
5:F:353:GLU:OE1	5:F:417:LYS:HD3	1.95	0.67
2:C:764:GLU:C	2:C:766:GLU:H	1.98	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:VAL:HG23	1:B:142:VAL:HG12	1.77	0.67
3:D:357:GLU:HB2	3:D:387:LEU:HD23	1.76	0.67
3:D:411:THR:HA	3:D:435:VAL:HG12	1.75	0.67
2:C:329:GLY:O	2:C:466:PHE:HE2	1.78	0.66
2:C:926:PHE:CZ	2:C:930:LYS:HD3	2.31	0.66
2:C:954:THR:HG23	2:C:965:GLU:OE2	1.95	0.66
2:C:1102:LEU:HD23	2:C:1108:PRO:HA	1.77	0.66
3:D:116:LEU:HD21	3:D:465:LEU:HD23	1.77	0.66
5:F:274:THR:HG21	5:F:295:MET:HE3	1.77	0.66
6:G:17:DT:N3	8:I:1:A:N6	1.91	0.66
2:C:261:ILE:CG2	2:C:291:ALA:HB3	2.25	0.66
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	1.76	0.66
2:C:922:PHE:CE2	2:C:964:LYS:HB2	2.30	0.66
1:A:64:GLU:OE2	2:C:830:LYS:NZ	2.26	0.65
2:C:214:TYR:O	2:C:218:VAL:HG23	1.97	0.65
6:G:18:DT:C2	8:I:0:A:N1	2.64	0.65
1:A:106:PRO:HG3	1:A:134:GLU:HG2	1.77	0.65
5:F:370:LYS:HG2	5:F:375:LEU:HD23	1.77	0.65
3:D:832:ARG:HD2	3:D:833:GLU:H	1.62	0.65
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.78	0.65
3:D:949:ILE:HD11	3:D:1023:MET:CE	2.26	0.65
3:D:65:ARG:CG	3:D:66:GLN:H	2.10	0.65
3:D:1242:HIS:CD2	11:D:2005:UTP:O3B	2.50	0.65
1:B:112:ARG:NH1	1:B:126:ASP:OD1	2.30	0.65
2:C:627:ARG:CZ	2:C:640:ARG:HG3	2.26	0.65
3:D:266:GLU:OE2	3:D:315:ARG:HG3	1.97	0.64
3:D:1140:ILE:CG2	3:D:1144:LEU:HD12	2.27	0.64
3:D:237:LYS:N	3:D:240:GLU:OE1	2.29	0.64
2:C:1:MET:HB2	2:C:898:GLY:O	1.97	0.64
2:C:757:GLY:HA2	2:C:789:SER:OG	1.97	0.64
1:B:18:ARG:O	1:B:207:PRO:HD3	1.97	0.64
2:C:302:VAL:O	2:C:305:PRO:HD2	1.98	0.64
5:F:168:LYS:CG	5:F:172:ARG:HH21	2.09	0.64
2:C:480:THR:HG22	2:C:482:GLU:H	1.62	0.64
2:C:1070:ILE:CG2	3:D:655:PRO:HB2	2.28	0.64
1:B:65:PHE:CD2	3:D:809:PRO:HB2	2.32	0.64
2:C:740:GLU:HB3	2:C:805:ARG:HH12	1.63	0.63
3:D:236:TYR:CE1	3:D:242:LEU:HD12	2.33	0.63
3:D:65:ARG:HG2	3:D:66:GLN:H	1.63	0.63
4:E:70:THR:OG1	4:E:72:ARG:HG3	1.96	0.63
2:C:170:PRO:HD2	2:C:267:TYR:HE1	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:182:VAL:HG11	2:C:221:LEU:HG	1.81	0.63
5:F:329:TYR:CE2	5:F:333:ILE:HD11	2.34	0.63
2:C:55:GLU:O	2:C:359:MET:HE1	1.99	0.63
1:B:44:LEU:HD13	1:B:199:ILE:HD13	1.79	0.63
1:B:124:ASN:ND2	1:B:127:LEU:HD22	2.13	0.63
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.33	0.63
2:C:911:GLU:OE1	3:D:1062:ARG:NH1	2.32	0.63
3:D:1493:LYS:HA	3:D:1493:LYS:CE	2.23	0.63
2:C:709:GLU:OE2	2:C:824:ARG:NH1	2.32	0.63
2:C:769:PRO:CG	3:D:65:ARG:NH2	2.62	0.63
3:D:1263:PHE:O	3:D:1375:MET:HE2	1.99	0.63
3:D:1493:LYS:HZ1	3:D:1496:GLU:HG3	1.63	0.63
6:G:11:DG:C2'	6:G:12:DG:H5"	2.28	0.63
1:B:101:LEU:HB2	1:B:114:PHE:CD1	2.33	0.63
5:F:274:THR:OG1	5:F:295:MET:CE	2.47	0.63
2:C:524:VAL:CG1	2:C:528:GLU:HB2	2.28	0.62
5:F:362:SER:OG	5:F:365:GLU:HG2	1.99	0.62
5:F:375:LEU:HD12	5:F:375:LEU:O	1.98	0.62
1:B:138:LEU:HD11	1:B:140:MET:HE2	1.82	0.62
3:D:1156:LEU:HD23	3:D:1182:GLU:OE2	1.99	0.62
3:D:1087:ARG:CB	3:D:1237:THR:CG2	2.78	0.62
3:D:1241:PHE:O	3:D:1243:THR:N	2.26	0.62
2:C:627:ARG:NH2	2:C:640:ARG:HG3	2.13	0.62
3:D:235:ALA:HB2	3:D:320:ALA:O	1.99	0.62
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.81	0.62
3:D:14:SER:HB3	3:D:511:TRP:CZ2	2.35	0.62
3:D:1258:ARG:HH21	3:D:1351:GLU:HG3	1.65	0.62
1:B:101:LEU:HD21	1:B:109:VAL:HG11	1.79	0.62
3:D:1044:LEU:H	3:D:1044:LEU:HD12	1.65	0.62
3:D:34:TYR:CZ	3:D:35:ARG:HG3	2.34	0.61
3:D:322:VAL:HG22	3:D:335:LEU:HD23	1.78	0.61
1:A:70:GLY:N	2:C:607:ASP:OD1	2.28	0.61
1:A:226:SER:O	1:A:228:PRO:HD3	1.99	0.61
2:C:764:GLU:O	2:C:766:GLU:N	2.28	0.61
3:D:65:ARG:HG2	3:D:66:GLN:N	2.16	0.61
4:E:50:THR:HG22	4:E:51:LEU:H	1.65	0.61
3:D:1492:LEU:HD13	3:D:1493:LYS:HZ1	1.66	0.61
3:D:405:ASP:N	3:D:423:ASP:OD1	2.25	0.61
5:F:193:ARG:NH1	7:H:7:DC:H5	1.99	0.61
5:F:265:VAL:O	5:F:269:ASN:ND2	2.30	0.61
6:G:17:DT:O2	8:I:1:A:C2	2.53	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:930:LYS:HE3	2:C:935:GLY:HA2	1.83	0.61
5:F:168:LYS:O	5:F:172:ARG:HG2	2.00	0.61
3:D:1108:ARG:HD2	3:D:1198:TYR:O	2.01	0.61
1:B:143:ARG:HG2	1:B:143:ARG:NH1	2.16	0.61
2:C:280:LYS:HE3	2:C:309:TYR:CZ	2.36	0.61
2:C:1058:ASP:OD2	3:D:621:LYS:HE2	2.00	0.60
3:D:875:THR:HG21	3:D:902:LEU:HD21	1.82	0.60
5:F:354:LEU:HD23	5:F:418:LEU:HD21	1.83	0.60
3:D:1277:ILE:HG22	3:D:1278:ASP:H	1.65	0.60
2:C:580:MET:HB3	2:C:584:GLU:CD	2.21	0.60
2:C:144:PRO:HG2	2:C:165:LEU:CD2	2.31	0.60
2:C:196:LEU:HD22	2:C:196:LEU:O	2.02	0.60
3:D:1112:CYS:SG	3:D:1114:THR:HG22	2.42	0.60
3:D:218:LYS:HG2	3:D:338:GLU:CG	2.21	0.60
3:D:1197:ARG:HG2	3:D:1198:TYR:CD2	2.37	0.60
3:D:236:TYR:CZ	3:D:242:LEU:HD12	2.37	0.60
3:D:17:LYS:HA	3:D:20:SER:OG	2.02	0.60
3:D:258:VAL:HG13	3:D:273:ARG:HG3	1.83	0.60
2:C:926:PHE:HE1	2:C:929:ARG:HH11	1.50	0.59
3:D:741:ASP:OD1	3:D:743:ASP:OD1	2.20	0.59
3:D:834:THR:OG1	3:D:838:ARG:HD2	2.02	0.59
1:A:97:VAL:HG13	1:A:98:THR:H	1.65	0.59
1:B:138:LEU:HD11	1:B:140:MET:CE	2.32	0.59
3:D:514:LEU:HD13	3:D:517:VAL:HG22	1.83	0.59
5:F:104:ARG:HG2	5:F:108:GLU:OE2	2.01	0.59
3:D:44:LEU:HB3	3:D:525:ARG:HH21	1.68	0.59
3:D:135:LEU:CD2	3:D:463:GLN:HG2	2.33	0.59
2:C:683:ASN:HB3	2:C:872:ASN:HD22	1.65	0.59
3:D:860:LEU:O	3:D:876:SER:HB2	2.02	0.59
3:D:1271:LYS:HG3	3:D:1272:ALA:O	2.01	0.59
3:D:1047:LYS:HB3	3:D:1048:PRO:CD	2.33	0.59
1:A:23:PHE:CD1	1:A:211:LEU:HD23	2.38	0.59
2:C:194:VAL:HG22	2:C:221:LEU:HD23	1.85	0.59
3:D:1044:LEU:HD12	3:D:1044:LEU:N	2.17	0.59
3:D:1347:TYR:O	3:D:1351:GLU:HB2	2.03	0.59
6:G:18:DT:N3	8:I:0:A:N6	2.07	0.59
2:C:134:ARG:NH1	2:C:392:SER:O	2.36	0.59
3:D:478:LEU:O	3:D:481:MET:HB2	2.03	0.59
3:D:809:PRO:HG3	3:D:829:VAL:HG11	1.83	0.59
5:F:101:GLU:HG2	5:F:105:LYS:HE2	1.84	0.59
2:C:32:ALA:HB2	2:C:73:LEU:CD1	2.30	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:373:PRO:HA	3:D:376:GLU:OE2	2.04	0.58
3:D:963:TYR:CD2	3:D:1002:LYS:HD3	2.38	0.58
2:C:64:LEU:HD22	2:C:100:LEU:HD11	1.84	0.58
2:C:1059:ASP:OD1	2:C:1062:GLY:N	2.25	0.58
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.85	0.58
2:C:212:GLY:CA	2:C:218:VAL:HG21	2.32	0.58
3:D:1047:LYS:HB3	3:D:1048:PRO:HD2	1.83	0.58
3:D:823:LEU:HD11	3:D:837:GLY:HA2	1.85	0.58
6:G:18:DT:H2"	6:G:19:DG:O4'	2.04	0.58
2:C:376:ARG:HB2	2:C:377:PRO:HD3	1.85	0.58
3:D:314:PRO:HD2	3:D:317:VAL:HG13	1.86	0.58
3:D:455:ARG:HH12	3:D:463:GLN:HE21	1.52	0.58
5:F:329:TYR:HE2	5:F:333:ILE:HD11	1.69	0.58
2:C:776:SER:OG	5:F:373:LYS:NZ	2.36	0.58
3:D:64:LYS:HB3	5:F:378:GLY:HA3	1.85	0.58
3:D:351:MET:HE1	3:D:368:VAL:HG11	1.84	0.58
2:C:32:ALA:CB	2:C:73:LEU:HD12	2.31	0.58
2:C:722:ILE:HD12	2:C:821:GLU:CD	2.24	0.58
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.85	0.57
1:A:97:VAL:CG1	1:A:98:THR:N	2.67	0.57
6:G:18:DT:H2'	6:G:19:DG:H8	1.69	0.57
1:A:39:PRO:HG3	1:B:39:PRO:CG	2.33	0.57
2:C:480:THR:HG22	2:C:481:ASP:N	2.18	0.57
5:F:96:LEU:O	5:F:100:VAL:HG23	2.04	0.57
5:F:82:ARG:HH21	7:H:9:DA:H61	1.52	0.57
2:C:638:ASP:OD1	2:C:640:ARG:HD2	2.04	0.57
2:C:740:GLU:HB3	2:C:805:ARG:NH1	2.19	0.57
2:C:143:SER:O	2:C:147:TYR:OH	2.18	0.57
2:C:150:PRO:HD3	2:C:322:VAL:HG11	1.86	0.57
2:C:999:HIS:HB3	2:C:1004:LYS:NZ	2.20	0.57
7:H:17:DC:H2"	7:H:18:DG:H5'	1.86	0.57
1:A:137:ARG:HH11	1:A:137:ARG:HG2	1.70	0.56
3:D:1154:GLU:HG2	3:D:1159:ARG:CA	2.31	0.56
2:C:261:ILE:HG21	2:C:291:ALA:HB3	1.88	0.56
2:C:429:ASP:OD1	3:D:1048:PRO:HB3	2.05	0.56
2:C:858:MET:HG2	2:C:867:VAL:O	2.05	0.56
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.88	0.56
3:D:817:GLU:OE1	3:D:817:GLU:HA	2.06	0.56
5:F:274:THR:OG1	5:F:295:MET:HE3	2.05	0.56
2:C:396:ASP:HA	2:C:633:GLN:NE2	2.20	0.56
2:C:766:GLU:CB	2:C:767:PRO:CD	2.83	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:144:PRO:HG2	2:C:165:LEU:HD23	1.87	0.56
2:C:240:THR:HG22	2:C:248:PRO:HG3	1.88	0.56
1:A:64:GLU:HG2	1:A:76:VAL:HG22	1.87	0.56
2:C:987:ILE:HD11	3:D:946:GLY:HA2	1.88	0.56
3:D:1284:GLU:HG2	3:D:1291:SER:HB3	1.88	0.56
3:D:664:LYS:HB2	3:D:666:ILE:HG13	1.88	0.56
2:C:614:ARG:HH21	2:C:614:ARG:HG3	1.70	0.56
3:D:181:ASP:HB2	3:D:205:TYR:CG	2.40	0.56
3:D:828:LYS:HG2	3:D:833:GLU:HB3	1.88	0.56
5:F:101:GLU:OE1	5:F:105:LYS:HE3	2.06	0.56
1:B:83:LYS:HE2	1:B:168:ASP:HB2	1.86	0.56
2:C:182:VAL:HG21	2:C:193:LEU:HD23	1.87	0.56
3:D:1492:LEU:HD13	3:D:1493:LYS:NZ	2.20	0.56
2:C:853:LEU:HB2	2:C:858:MET:HE2	1.88	0.55
3:D:131:LYS:O	3:D:456:MET:HG2	2.05	0.55
3:D:983:LEU:HA	3:D:987:GLU:OE2	2.07	0.55
2:C:150:PRO:HA	2:C:158:TYR:HD1	1.72	0.55
1:A:198:ARG:HD3	2:C:934:PHE:CZ	2.42	0.55
2:C:1001:VAL:HG13	3:D:630:VAL:HB	1.88	0.55
3:D:996:TRP:HB3	3:D:1044:LEU:HD11	1.88	0.55
3:D:1444:THR:O	3:D:1448:THR:HG23	2.05	0.55
2:C:56:GLU:HB2	2:C:359:MET:HE3	1.87	0.55
3:D:564:GLU:OE2	5:F:140:ARG:NH2	2.40	0.55
3:D:907:GLU:OE1	3:D:909:ASN:N	2.38	0.55
2:C:182:VAL:CG1	2:C:221:LEU:HG	2.37	0.55
2:C:214:TYR:HB3	2:C:217:LEU:HD12	1.89	0.55
2:C:999:HIS:HB3	2:C:1004:LYS:HZ2	1.71	0.55
3:D:1036:ARG:HH22	3:D:1246:VAL:HG11	1.71	0.55
3:D:984:THR:OG1	3:D:987:GLU:HG3	2.07	0.55
3:D:1386:ASP:OD2	3:D:1413:THR:HG22	2.07	0.55
5:F:122:LEU:HB2	5:F:127:ILE:HD11	1.89	0.55
6:G:20:DT:H2'	6:G:20:DT:O2	2.06	0.55
2:C:1043:TYR:CD1	3:D:763:MET:HG2	2.42	0.54
3:D:65:ARG:CG	3:D:66:GLN:N	2.69	0.54
3:D:1336:LEU:HB2	3:D:1344:VAL:HG21	1.88	0.54
2:C:370:ALA:O	5:F:280:GLN:NE2	2.29	0.54
5:F:271:LEU:HD22	5:F:307:THR:HG21	1.89	0.54
5:F:287:THR:HG22	5:F:288:TYR:H	1.71	0.54
3:D:231:VAL:HG13	3:D:242:LEU:O	2.07	0.54
3:D:1339:LYS:HB3	3:D:1343:ALA:CB	2.37	0.54
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1492:LEU:CD1	3:D:1493:LYS:NZ	2.70	0.54
2:C:577:PRO:HG2	2:C:580:MET:HG2	1.88	0.54
3:D:1046:GLN:HA	3:D:1052:THR:HA	1.89	0.54
1:A:206:THR:HB	1:A:209:GLU:HG3	1.89	0.54
2:C:774:LEU:HD22	5:F:350:LEU:HD11	1.90	0.54
1:B:80:LEU:HD13	3:D:867:ARG:HD3	1.90	0.54
2:C:394:PHE:CE2	2:C:632:ASN:CG	2.80	0.54
2:C:880:MET:HB3	3:D:1061:PHE:CE2	2.42	0.54
3:D:1386:ASP:H	3:D:1413:THR:HG23	1.73	0.54
3:D:1252:ILE:HG23	3:D:1252:ILE:O	2.07	0.54
1:B:179:PHE:HB3	1:B:197:LEU:CD2	2.38	0.54
3:D:236:TYR:HA	3:D:240:GLU:OE1	2.08	0.54
3:D:1040:GLY:O	3:D:1060:SER:HB3	2.07	0.54
2:C:211:LEU:HD23	2:C:311:PHE:CD2	2.43	0.53
1:B:26:GLU:HB3	1:B:194:LYS:HG3	1.91	0.53
2:C:1058:ASP:OD1	2:C:1084:SER:HB2	2.08	0.53
3:D:231:VAL:O	3:D:236:TYR:OH	2.25	0.53
3:D:520:LEU:O	3:D:525:ARG:NH1	2.39	0.53
3:D:963:TYR:HE2	3:D:1002:LYS:HD3	1.67	0.53
5:F:345:ALA:O	5:F:349:LEU:HG	2.08	0.53
2:C:170:PRO:HD2	2:C:267:TYR:CD1	2.43	0.53
2:C:261:ILE:HG22	2:C:262:ALA:N	2.22	0.53
2:C:394:PHE:CE2	2:C:632:ASN:CB	2.90	0.53
2:C:764:GLU:C	2:C:766:GLU:N	2.62	0.53
3:D:59:ALA:HB2	3:D:78:VAL:HG21	1.90	0.53
3:D:1154:GLU:CG	3:D:1159:ARG:HA	2.34	0.53
3:D:1495:ILE:HG12	4:E:88:GLU:CD	2.28	0.53
1:B:102:LYS:HG2	1:B:139:ASN:OD1	2.08	0.53
2:C:614:ARG:HG3	2:C:614:ARG:NH2	2.24	0.53
3:D:111:LYS:HG3	3:D:1452:ILE:HD11	1.89	0.53
5:F:279:GLN:O	5:F:279:GLN:HG2	2.08	0.53
1:A:106:PRO:CG	1:A:134:GLU:HG2	2.38	0.53
1:B:73:GLU:OE1	1:B:73:GLU:N	2.30	0.53
3:D:1084:THR:CG2	3:D:1238:MET:HA	2.38	0.53
1:A:100:LEU:CD2	1:A:141:GLU:HG2	2.39	0.53
2:C:805:ARG:HG3	2:C:823:VAL:HG22	1.90	0.53
3:D:1208:ASP:OD1	3:D:1208:ASP:C	2.47	0.53
1:A:196:THR:HG21	2:C:934:PHE:CE2	2.44	0.53
2:C:154:ARG:HH21	2:C:157:ARG:HG3	1.74	0.53
2:C:617:ASP:OD1	2:C:617:ASP:N	2.41	0.53
3:D:1263:PHE:HA	3:D:1375:MET:CE	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1276:GLU:O	3:D:1277:ILE:HD13	2.08	0.53
5:F:368:VAL:HG21	5:F:400:ILE:HD11	1.90	0.53
1:B:138:LEU:HD21	1:B:140:MET:CE	2.39	0.53
2:C:150:PRO:HD3	2:C:322:VAL:CG1	2.39	0.53
3:D:1191:PRO:HD2	3:D:1369:GLU:OE1	2.09	0.52
2:C:329:GLY:O	2:C:466:PHE:CE2	2.62	0.52
2:C:1100:GLN:HG3	3:D:9:ARG:HH21	1.75	0.52
2:C:258:TYR:CD2	2:C:262:ALA:HB3	2.44	0.52
2:C:132:ALA:HB1	2:C:394:PHE:CE1	2.41	0.52
3:D:1386:ASP:HB3	3:D:1412:LYS:HD2	1.91	0.52
2:C:593:ALA:HB1	2:C:659:PRO:HD2	1.92	0.52
1:B:179:PHE:HB3	1:B:197:LEU:HD23	1.91	0.52
3:D:15:PRO:O	3:D:19:ARG:HG3	2.09	0.52
3:D:218:LYS:CG	3:D:338:GLU:HG2	2.23	0.52
3:D:689:ASP:CG	4:E:51:LEU:HD11	2.30	0.52
2:C:84:ARG:HD3	2:C:629:TYR:OH	2.09	0.52
3:D:114:THR:CG2	3:D:498:VAL:HG21	2.39	0.52
3:D:892:ASP:OD1	3:D:894:LYS:HD2	2.08	0.52
2:C:462:ASP:OD2	2:C:468:ARG:NH1	2.40	0.52
5:F:274:THR:CG2	5:F:295:MET:HE3	2.39	0.52
1:A:112:ARG:HG2	1:A:125:PRO:O	2.09	0.52
2:C:359:MET:O	2:C:360:LEU:HD12	2.10	0.52
6:G:18:DT:C2'	6:G:19:DG:O4'	2.57	0.52
3:D:495:ARG:O	3:D:499:VAL:HG23	2.10	0.52
1:A:44:LEU:O	1:A:174:VAL:HG21	2.10	0.51
2:C:260:LEU:O	2:C:261:ILE:HD12	2.10	0.51
2:C:359:MET:C	2:C:360:LEU:HD12	2.30	0.51
2:C:575:GLN:HG3	2:C:670:GLN:HA	1.92	0.51
3:D:135:LEU:HD23	3:D:463:GLN:HG2	1.91	0.51
3:D:317:VAL:HG23	3:D:339:TRP:HB3	1.91	0.51
3:D:899:LEU:HD22	3:D:917:GLN:HB3	1.93	0.51
3:D:1281:VAL:HG23	3:D:1317:ASP:O	2.10	0.51
2:C:418:LEU:H	2:C:418:LEU:HD12	1.75	0.51
1:B:90:LEU:O	1:B:92:PRO:HD3	2.10	0.51
3:D:314:PRO:HB2	3:D:317:VAL:CG1	2.40	0.51
2:C:340:MET:CE	2:C:382:ILE:HD13	2.40	0.51
2:C:587:VAL:O	2:C:591:SER:HB3	2.09	0.51
3:D:134:VAL:HG23	3:D:149:LYS:HA	1.93	0.51
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.10	0.51
6:G:17:DT:N3	8:I:1:A:C6	2.61	0.51
6:G:18:DT:H2"	6:G:19:DG:C5'	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:PHE:N	1:A:23:PHE:CD2	2.77	0.51
5:F:260:ILE:HG22	5:F:265:VAL:HG23	1.92	0.51
1:B:188:GLN:HG2	1:B:189:ARG:N	2.26	0.51
3:D:945:SER:OG	3:D:947:ILE:HG12	2.11	0.51
6:G:9:DC:H2"	6:G:10:DC:OP2	2.11	0.51
1:B:47:SER:HB3	1:B:217:ILE:HD13	1.93	0.51
2:C:269:LEU:O	2:C:288:ARG:HD2	2.11	0.51
5:F:274:THR:OG1	5:F:295:MET:HE1	2.10	0.51
2:C:136:ILE:CB	2:C:336:VAL:HG13	2.40	0.51
3:D:204:LEU:HD22	3:D:441:ARG:NH1	2.25	0.51
5:F:222:ARG:HA	5:F:222:ARG:CZ	2.40	0.51
6:G:12:DG:H8	6:G:12:DG:C5'	2.23	0.51
3:D:1263:PHE:HA	3:D:1375:MET:HE1	1.93	0.51
5:F:393:THR:HG22	5:F:395:GLU:N	2.24	0.51
2:C:758:ARG:HH21	2:C:788:THR:HB	1.75	0.50
2:C:760:SER:HB2	2:C:786:LYS:HE3	1.93	0.50
2:C:765:SER:O	2:C:766:GLU:O	2.29	0.50
1:A:11:PHE:CD1	1:B:225:PHE:HA	2.47	0.50
2:C:230:ARG:HG3	2:C:233:GLU:HG3	1.93	0.50
2:C:499:ALA:HB2	2:C:533:ASP:HB2	1.93	0.50
2:C:563:ASN:O	2:C:566:THR:HB	2.12	0.50
3:D:84:ILE:CD1	3:D:87:ARG:HD2	2.42	0.50
3:D:693:GLU:HB3	4:E:48:MET:HE1	1.94	0.50
1:A:23:PHE:CD1	1:A:211:LEU:CD2	2.95	0.50
1:A:57:TYR:CG	1:A:161:ARG:HD2	2.46	0.50
3:D:520:LEU:HD11	3:D:524:LEU:HD12	1.94	0.50
3:D:796:ARG:NH2	3:D:859:ASP:OD2	2.34	0.50
3:D:1493:LYS:HE3	3:D:1496:GLU:HB2	1.92	0.50
5:F:274:THR:CB	5:F:295:MET:HE3	2.40	0.50
1:B:80:LEU:HD22	3:D:844:ALA:CA	2.40	0.50
4:E:46:PRO:HB2	4:E:57:ASP:CB	2.41	0.50
3:D:142:LEU:HB2	3:D:161:LEU:HD11	1.93	0.50
3:D:1051:GLU:O	3:D:1051:GLU:HG2	2.11	0.50
3:D:1313:VAL:HG11	3:D:1319:VAL:HG11	1.92	0.50
3:D:236:TYR:HB3	3:D:313:MET:HG3	1.94	0.50
1:B:190:THR:HG22	1:B:190:THR:O	2.12	0.50
2:C:468:ARG:HA	2:C:486:MET:O	2.10	0.50
2:C:722:ILE:HD12	2:C:821:GLU:HG3	1.93	0.50
3:D:526:PRO:HB2	3:D:528:VAL:HG13	1.93	0.50
1:B:94:LEU:HD21	1:B:97:VAL:CG2	2.42	0.50
3:D:780:LYS:HE3	3:D:912:LYS:HD3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1263:PHE:HD2	3:D:1375:MET:HE1	1.77	0.50
2:C:361:MET:O	2:C:362:GLY:O	2.29	0.49
2:C:591:SER:O	2:C:592:LEU:HB2	2.12	0.49
2:C:888:THR:HG22	2:C:990:GLY:HA3	1.93	0.49
3:D:805:GLU:HG3	3:D:828:LYS:HB2	1.94	0.49
1:B:108:GLU:CG	1:B:131:THR:HG22	2.34	0.49
3:D:215:TYR:O	3:D:340:THR:HA	2.12	0.49
3:D:750:PRO:O	3:D:756:GLN:NE2	2.45	0.49
2:C:204:GLN:HB2	2:C:227:PHE:CZ	2.47	0.49
2:C:235:LEU:HD21	2:C:254:VAL:HG22	1.93	0.49
2:C:482:GLU:HG3	2:C:482:GLU:O	2.12	0.49
2:C:693:GLU:HG2	2:C:855:VAL:HB	1.95	0.49
2:C:861:LEU:HB3	2:C:862:PRO:HD2	1.94	0.49
2:C:1059:ASP:OD1	2:C:1059:ASP:C	2.50	0.49
3:D:351:MET:HG2	3:D:370:ALA:HB2	1.94	0.49
1:A:39:PRO:CG	1:B:39:PRO:HG3	2.42	0.49
2:C:216:GLU:HA	2:C:216:GLU:OE1	2.12	0.49
2:C:343:GLN:HA	2:C:343:GLN:NE2	2.26	0.49
3:D:231:VAL:O	3:D:231:VAL:HG22	2.12	0.49
2:C:150:PRO:HG3	2:C:322:VAL:HG21	1.94	0.49
2:C:405:ARG:O	2:C:405:ARG:HG2	2.12	0.49
2:C:598:GLU:O	2:C:651:LYS:HG3	2.12	0.49
1:A:89:PHE:HD2	1:A:94:LEU:O	1.95	0.49
1:A:215:VAL:HG13	1:B:222:LEU:HD22	1.95	0.49
2:C:603:VAL:HG23	2:C:647:GLN:O	2.13	0.49
2:C:1056:LYS:HG2	3:D:625:TYR:HD1	1.77	0.49
3:D:215:TYR:HE1	3:D:381:ALA:H	1.58	0.49
3:D:1364:HIS:ND1	3:D:1366:LYS:CB	2.75	0.49
1:A:96:THR:HB	1:A:145:ASP:OD1	2.12	0.49
2:C:77:PRO:HB2	2:C:78:PHE:CD1	2.47	0.49
2:C:396:ASP:HA	2:C:633:GLN:HE22	1.78	0.49
2:C:571:LEU:HD22	2:C:700:TYR:HA	1.93	0.49
3:D:1353:GLN:HA	3:D:1353:GLN:OE1	2.12	0.49
3:D:65:ARG:HH11	3:D:65:ARG:CB	2.19	0.49
3:D:1377:LYS:HE3	3:D:1378:TYR:CZ	2.47	0.49
7:H:7:DC:H6	7:H:7:DC:H5'	1.78	0.49
2:C:679:PHE:H	2:C:683:ASN:HD22	1.59	0.49
2:C:1053:LEU:HA	3:D:621:LYS:HD2	1.95	0.49
2:C:539:VAL:O	2:C:539:VAL:HG12	2.12	0.48
2:C:679:PHE:N	2:C:683:ASN:HD22	2.10	0.48
5:F:278:LEU:HD11	5:F:294:ALA:CB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:ILE:O	1:B:163:ASN:HB2	2.13	0.48
3:D:103:TRP:CZ2	3:D:1444:THR:HG22	2.49	0.48
5:F:193:ARG:NH1	7:H:7:DC:C5	2.79	0.48
3:D:1386:ASP:N	3:D:1413:THR:HG23	2.28	0.48
5:F:238:TYR:OH	7:H:1:DT:H73	2.14	0.48
5:F:353:GLU:HB3	5:F:418:LEU:HD11	1.95	0.48
1:B:111:ALA:HB3	1:B:125:PRO:HA	1.95	0.48
2:C:304:LEU:HB3	2:C:305:PRO:HD3	1.95	0.48
3:D:465:LEU:HD12	3:D:513:ILE:HD13	1.95	0.48
5:F:323:ASP:CB	6:G:19:DG:H1	2.26	0.48
2:C:717:LEU:CD2	2:C:763:GLY:HA2	2.44	0.48
2:C:774:LEU:HD21	5:F:421:PHE:HB2	1.96	0.48
2:C:952:LEU:HA	2:C:952:LEU:HD23	1.64	0.48
3:D:103:TRP:HB3	3:D:1448:THR:HG21	1.95	0.48
3:D:1154:GLU:CD	3:D:1159:ARG:HB2	2.33	0.48
5:F:400:ILE:HA	5:F:403:LYS:CG	2.41	0.48
2:C:713:ARG:CZ	3:D:533:GLY:HA3	2.44	0.48
3:D:654:LYS:HB3	3:D:655:PRO:HD3	1.95	0.48
5:F:383:LEU:HD12	5:F:394:ARG:NH2	2.28	0.48
1:A:57:TYR:HE1	1:A:163:ASN:HB2	1.78	0.48
3:D:1410:GLU:O	3:D:1410:GLU:HG2	2.14	0.48
5:F:154:LYS:O	5:F:158:GLU:HG3	2.13	0.48
2:C:460:ARG:CD	2:C:485:TYR:CZ	2.94	0.48
3:D:792:ILE:HD13	3:D:941:PHE:CE1	2.49	0.48
3:D:1339:LYS:HB3	3:D:1343:ALA:HB3	1.96	0.48
1:A:198:ARG:HD3	2:C:934:PHE:CE1	2.49	0.48
2:C:56:GLU:HB2	2:C:359:MET:CE	2.43	0.48
2:C:267:TYR:CE2	2:C:290:LEU:HG	2.49	0.48
3:D:147:VAL:HG21	3:D:161:LEU:HD21	1.96	0.48
3:D:1047:LYS:HG2	3:D:1053:PHE:CZ	2.49	0.48
1:B:206:THR:CG2	1:B:209:GLU:H	2.16	0.48
2:C:787:ASP:OD2	2:C:791:ARG:NH2	2.47	0.48
3:D:792:ILE:HD13	3:D:941:PHE:CD1	2.49	0.48
3:D:1276:GLU:C	3:D:1277:ILE:HD13	2.34	0.48
3:D:1486:VAL:HG22	4:E:22:VAL:HG13	1.93	0.48
1:A:128:HIS:O	1:A:129:ILE:HD13	2.13	0.47
1:B:20:TYR:OH	1:B:22:GLU:HG2	2.13	0.47
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.14	0.47
1:B:49:PRO:CA	1:B:148:VAL:HG12	2.38	0.47
2:C:340:MET:HE2	2:C:382:ILE:HD13	1.97	0.47
2:C:1101:THR:OG1	2:C:1109:VAL:O	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1263:PHE:CD2	3:D:1375:MET:HE1	2.49	0.47
3:D:1495:ILE:HD11	4:E:88:GLU:HB2	1.97	0.47
2:C:249:LYS:HB3	2:C:252:LYS:HB2	1.95	0.47
2:C:775:ARG:HH21	5:F:422:LEU:HD23	1.80	0.47
2:C:862:PRO:HA	2:C:975:TYR:CE2	2.49	0.47
3:D:181:ASP:HB2	3:D:205:TYR:CD1	2.49	0.47
3:D:1258:ARG:NH2	3:D:1351:GLU:HG3	2.28	0.47
2:C:26:TYR:OH	2:C:119:PRO:O	2.14	0.47
2:C:168:ARG:O	2:C:267:TYR:HA	2.13	0.47
2:C:243:ARG:HD2	2:C:256:TYR:CE1	2.49	0.47
3:D:664:LYS:C	3:D:666:ILE:H	2.17	0.47
3:D:704:ARG:HB2	3:D:745:MET:HE2	1.95	0.47
3:D:1240:THR:CG2	3:D:1251:ASP:OD2	2.63	0.47
3:D:1249:ALA:O	3:D:1250:ALA:HB3	2.15	0.47
3:D:1384:PRO:HB3	3:D:1389:LEU:O	2.13	0.47
5:F:82:ARG:HB2	7:H:8:DG:O6	2.14	0.47
5:F:358:LEU:HD13	5:F:370:LYS:HE3	1.96	0.47
2:C:480:THR:HG22	2:C:481:ASP:H	1.78	0.47
3:D:126:VAL:O	3:D:457:GLY:N	2.42	0.47
8:I:0:A:HO2'	8:I:1:A:P	2.31	0.47
1:A:47:SER:O	1:A:49:PRO:HD3	2.14	0.47
2:C:13:ILE:HD13	2:C:483:VAL:HG21	1.97	0.47
5:F:130:VAL:HG21	5:F:159:ILE:CG2	2.41	0.47
5:F:277:GLN:O	5:F:281:GLU:HG2	2.14	0.47
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.96	0.47
1:A:206:THR:HG22	1:A:208:LEU:N	2.29	0.47
2:C:181:VAL:HA	2:C:220:GLY:O	2.15	0.47
2:C:214:TYR:CB	2:C:217:LEU:HD12	2.45	0.47
2:C:1067:TYR:CE2	2:C:1071:ILE:HD13	2.50	0.47
3:D:407:VAL:HG12	5:F:172:ARG:HH12	1.78	0.47
3:D:776:GLU:OE2	3:D:1362:LYS:HD3	2.14	0.47
3:D:876:SER:OG	3:D:879:ARG:HG3	2.15	0.47
3:D:1047:LYS:CG	3:D:1053:PHE:CE1	2.96	0.47
2:C:711:GLU:OE2	2:C:816:LYS:HE3	2.14	0.47
5:F:101:GLU:OE1	5:F:105:LYS:CE	2.63	0.47
5:F:194:LEU:HB2	7:H:6:DT:O2	2.15	0.47
1:A:39:PRO:CG	1:B:39:PRO:CG	2.92	0.47
1:A:137:ARG:HG2	1:A:137:ARG:NH1	2.29	0.47
2:C:472:ARG:HD2	2:C:480:THR:O	2.15	0.47
2:C:976:ASP:OD1	2:C:978:ARG:HD3	2.14	0.47
3:D:236:TYR:HB3	3:D:313:MET:CG	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:422:ALA:H	3:D:427:VAL:HG13	1.80	0.47
5:F:95:THR:HG22	5:F:96:LEU:N	2.30	0.47
8:I:2:U:C2'	8:I:3:U:H5'	2.45	0.47
1:A:38:ASN:HB3	1:A:39:PRO:HD3	1.96	0.46
3:D:871:LYS:NZ	3:D:897:TRP:HE1	2.13	0.46
3:D:1014:ASN:OD1	3:D:1014:ASN:N	2.48	0.46
2:C:99:GLN:O	2:C:99:GLN:HG3	2.15	0.46
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.55	0.46
2:C:69:LEU:HB2	2:C:97:ARG:O	2.14	0.46
3:D:175:VAL:CG1	3:D:193:PRO:HD2	2.45	0.46
3:D:586:ARG:NH2	6:G:10:DC:H5"	2.30	0.46
3:D:895:VAL:HG11	3:D:922:LEU:HD21	1.96	0.46
3:D:959:GLU:O	3:D:963:TYR:HD1	1.99	0.46
3:D:983:LEU:HB3	3:D:987:GLU:HB2	1.98	0.46
3:D:1122:LEU:HD22	3:D:1140:ILE:HD13	1.97	0.46
3:D:1272:ALA:HA	3:D:1326:THR:HB	1.96	0.46
5:F:197:SER:HA	5:F:200:LYS:HE2	1.98	0.46
1:A:6:LEU:HD11	1:A:192:LEU:HD13	1.98	0.46
1:B:65:PHE:HD2	3:D:809:PRO:HB2	1.78	0.46
2:C:194:VAL:CG1	2:C:221:LEU:O	2.64	0.46
2:C:419:THR:HG22	2:C:420:ARG:H	1.80	0.46
2:C:486:MET:HE1	2:C:531:PHE:CE1	2.50	0.46
2:C:103:LYS:HD2	2:C:104:ASP:H	1.80	0.46
2:C:114:PHE:CD2	5:F:283:GLY:HA2	2.50	0.46
2:C:374:ASN:CG	5:F:276:ARG:HD2	2.33	0.46
2:C:569:VAL:HG21	2:C:1000:MET:HE1	1.97	0.46
3:D:284:LEU:HD22	3:D:288:MET:CE	2.45	0.46
3:D:586:ARG:O	3:D:586:ARG:NH1	2.48	0.46
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.97	0.46
1:A:191:ASP:OD1	2:C:938:LYS:NZ	2.29	0.46
2:C:428:ARG:NH2	2:C:447:ALA:O	2.48	0.46
2:C:466:PHE:N	2:C:466:PHE:CD1	2.84	0.46
6:G:18:DT:C2'	6:G:19:DG:H5'	2.40	0.46
2:C:182:VAL:CG2	2:C:193:LEU:HD23	2.45	0.46
2:C:194:VAL:HG11	2:C:221:LEU:O	2.16	0.46
1:A:185:ARG:NH2	1:A:187:GLY:O	2.49	0.46
2:C:164:PRO:CA	2:C:269:LEU:HD12	2.43	0.46
5:F:140:ARG:HE	5:F:140:ARG:HB2	1.52	0.46
2:C:136:ILE:HD13	2:C:392:SER:HA	1.97	0.46
2:C:290:LEU:O	2:C:301:GLU:HB2	2.16	0.46
2:C:322:VAL:CG1	2:C:323:ASP:N	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:769:PRO:HG3	3:D:65:ARG:CZ	2.46	0.46
3:D:618:LEU:HD12	3:D:618:LEU:HA	1.64	0.46
2:C:162:ILE:HG21	2:C:290:LEU:HD21	1.98	0.46
2:C:911:GLU:OE2	3:D:1062:ARG:HD3	2.16	0.46
3:D:4:GLU:OE2	3:D:6:ARG:HD3	2.16	0.46
3:D:46:ASP:OD1	3:D:48:ARG:HB2	2.17	0.45
3:D:361:VAL:O	3:D:382:GLU:HA	2.16	0.45
1:B:79:ILE:HA	1:B:82:LEU:HD12	1.97	0.45
1:B:95:GLN:NE2	1:B:146:ARG:HD2	2.31	0.45
3:D:471:GLU:H	3:D:471:GLU:HG2	1.58	0.45
1:B:208:LEU:HD12	1:B:208:LEU:O	2.16	0.45
2:C:722:ILE:HD12	2:C:821:GLU:CG	2.47	0.45
2:C:838:LYS:HE3	3:D:741:ASP:O	2.17	0.45
2:C:882:LEU:HD23	2:C:882:LEU:HA	1.66	0.45
3:D:553:ARG:HD2	3:D:570:GLU:OE2	2.15	0.45
2:C:198:ARG:NH2	2:C:203:ASP:OD1	2.49	0.45
1:A:206:THR:HG22	1:A:209:GLU:H	1.81	0.45
3:D:103:TRP:HB3	3:D:1448:THR:CG2	2.46	0.45
3:D:455:ARG:HH12	3:D:463:GLN:NE2	2.14	0.45
1:B:95:GLN:O	1:B:96:THR:HB	2.17	0.45
2:C:486:MET:HE1	2:C:494:TYR:CD2	2.52	0.45
2:C:797:GLY:O	2:C:829:GLN:NE2	2.49	0.45
2:C:911:GLU:CD	3:D:1062:ARG:HH11	2.19	0.45
3:D:135:LEU:O	3:D:149:LYS:HE3	2.17	0.45
3:D:486:ARG:HA	3:D:489:ARG:NH2	2.31	0.45
3:D:1248:GLY:O	3:D:1249:ALA:O	2.33	0.45
3:D:1261:GLU:OE1	3:D:1268:PRO:HA	2.16	0.45
3:D:1265:ALA:O	3:D:1333:HIS:HE1	2.00	0.45
1:B:141:GLU:OE1	1:B:161:ARG:NH2	2.50	0.45
2:C:184:MET:HB2	2:C:193:LEU:HD13	1.99	0.45
2:C:593:ALA:HB1	2:C:659:PRO:CD	2.47	0.45
3:D:134:VAL:CG2	3:D:151:GLN:H	2.30	0.45
3:D:972:LEU:HD12	3:D:972:LEU:HA	1.64	0.45
3:D:1092:GLY:HA3	6:G:14:DA:O4'	2.16	0.45
2:C:44:ILE:HD13	2:C:44:ILE:HA	1.61	0.45
2:C:206:THR:O	2:C:210:GLU:HB2	2.16	0.45
2:C:501:THR:HG21	2:C:513:VAL:HB	1.99	0.45
3:D:1364:HIS:CE1	3:D:1366:LYS:HB2	2.50	0.45
3:D:17:LYS:HE2	3:D:17:LYS:HB2	1.58	0.45
3:D:804:LEU:HB2	3:D:806:PHE:HE2	1.81	0.45
5:F:207:LEU:HD23	5:F:207:LEU:HA	1.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LYS:HE3	1:A:107:LYS:HB2	1.75	0.45
1:B:71:VAL:HG22	1:B:132:LEU:HG	1.99	0.45
2:C:470:PRO:CD	2:C:485:TYR:CE2	2.97	0.45
3:D:1144:LEU:O	3:D:1147:ARG:HG3	2.17	0.45
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	1.99	0.45
1:B:13:VAL:HG13	1:B:23:PHE:CE1	2.52	0.44
1:B:59:GLU:HB2	1:B:139:ASN:HB3	2.00	0.44
2:C:293:PHE:HD1	2:C:298:PHE:CE2	2.35	0.44
3:D:1036:ARG:NH2	3:D:1042:ARG:O	2.44	0.44
5:F:127:ILE:O	5:F:131:VAL:HG23	2.17	0.44
1:A:32:PHE:HA	1:A:35:THR:HB	1.99	0.44
3:D:399:ARG:NH1	3:D:448:GLU:OE2	2.51	0.44
3:D:880:ILE:HD13	3:D:880:ILE:HA	1.85	0.44
3:D:269:PHE:CE2	3:D:283:PHE:HD1	2.35	0.44
3:D:1216:SER:OG	4:E:16:LYS:HG2	2.17	0.44
4:E:54:LEU:C	4:E:55:PHE:HD2	2.20	0.44
5:F:114:LYS:O	5:F:117:SER:HB3	2.17	0.44
1:A:100:LEU:HD23	1:A:141:GLU:HG2	2.00	0.44
1:A:186:LEU:O	1:A:188:GLN:OE1	2.36	0.44
1:B:80:LEU:HB3	3:D:867:ARG:HH21	1.81	0.44
2:C:607:ASP:HB3	2:C:610:ARG:H	1.82	0.44
3:D:270:LEU:HD23	3:D:270:LEU:C	2.36	0.44
3:D:851:LEU:HD11	3:D:855:HIS:HE1	1.82	0.44
3:D:1478:SER:O	3:D:1482:ARG:HB2	2.17	0.44
5:F:229:TYR:CZ	5:F:230:LYS:HD3	2.52	0.44
1:A:29:GLU:O	1:A:32:PHE:HB2	2.17	0.44
2:C:580:MET:SD	2:C:584:GLU:HG3	2.57	0.44
3:D:204:LEU:HD23	3:D:204:LEU:HA	1.85	0.44
3:D:632:VAL:O	3:D:727:GLN:HA	2.16	0.44
1:A:11:PHE:CE1	1:B:225:PHE:HA	2.53	0.44
2:C:715:THR:HG22	2:C:716:LYS:N	2.32	0.44
3:D:174:GLY:HA2	3:D:389:GLU:OE2	2.18	0.44
5:F:82:ARG:NH2	7:H:9:DA:H61	2.15	0.44
2:C:100:LEU:HD23	2:C:367:LEU:O	2.18	0.44
3:D:12:LEU:HD23	3:D:12:LEU:HA	1.79	0.44
3:D:1232:PRO:O	3:D:1236:LEU:HG	2.18	0.44
3:D:1353:GLN:NE2	3:D:1365:ASP:OD2	2.38	0.44
5:F:361:LEU:HB2	5:F:366:ALA:HB2	1.99	0.44
6:G:19:DG:H2"	6:G:20:DT:O5'	2.18	0.44
2:C:462:ASP:HB3	2:C:468:ARG:HD2	2.00	0.44
3:D:1197:ARG:HB2	3:D:1398:TRP:CZ2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1386:ASP:N	3:D:1413:THR:CG2	2.81	0.44
1:B:85:LEU:HG	1:B:87:VAL:HG23	1.99	0.44
2:C:374:ASN:OD1	2:C:376:ARG:HG2	2.18	0.44
3:D:191:LEU:HB2	3:D:195:VAL:HG12	2.00	0.44
3:D:473:LEU:HD21	3:D:495:ARG:HH21	1.81	0.44
4:E:14:ASP:OD2	4:E:18:ARG:NH1	2.45	0.44
1:A:57:TYR:CE1	1:A:163:ASN:HB2	2.53	0.43
3:D:468:LEU:HD23	3:D:468:LEU:HA	1.77	0.43
2:C:269:LEU:HD12	2:C:269:LEU:HA	1.78	0.43
2:C:879:ARG:HD2	2:C:879:ARG:N	2.32	0.43
2:C:910:LYS:O	2:C:914:ILE:HG13	2.18	0.43
3:D:387:LEU:N	3:D:387:LEU:HD22	2.33	0.43
5:F:229:TYR:CE1	5:F:230:LYS:HD3	2.53	0.43
5:F:382:THR:OG1	5:F:385:GLU:HG3	2.18	0.43
2:C:10:ARG:NH2	2:C:12:VAL:HG12	2.33	0.43
2:C:394:PHE:CZ	2:C:632:ASN:CG	2.91	0.43
2:C:405:ARG:HD2	2:C:442:GLU:OE2	2.19	0.43
2:C:774:LEU:HD22	5:F:350:LEU:CD1	2.49	0.43
3:D:248:PRO:HG3	3:D:308:LYS:HG3	1.99	0.43
3:D:473:LEU:HD21	3:D:495:ARG:NH2	2.32	0.43
3:D:1284:GLU:O	3:D:1284:GLU:HG3	2.17	0.43
4:E:54:LEU:O	4:E:55:PHE:HD2	2.01	0.43
2:C:137:VAL:HG12	2:C:138:SER:O	2.19	0.43
2:C:197:LEU:HD12	2:C:221:LEU:HD21	2.00	0.43
3:D:129:PHE:CZ	3:D:571:LYS:HB3	2.53	0.43
7:H:16:DC:H2"	7:H:17:DC:OP2	2.16	0.43
1:A:34:VAL:HG22	1:B:42:ARG:CZ	2.49	0.43
2:C:409:ARG:HD2	2:C:452:ILE:HG22	2.00	0.43
2:C:627:ARG:NH1	2:C:640:ARG:HG3	2.34	0.43
2:C:679:PHE:HA	3:D:943:THR:HG23	2.00	0.43
2:C:722:ILE:O	2:C:722:ILE:HG22	2.18	0.43
3:D:130:SER:HB2	5:F:83:GLN:HE22	1.82	0.43
1:A:9:PRO:HD2	1:B:224:TYR:CD2	2.53	0.43
2:C:460:ARG:HD2	2:C:485:TYR:CE1	2.54	0.43
3:D:534:ARG:HD2	5:F:312:GLN:OE1	2.18	0.43
3:D:1385:GLY:CA	3:D:1413:THR:HG23	2.48	0.43
1:A:101:LEU:HD11	1:A:109:VAL:CG1	2.49	0.43
2:C:278:GLU:HG2	2:C:284:ARG:HA	2.00	0.43
2:C:545:ASN:HB3	2:C:583:LEU:HD22	2.01	0.43
2:C:575:GLN:HG3	2:C:670:GLN:HG3	2.00	0.43
2:C:582:GLY:N	2:C:584:GLU:OE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1057:SER:HB3	2:C:1058:ASP:H	1.38	0.43
3:D:122:GLU:HG2	3:D:152:LEU:HD11	2.00	0.43
3:D:371:ILE:HB	5:F:232:ARG:HH12	1.82	0.43
3:D:405:ASP:CB	3:D:423:ASP:OD1	2.66	0.43
3:D:576:GLU:OE2	5:F:80:PRO:HG3	2.19	0.43
3:D:1492:LEU:CD1	3:D:1493:LYS:HZ1	2.29	0.43
1:B:65:PHE:CE2	3:D:809:PRO:HB2	2.53	0.43
2:C:260:LEU:C	2:C:261:ILE:HD12	2.39	0.43
3:D:34:TYR:CE1	3:D:35:ARG:HG3	2.54	0.43
3:D:1152:GLU:HG2	3:D:1162:GLU:HB2	2.00	0.43
3:D:1197:ARG:HD2	3:D:1398:TRP:CE2	2.54	0.43
1:A:90:LEU:HD13	1:A:90:LEU:HA	1.66	0.43
1:B:99:LEU:HB2	1:B:142:VAL:HG22	2.00	0.43
2:C:144:PRO:CG	2:C:165:LEU:HD23	2.47	0.43
3:D:787:LEU:HD21	3:D:947:ILE:HG21	2.00	0.43
3:D:1195:GLN:O	3:D:1398:TRP:HZ3	2.02	0.43
1:B:197:LEU:HD23	1:B:197:LEU:HA	1.64	0.43
2:C:226:VAL:O	2:C:229:MET:HG2	2.19	0.43
2:C:627:ARG:NE	2:C:639:GLN:O	2.52	0.43
3:D:879:ARG:HB3	3:D:902:LEU:CD1	2.48	0.43
1:B:64:GLU:HA	1:B:165:ILE:HD13	2.01	0.42
1:B:101:LEU:HB2	1:B:114:PHE:CE1	2.54	0.42
2:C:202:TYR:OH	2:C:304:LEU:HB2	2.19	0.42
2:C:767:PRO:CB	2:C:771:GLU:HG2	2.49	0.42
2:C:939:ARG:HG2	2:C:939:ARG:H	1.40	0.42
2:C:1043:TYR:CG	3:D:763:MET:HG2	2.54	0.42
2:C:1066:ALA:HA	2:C:1077:PRO:HD2	2.01	0.42
3:D:536:ALA:HA	5:F:315:VAL:O	2.18	0.42
5:F:226:LYS:HB3	7:H:1:DT:H73	2.01	0.42
1:B:179:PHE:CB	1:B:197:LEU:HD23	2.48	0.42
2:C:258:TYR:CE2	2:C:293:PHE:HB2	2.54	0.42
2:C:436:GLY:HA2	2:C:538:GLN:O	2.19	0.42
2:C:673:LEU:HD12	2:C:673:LEU:HA	1.86	0.42
2:C:717:LEU:HD23	2:C:763:GLY:HA2	2.01	0.42
3:D:702:LEU:HD23	3:D:702:LEU:HA	1.65	0.42
1:A:79:ILE:CD1	1:A:165:ILE:HG21	2.49	0.42
1:B:92:PRO:O	1:B:146:ARG:NH1	2.43	0.42
2:C:54:ILE:HG21	2:C:355:VAL:HG11	2.01	0.42
2:C:469:THR:HG23	2:C:471:TYR:CE1	2.54	0.42
3:D:179:VAL:HB	3:D:183:GLU:CD	2.39	0.42
2:C:708:TYR:HB3	2:C:790:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:462:GLN:HB2	3:D:513:ILE:HG21	2.01	0.42
3:D:844:ALA:O	3:D:867:ARG:HB3	2.20	0.42
3:D:879:ARG:HB3	3:D:902:LEU:HD11	2.01	0.42
3:D:1278:ASP:O	3:D:1294:VAL:HG12	2.19	0.42
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.69	0.42
2:C:334:ARG:HB2	2:C:339:LEU:HD21	2.01	0.42
2:C:722:ILE:HD13	2:C:823:VAL:CG2	2.49	0.42
3:D:202:VAL:HG21	3:D:400:VAL:HG13	2.02	0.42
3:D:284:LEU:HD22	3:D:288:MET:HE2	2.00	0.42
3:D:335:LEU:HD23	3:D:335:LEU:HA	1.81	0.42
3:D:411:THR:HB	3:D:437:VAL:H	1.85	0.42
3:D:711:LEU:HD13	3:D:778:LEU:HD13	2.01	0.42
1:A:57:TYR:CD1	1:A:161:ARG:HD2	2.55	0.42
2:C:135:VAL:HG23	2:C:395:LYS:HG3	2.01	0.42
2:C:348:LEU:HA	2:C:348:LEU:HD12	1.79	0.42
2:C:391:LEU:HD23	2:C:391:LEU:HA	1.55	0.42
3:D:274:ARG:O	3:D:275:GLU:HB2	2.20	0.42
3:D:561:GLY:HA3	5:F:132:ARG:HD3	2.01	0.42
3:D:684:LYS:O	3:D:687:VAL:HG22	2.19	0.42
3:D:1296:SER:OG	3:D:1297:GLU:N	2.53	0.42
3:D:1493:LYS:HE3	3:D:1493:LYS:CA	2.34	0.42
1:A:206:THR:HG22	1:A:208:LEU:H	1.85	0.42
1:B:162:ILE:HG22	1:B:163:ASN:N	2.34	0.42
2:C:394:PHE:HE2	2:C:632:ASN:CB	2.19	0.42
2:C:875:GLY:O	2:C:879:ARG:HD3	2.19	0.42
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.82	0.42
3:D:715:ALA:HB3	3:D:764:LEU:HA	2.00	0.42
3:D:1046:GLN:OE1	3:D:1247:ALA:HB2	2.19	0.42
3:D:1493:LYS:HD2	3:D:1493:LYS:N	2.34	0.42
2:C:694:LEU:HD23	2:C:694:LEU:HA	1.76	0.42
1:A:228:PRO:HB3	1:B:13:VAL:HG21	2.01	0.42
1:B:86:VAL:HG12	1:B:123:MET:HG3	2.02	0.42
2:C:644:VAL:HG22	2:C:645:VAL:N	2.34	0.42
2:C:711:GLU:O	2:C:758:ARG:NH1	2.51	0.42
3:D:959:GLU:O	3:D:963:TYR:CD1	2.73	0.42
3:D:407:VAL:HA	3:D:422:ALA:CB	2.49	0.42
3:D:1283:ILE:CG1	3:D:1315:ASP:CG	2.84	0.42
5:F:315:VAL:HG22	5:F:316:SER:N	2.35	0.42
1:B:226:SER:O	1:B:228:PRO:HD3	2.19	0.41
2:C:174:LEU:HG	2:C:193:LEU:HD22	2.01	0.41
2:C:229:MET:HB2	2:C:233:GLU:CB	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:424:GLY:O	2:C:428:ARG:HD2	2.19	0.41
3:D:210:ARG:HA	3:D:345:TYR:O	2.19	0.41
3:D:428:LYS:HE2	3:D:428:LYS:HB3	1.85	0.41
3:D:897:TRP:HH2	3:D:902:LEU:HD22	1.83	0.41
3:D:1314:LYS:O	3:D:1317:ASP:HB2	2.20	0.41
4:E:46:PRO:HB2	4:E:57:ASP:HB3	2.00	0.41
6:G:12:DG:H5"	6:G:12:DG:C8	2.45	0.41
1:A:94:LEU:O	1:A:146:ARG:NH1	2.53	0.41
2:C:76:PRO:HA	2:C:77:PRO:HD3	1.93	0.41
2:C:129:ILE:HD11	2:C:386:PHE:CD2	2.55	0.41
2:C:926:PHE:HE1	2:C:929:ARG:NH1	2.17	0.41
3:D:23:TYR:CE2	3:D:89:ARG:HD3	2.54	0.41
3:D:156:GLU:CD	3:D:156:GLU:H	2.24	0.41
3:D:474:GLU:HG3	3:D:496:LEU:HD11	2.02	0.41
3:D:693:GLU:CB	4:E:48:MET:HE1	2.49	0.41
3:D:957:PRO:HG3	3:D:1007:VAL:HA	2.02	0.41
3:D:1286:THR:HG22	3:D:1287:GLU:N	2.35	0.41
8:I:2:U:O2'	8:I:3:U:H5'	2.20	0.41
1:A:11:PHE:O	1:B:228:PRO:HA	2.20	0.41
2:C:127:PHE:O	2:C:133:ASP:HA	2.21	0.41
2:C:473:ARG:HA	2:C:531:PHE:CD2	2.55	0.41
2:C:906:PHE:CE1	3:D:1067:VAL:HA	2.55	0.41
2:C:1001:VAL:CG1	3:D:630:VAL:HB	2.50	0.41
2:C:681:GLY:CA	3:D:939:PHE:CD2	3.03	0.41
3:D:501:ALA:CB	3:D:1452:ILE:HG22	2.48	0.41
3:D:1342:GLU:CD	3:D:1342:GLU:H	2.22	0.41
1:B:80:LEU:HD21	3:D:842:VAL:HG12	2.02	0.41
3:D:172:PRO:HB2	3:D:175:VAL:CG2	2.50	0.41
3:D:1099:VAL:HG13	3:D:1223:ILE:CD1	2.50	0.41
1:A:129:ILE:HD13	1:A:129:ILE:HA	1.84	0.41
1:B:206:THR:HG22	1:B:209:GLU:N	2.19	0.41
2:C:570:PRO:HD2	2:C:635:THR:HB	2.03	0.41
3:D:307:ALA:HB1	3:D:311:LEU:HD23	2.03	0.41
3:D:1161:GLU:CD	3:D:1164:ARG:HB2	2.41	0.41
3:D:1489:GLN:OE1	3:D:1489:GLN:HA	2.21	0.41
5:F:148:LYS:HE3	5:F:148:LYS:HB2	1.84	0.41
8:I:0:A:C2'	8:I:1:A:O5'	2.69	0.41
1:A:228:PRO:HB3	1:B:13:VAL:CG2	2.50	0.41
2:C:328:LEU:HD23	2:C:328:LEU:HA	1.71	0.41
2:C:595:LEU:HD21	2:C:623:TYR:HB3	2.03	0.41
2:C:678:PRO:HA	2:C:683:ASN:HD22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:625:TYR:CE1	3:D:751:LEU:HD11	2.55	0.41
3:D:832:ARG:HD3	3:D:832:ARG:HA	1.95	0.41
3:D:1028:ALA:O	3:D:1029:ARG:HG2	2.20	0.41
3:D:1312:LEU:HD21	3:D:1327:ARG:HG2	2.01	0.41
1:B:153:ALA:C	1:B:155:LYS:H	2.24	0.41
3:D:500:ARG:HH12	3:D:1390:LEU:HD21	1.84	0.41
5:F:287:THR:HG22	5:F:288:TYR:N	2.34	0.41
7:H:18:DG:H1'	7:H:19:DG:H5'	2.02	0.41
1:A:225:PHE:O	1:B:11:PHE:CE2	2.74	0.41
2:C:12:VAL:HG21	2:C:472:ARG:HD3	2.02	0.41
2:C:55:GLU:O	2:C:56:GLU:CB	2.52	0.41
2:C:69:LEU:HD23	2:C:69:LEU:HA	1.90	0.41
2:C:161:SER:HA	2:C:172:ILE:O	2.21	0.41
2:C:235:LEU:HD21	2:C:254:VAL:CG2	2.51	0.41
2:C:501:THR:HA	2:C:502:PRO:HD3	1.96	0.41
2:C:540:PHE:HB3	2:C:544:THR:HB	2.03	0.41
2:C:775:ARG:HH21	5:F:422:LEU:CD2	2.34	0.41
3:D:84:ILE:HD12	3:D:87:ARG:HD2	2.01	0.41
3:D:701:LEU:O	3:D:702:LEU:HD23	2.20	0.41
3:D:893:GLU:H	3:D:894:LYS:HZ3	1.67	0.41
3:D:1141:GLU:CD	3:D:1168:MET:HE1	2.40	0.41
3:D:1197:ARG:HB2	3:D:1398:TRP:CH2	2.56	0.41
3:D:1240:THR:HG21	3:D:1251:ASP:OD2	2.20	0.41
1:B:124:ASN:HD22	1:B:127:LEU:HD22	1.83	0.41
2:C:586:ARG:HA	2:C:586:ARG:HD2	1.86	0.41
2:C:880:MET:HB3	3:D:1061:PHE:CD2	2.56	0.41
3:D:1069:GLU:O	3:D:1073:SER:OG	2.39	0.41
3:D:1205:TYR:CZ	3:D:1366:LYS:HD3	2.55	0.41
1:A:10:VAL:HG23	1:A:10:VAL:O	2.21	0.40
2:C:100:LEU:CD2	2:C:367:LEU:O	2.69	0.40
2:C:197:LEU:HD23	2:C:197:LEU:HA	1.93	0.40
2:C:577:PRO:HB3	2:C:993:PHE:CG	2.57	0.40
3:D:103:TRP:O	3:D:107:ASP:HB3	2.21	0.40
3:D:169:TYR:OH	3:D:198:ARG:HB2	2.21	0.40
3:D:186:VAL:HG12	3:D:187:LYS:N	2.35	0.40
3:D:689:ASP:OD2	4:E:51:LEU:HD11	2.21	0.40
3:D:1099:VAL:O	3:D:1103:HIS:HB3	2.21	0.40
5:F:408:LEU:HD23	5:F:408:LEU:HA	1.89	0.40
1:A:22:GLU:C	1:A:23:PHE:CD2	2.95	0.40
1:A:115:LEU:HD23	1:A:115:LEU:HA	1.82	0.40
2:C:211:LEU:HD23	2:C:311:PHE:HD2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:681:GLY:HA2	3:D:939:PHE:CE2	2.56	0.40
2:C:926:PHE:CE2	2:C:930:LYS:HD3	2.56	0.40
3:D:216:VAL:HB	3:D:382:GLU:HG2	2.02	0.40
3:D:237:LYS:O	3:D:240:GLU:HB2	2.20	0.40
5:F:364:ARG:NH1	5:F:364:ARG:HB3	2.37	0.40
1:A:18:ARG:O	1:A:207:PRO:HD3	2.21	0.40
2:C:64:LEU:N	2:C:103:LYS:HE2	2.36	0.40
2:C:778:PHE:CD1	5:F:422:LEU:HD11	2.57	0.40
3:D:465:LEU:HD23	3:D:465:LEU:HA	1.81	0.40
4:E:46:PRO:HB2	4:E:57:ASP:HB2	2.03	0.40
6:G:18:DT:C4	8:I:0:A:N6	2.77	0.40
1:B:80:LEU:HD23	1:B:80:LEU:HA	1.95	0.40
2:C:53:PRO:HB3	2:C:67:ASP:OD1	2.21	0.40
2:C:98:LEU:HA	2:C:98:LEU:HD23	1.81	0.40
2:C:773:LEU:O	2:C:777:ILE:HG13	2.21	0.40
3:D:185:VAL:HG13	3:D:189:GLN:HB3	2.02	0.40
3:D:372:ASP:OD1	3:D:372:ASP:N	2.54	0.40
3:D:827:ILE:O	3:D:833:GLU:HA	2.22	0.40
3:D:1141:GLU:CG	3:D:1168:MET:HE1	2.51	0.40
3:D:1143:GLY:O	3:D:1147:ARG:CD	2.58	0.40
2:C:1095:LEU:HD23	3:D:582:LEU:HD22	2.03	0.40
3:D:659:LYS:HA	3:D:659:LYS:HD2	1.95	0.40
3:D:1305:LEU:HD23	3:D:1305:LEU:N	2.36	0.40
3:D:1441:GLN:HE21	3:D:1441:GLN:HB3	1.56	0.40
3:D:1493:LYS:HZ3	3:D:1496:GLU:HG3	1.84	0.40

All (2) 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)
3:D:985:ASP:N	3:D:1497:GLU:OE2[1_545]	2.09	0.11
3:D:34:TYR:OH	3:D:327:GLU:OE1[4_1359]	2.18	0.02

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	224/315 (71%)	221 (99%)	3 (1%)	0	100	100
1	B	220/315 (70%)	210 (96%)	9 (4%)	1 (0%)	29	60
2	C	1107/1119 (99%)	1078 (97%)	26 (2%)	3 (0%)	41	70
3	D	1498/1524 (98%)	1454 (97%)	39 (3%)	5 (0%)	41	70
4	E	92/99 (93%)	89 (97%)	2 (2%)	1 (1%)	14	41
5	F	344/423 (81%)	336 (98%)	5 (2%)	3 (1%)	17	46
All	All	3485/3795 (92%)	3388 (97%)	84 (2%)	13 (0%)	34	65

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	362	GLY
2	C	766	GLU
3	D	1242	HIS
3	D	1249	ALA
5	F	322	GLY
5	F	323	ASP
5	F	145	PRO
1	B	154	GLU
3	D	1244	GLY
3	D	320	ALA
4	E	94	PRO
2	C	415	PRO
3	D	530	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	199/273 (73%)	188 (94%)	11 (6%)	21	51
1	B	195/273 (71%)	190 (97%)	5 (3%)	46	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	930/941 (99%)	883 (95%)	47 (5%)	24	54
3	D	1258/1279 (98%)	1183 (94%)	75 (6%)	19	47
4	E	83/88 (94%)	81 (98%)	2 (2%)	49	78
5	F	298/371 (80%)	292 (98%)	6 (2%)	55	81
All	All	2963/3225 (92%)	2817 (95%)	146 (5%)	25	56

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	11	PHE
1	A	34	VAL
1	A	97	VAL
1	A	104	GLU
1	A	112	ARG
1	A	122	ILE
1	A	133	GLU
1	A	184	THR
1	A	186	LEU
1	A	189	ARG
1	B	34	VAL
1	B	186	LEU
1	B	189	ARG
1	B	199	ILE
1	B	206	THR
2	C	8	ARG
2	C	15	LEU
2	C	56	GLU
2	C	81	ASP
2	C	103	LYS
2	C	107	LEU
2	C	133	ASP
2	C	141	HIS
2	C	168	ARG
2	C	177	GLU
2	C	251	ASP
2	C	331	ARG
2	C	342	ASP
2	C	364	GLU
2	C	377	PRO
2	C	427	VAL

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Mol	Chain	Res	Type
2	C	429	ASP
2	C	434	HIS
2	C	449	ILE
2	C	454	SER
2	C	460	ARG
2	C	525	SER
2	C	557	ARG
2	C	575	GLN
2	C	583	LEU
2	C	586	ARG
2	C	589	ARG
2	C	591	SER
2	C	610	ARG
2	C	617	ASP
2	C	638	ASP
2	C	640	ARG
2	C	670	GLN
2	C	698	ASP
2	C	775	ARG
2	C	807	ARG
2	C	808	ARG
2	C	813	VAL
2	C	815	LEU
2	C	848	VAL
2	C	923	GLU
2	C	939	ARG
2	C	942	GLU
2	C	968	LEU
2	C	1001	VAL
2	C	1014	SER
2	C	1057	SER
3	D	30	GLU
3	D	68	PHE
3	D	81	THR
3	D	106	LYS
3	D	141	ILE
3	D	142	LEU
3	D	148	GLU
3	D	155	ASP
3	D	190	GLU
3	D	191	LEU
3	D	198	ARG

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Mol	Chain	Res	Type
3	D	200	ASP
3	D	230	TRP
3	D	231	VAL
3	D	256	GLU
3	D	272	LEU
3	D	276	ASP
3	D	312	ARG
3	D	325	GLU
3	D	362	GLU
3	D	372	ASP
3	D	411	THR
3	D	421	LEU
3	D	525	ARG
3	D	572	ARG
3	D	587	ARG
3	D	610	LYS
3	D	618	LEU
3	D	650	LEU
3	D	685	ASP
3	D	709	HIS
3	D	754	PHE
3	D	778	LEU
3	D	784	ASP
3	D	808	THR
3	D	817	GLU
3	D	832	ARG
3	D	864	VAL
3	D	867	ARG
3	D	875	THR
3	D	894	LYS
3	D	904	VAL
3	D	970	LYS
3	D	972	LEU
3	D	984	THR
3	D	1041	LEU
3	D	1051	GLU
3	D	1062	ARG
3	D	1073	SER
3	D	1130	ARG
3	D	1155	VAL
3	D	1162	GLU
3	D	1188	VAL

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Mol	Chain	Res	Type
3	D	1195	GLN
3	D	1208	ASP
3	D	1219	GLU
3	D	1221	VAL
3	D	1252	ILE
3	D	1271	LYS
3	D	1284	GLU
3	D	1288	GLU
3	D	1290	LEU
3	D	1296	SER
3	D	1301	LYS
3	D	1305	LEU
3	D	1307	LYS
3	D	1308	GLU
3	D	1313	VAL
3	D	1317	ASP
3	D	1351	GLU
3	D	1470	ARG
3	D	1493	LYS
3	D	1496	GLU
3	D	1499	ARG
3	D	1500	LYS
4	E	50	THR
4	E	89	MET
5	F	120	THR
5	F	186	HIS
5	F	205	ARG
5	F	364	ARG
5	F	377	ASP
5	F	415	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	63	HIS
1	B	212	ASN
2	C	343	GLN
2	C	683	ASN
2	C	834	GLN
3	D	294	HIS
3	D	463	GLN
3	D	611	GLN

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Mol	Chain	Res	Type
3	D	640	HIS
3	D	724	GLN
3	D	744	GLN
3	D	991	GLN
3	D	1195	GLN
3	D	1323	GLN
3	D	1333	HIS
3	D	1359	GLN
4	E	49	GLN
5	F	83	GLN
5	F	86	HIS
5	F	90	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	3/4 (75%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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	UTP	D	2005	9	22,30,30	4.89	6 (27%)	27,47,47	1.51	4 (14%)

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	UTP	D	2005	9	-	8/20/38/38	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	2005	UTP	O4'-C1'	15.35	1.62	1.41
11	D	2005	UTP	C2'-C1'	-14.04	1.32	1.53
11	D	2005	UTP	O4'-C4'	-7.09	1.29	1.45
11	D	2005	UTP	O2'-C2'	3.96	1.52	1.43
11	D	2005	UTP	C5'-C4'	2.96	1.60	1.51
11	D	2005	UTP	PA-O5'	2.27	1.68	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	D	2005	UTP	PB-O3A-PA	-4.03	118.99	132.83
11	D	2005	UTP	C3'-C2'-C1'	3.12	105.68	100.98
11	D	2005	UTP	O2'-C2'-C3'	2.58	120.17	111.82
11	D	2005	UTP	C2'-C3'-C4'	2.27	107.05	102.64

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	D	2005	UTP	C5'-O5'-PA-O1A
11	D	2005	UTP	C5'-O5'-PA-O3A
11	D	2005	UTP	C3'-C4'-C5'-O5'
11	D	2005	UTP	O4'-C4'-C5'-O5'
11	D	2005	UTP	C4'-C5'-O5'-PA
11	D	2005	UTP	C5'-O5'-PA-O2A
11	D	2005	UTP	PB-O3A-PA-O2A
11	D	2005	UTP	PB-O3A-PA-O1A

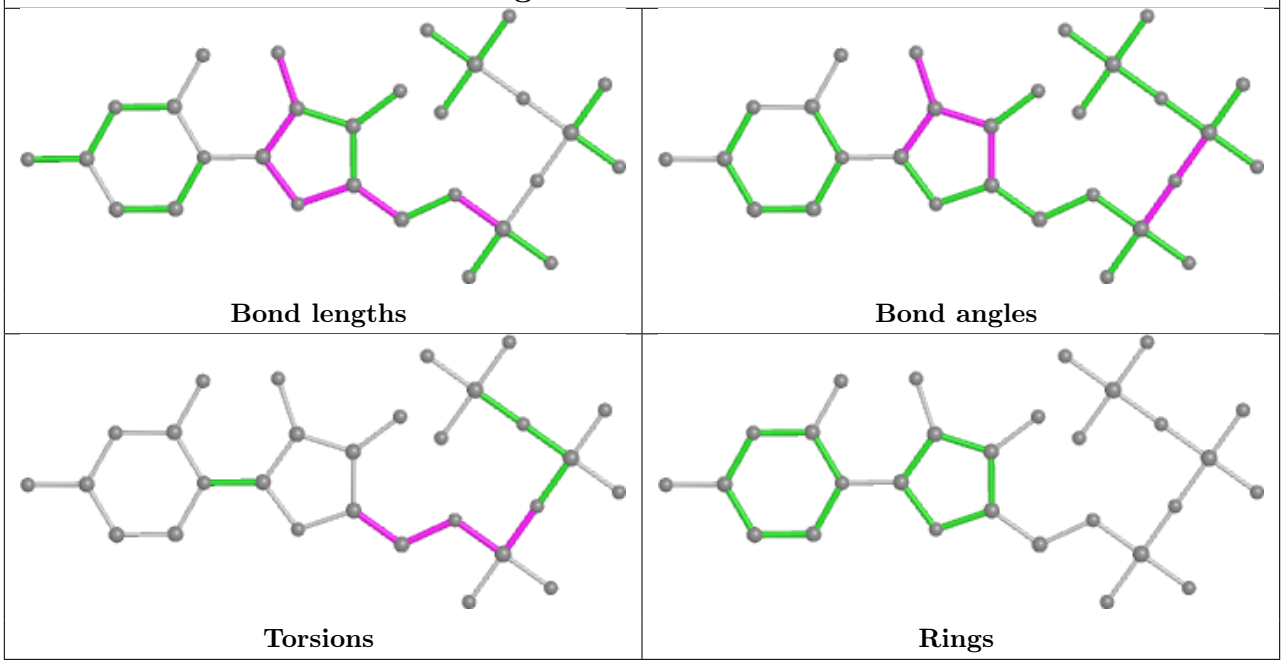
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	2005	UTP	1	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 then 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.

Ligand UTP D 2005



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	226/315 (71%)	-0.15	0	100	100	54, 77, 100, 109	0
1	B	222/315 (70%)	-0.21	0	100	100	52, 77, 106, 122	0
2	C	1111/1119 (99%)	0.27	70 (6%)	20	17	38, 80, 149, 164	0
3	D	1500/1524 (98%)	0.11	56 (3%)	41	38	36, 73, 127, 171	0
4	E	94/99 (94%)	-0.03	3 (3%)	47	44	48, 85, 133, 147	0
5	F	346/423 (81%)	0.03	12 (3%)	44	40	49, 93, 137, 149	0
6	G	15/21 (71%)	-0.08	0	100	100	49, 77, 152, 153	0
7	H	16/27 (59%)	-0.79	0	100	100	73, 99, 129, 129	0
8	I	4/4 (100%)	0.01	0	100	100	56, 62, 80, 107	0
All	All	3534/3847 (91%)	0.11	141 (3%)	38	35	36, 78, 138, 171	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	207	LEU	6.4
2	C	189	ARG	5.6
3	D	1287	GLU	5.5
2	C	66	LEU	5.5
3	D	1502	ALA	5.4
2	C	221	LEU	5.0
3	D	1495	ILE	4.9
2	C	107	LEU	4.8
2	C	242	LEU	4.7
2	C	64	LEU	4.6
3	D	1313	VAL	4.5
2	C	190	LYS	4.2
2	C	293	PHE	4.2
2	C	188	LYS	4.0
2	C	251	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
5	F	422	LEU	4.0
2	C	365	ASP	4.0
2	C	211	LEU	4.0
5	F	149	GLU	3.9
2	C	219	GLN	3.9
2	C	186	VAL	3.8
3	D	1245	GLY	3.8
3	D	1499	ARG	3.8
4	E	84	ARG	3.8
2	C	228	ALA	3.7
3	D	1288	GLU	3.7
3	D	1244	GLY	3.6
2	C	367	LEU	3.6
2	C	187	ASN	3.6
2	C	226	VAL	3.6
3	D	1297	GLU	3.6
2	C	358	ARG	3.5
2	C	814	GLU	3.5
3	D	1414	PRO	3.4
2	C	811	PRO	3.4
3	D	1300	SER	3.4
2	C	222	MET	3.4
5	F	148	LYS	3.3
2	C	249	LYS	3.2
5	F	420	ASP	3.2
2	C	98	LEU	3.2
2	C	372	LEU	3.2
2	C	362	GLY	3.1
5	F	147	LEU	3.1
3	D	1307	LYS	3.1
2	C	311	PHE	3.0
3	D	1128	VAL	3.0
2	C	158	TYR	3.0
2	C	191	PHE	3.0
3	D	971	LEU	3.0
3	D	361	VAL	3.0
2	C	236	ILE	2.9
2	C	238	LEU	2.9
3	D	337	LEU	2.9
3	D	191	LEU	2.9
2	C	296	GLY	2.8
3	D	339	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
3	D	322	VAL	2.8
2	C	153	ALA	2.8
2	C	366	SER	2.8
3	D	379	ALA	2.7
5	F	416	ARG	2.7
3	D	430	ASP	2.7
2	C	171	TRP	2.7
2	C	102	HIS	2.7
2	C	181	VAL	2.7
3	D	980	MET	2.7
2	C	300	ASP	2.6
2	C	810	ASP	2.6
3	D	1131	SER	2.6
2	C	250	ARG	2.6
3	D	241	ILE	2.6
2	C	205	GLU	2.5
2	C	196	LEU	2.5
2	C	253	ALA	2.5
3	D	310	LEU	2.5
3	D	235	ALA	2.5
2	C	364	GLU	2.4
3	D	1327	ARG	2.4
2	C	778	PHE	2.4
3	D	220	ARG	2.4
3	D	355	VAL	2.4
2	C	808	ARG	2.4
3	D	1318	TYR	2.4
3	D	336	PHE	2.4
2	C	244	PRO	2.4
3	D	1299	PHE	2.4
5	F	172	ARG	2.4
3	D	1240	THR	2.4
5	F	417	LYS	2.3
2	C	176	VAL	2.3
2	C	243	ARG	2.3
3	D	144	GLY	2.3
3	D	1304	LYS	2.3
2	C	729	LEU	2.3
2	C	254	VAL	2.3
5	F	142	ARG	2.3
2	C	195	LEU	2.3
3	D	409	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
3	D	371	ILE	2.3
3	D	321	GLN	2.3
5	F	159	ILE	2.3
3	D	360	ARG	2.3
2	C	10	ARG	2.2
3	D	1292	VAL	2.2
2	C	255	ALA	2.2
3	D	678	GLU	2.2
2	C	179	ASN	2.2
2	C	292	ARG	2.2
2	C	174	LEU	2.2
2	C	217	LEU	2.2
3	D	335	LEU	2.2
3	D	974	ILE	2.2
2	C	104	ASP	2.2
3	D	225	LEU	2.2
2	C	105	THR	2.2
2	C	115	LEU	2.1
3	D	1278	ASP	2.1
2	C	54	ILE	2.1
2	C	617	ASP	2.1
3	D	395	VAL	2.1
3	D	367	ILE	2.1
2	C	208	ALA	2.1
3	D	242	LEU	2.1
3	D	1129	THR	2.1
3	D	1243	THR	2.1
2	C	512	ARG	2.1
5	F	419	ARG	2.1
2	C	616	GLU	2.1
2	C	182	VAL	2.1
3	D	173	PRO	2.1
3	D	1319	VAL	2.0
5	F	392	VAL	2.0
3	D	161	LEU	2.0
3	D	1301	LYS	2.0
4	E	86	GLN	2.0
2	C	371	LYS	2.0
4	E	2	ALA	2.0
3	D	982	PHE	2.0
3	D	432	TYR	2.0
2	C	413	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

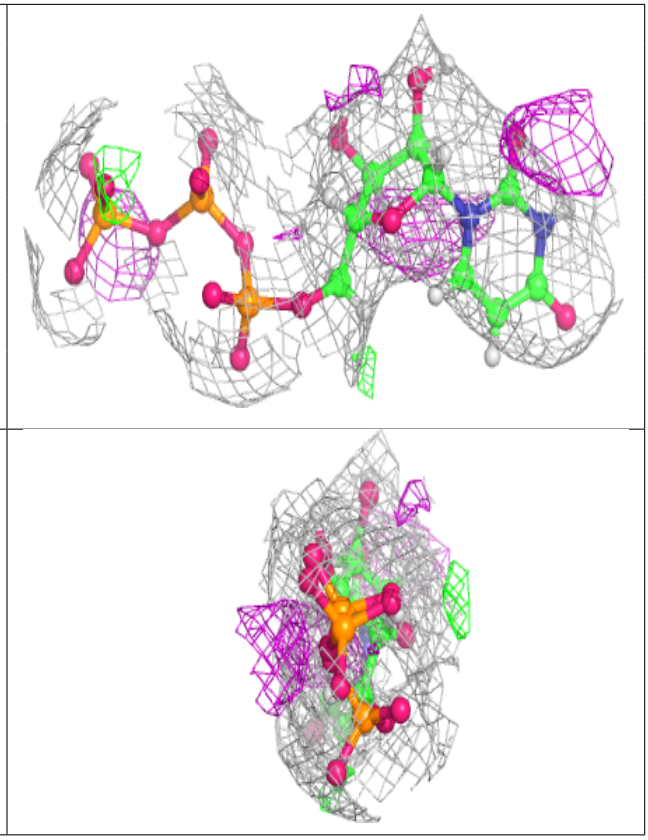
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	UTP	D	2005	29/29	0.90	0.18	53,71,98,110	0
9	MG	D	2002	1/1	0.94	0.36	65,65,65,65	0
10	ZN	D	2003	1/1	0.99	0.24	66,66,66,66	0
10	ZN	D	2004	1/1	0.99	0.12	103,103,103,103	0
9	MG	D	2001	1/1	0.99	0.24	40,40,40,40	0

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

Electron density around UTP D 2005:

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



6.5 Other polymers (i)

There are no such residues in this entry.