



Full wwPDB EM Model Validation Report ⓘ

Mar 5, 2020 – 02:10 PM EST

PDB ID : 6S1M
EMDB ID : EMD-10080
Title : Human polymerase delta holoenzyme Conformer 1
Authors : Lancey, C.; Hamdan, S.M.; De Biasio, A.
Deposited on : 2019-06-19
Resolution : 4.27 Å(reported)

This is a Full wwPDB EM Model Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.8

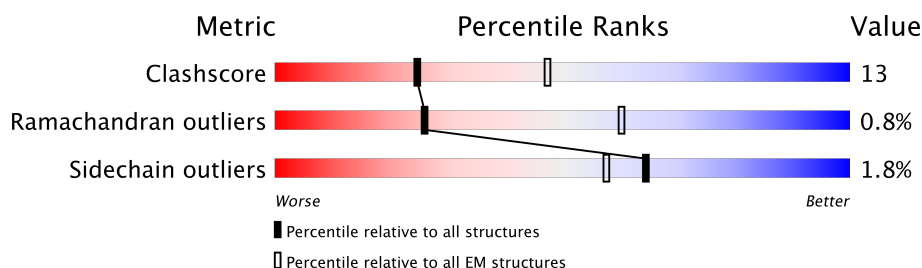
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.27 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)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1107	
2	B	469	
3	C	474	
4	D	137	
5	E	264	
5	F	264	
5	G	264	
6	P	25	
7	T	38	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 19726 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 polymerase delta catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1010	Total	C	N	O	S	1	0
			7926	5028	1405	1447	46		

- Molecule 2 is a protein called DNA polymerase delta subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	431	Total	C	N	O	S	0	0
			3304	2103	553	630	18		

- Molecule 3 is a protein called DNA polymerase delta subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	143	Total	C	N	O	S	0	0
			1130	715	196	214	5		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	MET	-	initiating methionine	UNP Q15054
C	-6	TRP	-	expression tag	UNP Q15054
C	-5	SER	-	expression tag	UNP Q15054
C	-4	HIS	-	expression tag	UNP Q15054
C	-3	PRO	-	expression tag	UNP Q15054
C	-2	GLN	-	expression tag	UNP Q15054
C	-1	PHE	-	expression tag	UNP Q15054
C	0	GLU	-	expression tag	UNP Q15054
C	1	LYS	-	expression tag	UNP Q15054

- Molecule 4 is a protein called DNA polymerase delta subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	66	Total	C	N	O	S	0	0
			554	359	97	94	4		

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-29	MET	-	initiating methionine	UNP Q9HCU8
D	-28	HIS	-	expression tag	UNP Q9HCU8
D	-27	HIS	-	expression tag	UNP Q9HCU8
D	-26	HIS	-	expression tag	UNP Q9HCU8
D	-25	HIS	-	expression tag	UNP Q9HCU8
D	-24	HIS	-	expression tag	UNP Q9HCU8
D	-23	HIS	-	expression tag	UNP Q9HCU8
D	-22	SER	-	expression tag	UNP Q9HCU8
D	-21	ARG	-	expression tag	UNP Q9HCU8
D	-20	ALA	-	expression tag	UNP Q9HCU8
D	-19	TRP	-	expression tag	UNP Q9HCU8
D	-18	ARG	-	expression tag	UNP Q9HCU8
D	-17	HIS	-	expression tag	UNP Q9HCU8
D	-16	PRO	-	expression tag	UNP Q9HCU8
D	-15	GLN	-	expression tag	UNP Q9HCU8
D	-14	PHE	-	expression tag	UNP Q9HCU8
D	-13	GLY	-	expression tag	UNP Q9HCU8
D	-12	GLY	-	expression tag	UNP Q9HCU8
D	-11	HIS	-	expression tag	UNP Q9HCU8
D	-10	HIS	-	expression tag	UNP Q9HCU8
D	-9	HIS	-	expression tag	UNP Q9HCU8
D	-8	HIS	-	expression tag	UNP Q9HCU8
D	-7	HIS	-	expression tag	UNP Q9HCU8
D	-6	HIS	-	expression tag	UNP Q9HCU8
D	-5	GLU	-	expression tag	UNP Q9HCU8
D	-4	ASN	-	expression tag	UNP Q9HCU8
D	-3	LEU	-	expression tag	UNP Q9HCU8
D	-2	TYR	-	expression tag	UNP Q9HCU8
D	-1	PHE	-	expression tag	UNP Q9HCU8
D	0	GLN	-	expression tag	UNP Q9HCU8
D	1	SER	-	expression tag	UNP Q9HCU8

- Molecule 5 is a protein called Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	251	Total	C	N	O	S	0	0
			1924	1211	314	383	16		
5	F	249	Total	C	N	O	S	0	0
			1913	1205	312	380	16		
5	G	249	Total	C	N	O	S	0	0
			1913	1204	314	379	16		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP P12004
E	-1	PRO	-	expression tag	UNP P12004
E	0	HIS	-	expression tag	UNP P12004
F	-2	GLY	-	expression tag	UNP P12004
F	-1	PRO	-	expression tag	UNP P12004
F	0	HIS	-	expression tag	UNP P12004
G	-2	GLY	-	expression tag	UNP P12004
G	-1	PRO	-	expression tag	UNP P12004
G	0	HIS	-	expression tag	UNP P12004

- Molecule 6 is a DNA chain called DNA primer.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	23	Total	C	N	O	P	0	0
			469	225	84	137	23		

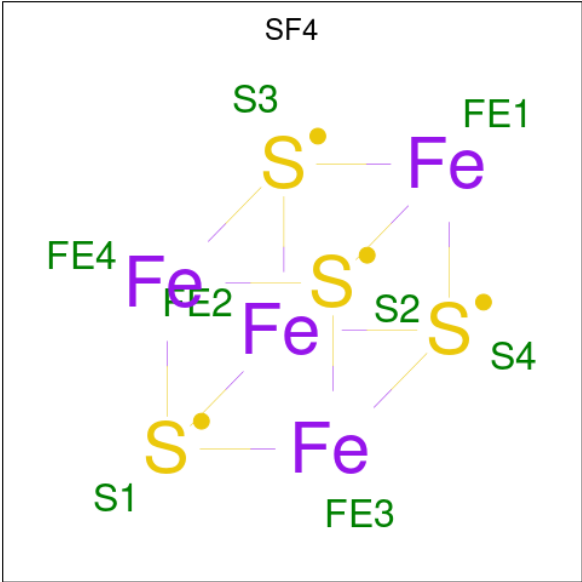
- Molecule 7 is a DNA chain called DNA template.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	27	Total	C	N	O	P	0	0
			555	266	100	162	27		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

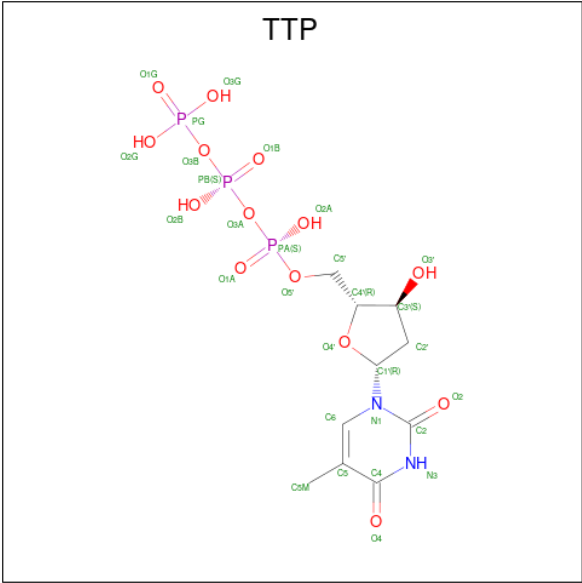
Mol	Chain	Residues	Atoms		AltConf
8	A	1	Total	Zn	0
			1	1	

- Molecule 9 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	Fe	S	0
			8	4	4	

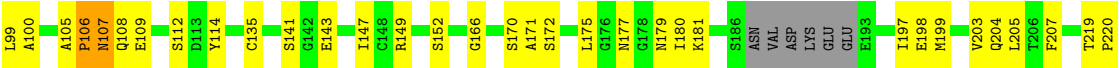
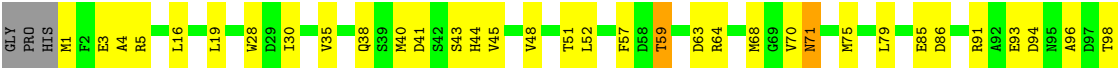
- Molecule 10 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).



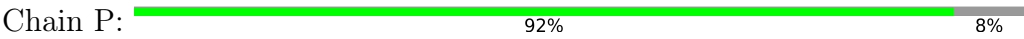
Mol	Chain	Residues	Atoms					AltConf
10	T	1	Total	C	N	O	P	0
			29	10	2	14	3	



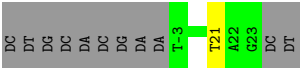
• Molecule 5: Proliferating cell nuclear antigen



• Molecule 6: DNA primer



• Molecule 7: DNA template



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	96612	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	600	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor

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: DOC, ZN, TTP, SF4

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	0.39	0/8094	0.64	0/10971
2	B	0.41	0/3380	0.61	0/4604
3	C	0.36	0/1149	0.58	0/1553
4	D	0.42	0/574	0.69	0/783
5	E	0.38	0/1949	0.63	0/2632
5	F	0.40	0/1937	0.62	0/2614
5	G	0.39	0/1938	0.64	0/2617
6	P	0.84	0/505	1.05	0/777
7	T	0.86	0/622	1.10	1/958 (0.1%)
All	All	0.43	0/20148	0.67	1/27509 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
7	T	21	DT	O4'-C1'-N1	5.26	111.68	108.00

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	7926	0	7967	193	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3304	0	3255	56	0
3	C	1130	0	1138	7	0
4	D	554	0	537	12	0
5	E	1924	0	1930	70	0
5	F	1913	0	1922	162	0
5	G	1913	0	1926	68	0
6	P	469	0	261	0	0
7	T	555	0	307	0	0
8	A	1	0	0	0	0
9	A	8	0	0	1	0
10	T	29	0	10	0	0
All	All	19726	0	19253	495	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 (495) 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)
1:A:861:VAL:CG1	1:A:985:ARG:HD3	1.40	1.51
1:A:688:GLY:HA2	1:A:691:LEU:CD2	1.43	1.49
1:A:995:LEU:CD1	5:F:124:GLU:CG	1.91	1.48
1:A:861:VAL:HG11	1:A:985:ARG:NE	1.27	1.46
1:A:861:VAL:CG1	1:A:985:ARG:CD	1.93	1.45
1:A:861:VAL:HG11	1:A:985:ARG:CZ	1.45	1.44
1:A:995:LEU:HD13	5:F:124:GLU:CG	0.94	1.41
1:A:861:VAL:HG13	1:A:985:ARG:CD	1.49	1.41
1:A:1007:LYS:CB	5:F:127:GLY:HA3	1.50	1.40
5:F:66:LEU:CD1	5:F:94:ASP:HA	1.54	1.36
1:A:995:LEU:CD1	5:F:124:GLU:HG3	1.53	1.33
1:A:995:LEU:CD2	5:F:122:ASP:O	1.81	1.27
5:F:66:LEU:HD11	5:F:94:ASP:CB	1.62	1.26
1:A:995:LEU:HD23	5:F:122:ASP:O	1.09	1.23
1:A:995:LEU:CD1	5:F:124:GLU:HG2	1.59	1.16
2:B:308:GLN:O	2:B:329:THR:HB	1.44	1.16
5:F:66:LEU:CD1	5:F:94:ASP:CA	2.23	1.15
1:A:1007:LYS:N	5:F:127:GLY:HA3	1.60	1.15
5:F:68:MET:SD	5:F:118:LEU:HD11	1.86	1.13
2:B:330:ASN:HB3	2:B:331:PRO:CD	1.77	1.13
1:A:1007:LYS:CA	5:F:127:GLY:HA3	1.78	1.12
1:A:1007:LYS:CB	5:F:127:GLY:CA	2.27	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:66:LEU:HD11	5:F:94:ASP:CA	1.82	1.10
1:A:688:GLY:O	1:A:691:LEU:HG	1.53	1.09
1:A:861:VAL:CG1	1:A:985:ARG:NE	2.08	1.09
1:A:995:LEU:HD22	5:F:124:GLU:CA	1.85	1.06
5:F:64:ARG:HD2	5:F:66:LEU:HD21	1.11	1.06
1:A:995:LEU:HD22	5:F:124:GLU:N	1.71	1.05
5:F:68:MET:SD	5:F:118:LEU:CD1	2.43	1.05
5:E:16:LEU:HD22	5:E:79:LEU:HD12	1.38	1.04
1:A:688:GLY:HA2	1:A:691:LEU:HD21	1.06	1.04
2:B:295:MET:HG2	2:B:329:THR:O	1.54	1.03
1:A:1007:LYS:N	5:F:127:GLY:CA	2.22	1.03
1:A:688:GLY:HA2	1:A:691:LEU:HD23	1.37	1.03
2:B:330:ASN:HB3	2:B:331:PRO:HD3	1.03	1.03
5:G:16:LEU:HD22	5:G:79:LEU:HD12	1.41	1.00
1:A:861:VAL:CG1	1:A:985:ARG:CZ	2.39	1.00
1:A:861:VAL:HG13	1:A:985:ARG:HD3	1.07	0.99
5:F:66:LEU:HD11	5:F:94:ASP:CG	1.81	0.99
1:A:688:GLY:CA	1:A:691:LEU:CD2	2.38	0.99
5:F:68:MET:CG	5:F:118:LEU:HD13	1.91	0.99
5:F:66:LEU:CD1	5:F:94:ASP:OD1	2.10	0.99
5:F:66:LEU:HD13	5:F:94:ASP:CA	1.91	0.98
5:F:68:MET:CB	5:F:118:LEU:HD13	1.94	0.97
1:A:995:LEU:CD2	5:F:123:VAL:C	2.33	0.97
5:F:66:LEU:HD13	5:F:94:ASP:HA	0.98	0.97
1:A:995:LEU:HD22	5:F:124:GLU:HA	1.46	0.97
5:F:64:ARG:HD2	5:F:66:LEU:CD2	1.95	0.96
1:A:995:LEU:HB3	5:F:123:VAL:HA	1.43	0.96
1:A:995:LEU:HD22	5:F:123:VAL:C	1.86	0.95
1:A:1005:PHE:HB3	5:F:129:PRO:CG	1.95	0.95
5:F:64:ARG:CD	5:F:66:LEU:HD21	1.95	0.95
1:A:1005:PHE:HB3	5:F:129:PRO:CD	1.99	0.93
1:A:995:LEU:CG	5:F:122:ASP:O	2.17	0.92
2:B:308:GLN:OE1	2:B:330:ASN:ND2	2.02	0.92
1:A:688:GLY:CA	1:A:691:LEU:HD21	1.96	0.92
1:A:861:VAL:HG11	1:A:985:ARG:CD	1.76	0.92
2:B:308:GLN:O	2:B:329:THR:CB	2.17	0.91
1:A:1007:LYS:H	5:F:127:GLY:CA	1.82	0.91
1:A:861:VAL:HG13	1:A:985:ARG:HD2	1.48	0.91
5:F:66:LEU:HD11	5:F:94:ASP:OD1	1.65	0.90
1:A:995:LEU:HB3	5:F:123:VAL:CA	2.01	0.90
1:A:995:LEU:HD13	5:F:124:GLU:HG2	0.92	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:330:ASN:CB	2:B:331:PRO:HD3	1.99	0.89
5:F:170:SER:HB3	5:F:179:ASN:HB3	1.51	0.89
5:E:170:SER:HB3	5:E:179:ASN:HB3	1.55	0.88
5:G:170:SER:HB3	5:G:179:ASN:HB3	1.54	0.88
1:A:861:VAL:HG12	1:A:985:ARG:HD3	1.54	0.87
1:A:1005:PHE:O	5:F:127:GLY:O	1.93	0.87
1:A:861:VAL:HG11	1:A:985:ARG:NH1	1.91	0.86
5:F:16:LEU:HD22	5:F:79:LEU:HD12	1.55	0.85
1:A:1005:PHE:HB3	5:F:129:PRO:HG2	1.57	0.85
2:B:295:MET:HG3	2:B:328:VAL:HG23	1.59	0.85
1:A:1003:LEU:HD21	5:F:40:MET:CE	2.09	0.83
1:A:164:LEU:HB3	1:A:190:VAL:HG11	1.59	0.83
1:A:1005:PHE:CB	5:F:129:PRO:HG2	2.09	0.81
1:A:1007:LYS:H	5:F:127:GLY:N	1.77	0.81
1:A:995:LEU:HD13	5:F:124:GLU:HG3	0.82	0.81
5:G:5:ARG:HB3	5:G:59:THR:HB	1.63	0.81
1:A:995:LEU:HD23	5:F:122:ASP:C	2.02	0.80
1:A:1002:LEU:HD12	5:F:234:PRO:HG2	1.62	0.80
5:E:5:ARG:HB3	5:E:59:THR:HB	1.64	0.79
1:A:188:LEU:HA	1:A:213:THR:O	1.83	0.79
5:F:68:MET:HB3	5:F:118:LEU:HD13	1.61	0.79
5:F:68:MET:SD	5:F:118:LEU:HD13	2.21	0.79
5:F:5:ARG:HB3	5:F:59:THR:HB	1.66	0.78
5:F:66:LEU:HD12	5:F:94:ASP:OD1	1.85	0.77
1:A:1038:GLN:HE22	2:B:273:VAL:HA	1.48	0.76
5:F:66:LEU:HD11	5:F:94:ASP:HB3	1.64	0.76
1:A:1003:LEU:HD21	5:F:40:MET:HE1	1.67	0.75
1:A:995:LEU:HD23	5:F:123:VAL:C	2.07	0.75
1:A:1078:ILE:HG13	9:A:1202:SF4:S1	2.26	0.74
1:A:861:VAL:CG1	1:A:985:ARG:NH1	2.50	0.74
5:E:147:ILE:HG23	5:E:180:ILE:HD12	1.69	0.74
1:A:995:LEU:CG	5:F:124:GLU:HG3	2.18	0.74
1:A:1005:PHE:CG	5:F:129:PRO:HG2	2.23	0.73
1:A:188:LEU:N	1:A:188:LEU:HD23	2.04	0.73
1:A:164:LEU:HB3	1:A:190:VAL:HG21	1.71	0.72
5:F:66:LEU:CD1	5:F:94:ASP:CB	2.53	0.72
1:A:1011:CYS:O	1:A:1098:ARG:NH1	2.22	0.71
1:A:688:GLY:CA	1:A:691:LEU:HD23	2.13	0.71
1:A:995:LEU:CD2	5:F:123:VAL:O	2.38	0.70
1:A:995:LEU:HD11	5:F:124:GLU:HG2	1.67	0.70
5:G:3:GLU:OE2	5:G:91:ARG:HD3	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:296:PRO:HD2	2:B:329:THR:HA	1.73	0.69
2:B:330:ASN:CB	2:B:331:PRO:CD	2.60	0.69
1:A:1007:LYS:H	5:F:127:GLY:HA3	1.40	0.69
1:A:995:LEU:CD2	5:F:124:GLU:N	2.51	0.68
5:F:69:GLY:HA3	5:F:121:LEU:HG	1.76	0.68
1:A:1024:ALA:HB2	1:A:1098:ARG:HB3	1.76	0.68
5:F:30:ILE:HD12	5:F:35:VAL:HG22	1.76	0.68
1:A:1006:ALA:C	5:F:127:GLY:O	2.32	0.67
1:A:1002:LEU:CD1	5:F:234:PRO:HG2	2.24	0.67
1:A:995:LEU:HB2	5:F:124:GLU:HG3	1.77	0.67
2:B:310:PRO:N	2:B:329:THR:HG22	2.09	0.67
5:E:3:GLU:OE2	5:E:91:ARG:HD3	1.95	0.67
5:G:30:ILE:HD12	5:G:35:VAL:HG22	1.76	0.67
2:B:309:GLN:C	2:B:329:THR:HG22	2.15	0.66
1:A:1091:ASP:OD1	1:A:1092:GLN:N	2.29	0.66
5:G:172:SER:HB3	5:G:177:ASN:HB3	1.78	0.66
5:E:170:SER:CB	5:E:179:ASN:HB3	2.27	0.65
5:E:172:SER:HB3	5:E:177:ASN:HB3	1.78	0.65
1:A:525:ARG:O	1:A:682:ARG:NH2	2.29	0.65
5:F:172:SER:HB3	5:F:177:ASN:HB3	1.79	0.64
5:G:170:SER:CB	5:G:179:ASN:HB3	2.27	0.64
5:G:41:ASP:OD2	5:G:43:SER:HB2	1.97	0.64
1:A:995:LEU:HD23	5:F:123:VAL:O	1.97	0.64
5:F:69:GLY:CA	5:F:121:LEU:HD12	2.28	0.64
5:E:30:ILE:HD12	5:E:35:VAL:HG22	1.80	0.63
5:G:52:LEU:HB3	5:G:244:MET:HE1	1.80	0.63
2:B:296:PRO:CD	2:B:329:THR:HA	2.28	0.62
1:A:688:GLY:O	1:A:691:LEU:CG	2.41	0.62
1:A:981:ALA:O	1:A:985:ARG:HG3	1.98	0.62
5:F:69:GLY:HA3	5:F:121:LEU:CD1	2.29	0.62
4:D:53:ASP:OD2	4:D:66:ARG:NH2	2.31	0.62
1:A:1005:PHE:HB3	5:F:129:PRO:HD3	1.80	0.61
5:F:170:SER:CB	5:F:179:ASN:HB3	2.29	0.61
2:B:73:TRP:NE1	2:B:175:ASP:OD2	2.33	0.60
4:D:42:GLU:OE2	4:D:96:ARG:NH2	2.34	0.60
1:A:995:LEU:CB	5:F:124:GLU:HG3	2.31	0.60
5:E:171:ALA:O	5:E:177:ASN:HB2	2.02	0.60
1:A:1003:LEU:HD21	5:F:40:MET:HE3	1.83	0.60
1:A:1013:ILE:HD12	1:A:1024:ALA:HB1	1.83	0.60
5:G:171:ALA:O	5:G:177:ASN:HB2	2.01	0.60
1:A:583:GLY:O	1:A:725:ARG:NH1	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:ARG:HH21	1:A:434:SER:HB2	1.66	0.60
1:A:188:LEU:H	1:A:188:LEU:HD23	1.65	0.59
5:G:64:ARG:HD2	5:G:94:ASP:HB3	1.84	0.59
1:A:1088:ASP:HA	1:A:1091:ASP:OD2	2.02	0.59
1:A:187:VAL:O	1:A:187:VAL:HG22	2.02	0.59
1:A:674:LEU:HD13	1:A:686:LEU:HB2	1.82	0.59
1:A:1005:PHE:CB	5:F:129:PRO:CG	2.71	0.59
1:A:525:ARG:HG2	1:A:682:ARG:HH22	1.67	0.59
5:F:3:GLU:OE2	5:F:91:ARG:HD3	2.03	0.59
5:G:4:ALA:HB1	5:G:57:PHE:CD2	2.38	0.59
4:D:61:CYS:SG	4:D:72:ARG:NH2	2.75	0.59
1:A:986:GLY:O	1:A:990:ARG:N	2.36	0.59
5:F:69:GLY:CA	5:F:121:LEU:CD1	2.81	0.59
5:F:135:CYS:SG	5:F:199:MET:HG2	2.43	0.59
1:A:357:LEU:HD11	1:A:374:GLU:HG2	1.85	0.58
2:B:184:GLN:HB2	2:B:398:CYS:HB3	1.85	0.58
5:F:51:THR:O	5:F:245:GLY:HA3	2.03	0.58
1:A:186:ALA:HB3	1:A:188:LEU:CD2	2.33	0.58
5:G:86:ASP:OD1	5:G:105:ALA:HA	2.04	0.58
1:A:995:LEU:CB	5:F:123:VAL:HA	2.26	0.58
5:E:141:SER:HB2	5:E:219:THR:HG23	1.86	0.58
1:A:1062:GLN:NE2	1:A:1068:ASP:O	2.37	0.58
1:A:1039:LYS:O	1:A:1040:GLU:HG2	2.04	0.57
1:A:161:MET:O	1:A:165:GLN:NE2	2.37	0.57
1:A:186:ALA:HB3	1:A:188:LEU:HD21	1.86	0.57
1:A:983:LEU:O	1:A:990:ARG:NH1	2.37	0.57
5:F:149:ARG:HH11	5:F:149:ARG:HG2	1.68	0.57
2:B:295:MET:HG3	2:B:328:VAL:CG2	2.33	0.57
1:A:628:GLN:HB3	1:A:629:LYS:HD3	1.86	0.57
2:B:134:VAL:HG11	2:B:141:ARG:HH11	1.70	0.57
2:B:1:MET:HG2	2:B:441:ASN:HD22	1.69	0.57
2:B:32:TYR:HH	2:B:332:TYR:HH	1.52	0.57
1:A:1056:THR:HG23	1:A:1060:ARG:HH21	1.70	0.57
5:G:51:THR:O	5:G:245:GLY:HA3	2.05	0.57
5:F:69:GLY:HA3	5:F:121:LEU:CG	2.34	0.56
5:G:107:ASN:O	5:G:109:GLU:OE1	2.23	0.56
5:E:170:SER:HB3	5:E:179:ASN:CB	2.34	0.56
1:A:539:THR:HA	1:A:558:GLN:HE21	1.69	0.56
5:F:171:ALA:O	5:F:177:ASN:HB2	2.05	0.56
5:F:52:LEU:HB3	5:F:244:MET:HE1	1.88	0.56
1:A:688:GLY:C	1:A:691:LEU:HG	2.24	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:68:MET:HB2	5:F:118:LEU:HD22	1.88	0.56
1:A:587:ILE:HD13	1:A:732:LYS:HD3	1.88	0.56
1:A:1026:CYS:O	1:A:1030:GLN:HG3	2.05	0.55
3:C:35:ASN:HA	3:C:38:LYS:HD2	1.88	0.55
5:F:16:LEU:HD13	5:F:79:LEU:CD1	2.35	0.55
5:E:40:MET:HE2	5:E:44:HIS:CG	2.42	0.55
1:A:142:HIS:NE2	1:A:289:ASP:OD1	2.37	0.55
5:E:135:CYS:SG	5:E:199:MET:HG2	2.46	0.55
5:F:93:GLU:HB2	5:F:96:ALA:HB3	1.89	0.55
2:B:307:PRO:O	2:B:309:GLN:NE2	2.37	0.55
2:B:296:PRO:HD2	2:B:329:THR:CA	2.36	0.55
1:A:995:LEU:HD22	5:F:123:VAL:O	2.03	0.55
5:G:28:TRP:HE3	5:G:35:VAL:HG11	1.70	0.55
5:E:86:ASP:OD1	5:E:105:ALA:HA	2.07	0.55
5:F:64:ARG:HD2	5:F:94:ASP:HB3	1.88	0.55
5:E:16:LEU:HD21	5:E:75:MET:CG	2.37	0.55
1:A:153:PRO:HD2	1:A:158:PRO:HG2	1.88	0.54
5:E:51:THR:O	5:E:245:GLY:HA3	2.07	0.54
5:F:141:SER:HB2	5:F:219:THR:HG23	1.89	0.54
5:G:19:LEU:CD2	5:G:48:VAL:HG11	2.38	0.54
2:B:298:GLU:HG3	2:B:347:GLN:HE21	1.73	0.54
2:B:356:SER:OG	2:B:357:SER:N	2.40	0.54
4:D:47:GLU:OE1	4:D:50:ARG:NH1	2.41	0.54
4:D:66:ARG:NH1	4:D:97:PHE:O	2.41	0.54
5:F:30:ILE:CD1	5:F:35:VAL:HG22	2.37	0.54
5:G:1:MET:H3	5:G:63:ASP:HB2	1.72	0.54
2:B:310:PRO:HA	2:B:328:VAL:O	2.08	0.53
2:B:404:CYS:SG	2:B:405:GLY:N	2.79	0.53
5:F:19:LEU:CD2	5:F:48:VAL:HG11	2.37	0.53
5:E:16:LEU:HD21	5:E:75:MET:HG2	1.90	0.53
5:E:93:GLU:HB2	5:E:96:ALA:HB3	1.89	0.53
5:G:147:ILE:HG23	5:G:180:ILE:HD12	1.91	0.53
3:C:110:ASP:OD1	3:C:110:ASP:N	2.42	0.53
1:A:164:LEU:CB	1:A:190:VAL:HG21	2.38	0.53
5:E:52:LEU:HB3	5:E:244:MET:HE1	1.91	0.53
5:E:30:ILE:HG13	5:E:68:MET:CE	2.39	0.53
5:G:170:SER:HB3	5:G:179:ASN:CB	2.33	0.53
5:G:30:ILE:HG13	5:G:68:MET:CE	2.39	0.53
5:E:4:ALA:HB1	5:E:57:PHE:CD2	2.44	0.52
1:A:1005:PHE:O	5:F:129:PRO:HD3	2.10	0.52
5:G:16:LEU:HD13	5:G:79:LEU:CD1	2.40	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:THR:HG22	1:A:457:MET:HB2	1.92	0.52
5:F:40:MET:HE2	5:F:44:HIS:CG	2.44	0.52
1:A:687:ASP:O	1:A:691:LEU:HD23	2.09	0.52
3:C:59:VAL:HG12	3:C:103:ILE:HG22	1.92	0.52
5:F:69:GLY:HA2	5:F:121:LEU:HD12	1.91	0.52
5:F:16:LEU:HD21	5:F:75:MET:CG	2.40	0.52
1:A:232:ARG:HH12	1:A:242:ALA:HB3	1.75	0.52
2:B:310:PRO:CD	2:B:329:THR:CG2	2.88	0.52
5:E:28:TRP:HE3	5:E:35:VAL:HG11	1.74	0.52
1:A:995:LEU:HG	5:F:122:ASP:O	2.05	0.52
5:F:172:SER:HB3	5:F:177:ASN:CB	2.40	0.52
5:E:135:CYS:HG	5:E:162:CYS:HG	1.57	0.51
5:F:135:CYS:HA	5:F:198:GLU:O	2.10	0.51
5:G:40:MET:HE2	5:G:44:HIS:CG	2.45	0.51
5:F:135:CYS:HG	5:F:162:CYS:HG	1.58	0.51
5:F:1:MET:H3	5:F:63:ASP:HB2	1.74	0.51
1:A:102:ASP:HB3	1:A:126:ARG:HB2	1.93	0.51
5:E:1:MET:H3	5:E:63:ASP:HB2	1.75	0.51
5:G:93:GLU:HB2	5:G:96:ALA:HB3	1.92	0.51
1:A:617:CYS:HB3	1:A:620:THR:HG22	1.91	0.51
5:G:135:CYS:HA	5:G:198:GLU:O	2.09	0.51
5:G:16:LEU:HD21	5:G:75:MET:CG	2.41	0.51
1:A:171:ALA:H	1:A:180:ARG:HG3	1.75	0.51
2:B:310:PRO:N	2:B:329:THR:CG2	2.73	0.51
5:G:40:MET:HE1	5:G:44:HIS:ND1	2.25	0.51
5:E:16:LEU:HD13	5:E:79:LEU:CD1	2.41	0.51
5:F:147:ILE:HG23	5:F:180:ILE:HD12	1.92	0.51
5:F:86:ASP:OD1	5:F:105:ALA:HA	2.11	0.51
1:A:164:LEU:HB3	1:A:190:VAL:CG1	2.37	0.50
5:F:28:TRP:CD1	5:F:28:TRP:N	2.79	0.50
1:A:995:LEU:HD13	5:F:124:GLU:CD	2.08	0.50
5:E:149:ARG:HG2	5:E:149:ARG:HH11	1.76	0.50
5:E:19:LEU:CD2	5:E:48:VAL:HG11	2.41	0.50
5:E:52:LEU:HD22	5:E:244:MET:HE1	1.93	0.50
1:A:736:GLU:HG3	1:A:751:VAL:HG23	1.94	0.50
5:G:141:SER:HB2	5:G:219:THR:HG23	1.93	0.50
5:F:143:GLU:O	5:F:147:ILE:HG13	2.12	0.50
1:A:1005:PHE:CD1	5:F:129:PRO:HG2	2.47	0.50
1:A:995:LEU:C	1:A:995:LEU:HD12	2.31	0.50
1:A:1007:LYS:H	5:F:127:GLY:H	1.58	0.49
1:A:1003:LEU:CD2	5:F:40:MET:HE3	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:984:LEU:HA	1:A:987:ASP:HB2	1.94	0.49
5:E:172:SER:HB3	5:E:177:ASN:CB	2.42	0.49
5:G:228:SER:HB2	5:G:236:VAL:HB	1.94	0.49
1:A:1021:HIS:CD2	1:A:1021:HIS:C	2.85	0.49
1:A:191:GLU:HB3	1:A:211:ARG:HB3	1.93	0.49
5:G:52:LEU:HB3	5:G:244:MET:CE	2.42	0.49
1:A:1039:LYS:O	1:A:1040:GLU:CG	2.61	0.49
1:A:995:LEU:CB	5:F:122:ASP:O	2.60	0.49
1:A:974:LEU:HD22	1:A:978:ARG:HD3	1.95	0.49
2:B:310:PRO:HD3	2:B:329:THR:HG21	1.94	0.49
5:F:69:GLY:HA3	5:F:121:LEU:HD12	1.94	0.49
5:G:143:GLU:O	5:G:147:ILE:HG13	2.12	0.49
1:A:587:ILE:HD12	1:A:754:GLY:HA3	1.94	0.48
5:E:28:TRP:CE3	5:E:35:VAL:HG11	2.47	0.48
5:E:30:ILE:CD1	5:E:35:VAL:HG22	2.43	0.48
5:G:28:TRP:CE3	5:G:35:VAL:HG11	2.46	0.48
1:A:964:LYS:HG3	1:A:965:PRO:HD3	1.95	0.48
5:G:203:VAL:HG12	5:G:204:GLN:N	2.28	0.48
1:A:865:GLN:NE2	1:A:985:ARG:HH11	2.10	0.48
1:A:1030:GLN:H	1:A:1031:PRO:CD	2.27	0.48
5:F:170:SER:HB3	5:F:179:ASN:CB	2.34	0.48
5:G:166:GLY:HA2	5:G:197:ILE:CD1	2.43	0.48
1:A:248:VAL:HG11	1:A:560:LEU:HD11	1.95	0.48
5:F:107:ASN:O	5:F:109:GLU:OE1	2.32	0.48
5:F:68:MET:CG	5:F:118:LEU:CD1	2.72	0.48
5:G:149:ARG:HH11	5:G:149:ARG:HG2	1.79	0.48
1:A:1030:GLN:HB2	1:A:1031:PRO:HD3	1.95	0.48
1:A:1039:LYS:O	1:A:1040:GLU:CB	2.62	0.48
1:A:421:LEU:HD22	1:A:421:LEU:H	1.78	0.48
2:B:99:LYS:H	2:B:155:THR:HB	1.77	0.48
5:G:207:PHE:CZ	5:G:235:LEU:HB2	2.49	0.48
1:A:995:LEU:CB	5:F:124:GLU:N	2.76	0.48
5:F:38:GLN:HA	5:F:48:VAL:O	2.13	0.48
5:F:40:MET:HE1	5:F:44:HIS:ND1	2.28	0.48
2:B:49:GLN:NE2	4:D:62:THR:OG1	2.46	0.47
3:C:6:TYR:OH	3:C:43:ASP:OD2	2.32	0.47
5:E:40:MET:HE1	5:E:44:HIS:ND1	2.28	0.47
1:A:1047:LEU:HB3	1:A:1089:LEU:HD13	1.96	0.47
2:B:18:SER:OG	2:B:19:ALA:N	2.45	0.47
5:F:166:GLY:HA2	5:F:197:ILE:HD12	1.96	0.47
5:F:4:ALA:HB1	5:F:57:PHE:CD2	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:VAL:HG11	2:B:315:MET:HB3	1.95	0.47
5:E:68:MET:O	5:E:70:VAL:HG23	2.14	0.47
5:F:68:MET:HG2	5:F:118:LEU:HD13	1.88	0.47
1:A:1088:ASP:O	1:A:1091:ASP:OD1	2.32	0.47
5:E:135:CYS:HA	5:E:198:GLU:O	2.14	0.47
5:F:27:CYS:O	5:F:27:CYS:SG	2.71	0.47
5:G:172:SER:HB3	5:G:177:ASN:CB	2.43	0.47
1:A:861:VAL:HG12	1:A:985:ARG:NH1	2.29	0.47
2:B:240:ARG:NH2	2:B:293:ASP:OD2	2.37	0.47
2:B:308:GLN:O	2:B:329:THR:CG2	2.62	0.47
2:B:309:GLN:HA	2:B:329:THR:HG21	1.96	0.47
5:F:16:LEU:HD21	5:F:75:MET:HG2	1.97	0.47
5:G:175:LEU:HD12	5:G:175:LEU:O	2.15	0.47
5:G:244:MET:HE2	5:G:244:MET:HB3	1.47	0.47
1:A:1054:LEU:HD23	2:B:107:ILE:HD13	1.96	0.47
1:A:1006:ALA:HA	5:F:127:GLY:H	1.79	0.47
5:F:110:LYS:HE3	5:G:180:ILE:HG21	1.96	0.47
1:A:360:CYS:SG	1:A:361:ALA:N	2.84	0.46
1:A:810:ALA:HA	1:A:825:ASP:O	2.15	0.46
4:D:50:ARG:HG3	4:D:101:LEU:HD21	1.96	0.46
5:F:241:ILE:O	5:F:244:MET:HB2	2.15	0.46
5:E:110:LYS:HE3	5:F:180:ILE:HG21	1.97	0.46
5:G:16:LEU:HD21	5:G:75:MET:HG2	1.97	0.46
2:B:310:PRO:HG3	2:B:329:THR:HG23	1.98	0.46
2:B:439:LEU:HG	2:B:450:ILE:HD11	1.98	0.46
5:E:166:GLY:HA2	5:E:197:ILE:CD1	2.45	0.46
2:B:309:GLN:C	2:B:329:THR:CG2	2.83	0.46
5:F:64:ARG:HB3	5:F:94:ASP:OD1	2.15	0.46
5:F:41:ASP:OD2	5:F:43:SER:HB2	2.15	0.46
2:B:83:CYS:HB3	2:B:140:GLN:HE22	1.80	0.46
5:E:166:GLY:HA2	5:E:197:ILE:HD12	1.98	0.46
3:C:104:GLN:NE2	3:C:106:ALA:O	2.49	0.46
4:D:79:GLU:HA	4:D:79:GLU:OE1	2.13	0.46
5:F:244:MET:HB3	5:F:244:MET:HE2	1.52	0.46
5:G:166:GLY:HA2	5:G:197:ILE:HD12	1.97	0.46
5:G:246:HIS:HD2	5:G:248:LYS:HG3	1.81	0.46
1:A:1030:GLN:H	1:A:1031:PRO:HD2	1.80	0.46
5:G:30:ILE:CD1	5:G:35:VAL:HG22	2.43	0.46
1:A:163:ASP:HA	1:A:166:ARG:HB2	1.98	0.45
5:G:38:GLN:HA	5:G:48:VAL:O	2.16	0.45
5:E:52:LEU:HB3	5:E:244:MET:CE	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:207:PHE:CZ	5:F:235:LEU:HB2	2.51	0.45
1:A:688:GLY:HA2	1:A:691:LEU:CG	2.34	0.45
1:A:843:LEU:HD22	1:A:867:VAL:HG11	1.99	0.45
1:A:164:LEU:HB3	1:A:190:VAL:CG2	2.46	0.45
5:E:244:MET:HE2	5:E:244:MET:HB3	1.58	0.45
5:E:246:HIS:HD2	5:E:248:LYS:HG3	1.82	0.45
1:A:1003:LEU:CD2	5:F:40:MET:CE	2.91	0.45
2:B:70:GLN:HG2	2:B:77:VAL:HG11	1.99	0.45
1:A:995:LEU:HB3	5:F:122:ASP:O	2.17	0.45
1:A:995:LEU:CD2	5:F:124:GLU:HA	2.32	0.45
1:A:1098:ARG:HG2	1:A:1098:ARG:NH2	2.31	0.45
5:E:41:ASP:OD2	5:E:43:SER:HB2	2.17	0.45
1:A:594:TYR:HB2	1:A:801:TYR:HB3	2.00	0.45
1:A:861:VAL:CG1	1:A:985:ARG:HH11	2.30	0.45
5:F:172:SER:CB	5:F:177:ASN:HB3	2.44	0.45
1:A:1002:LEU:HD21	5:F:47:LEU:HB2	1.99	0.45
5:F:52:LEU:HD22	5:F:244:MET:HE1	1.99	0.45
2:B:193:ASP:N	2:B:193:ASP:OD1	2.49	0.44
5:E:158:VAL:HB	5:E:209:LEU:HD21	1.99	0.44
5:E:64:ARG:HD2	5:E:94:ASP:HB3	1.98	0.44
5:F:166:GLY:HA2	5:F:197:ILE:CD1	2.47	0.44
5:E:16:LEU:CD2	5:E:75:MET:HG2	2.48	0.44
5:E:205:LEU:HD11	5:E:230:SER:O	2.18	0.44
5:G:246:HIS:CD2	5:G:248:LYS:HG3	2.53	0.44
1:A:187:VAL:O	1:A:187:VAL:HG13	2.18	0.44
5:G:149:ARG:O	5:G:152:SER:HB2	2.16	0.44
2:B:161:VAL:HG23	2:B:176:TYR:HB3	2.00	0.44
2:B:246:ASN:H	2:B:297:GLY:HA3	1.82	0.44
5:F:158:VAL:HB	5:F:209:LEU:HD21	1.99	0.44
5:F:203:VAL:HG12	5:F:204:GLN:N	2.33	0.44
5:F:228:SER:HB2	5:F:236:VAL:HB	2.00	0.44
5:G:99:LEU:HD12	5:G:100:ALA:H	1.83	0.44
1:A:834:ARG:HH21	1:A:921:ARG:HH11	1.65	0.44
5:E:140:PRO:HG3	5:E:192:GLU:O	2.17	0.44
5:E:110:LYS:HA	5:F:181:LYS:O	2.18	0.44
1:A:830:GLU:HG3	1:A:965:PRO:HB3	1.99	0.44
5:E:146:ARG:HD3	5:E:149:ARG:NH2	2.33	0.44
5:E:228:SER:HB2	5:E:236:VAL:HB	1.98	0.44
5:E:246:HIS:CD2	5:E:248:LYS:HG3	2.53	0.44
5:G:108:GLN:O	5:G:108:GLN:HG3	2.18	0.44
1:A:421:LEU:HD22	1:A:421:LEU:N	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:45:VAL:HG12	5:F:251:LEU:HD12	2.00	0.43
1:A:467:TYR:O	1:A:472:TYR:OH	2.32	0.43
2:B:366:GLU:HG3	2:B:415:ILE:HD13	1.99	0.43
5:E:137:VAL:O	5:E:226:THR:HA	2.18	0.43
4:D:66:ARG:HG2	4:D:88:LEU:HD11	2.00	0.43
5:E:16:LEU:HD21	5:E:75:MET:SD	2.59	0.43
1:A:1098:ARG:HH21	1:A:1098:ARG:CG	2.32	0.43
1:A:815:SER:OG	1:A:819:ASP:OD2	2.35	0.43
2:B:90:LYS:HA	2:B:90:LYS:HD3	1.85	0.43
5:E:219:THR:N	5:E:220:PRO:HD2	2.33	0.43
5:G:172:SER:CB	5:G:177:ASN:HB3	2.47	0.43
1:A:137:VAL:HG22	1:A:286:LEU:HB2	2.00	0.43
5:E:135:CYS:CB	5:E:162:CYS:HG	2.31	0.43
5:E:38:GLN:HA	5:E:48:VAL:O	2.18	0.43
5:G:1:MET:N	5:G:94:ASP:OD2	2.50	0.43
3:C:128:ASN:OD1	3:C:128:ASN:N	2.51	0.43
5:F:110:LYS:HA	5:G:181:LYS:O	2.19	0.43
1:A:617:CYS:SG	1:A:618:TYR:N	2.92	0.43
5:G:5:ARG:CB	5:G:59:THR:HB	2.42	0.43
2:B:310:PRO:HD3	2:B:329:THR:CG2	2.48	0.43
2:B:417:GLY:N	2:B:421:GLN:O	2.51	0.43
5:E:241:ILE:O	5:E:244:MET:HB2	2.19	0.43
1:A:682:ARG:HA	1:A:685:VAL:HG22	2.01	0.43
5:E:46:SER:HB2	5:E:250:TYR:O	2.18	0.43
5:F:12:LEU:HD12	5:F:12:LEU:HA	1.86	0.43
5:F:16:LEU:HD21	5:F:75:MET:SD	2.59	0.43
5:G:241:ILE:HG22	5:G:244:MET:HB2	1.99	0.43
5:E:135:CYS:HB3	5:E:162:CYS:HG	1.83	0.43
2:B:328:VAL:C	2:B:329:THR:HG23	2.40	0.42
5:E:107:ASN:O	5:E:108:GLN:CB	2.67	0.42
1:A:1030:GLN:N	1:A:1031:PRO:CD	2.82	0.42
3:C:62:LEU:HD12	3:C:79:VAL:HG22	2.01	0.42
5:F:149:ARG:HG2	5:F:149:ARG:NH1	2.34	0.42
5:G:105:ALA:O	5:G:106:PRO:C	2.57	0.42
5:E:96:ALA:HB1	5:E:98:THR:HG23	2.02	0.42
5:F:60:TYR:O	5:F:61:ARG:HB2	2.19	0.42
4:D:61:CYS:HB2	4:D:69:ARG:HH21	1.85	0.42
5:G:203:VAL:CG1	5:G:204:GLN:N	2.82	0.42
5:G:64:ARG:HB3	5:G:94:ASP:OD1	2.19	0.42
5:G:71:ASN:C	5:G:71:ASN:HD22	2.23	0.42
1:A:1078:ILE:HD13	1:A:1078:ILE:HA	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:THR:HA	1:A:748:SER:HA	2.02	0.42
1:A:995:LEU:HB2	5:F:124:GLU:N	2.33	0.42
1:A:995:LEU:HB3	5:F:123:VAL:C	2.40	0.42
2:B:137:ASP:OD1	2:B:138:GLU:N	2.45	0.42
5:E:207:PHE:CZ	5:E:235:LEU:HB2	2.54	0.42
1:A:865:GLN:HE21	1:A:985:ARG:HD3	1.84	0.42
5:F:135:CYS:CB	5:F:162:CYS:HG	2.32	0.42
1:A:1027:GLU:HA	1:A:1030:GLN:NE2	2.34	0.42
1:A:682:ARG:O	1:A:686:LEU:HG	2.20	0.42
2:B:407:THR:HG21	2:B:427:THR:HB	2.01	0.42
5:F:52:LEU:HB3	5:F:244:MET:CE	2.49	0.42
5:G:135:CYS:SG	5:G:199:MET:HG2	2.59	0.42
2:B:360:ASP:OD1	2:B:363:GLU:N	2.50	0.42
1:A:240:SER:HA	1:A:241:PHE:HA	1.62	0.42
1:A:367:LYS:HE3	1:A:369:GLN:HE21	1.85	0.42
1:A:523:LEU:HD12	1:A:528:VAL:HB	2.02	0.42
5:E:17:GLU:HA	5:E:17:GLU:OE1	2.19	0.42
5:E:199:MET:CE	5:E:202:PRO:HG3	2.50	0.42
5:F:135:CYS:HB3	5:F:162:CYS:HG	1.85	0.42
5:F:16:LEU:CD2	5:F:75:MET:HG2	2.50	0.41
5:F:246:HIS:CD2	5:F:248:LYS:HG3	2.55	0.41
5:F:219:THR:N	5:F:220:PRO:HD2	2.34	0.41
1:A:597:PRO:HD2	1:A:766:SER:HA	2.02	0.41
2:B:35:SER:O	2:B:333:GLN:NE2	2.53	0.41
5:E:203:VAL:CG1	5:E:204:GLN:N	2.83	0.41
5:E:215:PHE:N	5:E:215:PHE:CD1	2.89	0.41
5:E:1:MET:N	5:E:94:ASP:OD2	2.49	0.41
5:F:17:GLU:OE1	5:F:17:GLU:HA	2.20	0.41
1:A:157:GLY:HA3	1:A:237:GLY:HA2	2.03	0.41
1:A:188:LEU:CA	1:A:213:THR:O	2.62	0.41
5:E:11:ILE:O	5:E:15:VAL:HG23	2.20	0.41
5:G:112:SER:HB3	5:G:114:TYR:HE1	1.86	0.41
1:A:400:ASN:HD21	1:A:446:THR:HG23	1.85	0.41
1:A:594:TYR:HE2	1:A:762:ARG:HH11	1.67	0.41
1:A:1082:ARG:HH22	4:D:107:LEU:HA	1.86	0.41
5:G:68:MET:O	5:G:70:VAL:HG23	2.21	0.41
1:A:260:ILE:HG22	1:A:297:SER:HB2	2.01	0.41
5:E:64:ARG:HB3	5:E:94:ASP:OD1	2.19	0.41
1:A:242:ALA:HA	1:A:243:PRO:HD3	1.96	0.41
1:A:385:ILE:HG21	1:A:421:LEU:HD12	2.02	0.41
5:G:219:THR:N	5:G:220:PRO:HD2	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1087:LYS:HD3	1:A:1087:LYS:HA	1.89	0.41
1:A:618:TYR:OH	1:A:711:LEU:O	2.31	0.41
5:G:1:MET:HB3	5:G:63:ASP:OD2	2.21	0.41
5:E:185:THR:OG1	5:E:194:ALA:HB1	2.21	0.41
5:F:40:MET:CE	5:F:44:HIS:CG	3.04	0.41
5:G:241:ILE:O	5:G:244:MET:HB2	2.21	0.41
1:A:186:ALA:C	1:A:188:LEU:HD23	2.41	0.40
1:A:651:VAL:HG12	1:A:652:ARG:HG2	2.03	0.40
1:A:736:GLU:OE2	1:A:751:VAL:N	2.39	0.40
2:B:185:LYS:HE3	2:B:185:LYS:HB2	1.86	0.40
4:D:105:TYR:O	4:D:107:LEU:N	2.54	0.40
5:G:112:SER:HB3	5:G:114:TYR:CE1	2.56	0.40
5:G:45:VAL:HG12	5:G:251:LEU:HD12	2.03	0.40
1:A:218:ARG:H	1:A:218:ARG:HG2	1.73	0.40
5:G:64:ARG:CD	5:G:94:ASP:HB3	2.50	0.40
5:F:99:LEU:HD12	5:F:100:ALA:H	1.86	0.40
1:A:1039:LYS:N	1:A:1039:LYS:HD3	2.33	0.40
2:B:312:HIS:HA	2:B:313:PRO:HD3	1.98	0.40
5:E:203:VAL:HG12	5:E:204:GLN:N	2.36	0.40
1:A:1002:LEU:HD13	5:F:234:PRO:CB	2.51	0.40
5:F:23:ILE:HB	5:F:72:LEU:HD12	2.04	0.40
5:G:205:LEU:HD11	5:G:230:SER:O	2.22	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 PDB entries followed by that with respect to all EM entries.

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	1003/1107 (91%)	932 (93%)	66 (7%)	5 (0%)	31	72
2	B	425/469 (91%)	394 (93%)	29 (7%)	2 (0%)	31	72
3	C	141/474 (30%)	131 (93%)	10 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	64/137 (47%)	49 (77%)	12 (19%)	3 (5%)	2	27
5	E	247/264 (94%)	224 (91%)	21 (8%)	2 (1%)	21	63
5	F	243/264 (92%)	223 (92%)	16 (7%)	4 (2%)	11	49
5	G	245/264 (93%)	224 (91%)	17 (7%)	4 (2%)	11	49
All	All	2368/2979 (80%)	2177 (92%)	171 (7%)	20 (1%)	26	63

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	330	ASN
4	D	79	GLU
5	E	242	ALA
5	F	242	ALA
5	G	242	ALA
1	A	85	PRO
5	E	59	THR
5	F	59	THR
5	F	61	ARG
1	A	756	THR
1	A	1021	HIS
1	A	1040	GLU
2	B	328	VAL
5	G	106	PRO
4	D	106	PRO
5	F	243	ASP
5	G	59	THR
5	G	243	ASP
4	D	105	TYR
1	A	1030	GLN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	857/944 (91%)	844 (98%)	13 (2%)	67	84
2	B	367/403 (91%)	362 (99%)	5 (1%)	69	85
3	C	125/413 (30%)	125 (100%)	0	100	100
4	D	59/120 (49%)	58 (98%)	1 (2%)	63	83
5	E	217/230 (94%)	211 (97%)	6 (3%)	47	71
5	F	216/230 (94%)	209 (97%)	7 (3%)	42	69
5	G	217/230 (94%)	212 (98%)	5 (2%)	53	76
All	All	2058/2570 (80%)	2021 (98%)	37 (2%)	64	82

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	LEU
1	A	190	VAL
1	A	676	LYS
1	A	701	TYR
1	A	889	ARG
1	A	910	ARG
1	A	993	THR
1	A	1019	LEU
1	A	1021	HIS
1	A	1038	GLN
1	A	1039	LYS
1	A	1074	ARG
1	A	1098	ARG
2	B	44	ARG
2	B	180	ASP
2	B	220	ASP
2	B	328	VAL
2	B	330	ASN
4	D	79	GLU
5	E	71	ASN
5	E	85	GLU
5	E	98	THR
5	E	192	GLU
5	E	224	THR
5	E	235	LEU
5	F	27	CYS
5	F	68	MET
5	F	71	ASN
5	F	85	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	F	98	THR
5	F	224	THR
5	F	235	LEU
5	G	71	ASN
5	G	85	GLU
5	G	98	THR
5	G	107	ASN
5	G	224	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	369	GLN
1	A	430	ASN
1	A	558	GLN
1	A	726	GLN
1	A	842	ASN
1	A	865	GLN
1	A	1021	HIS
1	A	1038	GLN
1	A	1043	HIS
1	A	1092	GLN
2	B	21	ASN
2	B	70	GLN
2	B	140	GLN
2	B	308	GLN
2	B	330	ASN
2	B	347	GLN
3	C	116	ASN
5	E	38	GLN
5	E	65	ASN
5	E	71	ASN
5	F	38	GLN
5	F	65	ASN
5	F	71	ASN
5	F	184	GLN
5	G	38	GLN
5	G	65	ASN
5	G	71	ASN
5	G	107	ASN
5	G	184	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\# Z > 2$
6	DOC	P	25	7,6	13,19,20	5.02	10 (76%)	13,26,29	1.90	4 (30%)

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
6	DOC	P	25	7,6	-	2/3/18/19	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	25	DOC	C3'-C2'	-8.32	1.30	1.54
6	P	25	DOC	O4'-C4'	-8.09	1.28	1.44
6	P	25	DOC	C6-N1	6.71	1.44	1.35
6	P	25	DOC	O4'-C1'	5.82	1.55	1.42
6	P	25	DOC	C4-N3	5.50	1.44	1.35
6	P	25	DOC	C2-N3	5.28	1.48	1.38
6	P	25	DOC	C6-C5	4.80	1.48	1.38
6	P	25	DOC	C4-N4	3.85	1.46	1.35
6	P	25	DOC	C5-C4	2.89	1.48	1.41
6	P	25	DOC	O5'-C5'	-2.38	1.41	1.44

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	P	25	DOC	C2-N3-C4	3.74	119.84	116.26
6	P	25	DOC	C3'-C2'-C1'	2.92	106.30	102.80
6	P	25	DOC	N4-C4-N3	2.59	120.56	116.48
6	P	25	DOC	C2'-C3'-C4'	2.23	106.92	102.73

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	P	25	DOC	C3'-C4'-C5'-O5'
6	P	25	DOC	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	SF4	A	1202	1	0,12,12	0.00	-	-		
10	TTP	T	101	-	22,30,30	4.00	11 (50%)	27,47,47	1.54	6 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SF4	A	1202	1	-	-	0/6/5/5
10	TTP	T	101	-	-	3/18/34/34	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	T	101	TTP	C2'-C3'	-11.55	1.22	1.52
10	T	101	TTP	O4'-C4'	-7.87	1.27	1.45
10	T	101	TTP	C4-N3	6.85	1.45	1.33
10	T	101	TTP	C2-N3	5.57	1.49	1.38
10	T	101	TTP	C3'-C4'	4.42	1.65	1.53
10	T	101	TTP	O4'-C1'	3.43	1.50	1.42
10	T	101	TTP	PG-O3B	3.37	1.65	1.60
10	T	101	TTP	O3'-C3'	2.93	1.49	1.43
10	T	101	TTP	C6-C5	2.84	1.48	1.40
10	T	101	TTP	O4-C4	-2.55	1.18	1.24
10	T	101	TTP	C2'-C1'	2.04	1.57	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	T	101	TTP	C4-N3-C2	5.22	119.55	115.14
10	T	101	TTP	C2'-C1'-N1	-2.50	108.51	114.27
10	T	101	TTP	O4'-C1'-N1	2.38	111.79	107.78
10	T	101	TTP	PB-O3A-PA	-2.15	125.72	132.57
10	T	101	TTP	PB-O3B-PG	-2.11	125.86	132.57
10	T	101	TTP	C3'-C2'-C1'	2.08	107.83	102.53

There are no chirality outliers.

All (3) torsion outliers are listed below:

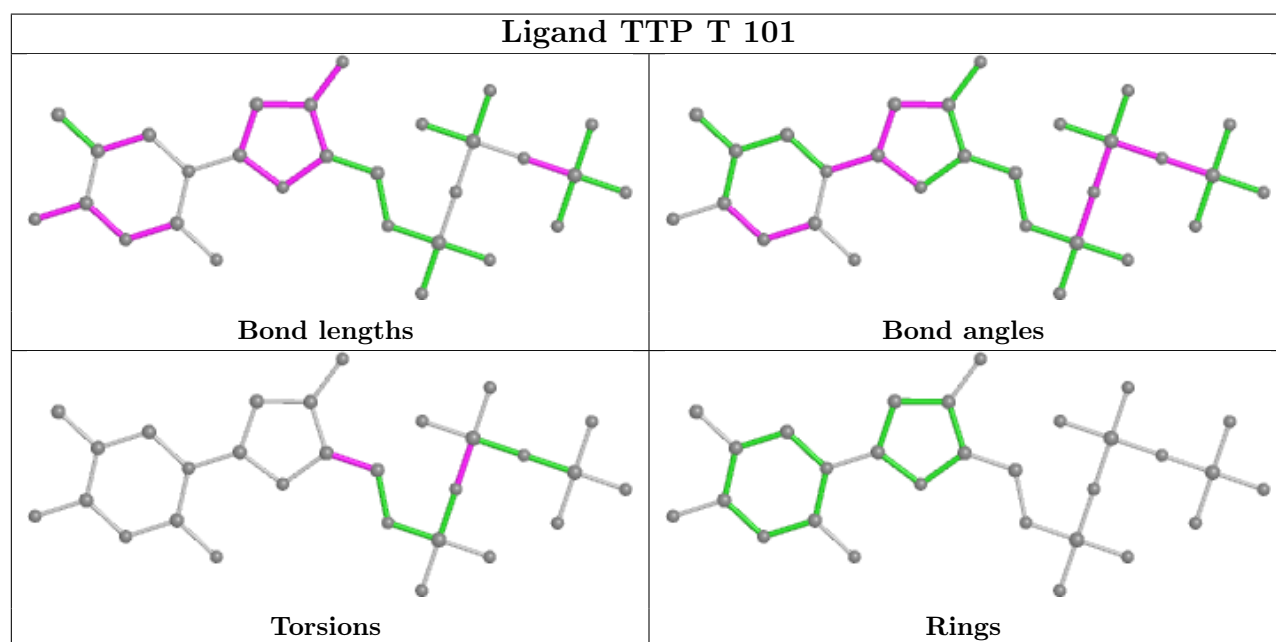
Mol	Chain	Res	Type	Atoms
10	T	101	TTP	O4'-C4'-C5'-O5'
10	T	101	TTP	C3'-C4'-C5'-O5'
10	T	101	TTP	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1202	SF4	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.