



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 4, 2021 – 12:11 PM JST

PDB ID : 7EH0
Title : Thermus thermophilus RNA polymerase transcription initiation complex containing a template-strand purine at position TSS-2, UpA RNA primer and CMPcPP
Authors : Li, L.; Zhang, Y.
Deposited on : 2021-03-27
Resolution : 2.81 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

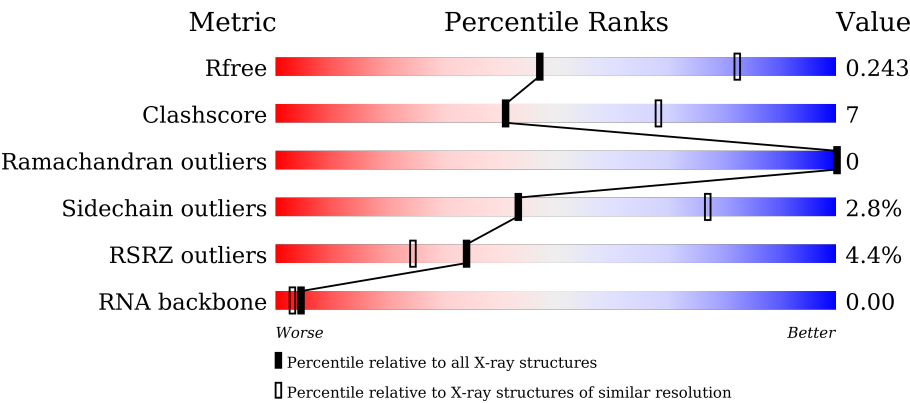
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.22
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.22

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	315	<div><div>2%</div><div><div></div><div>59%</div><div>13%</div><div>•</div><div>27%</div></div></div>
1	B	315	<div><div></div><div><div>55%</div><div>16%</div><div>29%</div></div></div>
2	C	1119	<div><div>3%</div><div><div></div><div>80%</div><div>18%</div><div>••</div></div></div>
3	D	1524	<div><div>6%</div><div><div></div><div>79%</div><div>17%</div><div>••</div></div></div>

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Mol	Chain	Length	Quality of chain
4	E	99	
5	F	443	
6	G	27	
7	H	19	
8	I	2	

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
11	2TM	D	2006	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 28596 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	224	Total	C	N	O	S	0	0	0
			1763	1127	306	328	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
			8768	5547	1562	1635	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1486	Total	C	N	O	S	0	1	0
			11726	7435	2063	2193	35			

- 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
			2807	1770	509	524	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 (27-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	25	Total	C	N	O	P	0	0	0
			516	246	99	147	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	17	Total	C	N	O	P	0	0	0
			349	167	67	99	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	2	Total	C	N	O	P	0	0	0
			39	19	7	12	1			

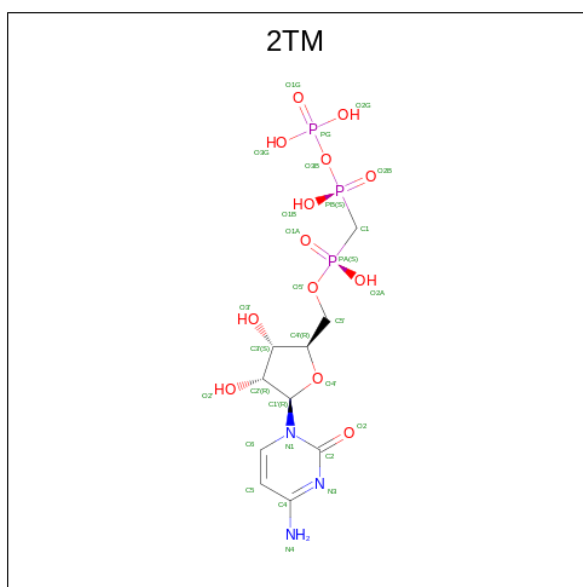
- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Mg 1 1	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: C₁₀H₁₈N₃O₁₃P₃).



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

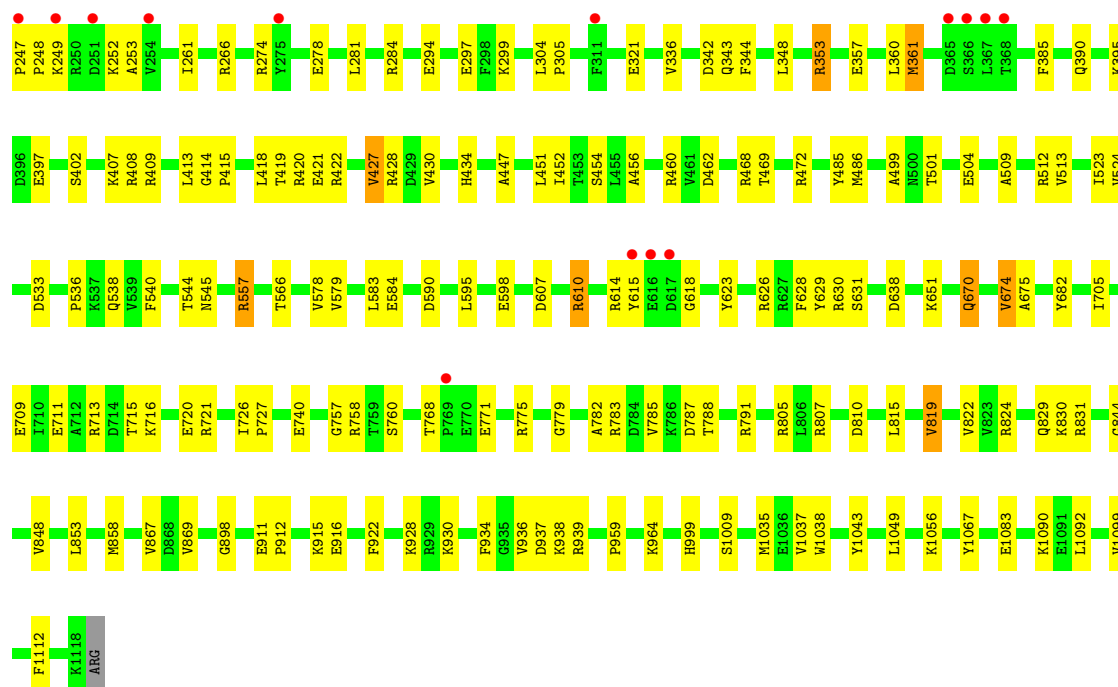
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	3	Total O 3 3	0	0
12	B	2	Total O 2 2	0	0

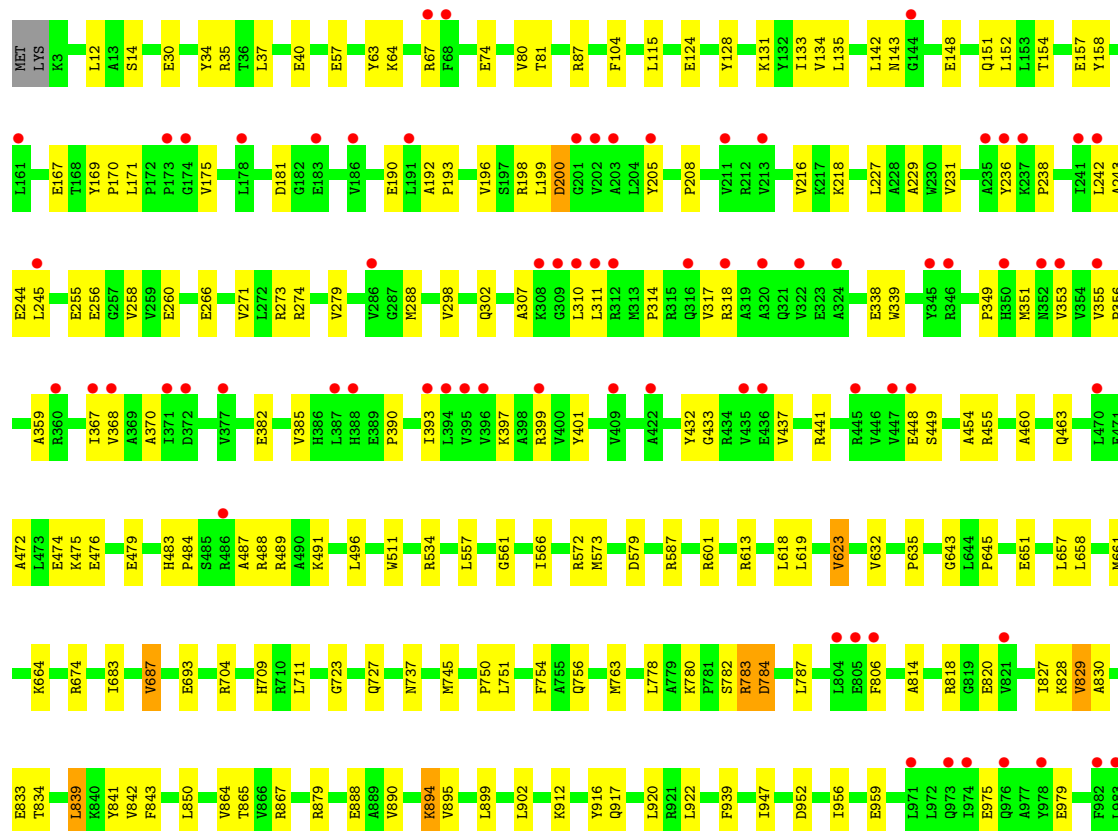
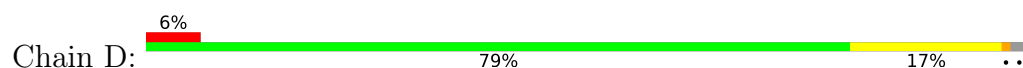
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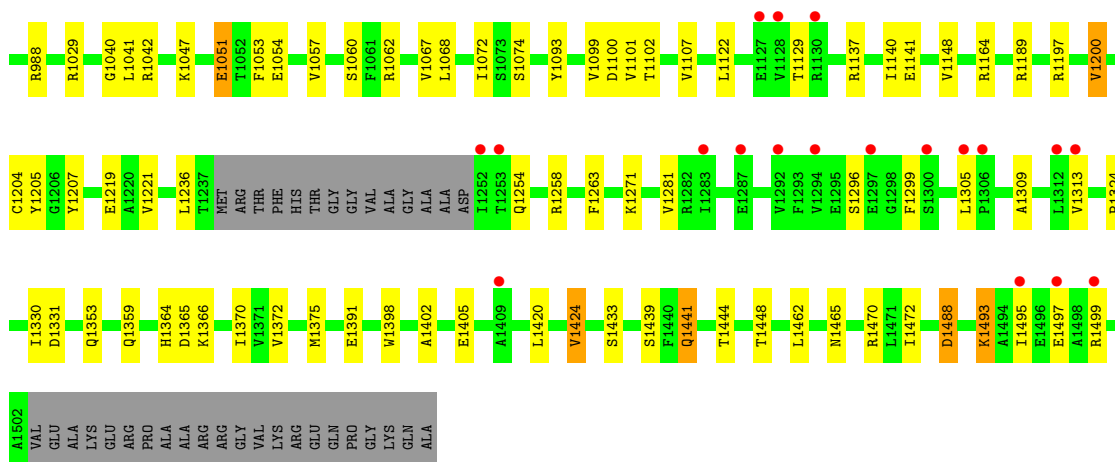
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	5	Total 5	O 5	0	0
12	D	9	Total 9	O 9	0	0
12	E	1	Total 1	O 1	0	0
12	F	2	Total 2	O 2	0	0




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





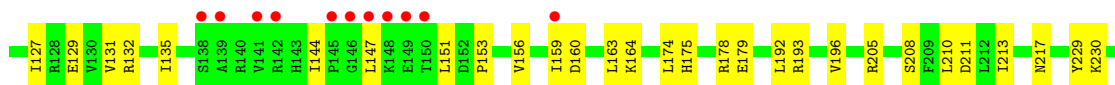
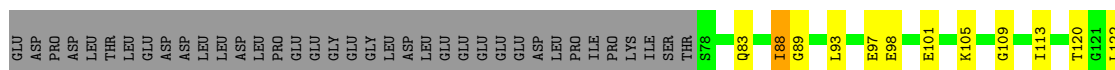
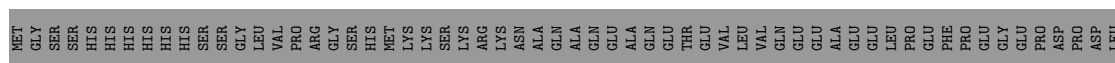
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:  82% 13% 5%



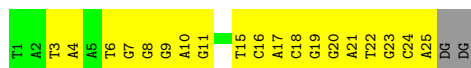
- Molecule 5: RNA polymerase sigma factor SigA

Chain F:  4% 63% 14% 22%



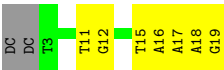
- Molecule 6: DNA (27-MER)

Chain G:  22% 70% 7%



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

Chain H:  53% 37% 11%



- Molecule 8: RNA (5'-R(*UP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	183.78Å 103.43Å 295.63Å 90.00° 98.95° 90.00°	Depositor
Resolution (Å)	48.75 – 2.81 48.75 – 2.81	Depositor EDS
% Data completeness (in resolution range)	94.8 (48.75-2.81) 94.9 (48.75-2.81)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.203 , 0.243 0.203 , 0.243	Depositor DCC
R_{free} test set	2292 reflections (1.80%)	wwPDB-VP
Wilson B-factor (Å ²)	61.8	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for $1/2^*h-3/2^*k,-1/2^*h-1/2^*k,-1/2^*h+1/2^*k-l$ 0.013 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	0.94	EDS
Total number of atoms	28596	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 2TM, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.31	0/1841	0.52	0/2504
1	B	0.31	0/1795	0.53	1/2442 (0.0%)
2	C	0.31	0/8935	0.49	0/12085
3	D	0.31	0/11935	0.50	0/16140
4	E	0.29	0/775	0.45	0/1045
5	F	0.29	0/2852	0.43	0/3837
6	G	0.71	0/580	0.95	0/895
7	H	0.73	0/392	0.91	0/604
8	I	0.34	0/43	0.82	0/65
All	All	0.33	0/29148	0.52	1/39617 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
3	D	0	3
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	8	ALA	C-N-CD	-6.62	106.04	120.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	7	LYS	Peptide
3	D	1207	TYR	Peptide
3	D	782	SER	Peptide
3	D	829	VAL	Peptide

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	30	0
1	B	1763	0	1810	36	0
2	C	8768	0	8866	128	0
3	D	11726	0	11947	181	0
4	E	761	0	778	10	0
5	F	2807	0	2882	42	0
6	G	516	0	283	17	0
7	H	349	0	193	6	0
8	I	39	0	22	2	0
9	B	1	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	3	0
12	A	3	0	0	0	0
12	B	2	0	0	0	0
12	C	5	0	0	0	0
12	D	9	0	0	0	0
12	E	1	0	0	0	0
12	F	2	0	0	0	0
All	All	28596	0	28658	403	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 7.

All (403) 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:628:PHE:H	2:C:638:ASP:HB3	1.37	0.89
2:C:775:ARG:HH22	2:C:782:ALA:H	1.28	0.81
3:D:828:LYS:HA	3:D:833:GLU:HA	1.63	0.80
3:D:134:VAL:HG22	3:D:151:GLN:H	1.51	0.76
2:C:709:GLU:OE2	2:C:824:ARG:NH1	2.21	0.74
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.22	0.72
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.71	0.72
2:C:428:ARG:NH2	2:C:447:ALA:O	2.22	0.72
2:C:24:GLU:OE2	2:C:27:ARG:NH2	2.23	0.71
3:D:1488:ASP:OD1	3:D:1488:ASP:N	2.22	0.70
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.73	0.70
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.73	0.70
5:F:397:ILE:HD12	5:F:400:ILE:HD11	1.73	0.70
1:B:80:LEU:HD21	3:D:842:VAL:HG12	1.74	0.69
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.74	0.69
2:C:212:GLY:HA2	2:C:218:VAL:HG11	1.75	0.68
2:C:194:VAL:HG22	2:C:221:LEU:HD12	1.76	0.67
3:D:244:GLU:HG3	3:D:310:LEU:HG	1.76	0.67
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.75	0.67
5:F:400:ILE:HG22	5:F:403:LYS:HE2	1.76	0.67
1:B:7:LYS:HD2	1:B:8:ALA:H	1.58	0.67
3:D:1101:VAL:HG23	3:D:1102:THR:HG23	1.75	0.67
2:C:229:MET:HB2	2:C:233:GLU:HB2	1.77	0.66
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.77	0.66
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.77	0.65
2:C:50:GLU:OE2	2:C:168:ARG:NH1	2.30	0.65
6:G:23:DG:H2''	6:G:24:DC:H5''	1.78	0.65
2:C:418:LEU:HD11	2:C:427:VAL:HG11	1.79	0.65
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.79	0.64
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.79	0.64
3:D:566:ILE:HD11	5:F:192:LEU:HD21	1.80	0.64
1:B:216:GLU:OE1	1:B:219:ARG:NH2	2.30	0.63
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.80	0.63
2:C:353:ARG:NH1	2:C:357:GLU:OE2	2.32	0.63
4:E:45:ARG:NH1	4:E:56:ASP:OD2	2.32	0.62
2:C:81:ASP:OD1	2:C:81:ASP:N	2.33	0.62
7:H:15:DT:H2'	7:H:16:DA:C8	2.35	0.61
1:A:209:GLU:O	1:A:213:GLN:HG2	2.01	0.61
3:D:975:GLU:O	3:D:979:GLU:HG2	1.99	0.61
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.83	0.61
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.83	0.60
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:197:LEU:HD12	2:C:221:LEU:HD11	1.83	0.60
2:C:294:GLU:HB3	2:C:299:LYS:HE2	1.83	0.60
1:B:179:PHE:HB3	1:B:197:LEU:HD12	1.83	0.60
3:D:657:LEU:HG	3:D:661:MET:HE2	1.84	0.60
3:D:658:LEU:HA	3:D:661:MET:HE3	1.84	0.60
1:B:7:LYS:HD2	1:B:8:ALA:N	2.17	0.60
1:A:4:SER:O	1:A:189:ARG:NH2	2.32	0.60
3:D:864:VAL:HG12	3:D:865:THR:H	1.67	0.59
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.84	0.59
3:D:1029:ARG:NH1	11:D:2006:2TM:O1G	2.23	0.59
1:B:94:LEU:O	1:B:146:ARG:NH2	2.35	0.59
2:C:124:ASP:OD2	2:C:407:LYS:NZ	2.31	0.59
2:C:713:ARG:HA	2:C:819:VAL:HA	1.84	0.59
3:D:787:LEU:HD21	3:D:947:ILE:HG21	1.83	0.58
2:C:390:GLN:HB3	2:C:415:PRO:HD3	1.85	0.58
5:F:326:ASP:HB2	7:H:19:DG:H22	1.69	0.58
2:C:224:GLU:CD	2:C:224:GLU:H	2.06	0.58
2:C:727:PRO:HB3	2:C:783:ARG:HD3	1.84	0.58
3:D:231:VAL:O	3:D:236:TYR:OH	2.21	0.58
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.04	0.58
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.85	0.58
3:D:57:GLU:HG3	3:D:64:LYS:HG2	1.86	0.58
1:A:220:GLU:O	1:A:223:THR:HB	2.04	0.58
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.86	0.58
3:D:181:ASP:HB2	3:D:205:TYR:CD2	2.39	0.58
3:D:1441:GLN:HG2	7:H:12:DG:H5''	1.86	0.58
2:C:249:LYS:HB3	2:C:252:LYS:HB2	1.85	0.57
1:A:112:ARG:HG3	1:A:125:PRO:HB2	1.87	0.57
2:C:129:ILE:HB	2:C:134:ARG:HD2	1.86	0.57
7:H:17:DA:H2'	7:H:18:DA:C8	2.40	0.57
1:A:57:TYR:CG	1:A:161:ARG:HD2	2.40	0.57
5:F:289:GLU:OE1	5:F:289:GLU:N	2.37	0.56
3:D:135:LEU:HD23	3:D:463:GLN:HG2	1.87	0.56
2:C:35:PRO:HG2	2:C:38:LYS:HD2	1.87	0.56
3:D:561:GLY:HA3	5:F:132:ARG:HD3	1.87	0.56
3:D:864:VAL:HG12	3:D:865:THR:N	2.19	0.56
5:F:93:LEU:HD11	6:G:6:DT:H2''	1.86	0.56
2:C:805:ARG:HH21	2:C:807:ARG:HD3	1.71	0.56
3:D:255:GLU:OE1	3:D:274:ARG:NH2	2.29	0.56
2:C:136:ILE:HB	2:C:336:VAL:HG13	1.86	0.56
2:C:598:GLU:O	2:C:651:LYS:NZ	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:674:VAL:HG22	2:C:869:VAL:HG22	1.87	0.55
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.88	0.55
2:C:614:ARG:NH2	2:C:618:GLY:O	2.40	0.55
2:C:775:ARG:HH22	2:C:782:ALA:N	2.02	0.55
3:D:208:PRO:HA	3:D:390:PRO:HA	1.88	0.54
3:D:534:ARG:NH2	5:F:313:GLU:O	2.40	0.54
3:D:841:TYR:HB2	3:D:864:VAL:HG13	1.90	0.54
5:F:370:LYS:HB3	5:F:376:ILE:HG12	1.90	0.54
1:B:132:LEU:HD21	1:B:138:LEU:HB2	1.89	0.54
3:D:1281:VAL:HG21	3:D:1313:VAL:HG21	1.88	0.54
3:D:455:ARG:HB2	3:D:460:ALA:HB2	1.90	0.54
3:D:489:ARG:NH1	3:D:1391:GLU:OE2	2.41	0.54
2:C:504:GLU:HG2	2:C:509:ALA:HB2	1.90	0.54
2:C:853:LEU:HB2	2:C:858:MET:CE	2.37	0.54
3:D:1372:VAL:HA	3:D:1375:MET:HE3	1.90	0.54
1:A:185:ARG:NH2	1:A:187:GLY:O	2.41	0.54
4:E:50:THR:HG22	4:E:53:GLY:O	2.07	0.54
3:D:142:LEU:HD23	3:D:143:ASN:HB2	1.90	0.53
1:A:154:GLU:CD	1:A:154:GLU:H	2.11	0.53
2:C:266:ARG:NH1	6:G:11:DG:N7	2.53	0.53
6:G:15:DT:H2''	6:G:16:DC:H2'	1.91	0.53
2:C:768:THR:OG1	2:C:771:GLU:OE1	2.26	0.53
2:C:726:ILE:HD11	2:C:757:GLY:HA3	1.91	0.53
2:C:1056:LYS:HE2	3:D:751:LEU:HG	1.91	0.53
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.91	0.53
6:G:8:DG:H2''	6:G:9:DG:H5''	1.89	0.53
1:B:32:PHE:HA	1:B:35:THR:HB	1.90	0.53
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.91	0.53
1:B:128:HIS:HE1	1:B:131:THR:HG23	1.74	0.53
2:C:501:THR:HG21	2:C:513:VAL:HG13	1.89	0.53
3:D:1205:TYR:O	3:D:1366:LYS:HD3	2.09	0.53
3:D:367:ILE:HG22	3:D:368:VAL:HG23	1.89	0.52
3:D:572:ARG:NH1	5:F:83:GLN:HB3	2.24	0.52
3:D:843:PHE:CE2	3:D:864:VAL:HG11	2.43	0.52
5:F:163:LEU:HD13	5:F:174:LEU:HD13	1.91	0.52
2:C:390:GLN:HG2	2:C:414:GLY:HA2	1.90	0.52
3:D:63:TYR:OH	3:D:74:GLU:OE2	2.23	0.52
3:D:236:TYR:CE2	3:D:242:LEU:HD12	2.45	0.52
2:C:1043:TYR:CG	3:D:763:MET:HG2	2.45	0.52
7:H:15:DT:H2'	7:H:16:DA:H8	1.74	0.52
2:C:922:PHE:CD2	2:C:964:LYS:HG3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.92	0.52
2:C:536:PRO:HB3	3:D:1067:VAL:HG21	1.93	0.51
3:D:231:VAL:HG23	3:D:243:ALA:HA	1.93	0.51
3:D:879:ARG:HD3	3:D:902:LEU:O	2.11	0.51
3:D:988:ARG:NH2	3:D:1054:GLU:OE2	2.43	0.51
2:C:915:LYS:NZ	3:D:952:ASP:OD2	2.37	0.51
3:D:487:ALA:O	3:D:491:LYS:HG2	2.11	0.51
2:C:758:ARG:HH21	2:C:788:THR:HB	1.76	0.51
3:D:827:ILE:O	3:D:834:THR:N	2.38	0.51
1:A:20:TYR:OH	1:A:198:ARG:HD2	2.10	0.51
1:A:183:ASP:HA	2:C:938:LYS:HE3	1.93	0.51
3:D:843:PHE:HE2	3:D:864:VAL:HG11	1.76	0.51
2:C:607:ASP:HB2	2:C:610:ARG:NH2	2.26	0.51
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	1.94	0.51
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.93	0.50
3:D:899:LEU:HD22	3:D:917:GLN:HB3	1.94	0.50
2:C:1083:GLU:OE2	3:D:87:ARG:NH2	2.44	0.50
3:D:317:VAL:HG23	3:D:339:TRP:HB3	1.94	0.50
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.93	0.50
1:A:198:ARG:HD3	2:C:934:PHE:CZ	2.47	0.50
3:D:200:ASP:O	3:D:397:LYS:HG2	2.12	0.50
1:A:222:LEU:HD11	1:B:218:LEU:HG	1.93	0.50
3:D:483:HIS:CE1	3:D:488:ARG:HD3	2.46	0.50
1:B:141:GLU:OE1	1:B:161:ARG:NH2	2.45	0.50
2:C:118:ILE:HD11	2:C:344:PHE:CE2	2.47	0.50
2:C:397:GLU:HG3	2:C:631:SER:HB2	1.93	0.49
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	1.94	0.49
1:B:90:LEU:HD12	1:B:119:ASP:HA	1.92	0.49
3:D:236:TYR:CZ	3:D:242:LEU:HD12	2.47	0.49
3:D:1047:LYS:HD3	3:D:1051:GLU:HG2	1.95	0.49
3:D:432:TYR:O	3:D:448:GLU:HA	2.12	0.49
3:D:683:ILE:HG23	3:D:687:VAL:HG11	1.95	0.49
3:D:1296:SER:HB3	3:D:1299:PHE:HB2	1.95	0.49
5:F:208:SER:HB3	5:F:211:ASP:OD2	2.11	0.49
2:C:281:LEU:HD13	2:C:305:PRO:HB2	1.94	0.49
3:D:349:PRO:HB3	5:F:97:GLU:HG3	1.94	0.49
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.94	0.49
3:D:827:ILE:HG12	3:D:834:THR:O	2.12	0.49
2:C:1067:TYR:OH	3:D:674[B]:ARG:NH1	2.45	0.49
3:D:34:TYR:CZ	3:D:35:ARG:HG3	2.47	0.49
3:D:208:PRO:HG2	3:D:353:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:894:LYS:H	3:D:894:LYS:HD2	1.78	0.49
2:C:101:ILE:HG12	2:C:108:ILE:HG12	1.95	0.49
2:C:760:SER:HB2	2:C:788:THR:HG21	1.95	0.49
3:D:288:MET:HG2	3:D:307:ALA:HB2	1.94	0.49
5:F:135:ILE:HD11	5:F:178:ARG:HB3	1.95	0.49
5:F:88:ILE:HG23	5:F:193:ARG:HG2	1.95	0.48
2:C:721:ARG:HH22	2:C:785:VAL:HG11	1.77	0.48
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.47	0.48
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.13	0.48
2:C:740:GLU:HB3	2:C:805:ARG:HH12	1.78	0.48
3:D:256:GLU:O	3:D:274:ARG:NH1	2.46	0.48
3:D:1236:LEU:HA	3:D:1359:GLN:HG3	1.96	0.48
2:C:121:MET:SD	2:C:125:GLY:HA2	2.53	0.48
3:D:67:ARG:HB3	5:F:377:ASP:O	2.13	0.48
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.49	0.48
3:D:274:ARG:NH2	3:D:279:VAL:HG21	2.28	0.48
3:D:613:ARG:HG3	3:D:618:LEU:HD23	1.96	0.48
1:B:128:HIS:CE1	1:B:131:THR:HG23	2.48	0.48
2:C:937:ASP:OD1	2:C:939:ARG:HD3	2.13	0.48
2:C:999:HIS:CE1	8:I:1:U:H4'	2.49	0.48
2:C:716:LYS:HE3	3:D:37:LEU:HG	1.96	0.48
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.47	0.48
3:D:128:TYR:OH	3:D:579:ASP:OD2	2.26	0.48
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.30	0.48
3:D:298:VAL:HG12	3:D:302:GLN:NE2	2.29	0.48
1:A:10:VAL:HG12	1:A:26:GLU:O	2.14	0.48
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.96	0.48
2:C:210:GLU:HG2	2:C:304:LEU:HD21	1.96	0.48
3:D:1047:LYS:HG2	3:D:1053:PHE:CZ	2.49	0.48
3:D:1271:LYS:HD3	3:D:1331:ASP:HB2	1.95	0.48
3:D:472:ALA:O	3:D:476:GLU:HG2	2.14	0.47
4:E:52:GLU:OE1	4:E:52:GLU:N	2.40	0.47
5:F:122:LEU:HD21	5:F:159:ILE:HD12	1.96	0.47
2:C:409:ARG:HD2	2:C:452:ILE:HG22	1.95	0.47
3:D:956:ILE:HD11	3:D:1062:ARG:HD3	1.96	0.47
3:D:959:GLU:OE1	3:D:959:GLU:N	2.37	0.47
3:D:433:GLY:HA2	3:D:449:SER:H	1.79	0.47
3:D:437:VAL:HG11	5:F:175:HIS:CD2	2.49	0.47
2:C:402:SER:HA	2:C:566:THR:HG23	1.96	0.47
3:D:834:THR:HG21	3:D:839:LEU:HD21	1.96	0.47
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:615:TYR:OH	2:C:623:TYR:OH	2.22	0.47
2:C:740:GLU:HB3	2:C:805:ARG:NH1	2.30	0.47
3:D:12:LEU:HD21	3:D:104:PHE:CZ	2.49	0.47
3:D:658:LEU:HD11	3:D:674[A]:ARG:HH11	1.79	0.47
5:F:362:SER:OG	5:F:365:GLU:HG2	2.14	0.47
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.96	0.47
6:G:24:DC:H2'	6:G:25:DA:C8	2.50	0.47
2:C:807:ARG:HB2	2:C:810:ASP:OD2	2.15	0.47
2:C:1035:MET:HG2	2:C:1038:TRP:CZ3	2.50	0.47
1:B:104:GLU:OE2	1:B:137:ARG:NH1	2.48	0.47
2:C:630:ARG:HG3	2:C:705:ILE:HB	1.96	0.46
1:B:73:GLU:HB3	1:B:77:GLU:HB3	1.98	0.46
2:C:20:GLU:O	2:C:24:GLU:HB2	2.16	0.46
3:D:1053:PHE:CE2	3:D:1072:ILE:HG23	2.50	0.46
5:F:196:VAL:HG22	5:F:213:ILE:HD13	1.96	0.46
2:C:557:ARG:HG3	2:C:844:GLY:HA3	1.97	0.46
3:D:829:VAL:HG12	3:D:830:ALA:H	1.81	0.46
3:D:1040:GLY:O	3:D:1060:SER:HB3	2.15	0.46
3:D:1499:ARG:NH2	4:E:80:VAL:HA	2.30	0.46
3:D:14:SER:HB3	3:D:511:TRP:CZ2	2.50	0.46
3:D:1364:HIS:CE1	3:D:1366:LYS:HG3	2.51	0.46
2:C:512:ARG:CZ	2:C:523:ILE:HG21	2.46	0.46
2:C:682:TYR:CE1	3:D:635:PRO:HD2	2.51	0.46
4:E:83:ASP:OD1	4:E:83:ASP:N	2.49	0.46
6:G:18:DC:H2''	6:G:19:DG:H8	1.81	0.46
3:D:664:LYS:NZ	3:D:693:GLU:OE1	2.48	0.46
1:B:26:GLU:HB3	1:B:194:LYS:HG3	1.98	0.45
3:D:67:ARG:NH2	5:F:379:ARG:HB3	2.31	0.45
3:D:133:ILE:HG13	3:D:152:LEU:HD12	1.98	0.45
1:A:64:GLU:HG3	1:A:79:ILE:HD12	1.98	0.45
2:C:787:ASP:OD2	2:C:791:ARG:NH2	2.47	0.45
3:D:192:ALA:HB1	3:D:193:PRO:HD2	1.98	0.45
3:D:1499:ARG:HH21	4:E:81:PRO:HD3	1.80	0.45
3:D:190:GLU:HA	3:D:196:VAL:HA	1.99	0.45
7:H:11:DT:H2''	7:H:12:DG:C8	2.51	0.45
3:D:1107:VAL:HA	3:D:1200:VAL:O	2.16	0.45
6:G:16:DC:H1'	6:G:17:DA:C8	2.51	0.45
1:A:228:PRO:HB3	1:B:13:VAL:HG21	1.98	0.45
2:C:1090:LYS:HD3	2:C:1090:LYS:HA	1.72	0.45
3:D:115:LEU:HD23	3:D:115:LEU:HA	1.81	0.45
3:D:1465:ASN:OD1	3:D:1470:ARG:NH1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.98	0.45
3:D:260:GLU:HB3	3:D:271:VAL:HB	1.98	0.45
2:C:419:THR:HG22	2:C:420:ARG:O	2.17	0.45
4:E:50:THR:HG23	4:E:52:GLU:H	1.82	0.45
1:B:77:GLU:OE1	3:D:867:ARG:NH1	2.41	0.44
2:C:127:PHE:O	2:C:133:ASP:HA	2.18	0.44
2:C:499:ALA:HB2	2:C:533:ASP:HB2	1.98	0.44
3:D:134:VAL:CG2	3:D:151:GLN:H	2.26	0.44
1:A:184:THR:O	1:A:192:LEU:HB2	2.17	0.44
3:D:258:VAL:HG12	3:D:273:ARG:O	2.18	0.44
5:F:144:ILE:HB	5:F:147:LEU:HD13	1.99	0.44
2:C:584:GLU:OE2	2:C:584:GLU:N	2.47	0.44
3:D:1101:VAL:HG11	3:D:1424:VAL:HG22	1.98	0.44
2:C:195:LEU:O	2:C:199:VAL:HG23	2.17	0.44
3:D:30:GLU:OE1	3:D:40:GLU:HG2	2.18	0.44
2:C:626:ARG:HG3	2:C:629:TYR:CD1	2.53	0.44
2:C:775:ARG:O	2:C:779:GLY:N	2.50	0.44
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.99	0.44
3:D:916:TYR:CE2	3:D:920:LEU:HD11	2.52	0.44
4:E:48:MET:N	4:E:55:PHE:O	2.42	0.44
1:B:101:LEU:HD21	1:B:109:VAL:HG11	2.00	0.44
2:C:911:GLU:O	2:C:915:LYS:HG2	2.18	0.44
3:D:1122:LEU:HD22	3:D:1140:ILE:HD13	2.00	0.44
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.17	0.44
5:F:229:TYR:CZ	5:F:230:LYS:HD3	2.52	0.44
1:B:110:LYS:HD3	1:B:128:HIS:HA	1.99	0.44
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	2.00	0.44
3:D:483:HIS:CG	3:D:484:PRO:HD2	2.52	0.44
3:D:1254:GLN:CB	3:D:1258:ARG:HB2	2.47	0.44
3:D:1093:TYR:OH	3:D:1441:GLN:OE1	2.20	0.44
5:F:101:GLU:O	5:F:105:LYS:HG3	2.17	0.44
6:G:3:DT:H2'	6:G:4:DA:C8	2.52	0.44
2:C:133:ASP:HB3	2:C:395:LYS:HD2	1.98	0.44
3:D:566:ILE:HD13	5:F:217:ASN:HB3	2.00	0.44
5:F:89:GLY:HA3	6:G:7:DG:C6	2.52	0.44
2:C:239:PHE:CD1	2:C:253:ALA:HA	2.53	0.43
2:C:15:LEU:HD12	2:C:583:LEU:HD11	2.01	0.43
3:D:573:MET:SD	5:F:210:LEU:HB3	2.58	0.43
3:D:1101:VAL:HG21	3:D:1424:VAL:HG22	1.99	0.43
3:D:1444:THR:O	3:D:1448:THR:HG23	2.18	0.43
1:B:111:ALA:HB3	1:B:125:PRO:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:274:ARG:NH1	2:C:284:ARG:HH22	2.15	0.43
2:C:1067:TYR:OH	3:D:674[A]:ARG:NH1	2.51	0.43
3:D:148:GLU:O	3:D:151:GLN:HB2	2.18	0.43
3:D:895:VAL:HG11	3:D:922:LEU:HD21	2.01	0.43
3:D:1197:ARG:HB2	3:D:1398:TRP:CH2	2.53	0.43
4:E:68:LEU:HD12	4:E:68:LEU:HA	1.80	0.43
1:A:179:PHE:HB3	1:A:197:LEU:HD23	2.01	0.43
1:B:71:VAL:HG22	1:B:132:LEU:HG	2.01	0.43
1:B:101:LEU:HB2	1:B:114:PHE:CD1	2.53	0.43
3:D:780:LYS:HE3	3:D:912:LYS:HD3	2.00	0.43
5:F:160:ASP:OD2	5:F:164:LYS:HE2	2.17	0.43
6:G:20:DG:H2''	6:G:21:DA:C8	2.54	0.43
1:B:101:LEU:HB2	1:B:114:PHE:CE1	2.53	0.43
2:C:912:PRO:O	2:C:916:GLU:HG3	2.18	0.43
3:D:14:SER:HB3	3:D:511:TRP:CE2	2.53	0.43
3:D:890:VAL:HB	3:D:922:LEU:HD13	2.00	0.43
2:C:768:THR:O	2:C:771:GLU:N	2.51	0.43
3:D:1053:PHE:CZ	3:D:1072:ILE:HD12	2.54	0.43
3:D:1366:LYS:O	3:D:1370:ILE:HG12	2.18	0.43
1:A:54:THR:HG21	1:A:145:ASP:HB2	1.99	0.43
2:C:468:ARG:HA	2:C:486:MET:O	2.18	0.43
3:D:142:LEU:HD11	3:D:157:GLU:HB3	1.99	0.43
3:D:167:GLU:OE2	3:D:198:ARG:NH1	2.52	0.43
3:D:658:LEU:HD23	3:D:661:MET:HE1	1.99	0.43
3:D:737:ASN:ND2	11:D:2006:2TM:O3'	2.51	0.43
11:D:2006:2TM:O4'	8:I:2:A:H2'	2.19	0.43
5:F:129:GLU:HB3	5:F:151:LEU:HD21	2.00	0.43
1:A:176:ARG:HG3	1:A:177:VAL:N	2.34	0.43
1:B:76:VAL:O	1:B:80:LEU:HG	2.19	0.43
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.86	0.43
2:C:930:LYS:HA	2:C:930:LYS:HD2	1.83	0.43
5:F:127:ILE:O	5:F:131:VAL:HG23	2.19	0.43
2:C:469:THR:OG1	2:C:538:GLN:NE2	2.52	0.43
5:F:392:VAL:HG11	5:F:396:ARG:HG2	2.00	0.43
1:A:150:TYR:CE2	1:A:152:PRO:HG3	2.54	0.42
2:C:420:ARG:C	2:C:422:ARG:H	2.22	0.42
3:D:818:ARG:HE	3:D:820:GLU:CD	2.21	0.42
2:C:675:ALA:HB2	2:C:867:VAL:HG11	2.01	0.42
3:D:1148:VAL:HA	3:D:1164:ARG:O	2.19	0.42
2:C:460:ARG:HD2	2:C:485:TYR:CZ	2.54	0.42
3:D:711:LEU:HD13	3:D:778:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:12:LEU:HD23	3:D:12:LEU:HA	1.81	0.42
3:D:475:LYS:O	3:D:479:GLU:HG2	2.19	0.42
1:A:70:GLY:N	2:C:607:ASP:OD1	2.51	0.42
2:C:274:ARG:HH12	2:C:284:ARG:HH22	1.66	0.42
3:D:131:LYS:NZ	3:D:154:THR:HG22	2.34	0.42
3:D:645:PRO:HB3	3:D:723:GLY:O	2.20	0.42
3:D:806:PHE:HB2	3:D:829:VAL:HG22	2.02	0.42
6:G:18:DC:H2''	6:G:19:DG:C8	2.55	0.42
2:C:1009:SER:HB3	3:D:651:GLU:O	2.20	0.42
3:D:216:VAL:HG22	3:D:382:GLU:HG3	2.00	0.42
5:F:373:LYS:HA	5:F:373:LYS:HD3	1.78	0.42
1:A:133:GLU:HG2	1:A:134:GLU:H	1.84	0.42
1:A:218:LEU:HG	1:B:222:LEU:HD11	2.02	0.42
1:A:226:SER:O	1:A:228:PRO:HD3	2.20	0.42
2:C:17:PRO:HB2	2:C:20:GLU:HB3	2.01	0.42
2:C:243:ARG:NH1	6:G:9:DG:O6	2.53	0.42
2:C:628:PHE:H	2:C:638:ASP:CB	2.20	0.42
2:C:670:GLN:HE21	2:C:670:GLN:HA	1.85	0.42
2:C:829:GLN:OE1	2:C:831:ARG:NH2	2.49	0.42
3:D:1462:LEU:HD22	3:D:1472:ILE:HB	2.02	0.42
1:A:133:GLU:HG2	1:A:134:GLU:N	2.35	0.41
1:B:83:LYS:NZ	3:D:842:VAL:O	2.53	0.41
2:C:408:ARG:NH1	2:C:456:ALA:O	2.54	0.41
2:C:1090:LYS:HE2	2:C:1112:PHE:CZ	2.55	0.41
3:D:227:LEU:HD12	3:D:227:LEU:HA	1.92	0.41
3:D:351:MET:HG2	3:D:370:ALA:HB2	2.02	0.41
3:D:557:LEU:HD13	3:D:566:ILE:HG22	2.01	0.41
3:D:784:ASP:HB2	3:D:939:PHE:CE1	2.55	0.41
2:C:278:GLU:OE2	2:C:284:ARG:NH2	2.51	0.41
1:B:219:ARG:O	1:B:223:THR:HG23	2.20	0.41
2:C:154:ARG:NH1	2:C:178:PRO:HG3	2.35	0.41
5:F:109:GLY:O	5:F:113:ILE:HG13	2.20	0.41
2:C:720:GLU:HG2	2:C:760:SER:OG	2.21	0.41
2:C:1056:LYS:HB2	3:D:623:VAL:HG22	2.02	0.41
3:D:258:VAL:HG13	3:D:273:ARG:HG3	2.02	0.41
2:C:540:PHE:HB3	2:C:544:THR:HB	2.02	0.41
1:A:155:LYS:HA	1:A:155:LYS:HD2	1.82	0.41
2:C:413:LEU:HD21	2:C:451:LEU:HD13	2.02	0.41
3:D:601:ARG:HD3	5:F:318:GLU:HG2	2.03	0.41
3:D:783:ARG:H	3:D:783:ARG:HG2	1.45	0.41
5:F:237:THR:OG1	6:G:4:DA:H8	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:VAL:HG22	1:A:196:THR:HG23	2.02	0.41
1:B:57:TYR:CD1	1:B:161:ARG:HD2	2.55	0.41
2:C:118:ILE:HD11	2:C:344:PHE:HE2	1.84	0.41
3:D:850:LEU:HA	3:D:850:LEU:HD23	1.78	0.41
1:B:113:ASP:OD1	1:B:113:ASP:N	2.53	0.41
3:D:814:ALA:O	3:D:818:ARG:HG3	2.21	0.41
3:D:1402:ALA:O	3:D:1405:GLU:HG2	2.20	0.41
2:C:1:MET:HB2	2:C:898:GLY:O	2.21	0.41
2:C:361:MET:H	2:C:361:MET:HG2	1.53	0.41
2:C:545:ASN:HB3	2:C:583:LEU:HD23	2.03	0.41
3:D:229:ALA:HB1	3:D:245:LEU:HD12	2.01	0.41
3:D:1353:GLN:NE2	3:D:1365:ASP:OD1	2.44	0.41
5:F:88:ILE:HD12	5:F:88:ILE:HA	1.87	0.41
5:F:105:LYS:HD3	5:F:179:GLU:HG2	2.03	0.41
6:G:9:DG:H2''	6:G:10:DA:C8	2.56	0.41
3:D:171:LEU:HD11	3:D:393:ILE:HD11	2.02	0.41
3:D:310:LEU:H	3:D:310:LEU:HD12	1.86	0.41
3:D:750:PRO:O	3:D:756:GLN:NE2	2.54	0.41
2:C:578:VAL:HG23	2:C:579:VAL:HG23	2.04	0.40
3:D:169:TYR:HA	3:D:170:PRO:HD3	1.93	0.40
3:D:704:ARG:HB2	3:D:745:MET:HG2	2.02	0.40
1:A:196:THR:HG21	2:C:934:PHE:HE1	1.86	0.40
2:C:205:GLU:O	2:C:209:ARG:HG2	2.22	0.40
3:D:1305:LEU:HD13	3:D:1309:ALA:HB3	2.02	0.40
3:D:1420:LEU:HD12	3:D:1420:LEU:HA	1.97	0.40
5:F:193:ARG:HB3	6:G:7:DG:H5''	2.02	0.40
2:C:928:LYS:HB2	2:C:928:LYS:HE3	1.76	0.40
3:D:314:PRO:HB2	3:D:317:VAL:HG12	2.02	0.40
6:G:22:DT:H2''	6:G:23:DG:H5'	2.03	0.40
2:C:830:LYS:HB3	2:C:830:LYS:HE2	1.87	0.40
3:D:399:ARG:HB3	3:D:401:TYR:CZ	2.56	0.40
3:D:619:LEU:HD11	3:D:1439:SER:HB2	2.04	0.40
3:D:1263:PHE:HD1	3:D:1375:MET:HE2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	221 (96%)	8 (4%)	0	100	100
1	B	222/315 (70%)	218 (98%)	4 (2%)	0	100	100
2	C	1108/1119 (99%)	1075 (97%)	33 (3%)	0	100	100
3	D	1483/1524 (97%)	1444 (97%)	39 (3%)	0	100	100
4	E	92/99 (93%)	90 (98%)	2 (2%)	0	100	100
5	F	344/443 (78%)	339 (98%)	5 (2%)	0	100	100
All	All	3478/3815 (91%)	3387 (97%)	91 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	200/273 (73%)	195 (98%)	5 (2%)	47	80
1	B	196/273 (72%)	189 (96%)	7 (4%)	35	69
2	C	935/941 (99%)	904 (97%)	31 (3%)	38	72
3	D	1250/1279 (98%)	1223 (98%)	27 (2%)	52	83
4	E	83/88 (94%)	82 (99%)	1 (1%)	71	92
5	F	301/388 (78%)	290 (96%)	11 (4%)	34	68
All	All	2965/3242 (92%)	2883 (97%)	82 (3%)	43	77

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	THR
1	A	112	ARG
1	A	205	VAL
1	A	223	THR
1	A	229	GLN
1	B	6	LEU
1	B	7	LYS
1	B	34	VAL
1	B	55	SER
1	B	93	SER
1	B	96	THR
1	B	154	GLU
2	C	1	MET
2	C	11	GLU
2	C	33	ASP
2	C	141	HIS
2	C	174	LEU
2	C	200	LEU
2	C	206	THR
2	C	261	ILE
2	C	297	GLU
2	C	321	GLU
2	C	342	ASP
2	C	348	LEU
2	C	353	ARG
2	C	360	LEU
2	C	361	MET
2	C	421	GLU
2	C	427	VAL
2	C	430	VAL
2	C	434	HIS
2	C	454	SER
2	C	524	VAL
2	C	557	ARG
2	C	590	ASP
2	C	595	LEU
2	C	610	ARG
2	C	670	GLN
2	C	674	VAL
2	C	715	THR
2	C	815	LEU
2	C	819	VAL

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Mol	Chain	Res	Type
2	C	848	VAL
3	D	80	VAL
3	D	81	THR
3	D	175	VAL
3	D	199	LEU
3	D	200	ASP
3	D	623	VAL
3	D	632	VAL
3	D	687	VAL
3	D	709	HIS
3	D	754	PHE
3	D	783	ARG
3	D	784	ASP
3	D	839	LEU
3	D	894	LYS
3	D	1041	LEU
3	D	1051	GLU
3	D	1074	SER
3	D	1100	ASP
3	D	1129	THR
3	D	1200	VAL
3	D	1219	GLU
3	D	1221	VAL
3	D	1424	VAL
3	D	1433	SER
3	D	1441	GLN
3	D	1488	ASP
3	D	1493	LYS
4	E	93	TYR
5	F	88	ILE
5	F	98	GLU
5	F	120	THR
5	F	205	ARG
5	F	273	ARG
5	F	279	GLN
5	F	315	VAL
5	F	369	LEU
5	F	392	VAL
5	F	405	LEU
5	F	420	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	737	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	1/2 (50%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 7 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	2006	-	24,30,30	4.62	14 (58%)	30,47,47	1.53	3 (10%)

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	2006	-	-	3/17/38/38	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	2006	2TM	PA-O5'	8.98	1.70	1.57
11	D	2006	2TM	C6-N1	8.92	1.46	1.35
11	D	2006	2TM	O4'-C1'	-7.19	1.31	1.41
11	D	2006	2TM	C2'-C1'	6.73	1.64	1.53
11	D	2006	2TM	C2-N3	6.73	1.51	1.38
11	D	2006	2TM	C2'-C3'	-6.64	1.35	1.53
11	D	2006	2TM	O4'-C4'	5.93	1.58	1.45
11	D	2006	2TM	C6-C5	5.42	1.50	1.38
11	D	2006	2TM	C4-N3	5.41	1.44	1.35
11	D	2006	2TM	PB-O3B	3.84	1.62	1.58
11	D	2006	2TM	C5-C4	3.78	1.50	1.41
11	D	2006	2TM	C5'-C4'	-3.56	1.40	1.51
11	D	2006	2TM	C4-N4	3.24	1.44	1.35
11	D	2006	2TM	O3'-C3'	3.13	1.50	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	2006	2TM	C3'-C2'-C1'	4.80	108.20	100.98
11	D	2006	2TM	C2-N3-C4	4.26	120.66	116.34
11	D	2006	2TM	C2'-C3'-C4'	2.64	107.77	102.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

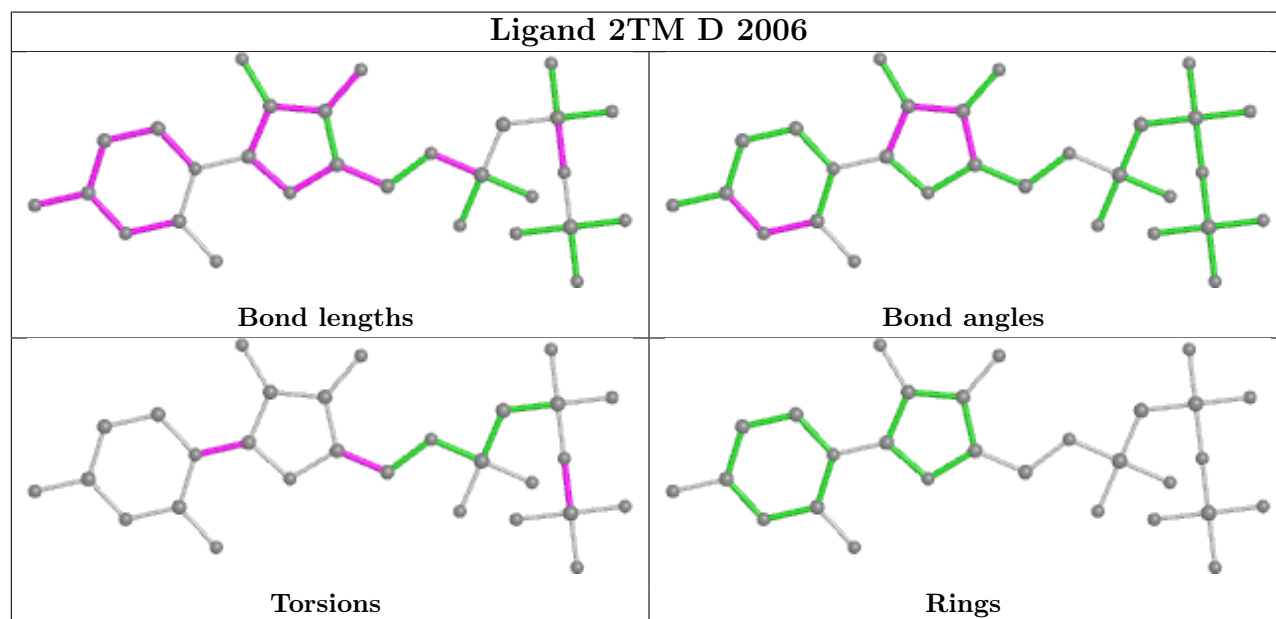
Mol	Chain	Res	Type	Atoms
11	D	2006	2TM	C2'-C1'-N1-C6
11	D	2006	2TM	PB-O3B-PG-O1G
11	D	2006	2TM	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	2006	2TM	3	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.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	231/315 (73%)	-0.15	7 (3%) 50 40	48, 64, 90, 139	0
1	B	224/315 (71%)	-0.10	1 (0%) 92 91	49, 73, 100, 114	0
2	C	1112/1119 (99%)	-0.04	37 (3%) 46 36	32, 60, 118, 143	0
3	D	1486/1524 (97%)	0.17	91 (6%) 21 13	27, 62, 123, 151	0
4	E	94/99 (94%)	-0.26	0 100 100	40, 63, 96, 104	0
5	F	346/443 (78%)	0.19	18 (5%) 27 18	41, 80, 121, 143	0
6	G	25/27 (92%)	-0.17	0 100 100	75, 114, 164, 170	0
7	H	17/19 (89%)	-0.15	0 100 100	70, 89, 162, 167	0
8	I	2/2 (100%)	3.44	2 (100%) 0 0	78, 78, 78, 83	2 (100%)
All	All	3537/3863 (91%)	0.05	156 (4%) 34 24	27, 65, 121, 170	2 (0%)

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	232	ALA	6.0
3	D	203	ALA	5.9
5	F	149	GLU	5.3
2	C	365	ASP	5.1
3	D	1127	GLU	4.9
8	I	1	U	4.5
1	A	231	ALA	4.5
3	D	974	ILE	4.4
3	D	1297	GLU	4.4
1	A	233	VAL	4.4
1	A	234	ALA	4.4
5	F	138	SER	4.3
3	D	422	ALA	4.3
3	D	144	GLY	4.3
3	D	202	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
5	F	141	VAL	4.2
3	D	201	GLY	4.2
3	D	368	VAL	4.2
2	C	207	LEU	4.1
5	F	146	GLY	4.0
3	D	393	ILE	4.0
3	D	241	ILE	3.9
3	D	236	TYR	3.9
2	C	104	ASP	3.9
2	C	221	LEU	3.8
3	D	310	LEU	3.8
3	D	976	GLN	3.7
3	D	395	VAL	3.5
3	D	1287	GLU	3.5
5	F	145	PRO	3.5
2	C	198	ARG	3.4
3	D	1313	VAL	3.4
3	D	367	ILE	3.4
3	D	312	ARG	3.4
3	D	360	ARG	3.4
2	C	189	ARG	3.3
5	F	325	LYS	3.3
3	D	1128	VAL	3.3
2	C	64	LEU	3.3
3	D	1499	ARG	3.2
3	D	211	VAL	3.2
3	D	174	GLY	3.2
5	F	142	ARG	3.2
3	D	352	ASN	3.2
3	D	445	ARG	3.1
3	D	309	GLY	3.1
3	D	242	LEU	3.1
5	F	324	GLU	3.1
3	D	320	ALA	3.1
3	D	191	LEU	3.0
3	D	173	PRO	3.0
3	D	205	TYR	3.0
2	C	176	VAL	3.0
2	C	205	GLU	3.0
3	D	186	VAL	2.9
3	D	983	LEU	2.9
3	D	470	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
5	F	150	THR	2.9
2	C	251	ASP	2.8
2	C	249	LYS	2.8
3	D	324	ALA	2.8
3	D	447	VAL	2.8
3	D	316	GLN	2.8
3	D	355	VAL	2.8
5	F	147	LEU	2.8
2	C	188	LYS	2.8
3	D	387	LEU	2.8
5	F	376	ILE	2.7
3	D	804	LEU	2.7
3	D	286	VAL	2.6
2	C	366	SER	2.6
3	D	345	TYR	2.6
2	C	617	ASP	2.6
3	D	821	VAL	2.6
3	D	245	LEU	2.6
3	D	1252	ILE	2.6
3	D	178	LEU	2.6
3	D	1497	GLU	2.6
3	D	1130	ARG	2.5
3	D	1292	VAL	2.5
3	D	971	LEU	2.5
3	D	1294	VAL	2.5
3	D	396	VAL	2.5
3	D	68	PHE	2.5
3	D	1253	THR	2.5
2	C	247	PRO	2.5
1	B	138	LEU	2.5
3	D	350	HIS	2.5
3	D	235	ALA	2.5
2	C	203	ASP	2.5
2	C	254	VAL	2.4
2	C	227	PHE	2.4
2	C	311	PHE	2.4
3	D	409	VAL	2.4
5	F	148	LYS	2.4
3	D	67	ARG	2.4
5	F	414	ARG	2.4
3	D	435	VAL	2.4
5	F	379	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	105	THR	2.4
8	I	2	A	2.4
2	C	103	LYS	2.4
3	D	1300	SER	2.4
3	D	806	PHE	2.3
2	C	275	TYR	2.3
3	D	161	LEU	2.3
2	C	368	THR	2.3
3	D	322	VAL	2.3
2	C	769	PRO	2.3
3	D	346	ARG	2.3
2	C	219	GLN	2.3
3	D	213	VAL	2.3
5	F	377	ASP	2.3
2	C	235	LEU	2.3
2	C	242	LEU	2.3
3	D	308	LYS	2.3
5	F	422	LEU	2.3
2	C	238	LEU	2.3
2	C	615	TYR	2.3
1	A	4	SER	2.3
3	D	388	HIS	2.3
3	D	1283	ILE	2.3
3	D	1495	ILE	2.3
2	C	191	PHE	2.3
2	C	226	VAL	2.2
3	D	353	VAL	2.2
3	D	1306	PRO	2.2
2	C	616	GLU	2.2
5	F	159	ILE	2.2
3	D	805	GLU	2.2
3	D	1305	LEU	2.2
3	D	486	ARG	2.2
3	D	973	GLN	2.2
3	D	978	TYR	2.2
1	A	230	ALA	2.2
3	D	311	LEU	2.2
2	C	228	ALA	2.2
3	D	183	GLU	2.2
3	D	371	ILE	2.1
5	F	139	ALA	2.1
2	C	367	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	D	982	PHE	2.1
3	D	436	GLU	2.1
3	D	448	GLU	2.1
3	D	318	ARG	2.1
3	D	1312	LEU	2.1
3	D	377	VAL	2.1
1	A	138	LEU	2.0
3	D	372	ASP	2.0
3	D	1409	ALA	2.0
3	D	399	ARG	2.0
2	C	190	LYS	2.0
3	D	237	LYS	2.0
2	C	246	ASP	2.0
2	C	154	ARG	2.0
3	D	394	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

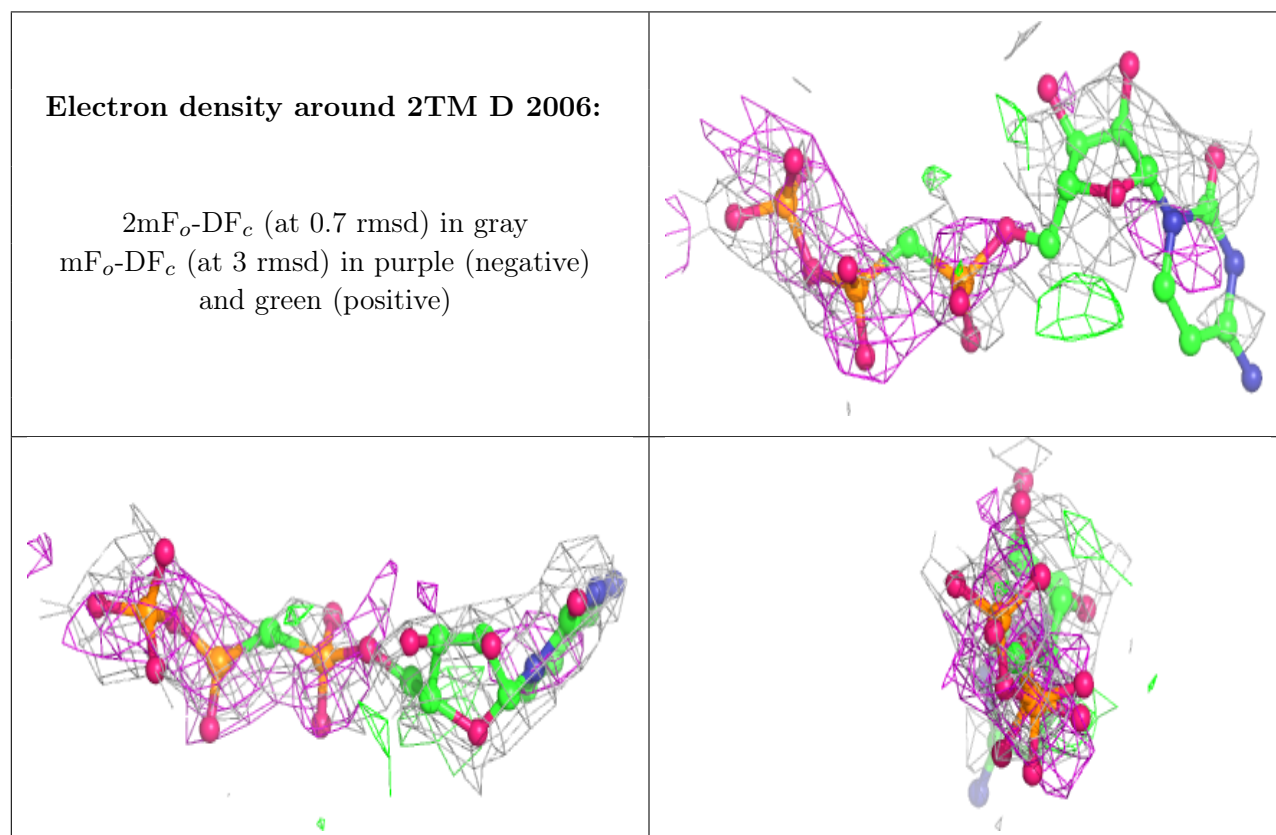
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	MG	D	2005	1/1	0.66	0.14	65,65,65,65	0
11	2TM	D	2006	29/29	0.73	0.41	63,80,103,108	29
9	MG	B	2001	1/1	0.84	0.13	77,77,77,77	0
9	MG	F	2001	1/1	0.91	0.09	69,69,69,69	0
9	MG	D	2003	1/1	0.95	0.26	40,40,40,40	0
10	ZN	D	2001	1/1	0.99	0.18	49,49,49,49	0
10	ZN	D	2002	1/1	0.99	0.10	92,92,92,92	0
9	MG	D	2004	1/1	0.99	0.52	59,59,59,59	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.