Full wwPDB X-ray Structure Validation Report ⓘ

Jul 16, 2024 – 04:21 PM JST

PDB ID	:	8W8P
Title	:	Thermus thermophilus initiation transcription complex containing CMPcPP in the post-translocated state
Authors	:	Li, L.; Zhang, Y.
Deposited on	:	2023-09-04
Resolution	:	3.17 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:

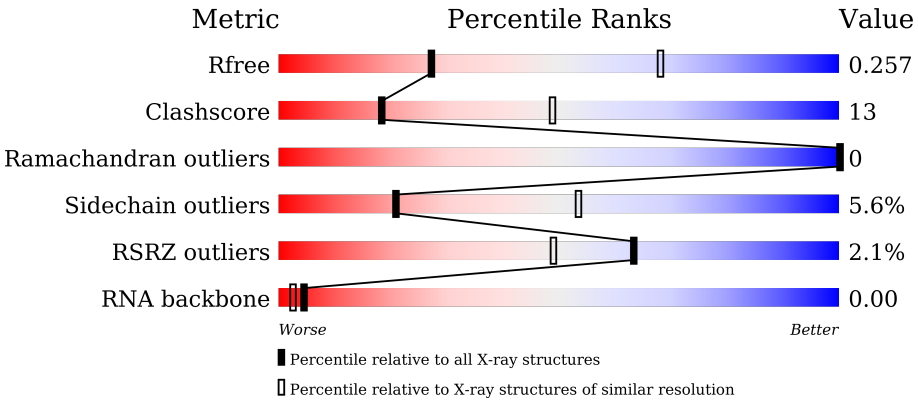
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.17 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.



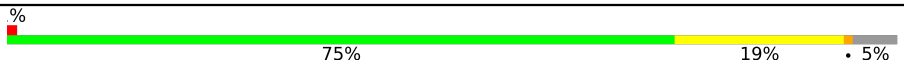
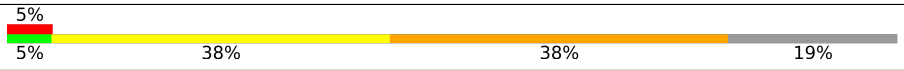
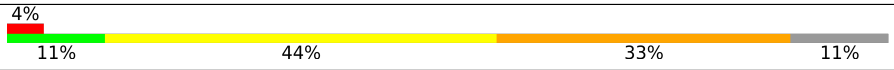
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)
RNA backbone	3102	1073 (3.50-2.82)

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	50% 20% 27%
1	B	315	2% 48% 23% 28%
2	C	1119	65% 32%
3	D	1524	3% 65% 31%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	99	
5	F	443	
6	G	21	
7	H	27	
8	I	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	MG	D	1604	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 28769 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	231	Total	C	N	O	S	0	0	0
			1809	1155	315	337	2			
1	B	227	Total	C	N	O	S	0	0	0
			1789	1143	310	334	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1112	Total	C	N	O	S	0	0	0
			8771	5547	1565	1635	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1497	Total	C	N	O	S	0	1	0
			11817	7488	2085	2208	36			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2804	1769	509	522	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	expression tag	UNP Q5SKW1
F	-18	GLY	-	expression tag	UNP Q5SKW1
F	-17	SER	-	expression tag	UNP Q5SKW1
F	-16	SER	-	expression tag	UNP Q5SKW1
F	-15	HIS	-	expression tag	UNP Q5SKW1
F	-14	HIS	-	expression tag	UNP Q5SKW1
F	-13	HIS	-	expression tag	UNP Q5SKW1
F	-12	HIS	-	expression tag	UNP Q5SKW1
F	-11	HIS	-	expression tag	UNP Q5SKW1
F	-10	HIS	-	expression tag	UNP Q5SKW1
F	-9	SER	-	expression tag	UNP Q5SKW1
F	-8	SER	-	expression tag	UNP Q5SKW1
F	-7	GLY	-	expression tag	UNP Q5SKW1
F	-6	LEU	-	expression tag	UNP Q5SKW1
F	-5	VAL	-	expression tag	UNP Q5SKW1
F	-4	PRO	-	expression tag	UNP Q5SKW1
F	-3	ARG	-	expression tag	UNP Q5SKW1
F	-2	GLY	-	expression tag	UNP Q5SKW1
F	-1	SER	-	expression tag	UNP Q5SKW1
F	0	HIS	-	expression tag	UNP Q5SKW1

- Molecule 6 is a DNA chain called DNA (21-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	17	Total	C	N	O	P	0	0	0
			347	165	66	100	16			

- Molecule 7 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	24	Total	C	N	O	P	0	0	0
			495	236	94	142	23			

- Molecule 8 is a RNA chain called RNA (5'-(GTP)GA-3').

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

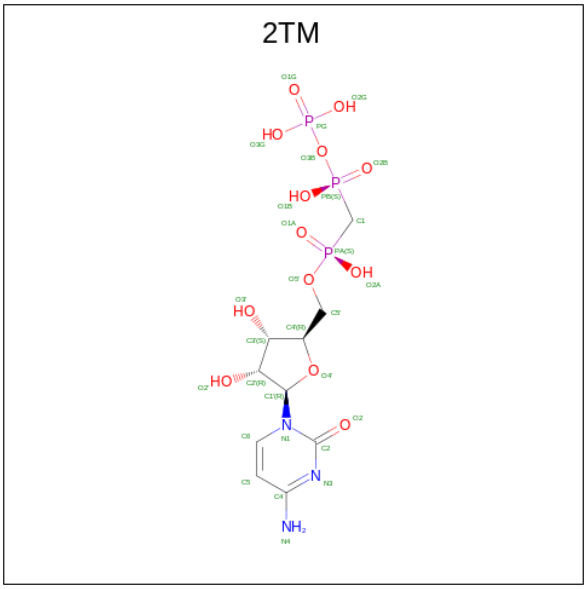
- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	2	Total Mg 2 2	0	0
9	D	3	Total Mg 3 3	0	0
9	F	1	Total Mg 1 1	0	0

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

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

- Molecule 11 is 5'-O-[(S)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]methyl}phosphoryl]cytidine (three-letter code: 2TM) (formula: $C_{10}H_{18}N_3O_{13}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	D	1	Total C N O P 29 10 3 13 3	0	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	3	Total O 3 3	0	0
12	B	4	Total O 4 4	0	0

Continued on next page...

Continued from previous page...

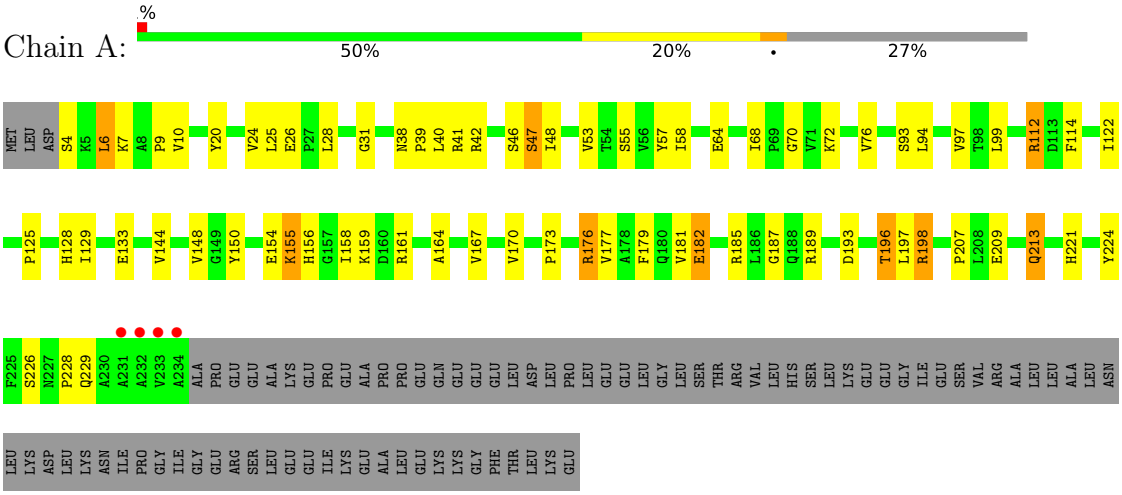
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	19	Total O 19 19	0	0
12	D	24	Total O 24 24	0	0
12	E	2	Total O 2 2	0	0
12	F	1	Total O 1 1	0	0
12	G	5	Total O 5 5	0	0
12	H	1	Total O 1 1	0	0
12	I	3	Total O 3 3	0	0

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.

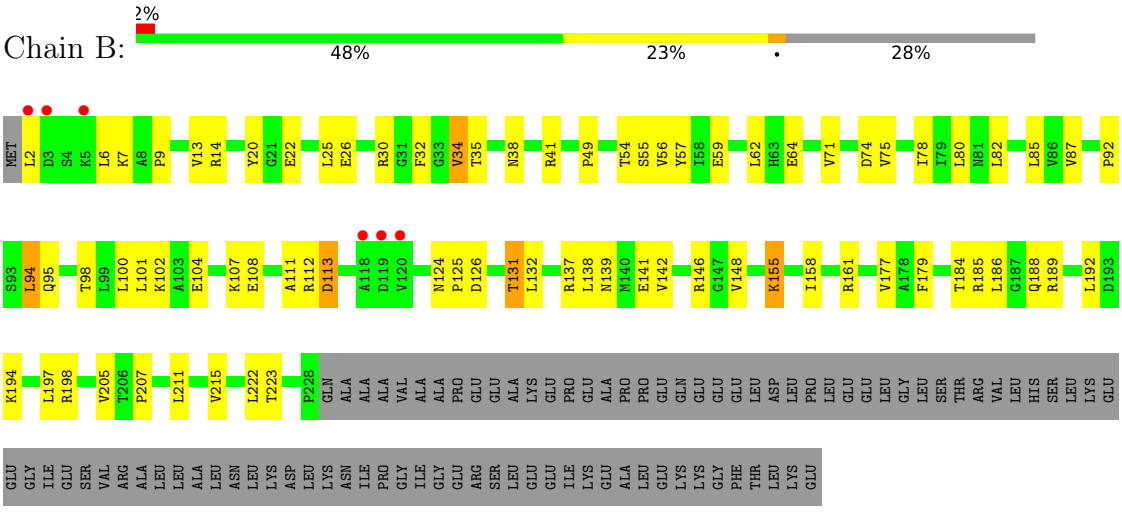
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



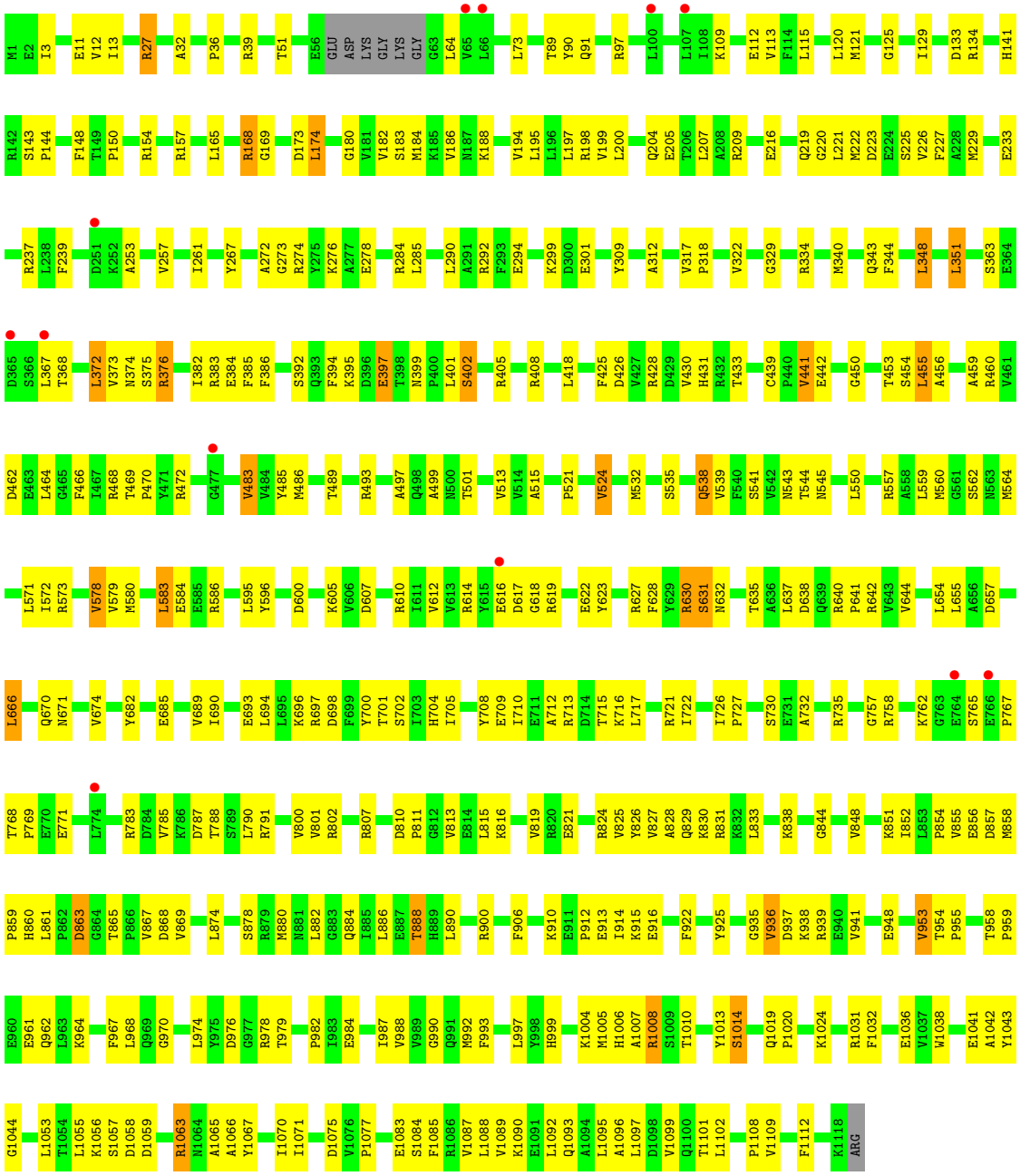
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:

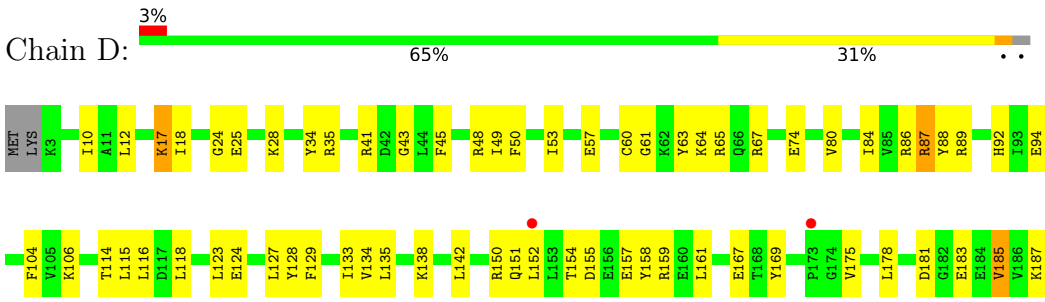


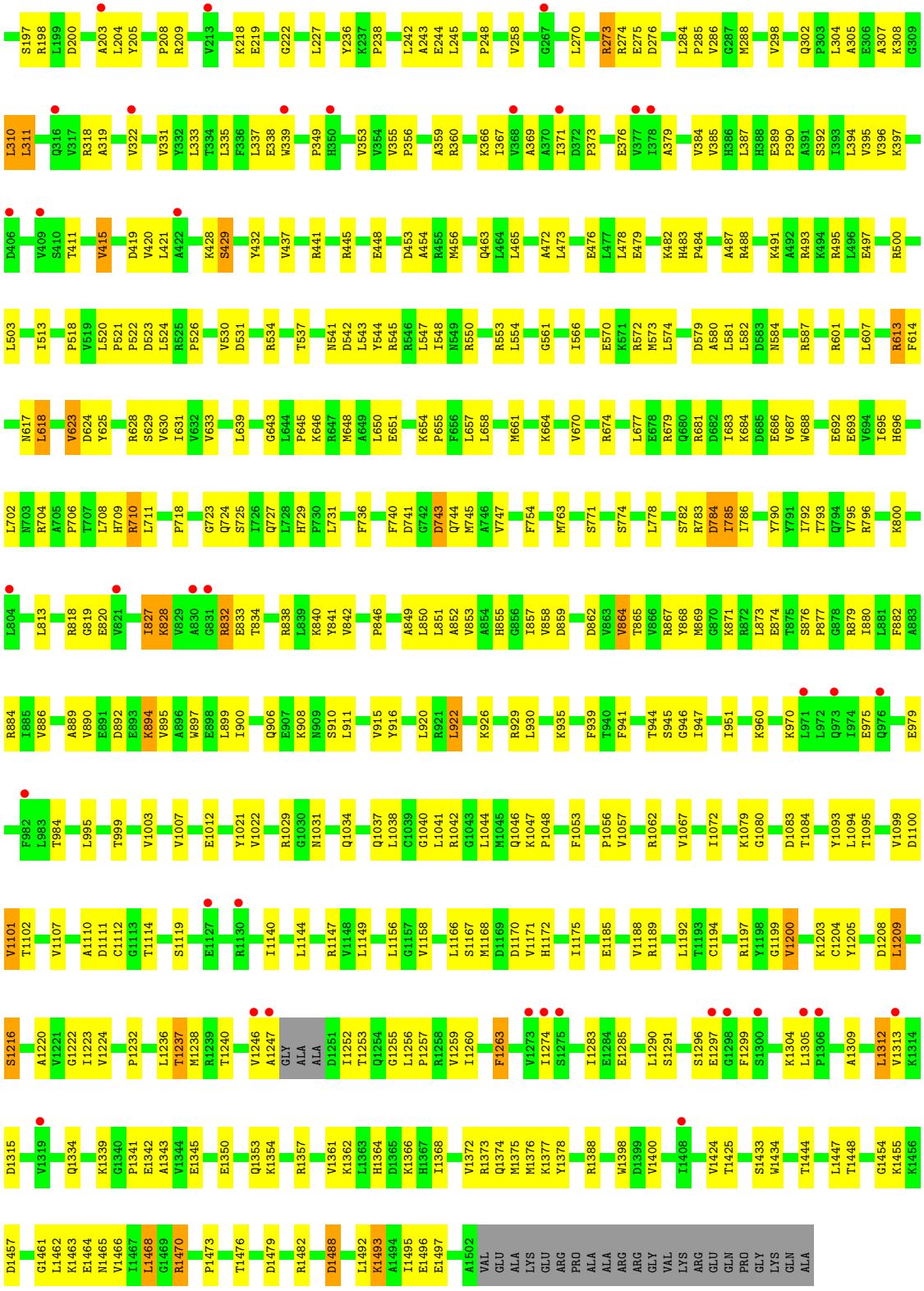
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C:



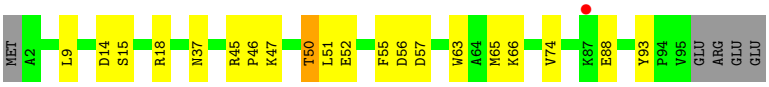
• Molecule 3: DNA-directed RNA polymerase subunit beta'





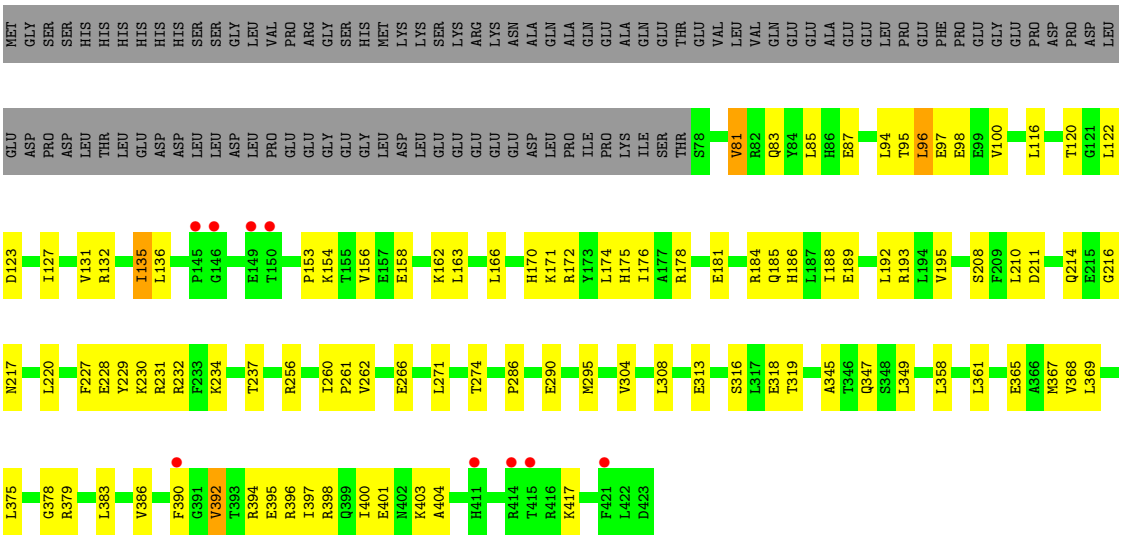
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:



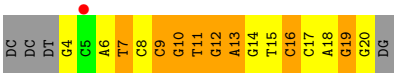
• Molecule 5: RNA polymerase sigma factor SigA

Chain F:



• Molecule 6: DNA (21-MER)

Chain G:



• Molecule 7: DNA (27-MER)

Chain H:

• Molecule 8: RNA (5'-(GTP)GA-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	184.68Å 103.89Å 294.61Å 90.00° 98.97° 90.00°	Depositor
Resolution (Å)	39.76 – 3.17 39.75 – 3.17	Depositor EDS
% Data completeness (in resolution range)	94.4 (39.76-3.17) 94.5 (39.75-3.17)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 3.18Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.211 , 0.257 0.211 , 0.257	Depositor DCC
R_{free} test set	2014 reflections (2.26%)	wwPDB-VP
Wilson B-factor (Å^2)	57.6	Xtriage
Anisotropy	0.957	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 38.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.025 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h+1/2*k-l 0.025 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h-1/2*k-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	28769	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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: ZN, 2TM, MG, 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	0.50	0/1841	0.66	0/2504
1	B	0.45	0/1821	0.60	0/2476
2	C	0.48	0/8938	0.63	0/12088
3	D	0.48	0/12027	0.62	0/16261
4	E	0.46	0/775	0.59	0/1045
5	F	0.45	0/2849	0.61	0/3833
6	G	0.64	0/389	1.60	13/599 (2.2%)
7	H	0.76	0/556	1.47	12/858 (1.4%)
8	I	0.51	0/50	1.36	1/76 (1.3%)
All	All	0.49	0/29246	0.68	26/39740 (0.1%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	H	3	DT	P-O3'-C3'	-11.83	105.51	119.70
7	H	15	DT	P-O3'-C3'	-11.29	106.15	119.70
6	G	15	DT	P-O3'-C3'	-10.58	107.01	119.70
6	G	14	DG	P-O3'-C3'	-10.02	107.67	119.70
6	G	9	DC	P-O3'-C3'	-9.74	108.01	119.70
6	G	17	DC	P-O3'-C3'	-8.96	108.95	119.70
6	G	16	DC	P-O3'-C3'	-8.94	108.97	119.70
6	G	11	DT	P-O3'-C3'	-8.64	109.33	119.70
6	G	19	DG	P-O3'-C3'	-8.32	109.72	119.70
7	H	13	DT	P-O3'-C3'	-8.29	109.75	119.70
7	H	8	DG	P-O3'-C3'	-8.00	110.10	119.70
8	I	6	G	P-O3'-C3'	-7.86	110.27	119.70
7	H	2	DA	P-O3'-C3'	-7.82	110.32	119.70
7	H	9	DG	P-O3'-C3'	-7.77	110.38	119.70
6	G	8	DC	P-O3'-C3'	-7.63	110.54	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	H	4	DA	P-O3'-C3'	-7.54	110.65	119.70
6	G	12	DG	P-O3'-C3'	-7.35	110.88	119.70
7	H	6	DT	P-O3'-C3'	-7.26	110.99	119.70
7	H	7	DG	P-O3'-C3'	-6.91	111.41	119.70
7	H	1	DT	P-O3'-C3'	-6.77	111.58	119.70
6	G	18	DA	P-O3'-C3'	-6.67	111.69	119.70
7	H	14	DG	P-O3'-C3'	-6.67	111.70	119.70
6	G	10	DG	P-O3'-C3'	-6.26	112.19	119.70
6	G	7	DT	P-O3'-C3'	-6.25	112.20	119.70
6	G	13	DA	P-O3'-C3'	-5.82	112.72	119.70
7	H	5	DA	P-O3'-C3'	-5.31	113.33	119.70

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	1809	0	1863	49	0
1	B	1789	0	1841	50	0
2	C	8771	0	8868	275	0
3	D	11817	0	12044	352	0
4	E	761	0	778	13	0
5	F	2804	0	2880	67	0
6	G	347	0	192	13	0
7	H	495	0	272	27	0
8	I	77	0	34	1	0
9	B	2	0	0	0	0
9	D	3	0	0	0	0
9	F	1	0	0	0	0
10	D	2	0	0	0	0
11	D	29	0	14	4	0
12	A	3	0	0	0	0
12	B	4	0	0	1	0
12	C	19	0	0	7	0
12	D	24	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	E	2	0	0	0	0
12	F	1	0	0	0	0
12	G	5	0	0	0	0
12	H	1	0	0	0	0
12	I	3	0	0	0	0
All	All	28769	0	28786	766	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 (766) 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)
2:C:1057:SER:HA	12:C:1202:HOH:O	1.44	1.18
2:C:993:PHE:HB3	12:C:1201:HOH:O	1.46	1.15
3:D:236:TYR:CE2	3:D:322:VAL:HG21	1.95	1.02
2:C:579:VAL:HG23	12:C:1206:HOH:O	1.60	1.01
3:D:1102:THR:HG22	3:D:1222:GLY:CA	1.97	0.92
7:H:8:DG:H2"	7:H:9:DG:H5"	1.52	0.92
3:D:236:TYR:CD2	3:D:322:VAL:HG21	2.06	0.90
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.51	0.90
3:D:1102:THR:CG2	3:D:1222:GLY:CA	2.50	0.90
2:C:693:GLU:OE2	2:C:855:VAL:HG21	1.73	0.89
2:C:628:PHE:H	2:C:638:ASP:HB3	1.39	0.88
3:D:1102:THR:HG22	3:D:1222:GLY:HA3	1.57	0.86
2:C:769:PRO:HG3	3:D:65:ARG:HH12	1.40	0.86
1:B:185:ARG:HH22	3:D:692:GLU:HG3	1.42	0.84
1:B:80:LEU:HD21	3:D:842:VAL:HG12	1.60	0.83
2:C:693:GLU:HG2	2:C:696:LYS:HD2	1.59	0.82
5:F:120:THR:HG23	5:F:122:LEU:H	1.42	0.82
5:F:95:THR:HB	5:F:98:GLU:HG3	1.62	0.81
3:D:1216:SER:HB3	4:E:15:SER:HA	1.63	0.80
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.65	0.78
2:C:198:ARG:HE	2:C:227:PHE:HA	1.48	0.78
2:C:395:LYS:HD3	2:C:397:GLU:HG2	1.66	0.78
6:G:4:DG:H1	7:H:24:DC:H42	1.29	0.78
2:C:397:GLU:HG3	2:C:632:ASN:HB2	1.68	0.76
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.66	0.76
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.67	0.75
3:D:244:GLU:HG3	3:D:310:LEU:HD22	1.69	0.74
2:C:144:PRO:HB2	2:C:273:GLY:HA3	1.69	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:GLU:OE2	2:C:830:LYS:NZ	2.20	0.74
2:C:428:ARG:HB3	2:C:450:GLY:HA3	1.67	0.74
3:D:1102:THR:CG2	3:D:1222:GLY:HA2	2.17	0.74
5:F:316:SER:HB3	5:F:319:THR:HG23	1.69	0.74
2:C:802:ARG:HB2	2:C:826:TYR:HB2	1.68	0.74
3:D:187:LYS:HA	12:D:1701:HOH:O	1.88	0.73
2:C:32:ALA:HB2	2:C:73:LEU:HD12	1.71	0.72
5:F:395:GLU:OE2	5:F:398:ARG:NH2	2.23	0.72
2:C:274:ARG:NH2	2:C:285:LEU:O	2.23	0.71
2:C:1019:GLN:NE2	3:D:617:ASN:HB3	2.05	0.71
2:C:1019:GLN:HE22	3:D:617:ASN:HB3	1.55	0.71
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	1.72	0.71
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.23	0.71
6:G:9:DC:H2'	6:G:10:DG:C8	2.25	0.71
6:G:12:DG:H2'	6:G:13:DA:C8	2.26	0.71
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.73	0.70
3:D:1044:LEU:HD23	3:D:1056:PRO:HB3	1.74	0.70
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.74	0.69
2:C:344:PHE:CD2	2:C:382:ILE:HD11	2.29	0.68
7:H:9:DG:H2"	7:H:10:DA:C8	2.28	0.68
3:D:792:ILE:HG13	3:D:793:THR:HG23	1.75	0.68
2:C:13:ILE:HD13	2:C:483:VAL:HG21	1.75	0.68
2:C:605:LYS:HD3	2:C:610:ARG:HH12	1.59	0.68
2:C:1067:TYR:OH	3:D:674[A]:ARG:NH1	2.27	0.68
5:F:116:LEU:O	5:F:120:THR:HG22	1.94	0.68
3:D:695:ILE:HD12	3:D:718:PRO:HG2	1.75	0.68
2:C:674:VAL:HG22	2:C:869:VAL:HG22	1.75	0.67
3:D:243:ALA:HB3	3:D:311:LEU:HD11	1.75	0.67
3:D:677:LEU:HD21	3:D:687:VAL:HG21	1.75	0.67
5:F:172:ARG:O	5:F:176:ILE:HG12	1.95	0.67
3:D:65:ARG:NH1	5:F:378:GLY:O	2.27	0.67
2:C:758:ARG:HH21	2:C:788:THR:HB	1.61	0.66
1:B:132:LEU:HD21	1:B:138:LEU:HB2	1.78	0.66
3:D:1102:THR:HG21	3:D:1222:GLY:O	1.96	0.66
3:D:1144:LEU:O	3:D:1147:ARG:HG3	1.96	0.66
3:D:236:TYR:HE2	3:D:322:VAL:HG21	1.58	0.66
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.78	0.66
3:D:18:ILE:HD13	3:D:518:PRO:HG3	1.76	0.65
3:D:543:LEU:HD13	3:D:581:LEU:HA	1.76	0.65
3:D:473:LEU:HD21	3:D:495:ARG:HH21	1.61	0.65
7:H:3:DT:H2'	7:H:4:DA:C8	2.31	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:706:PRO:HB2	3:D:708:LEU:HD21	1.78	0.65
2:C:150:PRO:HG3	2:C:322:VAL:HG21	1.77	0.65
2:C:204:GLN:NE2	2:C:222:MET:SD	2.69	0.65
2:C:859:PRO:O	2:C:867:VAL:HG22	1.97	0.65
7:H:12:DC:H1'	7:H:13:DT:C4	2.32	0.65
2:C:545:ASN:HB3	2:C:583:LEU:HD12	1.79	0.64
2:C:501:THR:HG21	2:C:513:VAL:HG13	1.80	0.64
2:C:612:VAL:HG22	2:C:622:GLU:HG3	1.78	0.64
3:D:12:LEU:HD21	3:D:104:PHE:CZ	2.32	0.64
2:C:726:ILE:HD11	2:C:757:GLY:HA3	1.80	0.64
3:D:889:ALA:HB1	3:D:930:LEU:HA	1.80	0.64
2:C:999:HIS:HB3	2:C:1004:LYS:NZ	2.13	0.63
2:C:557:ARG:HG3	2:C:844:GLY:HA3	1.79	0.63
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.80	0.63
1:B:111:ALA:HB3	1:B:125:PRO:HA	1.79	0.63
3:D:135:LEU:HD13	3:D:463:GLN:HG2	1.81	0.63
3:D:258:VAL:HG12	3:D:273:ARG:O	1.99	0.63
3:D:542:ASP:OD2	3:D:545:ARG:NH2	2.32	0.63
3:D:1236:LEU:HD12	3:D:1252:ILE:HD13	1.80	0.63
2:C:878:SER:HA	3:D:1034:GLN:OE1	1.99	0.63
3:D:573:MET:SD	5:F:210:LEU:HB3	2.39	0.63
3:D:566:ILE:HD11	5:F:192:LEU:HD21	1.81	0.62
3:D:133:ILE:HG13	3:D:152:LEU:HD12	1.80	0.62
3:D:208:PRO:HA	3:D:390:PRO:HA	1.80	0.62
3:D:1094:LEU:HD22	3:D:1260:ILE:HG12	1.80	0.62
3:D:1492:LEU:HD22	4:E:74:VAL:HG21	1.79	0.62
2:C:628:PHE:H	2:C:638:ASP:CB	2.12	0.62
3:D:838:ARG:NH1	3:D:874:GLU:OE1	2.31	0.62
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.82	0.62
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.82	0.62
2:C:1063:ARG:NH1	12:C:1202:HOH:O	2.31	0.61
3:D:645:PRO:HB3	3:D:723:GLY:O	2.00	0.61
3:D:657:LEU:O	3:D:661:MET:HB2	1.99	0.61
3:D:1199:GLY:O	3:D:1373:ARG:NH1	2.25	0.61
1:A:20:TYR:OH	1:A:198:ARG:HD2	2.00	0.61
2:C:468:ARG:HA	2:C:486:MET:O	2.00	0.61
2:C:1071:ILE:HD11	5:F:345:ALA:HB1	1.82	0.61
3:D:683:ILE:HG23	3:D:687:VAL:HG11	1.82	0.61
3:D:828:LYS:HA	3:D:833:GLU:HA	1.82	0.61
2:C:915:LYS:NZ	2:C:968:LEU:O	2.25	0.61
3:D:116:LEU:HB2	3:D:118:LEU:HD12	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:661:MET:HE1	3:D:677:LEU:HD11	1.82	0.61
3:D:1372:VAL:HA	3:D:1375:MET:HG3	1.83	0.61
1:B:56:VAL:HG21	1:B:82:LEU:HD13	1.82	0.60
2:C:197:LEU:HD12	2:C:221:LEU:HD11	1.81	0.60
2:C:1070:ILE:CG2	3:D:655:PRO:HB2	2.31	0.60
5:F:271:LEU:HA	5:F:295:MET:HE1	1.83	0.60
4:E:50:THR:HG1	4:E:55:PHE:HD2	1.49	0.60
3:D:285:PRO:HD2	3:D:288:MET:HE1	1.83	0.60
5:F:368:VAL:HG21	5:F:400:ILE:HD11	1.82	0.60
1:B:92:PRO:O	1:B:146:ARG:NH2	2.32	0.60
5:F:85:LEU:HB3	7:H:7:DG:N3	2.17	0.60
3:D:244:GLU:HG3	3:D:310:LEU:CD2	2.32	0.60
4:E:45:ARG:NH1	4:E:63:TRP:HH2	2.00	0.60
1:A:31:GLY:N	1:A:193:ASP:OD1	2.35	0.60
3:D:248:PRO:HG3	3:D:308:LYS:HG3	1.83	0.60
2:C:578:VAL:HG12	2:C:671:ASN:OD1	2.01	0.59
3:D:116:LEU:HD21	3:D:465:LEU:HD23	1.83	0.59
2:C:627:ARG:HA	2:C:638:ASP:HB2	1.83	0.59
2:C:910:LYS:O	2:C:914:ILE:HG13	2.02	0.59
3:D:270:LEU:HD12	3:D:284:LEU:HD11	1.83	0.59
1:A:25:LEU:HD23	1:A:28:LEU:HD11	1.85	0.59
1:A:150:TYR:CD1	2:C:696:LYS:HG2	2.37	0.59
1:A:185:ARG:NH2	1:A:187:GLY:O	2.35	0.59
1:B:20:TYR:C	1:B:207:PRO:HG2	2.22	0.59
2:C:550:LEU:HD23	2:C:906:PHE:HE2	1.66	0.59
2:C:882:LEU:HD11	3:D:1038:LEU:HD22	1.84	0.59
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.84	0.59
3:D:895:VAL:HG11	3:D:922:LEU:HD21	1.85	0.59
3:D:236:TYR:HB2	3:D:319:ALA:HB3	1.84	0.59
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.38	0.59
1:B:107:LYS:NZ	1:B:113:ASP:OD1	2.25	0.59
3:D:245:LEU:HD21	3:D:311:LEU:HD21	1.84	0.59
3:D:1102:THR:CG2	3:D:1222:GLY:C	2.71	0.59
3:D:1240:THR:CG2	12:D:1706:HOH:O	2.51	0.59
3:D:181:ASP:HB2	3:D:205:TYR:CD1	2.38	0.58
2:C:922:PHE:CD2	2:C:964:LYS:HG3	2.38	0.58
3:D:142:LEU:HB2	3:D:161:LEU:HD21	1.85	0.58
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.86	0.58
2:C:272:ALA:HA	2:C:464:LEU:HD23	1.85	0.58
2:C:578:VAL:HA	2:C:900:ARG:HG2	1.85	0.58
7:H:10:DA:H2"	7:H:11:DG:OP1	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:329:GLY:HA3	2:C:489:THR:HG23	1.85	0.58
3:D:1046:GLN:NE2	3:D:1246:VAL:O	2.37	0.58
3:D:1462:LEU:HD23	3:D:1473:PRO:HD2	1.85	0.58
5:F:237:THR:HG21	7:H:3:DT:H5'	1.86	0.58
1:B:98:THR:CG2	12:B:501:HOH:O	2.52	0.58
2:C:614:ARG:NH2	2:C:618:GLY:O	2.36	0.58
2:C:958:THR:N	2:C:961:GLU:OE1	2.24	0.58
2:C:878:SER:HB2	3:D:1029:ARG:HD2	1.86	0.57
2:C:1056:LYS:HB2	3:D:623:VAL:HG22	1.86	0.57
2:C:816:LYS:O	2:C:819:VAL:HG13	2.04	0.57
2:C:1093:GLN:O	2:C:1096:ALA:N	2.35	0.57
3:D:169:TYR:O	3:D:392:SER:HB2	2.04	0.57
7:H:10:DA:H2'	7:H:11:DG:C8	2.38	0.57
3:D:1479:ASP:OD1	3:D:1482:ARG:NH2	2.35	0.57
1:B:85:LEU:HA	1:B:124:ASN:HD21	1.70	0.57
2:C:700:TYR:CB	2:C:833:LEU:HD22	2.35	0.57
2:C:700:TYR:HB2	2:C:833:LEU:HD22	1.87	0.57
2:C:1059:ASP:O	2:C:1063:ARG:HB3	2.05	0.57
3:D:876:SER:OG	3:D:879:ARG:HG3	2.05	0.57
7:H:12:DC:H1'	7:H:13:DT:C5	2.39	0.57
3:D:200:ASP:O	3:D:397:LYS:HG2	2.05	0.57
3:D:353:VAL:HG12	3:D:355:VAL:H	1.69	0.57
7:H:15:DT:H2'	7:H:16:DC:C6	2.39	0.57
1:A:48:ILE:HG22	1:A:173:PRO:HD2	1.87	0.57
2:C:115:LEU:O	2:C:375:SER:HB2	2.04	0.57
1:A:6:LEU:HD23	1:A:7:LYS:H	1.68	0.57
3:D:411:THR:O	5:F:178:ARG:NH1	2.33	0.57
6:G:19:DG:H2'	6:G:20:DG:C8	2.39	0.57
3:D:298:VAL:HG12	3:D:302:GLN:NE2	2.20	0.56
3:D:318:ARG:NH1	3:D:338:GLU:OE1	2.37	0.56
1:B:57:TYR:CD1	1:B:161:ARG:HD2	2.40	0.56
2:C:884:GLN:O	2:C:888:THR:OG1	2.23	0.56
3:D:1444:THR:O	3:D:1448:THR:HG23	2.05	0.56
11:D:1606:2TM:H10	11:D:1606:2TM:C5'	2.35	0.56
1:A:41:ARG:HA	1:A:177:VAL:HG11	1.86	0.56
3:D:534:ARG:NH2	5:F:313:GLU:O	2.38	0.56
3:D:1434:TRP:HB3	3:D:1455:LYS:HD2	1.88	0.56
1:A:72:LYS:HG3	2:C:641:PRO:HG2	1.87	0.56
2:C:617:ASP:HB2	2:C:619:ARG:HG2	1.87	0.56
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.41	0.56
3:D:415:VAL:HG13	3:D:419:ASP:HB2	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:GLU:O	1:A:213:GLN:HG2	2.06	0.56
1:B:186:LEU:HB2	1:B:192:LEU:HD12	1.86	0.56
3:D:684:LYS:O	3:D:687:VAL:HG12	2.05	0.56
3:D:1296:SER:HB3	3:D:1299:PHE:HB2	1.87	0.55
2:C:1092:LEU:HD22	2:C:1097:LEU:HD12	1.89	0.55
3:D:167:GLU:OE2	3:D:198:ARG:NH1	2.39	0.55
3:D:1031:ASN:ND2	3:D:1034:GLN:HE21	2.04	0.55
3:D:1102:THR:HG22	3:D:1222:GLY:C	2.27	0.55
3:D:1111:ASP:OD1	3:D:1189:ARG:NH2	2.40	0.55
1:B:49:PRO:HA	1:B:148:VAL:HG12	1.88	0.55
2:C:690:ILE:HB	2:C:694:LEU:HD12	1.88	0.55
3:D:941:PHE:O	3:D:945:SER:HB3	2.06	0.55
3:D:1101:VAL:O	3:D:1374:GLN:HG3	2.06	0.55
2:C:36:PRO:HA	2:C:39:ARG:HG3	1.88	0.55
2:C:880:MET:SD	3:D:1037:GLN:NE2	2.80	0.55
2:C:1055:LEU:HD13	2:C:1066:ALA:HB2	1.89	0.55
2:C:627:ARG:NH1	2:C:640:ARG:HG2	2.21	0.55
3:D:975:GLU:O	3:D:979:GLU:HG2	2.07	0.55
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.89	0.55
2:C:1087:VAL:HG22	3:D:524:LEU:HD22	1.88	0.54
2:C:470:PRO:HD3	2:C:485:TYR:CE2	2.43	0.54
1:B:112:ARG:NH2	1:B:126:ASP:OD2	2.26	0.54
2:C:689:VAL:HG13	2:C:851:LYS:HB3	1.88	0.54
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.90	0.54
2:C:344:PHE:HD2	2:C:382:ILE:HD11	1.70	0.54
2:C:455:LEU:HD22	2:C:459:ALA:HB3	1.90	0.54
1:B:71:VAL:HG22	1:B:132:LEU:HG	1.89	0.54
2:C:27:ARG:NH2	2:C:27:ARG:HB3	2.23	0.54
2:C:194:VAL:HG22	2:C:221:LEU:HD12	1.89	0.54
3:D:208:PRO:HG3	3:D:387:LEU:HD22	1.90	0.54
3:D:916:TYR:CZ	3:D:920:LEU:HD11	2.43	0.54
5:F:256:ARG:HD3	5:F:260:ILE:HD12	1.88	0.54
7:H:12:DC:H2"	7:H:13:DT:OP2	2.08	0.54
3:D:869:MET:O	3:D:871:LYS:HG3	2.07	0.54
3:D:236:TYR:CD2	3:D:322:VAL:CG2	2.86	0.54
3:D:633:VAL:HB	3:D:740:PHE:CE2	2.43	0.54
11:D:1606:2TM:H10	11:D:1606:2TM:H1	1.90	0.54
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.90	0.54
1:A:154:GLU:CD	1:A:154:GLU:H	2.10	0.54
3:D:709:HIS:CD2	3:D:711:LEU:HB2	2.43	0.54
5:F:208:SER:HB3	5:F:211:ASP:OD2	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:787:ASP:OD2	2:C:791:ARG:NH2	2.39	0.54
2:C:1085:PHE:CE2	2:C:1088:LEU:HD23	2.43	0.54
3:D:657:LEU:HG	3:D:661:MET:CE	2.37	0.54
3:D:1263:PHE:HD2	3:D:1375:MET:HE2	1.73	0.54
5:F:166:LEU:HD13	5:F:170:HIS:HB3	1.90	0.54
2:C:134:ARG:NH1	2:C:392:SER:O	2.39	0.53
1:A:176:ARG:HG3	1:A:177:VAL:N	2.23	0.53
3:D:96:ALA:HB3	3:D:554:LEU:HD23	1.89	0.53
2:C:205:GLU:O	2:C:209:ARG:HG2	2.08	0.53
7:H:18:DC:H2'	7:H:19:DG:C8	2.42	0.53
2:C:976:ASP:OD1	2:C:978:ARG:HD3	2.08	0.53
1:B:102:LYS:HG2	1:B:139:ASN:OD1	2.07	0.53
2:C:572:ILE:HG13	2:C:573:ARG:HG3	1.90	0.53
2:C:713:ARG:HA	2:C:819:VAL:HA	1.90	0.53
2:C:984:GLU:HB2	3:D:944:THR:O	2.09	0.53
3:D:487:ALA:O	3:D:491:LYS:HG2	2.08	0.53
1:A:46:SER:O	1:A:47:SER:HB2	2.08	0.53
2:C:890:LEU:HD13	2:C:914:ILE:HG23	1.90	0.53
1:B:101:LEU:HD11	1:B:113:ASP:HB2	1.90	0.53
2:C:861:LEU:HD12	2:C:865:THR:HB	1.91	0.53
3:D:629:SER:OG	3:D:630:VAL:N	2.37	0.53
3:D:1046:GLN:NE2	3:D:1247:ALA:HA	2.24	0.53
2:C:829:GLN:OE1	2:C:831:ARG:NH2	2.42	0.53
2:C:856:GLU:HG2	2:C:857:ASP:OD1	2.08	0.52
2:C:708:TYR:HB3	2:C:790:LEU:HD21	1.91	0.52
2:C:1042:ALA:HB3	3:D:710:ARG:HB2	1.91	0.52
3:D:270:LEU:HD13	3:D:304:LEU:HD13	1.91	0.52
7:H:15:DT:H2"	7:H:16:DC:H5'	1.91	0.52
2:C:768:THR:OG1	2:C:771:GLU:OE1	2.27	0.52
2:C:888:THR:HG22	2:C:990:GLY:HA3	1.90	0.52
3:D:34:TYR:CE2	5:F:261:PRO:HD2	2.44	0.52
3:D:63:TYR:OH	3:D:74:GLU:OE2	2.28	0.52
1:A:4:SER:HA	1:A:189:ARG:HH22	1.75	0.52
2:C:607:ASP:HB3	2:C:610:ARG:HG2	1.92	0.52
1:A:133:GLU:OE2	2:C:605:LYS:HB3	2.09	0.52
3:D:646:LYS:HB3	3:D:688:TRP:CZ3	2.45	0.52
3:D:795:VAL:HG12	3:D:876:SER:HB3	1.91	0.52
3:D:945:SER:OG	3:D:947:ILE:HG12	2.10	0.52
3:D:1080:GLY:O	3:D:1084:THR:HG23	2.09	0.52
3:D:1197:ARG:HB2	3:D:1398:TRP:CH2	2.45	0.52
2:C:705:ILE:HG12	2:C:828:ALA:HB2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ILE:HG21	1:A:68:ILE:HD11	1.92	0.52
2:C:1053:LEU:CD1	3:D:1466:VAL:HG13	2.40	0.52
3:D:28:LYS:O	3:D:43:GLY:HA2	2.10	0.52
3:D:236:TYR:CE1	3:D:242:LEU:HD12	2.44	0.52
3:D:654:LYS:O	3:D:658:LEU:HG	2.10	0.52
3:D:1197:ARG:HD2	3:D:1398:TRP:CE2	2.45	0.52
2:C:173:ASP:O	2:C:184:MET:HA	2.09	0.51
2:C:727:PRO:HB3	2:C:783:ARG:HD3	1.92	0.51
3:D:553:ARG:HD2	3:D:570:GLU:CD	2.30	0.51
3:D:771:SER:HB2	3:D:778:LEU:HD22	1.92	0.51
4:E:9:LEU:HD13	4:E:65:MET:HE2	1.92	0.51
2:C:27:ARG:HB3	2:C:27:ARG:HH21	1.74	0.51
3:D:373:PRO:HA	3:D:376:GLU:HG3	1.93	0.51
3:D:785:ILE:HD13	3:D:935:LYS:HA	1.92	0.51
3:D:222:GLY:HA2	3:D:333:LEU:O	2.11	0.51
3:D:1102:THR:HG21	3:D:1222:GLY:C	2.31	0.51
1:A:156:HIS:NE2	1:A:167:VAL:O	2.36	0.51
1:B:64:GLU:O	1:B:75:VAL:HB	2.10	0.51
2:C:710:ILE:HD12	2:C:790:LEU:HB2	1.92	0.51
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.91	0.51
3:D:243:ALA:HB3	3:D:311:LEU:CD1	2.41	0.51
3:D:397:LYS:O	3:D:448:GLU:HG2	2.11	0.51
2:C:682:TYR:CZ	2:C:851:LYS:HE2	2.46	0.51
2:C:722:ILE:HD12	2:C:821:GLU:HG3	1.93	0.51
2:C:1085:PHE:HE2	2:C:1088:LEU:HD23	1.74	0.51
3:D:911:LEU:O	3:D:915:VAL:HG23	2.11	0.51
4:E:52:GLU:OE1	4:E:52:GLU:N	2.39	0.51
5:F:195:VAL:HG13	5:F:216:GLY:HA3	1.93	0.51
7:H:19:DG:H2"	7:H:20:DG:C8	2.46	0.51
1:B:59:GLU:CD	1:B:139:ASN:HD22	2.15	0.51
2:C:1008:ARG:NH1	3:D:624:ASP:OD1	2.40	0.51
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.92	0.51
3:D:1149:LEU:HG	3:D:1166:LEU:HD21	1.92	0.51
2:C:948:GLU:HG3	2:C:953:VAL:HG23	1.91	0.50
5:F:383:LEU:HD12	5:F:394:ARG:NH2	2.25	0.50
3:D:696:HIS:ND1	4:E:57:ASP:OD1	2.44	0.50
3:D:850:LEU:HD12	3:D:884:ARG:NH2	2.27	0.50
3:D:1156:LEU:O	3:D:1158:VAL:HG23	2.11	0.50
5:F:392:VAL:HG13	5:F:396:ARG:HB3	1.92	0.50
1:B:38:ASN:ND2	2:C:979:THR:HA	2.26	0.50
2:C:441:VAL:HG11	2:C:544:THR:HG21	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:539:VAL:HG21	3:D:1067:VAL:HG11	1.94	0.50
2:C:223:ASP:OD1	2:C:225:SER:OG	2.26	0.50
3:D:437:VAL:HG11	5:F:175:HIS:CD2	2.46	0.50
3:D:530:VAL:HG12	3:D:531:ASP:H	1.76	0.50
3:D:882:PHE:O	3:D:886:VAL:HG23	2.12	0.50
5:F:181:GLU:O	5:F:185:GLN:HG2	2.12	0.50
2:C:401:LEU:HD21	2:C:543:ASN:ND2	2.27	0.50
3:D:472:ALA:O	3:D:476:GLU:HG2	2.11	0.50
3:D:561:GLY:HA3	5:F:132:ARG:HD3	1.93	0.50
2:C:712:ALA:HB3	2:C:821:GLU:HG2	1.93	0.50
2:C:937:ASP:OD1	2:C:939:ARG:HD3	2.11	0.50
3:D:1220:ALA:O	3:D:1224:VAL:HG23	2.11	0.50
1:B:108:GLU:HG2	1:B:131:THR:HB	1.93	0.50
2:C:229:MET:HB2	2:C:233:GLU:HB2	1.93	0.49
3:D:45:PHE:HZ	3:D:541:ASN:HD21	1.60	0.49
3:D:631:ILE:HD11	3:D:743:ASP:HB2	1.94	0.49
3:D:1047:LYS:HG2	3:D:1053:PHE:CZ	2.47	0.49
3:D:1110:ALA:O	3:D:1203:LYS:HG2	2.11	0.49
4:E:37:ASN:OD1	4:E:37:ASN:N	2.44	0.49
5:F:81:VAL:O	5:F:85:LEU:HG	2.12	0.49
2:C:807:ARG:HB2	2:C:810:ASP:OD2	2.11	0.49
3:D:41:ARG:HE	3:D:48:ARG:CZ	2.25	0.49
3:D:493:ARG:O	3:D:497:GLU:HG3	2.11	0.49
3:D:851:LEU:O	3:D:855:HIS:HD2	1.95	0.49
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	1.94	0.49
1:A:42:ARG:NH1	2:C:978:ARG:HA	2.26	0.49
2:C:521:PRO:HG2	3:D:1072:ILE:HD11	1.94	0.49
3:D:970:LYS:HD3	3:D:995:LEU:HD13	1.94	0.49
2:C:278:GLU:HG2	2:C:284:ARG:HA	1.94	0.49
2:C:571:LEU:HD22	2:C:700:TYR:HA	1.93	0.49
7:H:12:DC:OP2	7:H:12:DC:H3'	2.12	0.49
1:A:57:TYR:CE1	1:A:161:ARG:HD2	2.47	0.49
3:D:288:MET:SD	3:D:307:ALA:HB2	2.52	0.49
3:D:1200:VAL:HG23	3:D:1373:ARG:NH1	2.27	0.49
5:F:135:ILE:HG13	5:F:181:GLU:HB2	1.94	0.49
1:B:22:GLU:HG2	1:B:198:ARG:HG2	1.95	0.49
1:A:155:LYS:O	1:A:155:LYS:HE3	2.12	0.49
2:C:829:GLN:OE1	2:C:831:ARG:NE	2.46	0.49
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.48	0.49
3:D:800:LYS:HE3	3:D:819:GLY:O	2.13	0.49
2:C:1070:ILE:HG21	3:D:655:PRO:HB2	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:926:LYS:HG2	3:D:929:ARG:NH2	2.28	0.48
1:A:57:TYR:CD1	1:A:161:ARG:HD2	2.47	0.48
3:D:1377:LYS:HE3	3:D:1378:TYR:CZ	2.47	0.48
6:G:6:DA:H2"	6:G:7:DT:C5'	2.43	0.48
1:A:181:VAL:HG12	2:C:938:LYS:HD2	1.96	0.48
2:C:564:MET:SD	2:C:997:LEU:HD11	2.54	0.48
2:C:1053:LEU:HD13	3:D:1466:VAL:HG13	1.94	0.48
2:C:469:THR:OG1	2:C:538:GLN:NE2	2.46	0.48
1:A:97:VAL:HG12	1:A:99:LEU:HD12	1.95	0.48
3:D:840:LYS:HE3	3:D:841:TYR:CZ	2.49	0.48
3:D:1107:VAL:HA	3:D:1200:VAL:O	2.14	0.48
5:F:95:THR:O	5:F:98:GLU:N	2.47	0.48
1:B:41:ARG:HG3	1:B:177:VAL:HG12	1.94	0.48
3:D:209:ARG:HG2	3:D:389:GLU:O	2.14	0.48
3:D:500:ARG:NH1	3:D:1388:ARG:O	2.47	0.48
7:H:3:DT:H2"	7:H:4:DA:H5'	1.95	0.48
2:C:11:GLU:HG2	2:C:535:SER:HB2	1.94	0.48
3:D:1232:PRO:HB3	3:D:1361:VAL:HG11	1.95	0.48
1:B:85:LEU:HG	1:B:87:VAL:HG23	1.96	0.48
2:C:937:ASP:OD1	2:C:938:LYS:N	2.47	0.48
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.94	0.48
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.95	0.48
3:D:45:PHE:O	3:D:86:ARG:NH2	2.47	0.48
5:F:237:THR:HG21	7:H:3:DT:C5'	2.44	0.48
2:C:560:MET:O	2:C:564:MET:HG3	2.14	0.48
2:C:600:ASP:O	2:C:616:GLU:HG2	2.14	0.48
2:C:1010:THR:HA	3:D:624:ASP:OD1	2.14	0.48
3:D:367:ILE:HD11	3:D:379:ALA:HB2	1.96	0.48
3:D:846:PRO:HB3	3:D:880:ILE:CG2	2.43	0.48
3:D:882:PHE:CE1	3:D:906:GLN:HG3	2.49	0.48
5:F:192:LEU:HD23	5:F:220:LEU:HD23	1.96	0.48
6:G:6:DA:H2'	6:G:7:DT:C6	2.49	0.48
2:C:709:GLU:OE2	2:C:824:ARG:NH1	2.46	0.47
3:D:227:LEU:HD13	3:D:331:VAL:CG2	2.44	0.47
3:D:483:HIS:CE1	3:D:488:ARG:HD3	2.49	0.47
3:D:1255:GLY:O	3:D:1259:VAL:HG23	2.13	0.47
1:B:104:GLU:OE2	1:B:137:ARG:NH1	2.47	0.47
5:F:184:ARG:O	5:F:188:ILE:HG13	2.14	0.47
3:D:1012:GLU:HB2	3:D:1021:TYR:OH	2.15	0.47
3:D:1168:MET:HE3	3:D:1171:VAL:HB	1.96	0.47
3:D:1205:TYR:O	3:D:1366:LYS:HD3	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1031:ARG:NE	6:G:16:DC:OP1	2.44	0.47
3:D:134:VAL:HG12	3:D:454:ALA:HB2	1.95	0.47
2:C:408:ARG:NH1	2:C:456:ALA:O	2.47	0.47
7:H:9:DG:H2"	7:H:10:DA:N7	2.29	0.47
2:C:726:ILE:HD11	2:C:757:GLY:CA	2.45	0.47
3:D:371:ILE:HG21	5:F:232:ARG:NH1	2.29	0.47
3:D:483:HIS:CG	3:D:484:PRO:HD2	2.50	0.47
3:D:782:SER:HA	3:D:786:ILE:HD12	1.97	0.47
1:A:41:ARG:NE	1:A:177:VAL:O	2.34	0.47
1:B:94:LEU:HD23	1:B:95:GLN:H	1.79	0.47
2:C:351:LEU:HD12	2:C:374:ASN:O	2.15	0.47
2:C:838:LYS:HE3	3:D:741:ASP:O	2.15	0.47
2:C:999:HIS:HB3	2:C:1004:LYS:HZ1	1.76	0.47
3:D:479:GLU:HA	3:D:482:LYS:HE2	1.97	0.47
3:D:890:VAL:HB	3:D:922:LEU:HD13	1.97	0.47
3:D:1167:SER:O	3:D:1171:VAL:HG23	2.15	0.47
5:F:96:LEU:O	5:F:100:VAL:HG23	2.14	0.47
5:F:367:MET:HB3	5:F:390:PHE:HZ	1.80	0.47
2:C:874:LEU:HD13	3:D:783:ARG:HB3	1.96	0.47
3:D:1305:LEU:HD13	3:D:1309:ALA:HB3	1.96	0.47
2:C:351:LEU:HD11	2:C:373:VAL:HG13	1.97	0.47
2:C:811:PRO:O	2:C:813:VAL:HG23	2.15	0.47
3:D:128:TYR:OH	3:D:579:ASP:OD2	2.25	0.47
3:D:1205:TYR:CE1	3:D:1366:LYS:HD2	2.49	0.47
6:G:19:DG:O5'	6:G:19:DG:H8	1.97	0.47
2:C:513:VAL:HB	2:C:524:VAL:O	2.15	0.47
3:D:581:LEU:HG	3:D:582:LEU:HD23	1.96	0.47
3:D:706:PRO:HB2	3:D:708:LEU:CD2	2.44	0.47
3:D:138:LYS:NZ	3:D:453:ASP:HB2	2.30	0.46
3:D:1291:SER:OG	3:D:1304:LYS:HG2	2.15	0.46
3:D:1341:PRO:HB3	3:D:1376:MET:HE2	1.98	0.46
4:E:14:ASP:OD2	4:E:18:ARG:NH1	2.42	0.46
1:B:26:GLU:HB3	1:B:194:LYS:HG3	1.97	0.46
2:C:642:ARG:HG3	2:C:654:LEU:HD21	1.98	0.46
2:C:1008:ARG:CZ	2:C:1020:PRO:HB3	2.45	0.46
3:D:100:ALA:HA	3:D:513:ILE:HD13	1.97	0.46
3:D:1350:GLU:O	3:D:1354:LYS:HG3	2.15	0.46
1:B:57:TYR:CG	1:B:161:ARG:HD2	2.51	0.46
1:A:99:LEU:HD21	1:A:122:ILE:HD11	1.96	0.46
1:B:6:LEU:HD12	1:B:7:LYS:H	1.80	0.46
2:C:144:PRO:HB2	2:C:273:GLY:CA	2.43	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:974:LEU:HD12	2:C:974:LEU:HA	1.79	0.46
3:D:192:ALA:HB1	3:D:193:PRO:HD2	1.96	0.46
2:C:583:LEU:HA	2:C:583:LEU:HD23	1.66	0.46
2:C:595:LEU:HD11	2:C:623:TYR:HB3	1.97	0.46
2:C:1032:PHE:CZ	2:C:1036:GLU:HB3	2.49	0.46
3:D:630:VAL:HA	3:D:744:GLN:HG2	1.96	0.46
1:A:70:GLY:N	2:C:607:ASP:OD1	2.48	0.46
1:B:100:LEU:HG	1:B:141:GLU:HG2	1.97	0.46
3:D:57:GLU:HA	3:D:64:LYS:HA	1.97	0.46
1:B:223:THR:HG22	1:B:223:THR:O	2.16	0.46
2:C:888:THR:HG22	2:C:990:GLY:CA	2.45	0.46
3:D:1463:LYS:HE2	3:D:1463:LYS:HB3	1.56	0.46
2:C:180:GLY:O	2:C:220:GLY:HA3	2.15	0.46
2:C:372:LEU:HD12	2:C:372:LEU:HA	1.69	0.46
2:C:399:ASN:H	2:C:402:SER:HG	1.64	0.46
2:C:497:ALA:HA	2:C:515:ALA:HA	1.98	0.46
3:D:686:GLU:CD	3:D:686:GLU:H	2.18	0.46
2:C:51:THR:OG1	2:C:348:LEU:HB3	2.16	0.46
2:C:276:LYS:HD2	2:C:466:PHE:HZ	1.81	0.46
2:C:1067:TYR:O	2:C:1071:ILE:HG12	2.15	0.46
3:D:1364:HIS:CE1	3:D:1366:LYS:HG3	2.51	0.46
5:F:163:LEU:HD13	5:F:174:LEU:HD13	1.98	0.46
2:C:97:ARG:HG3	2:C:112:GLU:HG3	1.98	0.45
2:C:1042:ALA:HB1	3:D:1224:VAL:HG22	1.98	0.45
3:D:134:VAL:HG22	3:D:151:GLN:O	2.16	0.45
3:D:708:LEU:N	3:D:708:LEU:HD23	2.29	0.45
1:A:228:PRO:HB3	1:B:13:VAL:HG21	1.96	0.45
2:C:294:GLU:HB3	2:C:299:LYS:HE2	1.97	0.45
3:D:154:THR:OG1	3:D:157:GLU:HG3	2.15	0.45
3:D:520:LEU:HD12	3:D:521:PRO:HD2	1.98	0.45
2:C:148:PHE:CZ	2:C:309:TYR:HB3	2.51	0.45
2:C:453:THR:HG22	12:C:1205:HOH:O	2.16	0.45
3:D:1003:VAL:O	3:D:1007:VAL:HG23	2.17	0.45
5:F:83:GLN:O	5:F:87:GLU:HG3	2.17	0.45
2:C:223:ASP:OD1	2:C:226:VAL:HG23	2.17	0.45
2:C:596:TYR:O	2:C:655:LEU:HD12	2.16	0.45
3:D:178:LEU:HG	3:D:193:PRO:HD3	1.98	0.45
3:D:242:LEU:HB3	3:D:311:LEU:O	2.17	0.45
3:D:643:GLY:HA3	3:D:727:GLN:HG3	1.98	0.45
3:D:790:TYR:CD1	3:D:1022:VAL:HG13	2.52	0.45
3:D:813:LEU:HD21	3:D:840:LYS:HA	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1274:ILE:HD11	3:D:1334:GLN:HB3	1.98	0.45
3:D:349:PRO:HB3	5:F:97:GLU:HG3	1.99	0.45
5:F:158:GLU:O	5:F:162:LYS:HG3	2.16	0.45
1:A:38:ASN:HB3	1:A:39:PRO:HD3	1.97	0.45
1:A:41:ARG:NH1	2:C:860:HIS:CE1	2.83	0.45
1:A:159:LYS:HG2	1:A:164:ALA:O	2.17	0.45
2:C:385:PHE:HD2	2:C:386:PHE:CD1	2.34	0.45
2:C:1014:SER:N	2:C:1019:GLN:O	2.50	0.45
3:D:916:TYR:CE1	3:D:920:LEU:HD11	2.52	0.45
3:D:1172:HIS:HA	3:D:1175:ILE:HD12	1.99	0.45
4:E:50:THR:HG22	4:E:51:LEU:H	1.81	0.45
1:A:112:ARG:HG2	1:A:125:PRO:O	2.17	0.45
2:C:584:GLU:HB3	2:C:666:LEU:H	1.81	0.45
3:D:219:GLU:HB2	3:D:339:TRP:CZ3	2.52	0.45
3:D:554:LEU:HD13	3:D:570:GLU:HB3	1.99	0.45
2:C:267:TYR:CE2	2:C:290:LEU:HG	2.52	0.45
2:C:825:VAL:HG12	2:C:827:VAL:HG23	1.99	0.45
3:D:1457:ASP:OD1	3:D:1464:GLU:HG2	2.16	0.45
5:F:386:VAL:HG12	5:F:397:ILE:HG12	1.99	0.45
1:A:9:PRO:HB3	1:A:26:GLU:C	2.36	0.45
2:C:290:LEU:O	2:C:301:GLU:HB2	2.17	0.45
2:C:685:GLU:HA	2:C:685:GLU:OE1	2.17	0.45
3:D:867:ARG:HA	3:D:871:LYS:O	2.17	0.45
1:B:32:PHE:HA	1:B:35:THR:HB	1.99	0.44
2:C:121:MET:SD	2:C:125:GLY:HA2	2.57	0.44
2:C:1007:ALA:O	3:D:651:GLU:HG2	2.17	0.44
3:D:10:ILE:O	3:D:1454:GLY:HA2	2.17	0.44
1:A:182:GLU:OE1	2:C:935:GLY:N	2.49	0.44
1:B:74:ASP:O	1:B:78:ILE:HG13	2.17	0.44
3:D:286:VAL:O	3:D:311:LEU:HA	2.17	0.44
2:C:261:ILE:HG23	2:C:290:LEU:HB2	1.99	0.44
2:C:769:PRO:HG3	3:D:65:ARG:NH1	2.20	0.44
2:C:1057:SER:O	2:C:1058:ASP:HB2	2.16	0.44
2:C:1083:GLU:OE2	3:D:87:ARG:NH2	2.50	0.44
3:D:1083:ASP:HB3	3:D:1253:THR:HG21	1.99	0.44
2:C:499:ALA:HA	2:C:532:MET:CE	2.48	0.44
2:C:1102:LEU:HD23	2:C:1108:PRO:HA	2.00	0.44
3:D:86:ARG:HB3	3:D:522:PRO:HG2	1.98	0.44
3:D:566:ILE:HG23	5:F:214:GLN:HE22	1.83	0.44
3:D:572:ARG:HH12	5:F:83:GLN:HB3	1.83	0.44
3:D:709:HIS:HD2	3:D:711:LEU:H	1.64	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1493:LYS:HZ2	3:D:1496:GLU:HG2	1.81	0.44
6:G:6:DA:H2"	6:G:7:DT:O5'	2.18	0.44
1:A:226:SER:O	1:A:228:PRO:HD3	2.18	0.44
1:B:155:LYS:HA	1:B:155:LYS:HD3	1.77	0.44
2:C:863:ASP:OD2	2:C:925:TYR:HE2	1.99	0.44
3:D:50:PHE:O	3:D:89:ARG:HD2	2.18	0.44
3:D:394:LEU:HG	3:D:396:VAL:HG23	1.99	0.44
3:D:566:ILE:HG12	5:F:217:ASN:ND2	2.33	0.44
1:B:30:ARG:NH2	2:C:854:PRO:HB3	2.33	0.44
2:C:1006:HIS:HB2	2:C:1024:LYS:HG3	1.99	0.44
2:C:1041:GLU:O	2:C:1044:GLY:N	2.44	0.44
3:D:432:TYR:O	3:D:448:GLU:HA	2.18	0.44
3:D:862:ASP:O	3:D:877:PRO:HD3	2.17	0.44
3:D:1194:CYS:HB2	3:D:1204:CYS:SG	2.56	0.44
3:D:1364:HIS:CD2	3:D:1366:LYS:HE2	2.52	0.44
1:A:48:ILE:HD13	1:A:48:ILE:HA	1.69	0.44
2:C:3:ILE:CD1	2:C:900:ARG:HB2	2.48	0.44
2:C:580:MET:HB3	2:C:584:GLU:CD	2.38	0.44
2:C:627:ARG:CZ	2:C:640:ARG:HG2	2.47	0.44
2:C:765:SER:O	2:C:767:PRO:HD3	2.17	0.44
5:F:229:TYR:CZ	5:F:230:LYS:HD3	2.53	0.44
2:C:207:LEU:HD13	2:C:221:LEU:HD21	1.99	0.44
2:C:987:ILE:HD11	3:D:946:GLY:HA2	2.00	0.44
2:C:1043:TYR:CE2	3:D:710:ARG:HG3	2.53	0.44
3:D:523:ASP:O	3:D:526:PRO:HG3	2.18	0.44
3:D:790:TYR:CE1	3:D:1022:VAL:HG13	2.52	0.44
3:D:960:LYS:NZ	3:D:1040:GLY:O	2.38	0.44
3:D:1238:MET:SD	11:D:1606:2TM:H6	2.58	0.44
3:D:1447:LEU:HD23	3:D:1447:LEU:HA	1.90	0.44
5:F:189:GLU:HA	5:F:192:LEU:HG	2.00	0.44
2:C:697:ARG:NH2	2:C:868:ASP:OD1	2.50	0.43
3:D:17:LYS:HB2	3:D:17:LYS:HE2	1.73	0.43
3:D:550:ARG:CZ	3:D:573:MET:HE3	2.48	0.43
3:D:828:LYS:NZ	3:D:833:GLU:HB3	2.32	0.43
3:D:1102:THR:HG21	3:D:1222:GLY:CA	2.40	0.43
5:F:127:ILE:O	5:F:131:VAL:HG23	2.19	0.43
5:F:154:LYS:O	5:F:158:GLU:HG3	2.18	0.43
5:F:262:VAL:O	5:F:266:GLU:HG3	2.18	0.43
1:B:62:LEU:HD23	1:B:62:LEU:HA	1.87	0.43
2:C:693:GLU:O	2:C:697:ARG:HG2	2.17	0.43
3:D:67:ARG:HE	5:F:379:ARG:HG2	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:784:ASP:HB2	3:D:939:PHE:CD2	2.54	0.43
3:D:818:ARG:HE	3:D:820:GLU:CD	2.21	0.43
3:D:832:ARG:NH1	3:D:833:GLU:HG2	2.33	0.43
2:C:858:MET:HG2	2:C:867:VAL:O	2.19	0.43
3:D:1285:GLU:HB2	3:D:1290:LEU:HD13	2.00	0.43
7:H:18:DC:H2"	7:H:19:DG:H5'	1.99	0.43
2:C:188:LYS:HB2	2:C:188:LYS:HE2	1.83	0.43
2:C:730:SER:OG	2:C:732:ALA:HB3	2.19	0.43
3:D:12:LEU:HD23	3:D:12:LEU:HA	1.70	0.43
3:D:185:VAL:HG11	3:D:203:ALA:HB2	2.00	0.43
2:C:439:CYS:HB2	2:C:541:SER:N	2.34	0.43
3:D:34:TYR:CZ	3:D:35:ARG:HG3	2.53	0.43
3:D:197:SER:OG	3:D:395:VAL:HG21	2.19	0.43
3:D:520:LEU:HD11	3:D:524:LEU:HD12	1.99	0.43
3:D:792:ILE:HD13	3:D:941:PHE:CD1	2.53	0.43
3:D:853:VAL:HG22	3:D:858:VAL:HG23	1.99	0.43
5:F:163:LEU:HD13	5:F:174:LEU:CD1	2.49	0.43
1:A:10:VAL:HG12	1:A:26:GLU:O	2.19	0.43
2:C:886:LEU:HD21	3:D:951:ILE:HG12	2.01	0.43
3:D:114:THR:HG23	3:D:495:ARG:HG2	2.00	0.43
3:D:704:ARG:HD3	3:D:736:PHE:O	2.19	0.43
5:F:304:VAL:O	5:F:308:LEU:HG	2.18	0.43
2:C:363:SER:O	2:C:367:LEU:HG	2.18	0.43
3:D:639:LEU:HA	3:D:729:HIS:CD2	2.54	0.43
3:D:664:LYS:NZ	3:D:693:GLU:OE1	2.24	0.43
3:D:892:ASP:OD1	3:D:894:LYS:HD2	2.19	0.43
3:D:1488:ASP:OD1	3:D:1488:ASP:N	2.38	0.43
2:C:312:ALA:O	2:C:317:VAL:HG13	2.19	0.43
2:C:1058:ASP:N	12:C:1202:HOH:O	2.51	0.43
3:D:796:ARG:NH2	3:D:859:ASP:OD2	2.46	0.43
4:E:46:PRO:HG3	4:E:66:LYS:HD2	2.01	0.43
1:B:34:VAL:HG21	2:C:978:ARG:HB3	2.00	0.43
1:B:185:ARG:HG3	1:B:189:ARG:O	2.18	0.43
2:C:1032:PHE:CE2	2:C:1036:GLU:HB3	2.54	0.43
3:D:123:LEU:O	3:D:127:LEU:HB2	2.19	0.43
3:D:285:PRO:HD2	3:D:288:MET:CE	2.47	0.43
3:D:478:LEU:HD21	3:D:500:ARG:NH2	2.34	0.43
3:D:704:ARG:HH22	11:D:1606:2TM:C1'	2.32	0.43
3:D:1084:THR:HB	3:D:1237:THR:O	2.19	0.43
2:C:1090:LYS:HE3	3:D:88:TYR:O	2.19	0.42
2:C:195:LEU:O	2:C:199:VAL:HG23	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:631:SER:HB3	2:C:635:THR:O	2.19	0.42
3:D:25:GLU:OE2	3:D:94:GLU:HB3	2.19	0.42
5:F:227:PHE:CE1	7:H:2:DA:H2	2.37	0.42
5:F:369:LEU:HD12	5:F:401:GLU:HG3	2.02	0.42
1:A:53:VAL:HG22	1:A:144:VAL:HG22	2.00	0.42
2:C:195:LEU:HD21	2:C:237:ARG:HG3	2.01	0.42
2:C:441:VAL:HG23	2:C:559:LEU:HA	2.02	0.42
2:C:693:GLU:CD	2:C:855:VAL:HG21	2.37	0.42
2:C:913:GLU:HA	2:C:916:GLU:CD	2.40	0.42
2:C:938:LYS:O	2:C:941:VAL:HB	2.20	0.42
2:C:953:VAL:HG11	2:C:962:GLN:HB3	2.01	0.42
2:C:1056:LYS:HD3	3:D:625:TYR:HD1	1.83	0.42
2:C:239:PHE:CD2	2:C:253:ALA:HA	2.54	0.42
2:C:762:LYS:HD2	2:C:783:ARG:O	2.18	0.42
3:D:204:LEU:HD22	3:D:441:ARG:CZ	2.49	0.42
3:D:702:LEU:HD23	3:D:702:LEU:HA	1.85	0.42
3:D:1140:ILE:O	3:D:1144:LEU:HB2	2.19	0.42
5:F:193:ARG:HB3	7:H:7:DG:H5"	2.01	0.42
1:A:99:LEU:HB3	1:A:114:PHE:CD2	2.54	0.42
2:C:109:LYS:HG2	2:C:368:THR:HG22	2.00	0.42
2:C:174:LEU:HA	2:C:183:SER:O	2.19	0.42
3:D:236:TYR:CE2	3:D:322:VAL:CG2	2.84	0.42
2:C:3:ILE:HD12	2:C:900:ARG:HB2	2.02	0.42
2:C:1008:ARG:NH1	2:C:1020:PRO:HB3	2.35	0.42
3:D:679:ARG:NH2	3:D:681:ARG:HD2	2.34	0.42
3:D:1353:GLN:O	3:D:1357:ARG:HG3	2.20	0.42
1:B:7:LYS:HA	1:B:7:LYS:HD3	1.88	0.42
2:C:431:HIS:ND1	2:C:433:THR:HG23	2.35	0.42
2:C:584:GLU:OE2	2:C:584:GLU:N	2.34	0.42
2:C:912:PRO:O	2:C:916:GLU:HG3	2.20	0.42
3:D:613:ARG:HG3	3:D:618:LEU:HD11	2.02	0.42
3:D:774:SER:HB3	3:D:1362:LYS:O	2.19	0.42
3:D:999:THR:O	3:D:1003:VAL:HG13	2.20	0.42
3:D:1167:SER:O	3:D:1170:ASP:HB2	2.20	0.42
3:D:1256:LEU:HB3	3:D:1257:PRO:HD3	2.00	0.42
6:G:7:DT:H3	7:H:21:DA:H61	1.68	0.42
2:C:922:PHE:HB2	2:C:967:PHE:CD2	2.55	0.42
3:D:553:ARG:HD3	5:F:214:GLN:HB3	2.02	0.42
3:D:864:VAL:HG13	3:D:865:THR:N	2.34	0.42
3:D:1048:PRO:O	3:D:1079:LYS:NZ	2.52	0.42
2:C:344:PHE:CE2	2:C:382:ILE:HD11	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:721:ARG:HH12	2:C:785:VAL:HG11	1.85	0.42
3:D:84:ILE:HD12	3:D:87:ARG:HD2	2.02	0.42
3:D:155:ASP:OD1	3:D:159:ARG:NH2	2.52	0.42
3:D:242:LEU:HB3	3:D:311:LEU:HD12	2.02	0.42
3:D:547:LEU:HA	3:D:547:LEU:HD12	1.71	0.42
3:D:868:TYR:HB3	3:D:873:LEU:HD11	2.02	0.42
3:D:1031:ASN:HD21	3:D:1034:GLN:HE21	1.65	0.42
3:D:1353:GLN:HG2	3:D:1368:ILE:CD1	2.49	0.42
1:A:41:ARG:HD2	1:A:177:VAL:HG12	2.00	0.42
1:A:221:HIS:HA	1:A:224:TYR:CE2	2.55	0.42
2:C:90:TYR:CD2	2:C:120:LEU:HB2	2.55	0.42
2:C:425:PHE:O	2:C:428:ARG:N	2.52	0.42
2:C:1065:ALA:CB	2:C:1077:PRO:HG3	2.50	0.42
3:D:763:MET:HB3	3:D:763:MET:HE2	1.88	0.42
3:D:951:ILE:HD11	3:D:1062:ARG:HG3	2.01	0.42
3:D:1342:GLU:CD	3:D:1342:GLU:H	2.22	0.42
1:A:150:TYR:CE1	2:C:696:LYS:HA	2.55	0.41
2:C:557:ARG:CG	2:C:844:GLY:HA3	2.49	0.41
2:C:1013:TYR:HE1	2:C:1020:PRO:HG3	1.85	0.41
3:D:1192:LEU:HD13	3:D:1345:GLU:HB3	2.02	0.41
3:D:1223:ILE:HD12	3:D:1223:ILE:HG23	1.71	0.41
1:B:9:PRO:HG2	1:B:25:LEU:HD11	2.02	0.41
2:C:154:ARG:HH21	2:C:157:ARG:HG3	1.85	0.41
2:C:216:GLU:HG2	2:C:219:GLN:HB2	2.01	0.41
2:C:382:ILE:O	2:C:383:ARG:C	2.58	0.41
2:C:630:ARG:HD2	2:C:705:ILE:O	2.20	0.41
2:C:690:ILE:HG12	2:C:852:ILE:HG12	2.02	0.41
7:H:18:DC:H4'	7:H:19:DG:OP1	2.20	0.41
1:B:132:LEU:HD21	1:B:138:LEU:CB	2.50	0.41
2:C:165:LEU:HB2	2:C:168:ARG:HG3	2.02	0.41
3:D:288:MET:HG2	3:D:305:ALA:HB1	2.02	0.41
3:D:319:ALA:HA	3:D:337:LEU:HD23	2.01	0.41
3:D:428:LYS:HE2	3:D:428:LYS:HB3	1.83	0.41
3:D:1312:LEU:HD12	3:D:1312:LEU:HA	1.94	0.41
6:G:11:DT:H2"	6:G:12:DG:C8	2.55	0.41
2:C:631:SER:HB2	2:C:637:LEU:HD11	2.02	0.41
2:C:800:VAL:HG22	2:C:827:VAL:HG22	2.02	0.41
3:D:60:CYS:SG	3:D:61:GLY:N	2.93	0.41
1:B:179:PHE:HB3	1:B:197:LEU:HD13	2.01	0.41
2:C:154:ARG:NH2	2:C:157:ARG:HG3	2.35	0.41
3:D:142:LEU:HD13	3:D:161:LEU:HD21	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:580:ALA:HA	3:D:584:ASN:HA	2.03	0.41
1:B:54:THR:OG1	1:B:158:ILE:HD11	2.20	0.41
2:C:89:THR:O	2:C:91:GLN:HG2	2.19	0.41
3:D:704:ARG:HB2	3:D:745:MET:HE2	2.03	0.41
3:D:827:ILE:HG12	3:D:834:THR:O	2.20	0.41
3:D:1095:THR:O	3:D:1099:VAL:HG23	2.20	0.41
1:A:128:HIS:CD2	1:A:129:ILE:N	2.88	0.41
1:B:177:VAL:HG13	1:B:197:LEU:HD11	2.02	0.41
2:C:586:ARG:HD2	2:C:586:ARG:HA	1.84	0.41
2:C:735:ARG:HH11	3:D:681:ARG:NH1	2.19	0.41
2:C:970:GLY:O	2:C:988:VAL:HA	2.21	0.41
3:D:115:LEU:HD23	3:D:115:LEU:HA	1.92	0.41
2:C:1005:MET:SD	3:D:648:MET:HG3	2.60	0.41
3:D:24:GLY:HA3	3:D:49:ILE:HG23	2.02	0.41
3:D:366:LYS:HD3	3:D:369:ALA:HB2	2.03	0.41
3:D:729:HIS:CE1	3:D:731:LEU:HB2	2.56	0.41
3:D:849:ALA:O	3:D:853:VAL:HG23	2.21	0.41
3:D:1034:GLN:HA	3:D:1037:GLN:HE21	1.86	0.41
3:D:1093:TYR:CE2	6:G:13:DA:H5'	2.56	0.41
3:D:1112:CYS:SG	3:D:1114:THR:HG22	2.60	0.41
2:C:13:ILE:HG21	2:C:483:VAL:HG11	2.02	0.41
2:C:129:ILE:HG13	2:C:386:PHE:HB3	2.03	0.41
2:C:317:VAL:HA	2:C:318:PRO:HD3	1.93	0.41
2:C:939:ARG:HG2	2:C:982:PRO:HD3	2.03	0.41
2:C:999:HIS:HB3	2:C:1004:LYS:HZ2	1.84	0.41
2:C:1071:ILE:HB	3:D:670:VAL:HG21	2.02	0.41
2:C:1101:THR:O	2:C:1109:VAL:N	2.53	0.41
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.53	0.41
3:D:871:LYS:NZ	3:D:897:TRP:HE1	2.18	0.41
3:D:882:PHE:HE2	3:D:900:ILE:HG23	1.86	0.41
3:D:1194:CYS:HB2	3:D:1204:CYS:CB	2.51	0.41
5:F:85:LEU:HD23	5:F:85:LEU:HA	1.82	0.41
5:F:274:THR:HG21	5:F:295:MET:HE2	2.03	0.41
5:F:383:LEU:HD13	5:F:398:ARG:HB2	2.02	0.41
7:H:10:DA:H3'	7:H:11:DG:N7	2.36	0.41
7:H:12:DC:H4'	7:H:13:DT:O5'	2.20	0.41
1:A:20:TYR:C	1:A:207:PRO:HG2	2.41	0.41
1:B:14:ARG:NH2	1:B:22:GLU:OE1	2.54	0.41
1:B:222:LEU:HD23	1:B:222:LEU:HA	1.85	0.41
2:C:954:THR:HA	2:C:955:PRO:HD3	1.91	0.41
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.75	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:544:TYR:O	3:D:548:ILE:HG13	2.21	0.41
3:D:1208:ASP:O	3:D:1209:LEU:HB2	2.21	0.41
3:D:1296:SER:OG	3:D:1297:GLU:N	2.54	0.41
1:B:211:LEU:O	1:B:215:VAL:HG13	2.21	0.40
2:C:292:ARG:HE	2:C:292:ARG:HB2	1.63	0.40
2:C:394:PHE:CE2	6:G:20:DG:H5"	2.56	0.40
2:C:405:ARG:HD2	2:C:442:GLU:CD	2.42	0.40
2:C:1066:ALA:O	2:C:1070:ILE:HG13	2.20	0.40
3:D:360:ARG:HG2	3:D:384:VAL:HG12	2.02	0.40
3:D:483:HIS:CD2	3:D:484:PRO:HD2	2.56	0.40
7:H:1:DT:O2	7:H:1:DT:O4'	2.37	0.40
1:A:42:ARG:NH2	1:B:34:VAL:HG22	2.35	0.40
2:C:340:MET:HE2	2:C:340:MET:HB3	1.94	0.40
2:C:1089:VAL:HG11	2:C:1112:PHE:CZ	2.57	0.40
3:D:129:PHE:CD1	3:D:456:MET:HB3	2.56	0.40
3:D:601:ARG:CD	5:F:318:GLU:HG2	2.51	0.40
3:D:1283:ILE:HG12	3:D:1315:ASP:HB2	2.02	0.40
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.21	0.40
5:F:286:PRO:HA	5:F:290:GLU:OE1	2.21	0.40
1:A:55:SER:HB2	1:A:158:ILE:HG22	2.03	0.40
2:C:276:LYS:HD2	2:C:466:PHE:CZ	2.56	0.40
2:C:1090:LYS:HE2	2:C:1112:PHE:CZ	2.57	0.40
3:D:709:HIS:O	3:D:711:LEU:N	2.55	0.40
3:D:908:LYS:HB3	3:D:908:LYS:HE2	1.97	0.40
3:D:1339:LYS:HB3	3:D:1343:ALA:CB	2.51	0.40
4:E:47:LYS:NZ	4:E:56:ASP:OD1	2.52	0.40
2:C:141:HIS:CD2	2:C:334:ARG:HD2	2.57	0.40
2:C:169:GLY:HA3	2:C:267:TYR:CD1	2.56	0.40
3:D:123:LEU:HG	3:D:127:LEU:HD12	2.03	0.40
3:D:1468:LEU:HD12	3:D:1470:ARG:HD2	2.04	0.40
5:F:123:ASP:O	5:F:127:ILE:HG13	2.22	0.40
5:F:228:GLU:OE2	5:F:231:ARG:NE	2.40	0.40
1:A:40:LEU:HD23	1:A:40:LEU:HA	1.89	0.40
2:C:376:ARG:HH11	2:C:376:ARG:HD2	1.78	0.40
2:C:671:ASN:HA	2:C:992:MET:O	2.21	0.40
2:C:701:THR:HA	2:C:831:ARG:O	2.22	0.40
2:C:993:PHE:CB	12:C:1201:HOH:O	2.28	0.40
3:D:25:GLU:HB2	3:D:92:HIS:CE1	2.56	0.40
3:D:421:LEU:HD11	3:D:429:SER:HB2	2.02	0.40
3:D:852:ALA:HB1	3:D:857:ILE:HB	2.02	0.40
8:I:6:G:C2'	8:I:7:A:H5'	2.51	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	229/315 (73%)	216 (94%)	13 (6%)	0	100	100
1	B	225/315 (71%)	212 (94%)	13 (6%)	0	100	100
2	C	1108/1119 (99%)	1050 (95%)	58 (5%)	0	100	100
3	D	1494/1524 (98%)	1411 (94%)	83 (6%)	0	100	100
4	E	92/99 (93%)	84 (91%)	8 (9%)	0	100	100
5	F	344/443 (78%)	334 (97%)	10 (3%)	0	100	100
All	All	3492/3815 (92%)	3307 (95%)	185 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	200/273 (73%)	185 (92%)	15 (8%)	13	42
1	B	200/273 (73%)	190 (95%)	10 (5%)	24	57
2	C	935/941 (99%)	878 (94%)	57 (6%)	18	50
3	D	1259/1279 (98%)	1191 (95%)	68 (5%)	22	55
4	E	83/88 (94%)	81 (98%)	2 (2%)	49	76
5	F	300/388 (77%)	286 (95%)	14 (5%)	26	60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2977/3242 (92%)	2811 (94%)	166 (6%)	21 53

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	47	SER
1	A	76	VAL
1	A	93	SER
1	A	94	LEU
1	A	112	ARG
1	A	148	VAL
1	A	155	LYS
1	A	170	VAL
1	A	176	ARG
1	A	182	GLU
1	A	196	THR
1	A	198	ARG
1	A	213	GLN
1	A	229	GLN
1	B	2	LEU
1	B	34	VAL
1	B	55	SER
1	B	94	LEU
1	B	113	ASP
1	B	131	THR
1	B	155	LYS
1	B	184	THR
1	B	188	GLN
1	B	205	VAL
2	C	27	ARG
2	C	64	LEU
2	C	113	VAL
2	C	133	ASP
2	C	143	SER
2	C	168	ARG
2	C	174	LEU
2	C	182	VAL
2	C	186	VAL
2	C	200	LEU
2	C	257	VAL
2	C	348	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	351	LEU
2	C	372	LEU
2	C	376	ARG
2	C	384	GLU
2	C	397	GLU
2	C	402	SER
2	C	418	LEU
2	C	426	ASP
2	C	430	VAL
2	C	441	VAL
2	C	454	SER
2	C	455	LEU
2	C	460	ARG
2	C	483	VAL
2	C	493	ARG
2	C	524	VAL
2	C	538	GLN
2	C	562	SER
2	C	578	VAL
2	C	583	LEU
2	C	630	ARG
2	C	631	SER
2	C	644	VAL
2	C	657	ASP
2	C	666	LEU
2	C	670	GLN
2	C	698	ASP
2	C	702	SER
2	C	715	THR
2	C	716	LYS
2	C	717	LEU
2	C	801	VAL
2	C	815	LEU
2	C	848	VAL
2	C	863	ASP
2	C	888	THR
2	C	936	VAL
2	C	953	VAL
2	C	1008	ARG
2	C	1014	SER
2	C	1063	ARG
2	C	1075	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	1084	SER
2	C	1095	LEU
2	C	1099	VAL
3	D	17	LYS
3	D	53	ILE
3	D	80	VAL
3	D	87	ARG
3	D	106	LYS
3	D	150	ARG
3	D	175	VAL
3	D	183	GLU
3	D	185	VAL
3	D	273	ARG
3	D	274	ARG
3	D	275	GLU
3	D	276	ASP
3	D	310	LEU
3	D	311	LEU
3	D	335	LEU
3	D	415	VAL
3	D	420	VAL
3	D	429	SER
3	D	445	ARG
3	D	503	LEU
3	D	537	THR
3	D	574	LEU
3	D	607	LEU
3	D	613	ARG
3	D	614	PHE
3	D	618	LEU
3	D	623	VAL
3	D	628	ARG
3	D	650	LEU
3	D	710	ARG
3	D	724	GLN
3	D	725	SER
3	D	743	ASP
3	D	747	VAL
3	D	754	PHE
3	D	784	ASP
3	D	785	ILE
3	D	827	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	828	LYS
3	D	832	ARG
3	D	864	VAL
3	D	894	LYS
3	D	899	LEU
3	D	910	SER
3	D	922	LEU
3	D	984	THR
3	D	1041	LEU
3	D	1100	ASP
3	D	1101	VAL
3	D	1119	SER
3	D	1185	GLU
3	D	1200	VAL
3	D	1209	LEU
3	D	1216	SER
3	D	1237	THR
3	D	1263	PHE
3	D	1312	LEU
3	D	1313	VAL
3	D	1400	VAL
3	D	1424	VAL
3	D	1425	THR
3	D	1433	SER
3	D	1468	LEU
3	D	1470	ARG
3	D	1476	THR
3	D	1488	ASP
3	D	1493	LYS
4	E	50	THR
4	E	93	TYR
5	F	81	VAL
5	F	94	LEU
5	F	96	LEU
5	F	135	ILE
5	F	136	LEU
5	F	171	LYS
5	F	186	HIS
5	F	234	LYS
5	F	347	GLN
5	F	349	LEU
5	F	358	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	F	375	LEU
5	F	392	VAL
5	F	417	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	163	ASN
2	C	1019	GLN
3	D	294	HIS
3	D	709	HIS
3	D	1034	GLN
3	D	1037	GLN
3	D	1046	GLN
3	D	1242	HIS

5.3.3 RNA (i)

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

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	I	7	A

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 9 ligands modelled in this entry, 8 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	2TM	D	1606	9	27,30,30	4.14	16 (59%)	39,47,47	1.17	3 (7%)

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	2TM	D	1606	9	-	2/19/38/38	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	1606	2TM	PB-O3B	8.24	1.67	1.58
11	D	1606	2TM	O4'-C1'	7.38	1.59	1.42
11	D	1606	2TM	O4'-C4'	-6.97	1.29	1.45
11	D	1606	2TM	PA-O5'	6.71	1.67	1.57
11	D	1606	2TM	C2-N3	6.41	1.49	1.36
11	D	1606	2TM	C4-N4	5.90	1.47	1.33
11	D	1606	2TM	C2'-C1'	-5.81	1.34	1.53
11	D	1606	2TM	C6-C5	5.69	1.48	1.35
11	D	1606	2TM	C4-N3	5.44	1.45	1.34
11	D	1606	2TM	C2-N1	4.07	1.48	1.40
11	D	1606	2TM	C6-N1	3.53	1.46	1.38
11	D	1606	2TM	O2-C2	-3.15	1.17	1.23
11	D	1606	2TM	O2'-C2'	3.05	1.50	1.43
11	D	1606	2TM	O3'-C3'	-2.51	1.37	1.43
11	D	1606	2TM	C5-C4	2.37	1.48	1.42
11	D	1606	2TM	C3'-C4'	2.30	1.58	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	D	1606	2TM	PB-O3B-PG	-3.25	121.15	132.62
11	D	1606	2TM	O2G-PG-O3B	3.06	114.91	104.64
11	D	1606	2TM	N4-C4-N3	2.37	122.13	117.97

There are no chirality outliers.

All (2) torsion outliers are listed below:

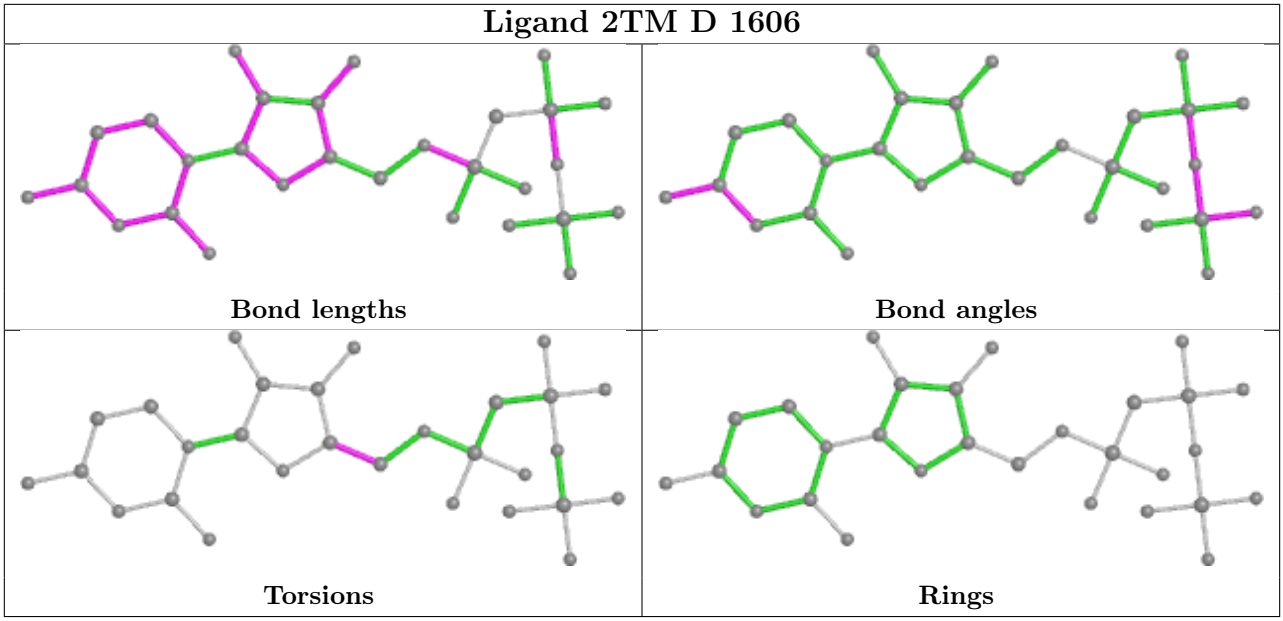
Mol	Chain	Res	Type	Atoms
11	D	1606	2TM	O4'-C4'-C5'-O5'
11	D	1606	2TM	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	1606	2TM	4	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.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	231/315 (73%)	-0.20	4 (1%)	70	57	36, 54, 76, 122	0
1	B	227/315 (72%)	-0.06	6 (2%)	56	40	37, 68, 91, 126	0
2	C	1112/1119 (99%)	-0.13	12 (1%)	80	70	21, 54, 99, 121	0
3	D	1497/1524 (98%)	-0.05	40 (2%)	54	38	20, 56, 108, 167	1 (0%)
4	E	94/99 (94%)	-0.22	1 (1%)	80	70	36, 59, 90, 96	0
5	F	346/443 (78%)	-0.02	9 (2%)	56	40	33, 65, 107, 125	0
6	G	17/21 (80%)	0.07	1 (5%)	22	12	36, 67, 142, 143	0
7	H	24/27 (88%)	0.07	1 (4%)	36	21	53, 84, 122, 154	0
8	I	2/3 (66%)	-0.10	0	100	100	38, 38, 38, 39	0
All	All	3550/3866 (91%)	-0.08	74 (2%)	63	49	20, 57, 105, 167	1 (0%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	149	GLU	4.0
3	D	203	ALA	3.9
3	D	1297	GLU	3.9
3	D	322	VAL	3.8
3	D	267	GLY	3.7
2	C	107	LEU	3.6
1	A	231	ALA	3.4
3	D	1305	LEU	3.4
3	D	1298	GLY	3.3
5	F	415	THR	3.2
3	D	409	VAL	3.2
2	C	365	ASP	3.2
1	A	234	ALA	3.1
1	A	232	ALA	3.1
1	B	2	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	D	1127	GLU	3.1
3	D	350	HIS	3.0
5	F	414	ARG	3.0
3	D	1306	PRO	2.9
3	D	821	VAL	2.8
3	D	377	VAL	2.8
5	F	421	PHE	2.8
3	D	1273	VAL	2.8
2	C	65	VAL	2.8
3	D	1130	ARG	2.7
3	D	831	GLY	2.7
1	B	3	ASP	2.7
1	B	118	ALA	2.7
3	D	1313	VAL	2.7
3	D	982	PHE	2.6
3	D	1247	ALA	2.6
3	D	973	GLN	2.6
3	D	368	VAL	2.6
2	C	66	LEU	2.6
3	D	1408	ILE	2.6
5	F	411	HIS	2.6
3	D	971	LEU	2.6
3	D	378	ILE	2.6
2	C	764	GLU	2.6
2	C	766	GLU	2.5
3	D	1300	SER	2.5
1	A	233	VAL	2.5
1	B	119	ASP	2.5
3	D	1319	VAL	2.5
2	C	774	LEU	2.5
3	D	152	LEU	2.4
1	B	120	VAL	2.4
3	D	830	ALA	2.4
3	D	173	PRO	2.4
3	D	422	ALA	2.4
2	C	616	GLU	2.4
3	D	976	GLN	2.3
5	F	146	GLY	2.3
3	D	406	ASP	2.3
7	H	24	DC	2.3
1	B	5	LYS	2.2
3	D	213	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	F	145	PRO	2.2
5	F	390	PHE	2.2
3	D	1246	VAL	2.2
2	C	367	LEU	2.2
5	F	150	THR	2.2
2	C	100	LEU	2.1
3	D	804	LEU	2.1
3	D	191	LEU	2.1
3	D	1275	SER	2.1
4	E	87	LYS	2.1
3	D	339	TRP	2.1
6	G	5	DC	2.1
2	C	251	ASP	2.1
3	D	316	GLN	2.1
3	D	371	ILE	2.0
2	C	477	GLY	2.0
3	D	1274	ILE	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
9	MG	D	1604	1/1	0.78	0.52	42,42,42,42	0
9	MG	D	1605	1/1	0.82	0.19	59,59,59,59	0
9	MG	B	401	1/1	0.85	0.10	73,73,73,73	0
11	2TM	D	1606	29/29	0.87	0.26	26,37,62,75	29
9	MG	D	1603	1/1	0.91	0.15	27,27,27,27	0
9	MG	B	402	1/1	0.92	0.45	44,44,44,44	0

Continued on next page...

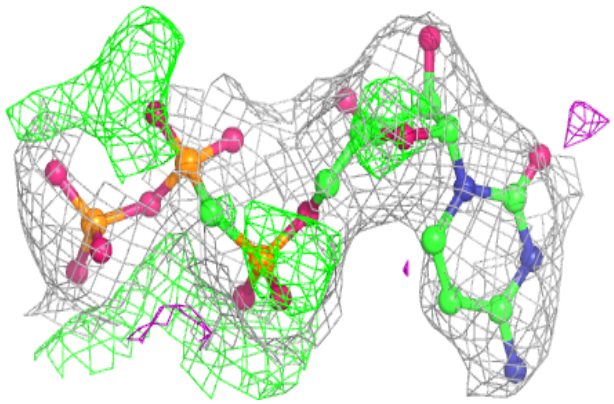
Continued from previous page...

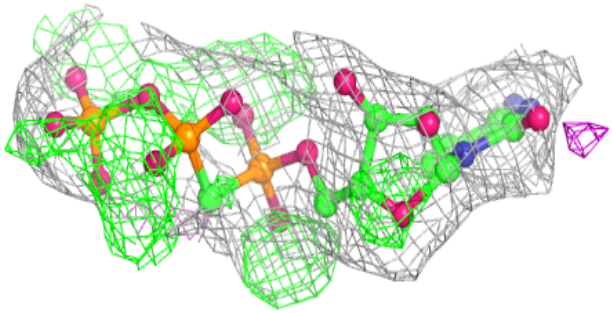
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	MG	F	501	1/1	0.94	0.07	65,65,65,65	0
10	ZN	D	1602	1/1	0.99	0.05	57,57,57,57	0
10	ZN	D	1601	1/1	0.99	0.15	46,46,46,46	0

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 2TM D 1606:

$2mF_o$-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

There are no such residues in this entry.