



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 11:57 PM UTC

PDB ID : 7EH0 / pdb_00007eh0
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 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:

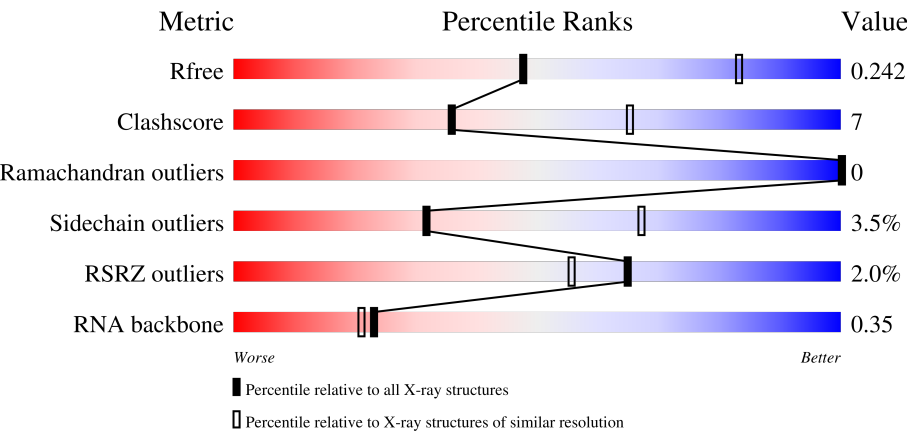
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)
RNA backbone	3983	1114 (3.00-2.60)

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	% 59%14%•27%
1	B	315	% 54%17%•29%
2	C	1119	% 79%19%••

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Mol	Chain	Length	Quality of chain
3	D	1524	3% 78% 18% ••
4	E	99	% 80% 15% 5%
5	F	443	2% 63% 15% 22%
6	G	27	22% 70% 7%
7	H	19	11% 47% 42% 11%
8	I	2	100% 100%

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			

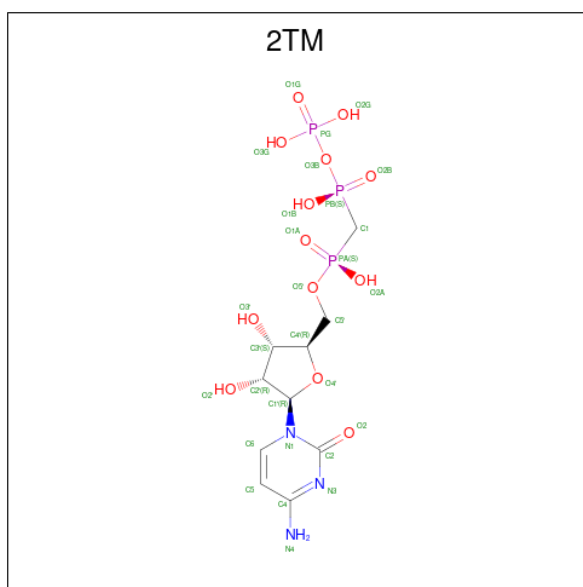
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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 (CCD ID: 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 (CCD ID: 2TM) (formula: C₁₀H₁₈N₃O₁₃P₃).



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

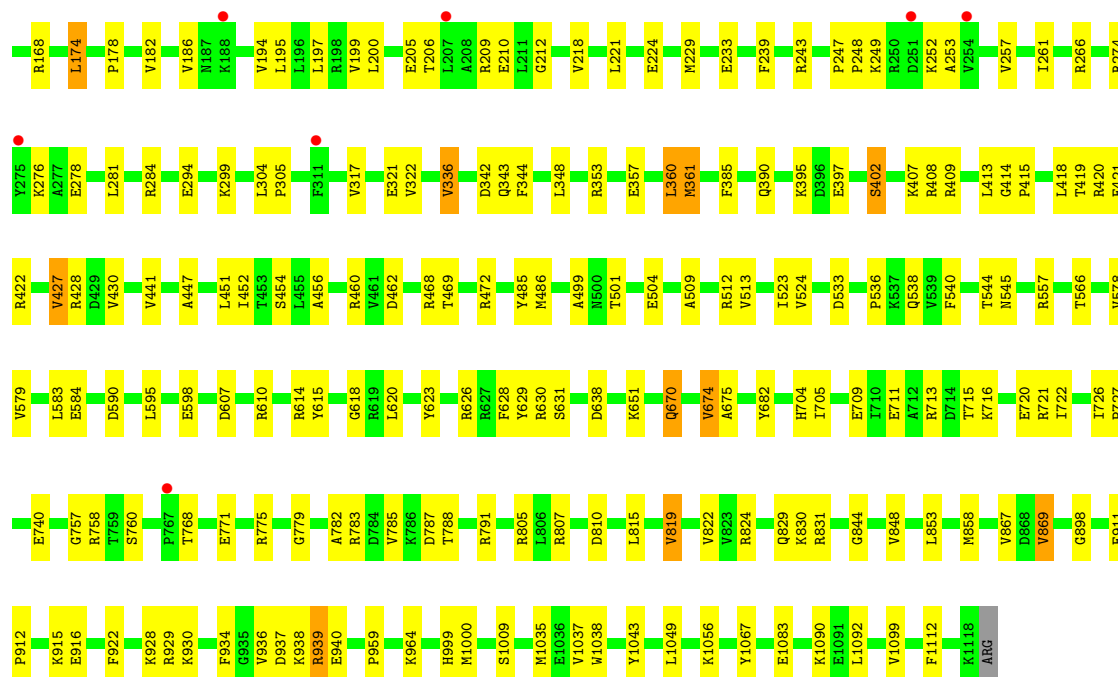
- Molecule 12 is water.

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

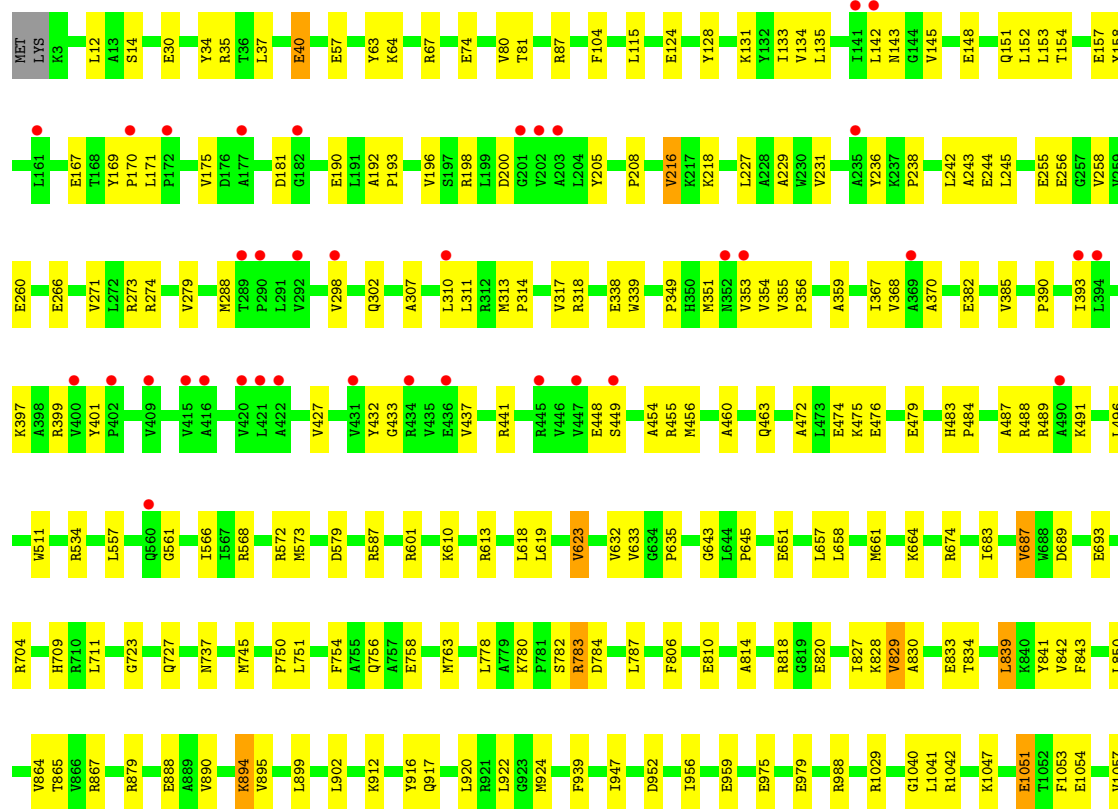
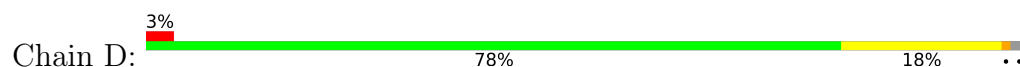
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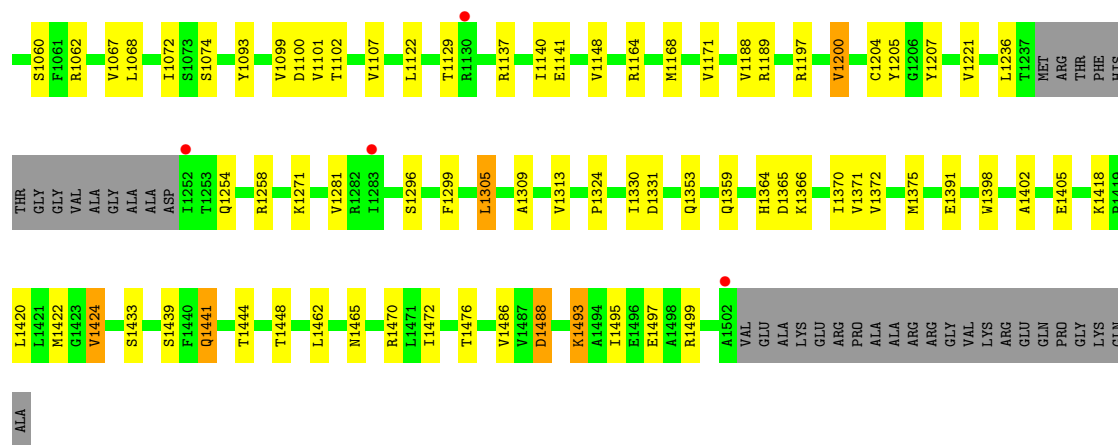
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	5	Total 5	O 5	0	0
12	D	9	Total 9	O 9	0	0
12	E	1	Total 1	O 1	0	0
12	F	2	Total 2	O 2	0	0

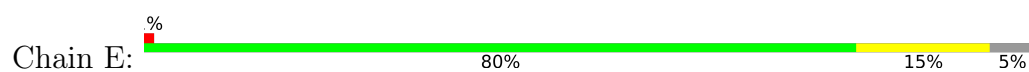


• Molecule 3: DNA-directed RNA polymerase subunit beta'

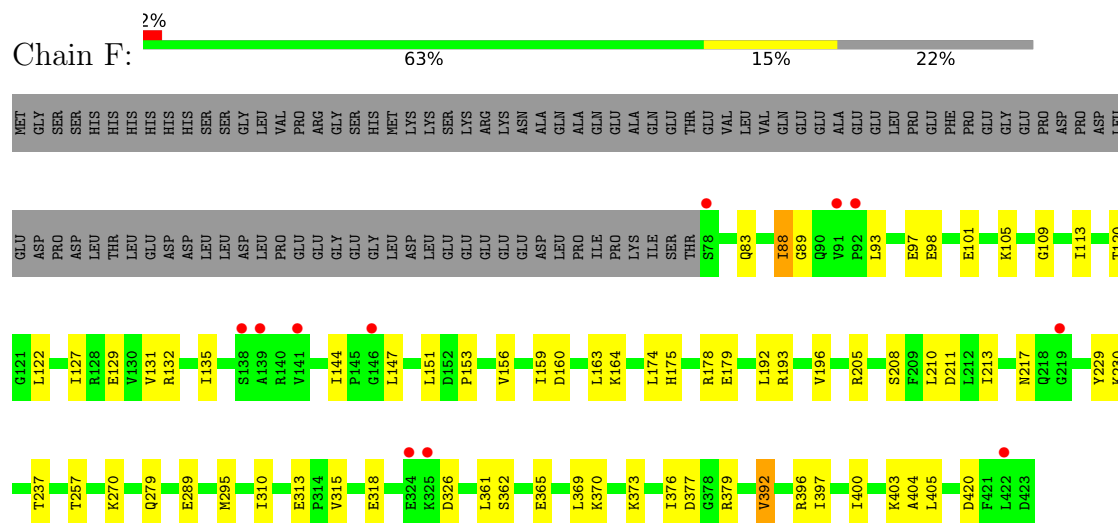




- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 5: RNA polymerase sigma factor SigA

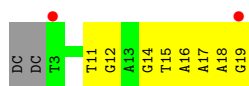


- Molecule 6: DNA (27-MER)



- 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')





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

Chain I:
100%
100%



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 , 0.242	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 , 42.4	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: 2TM, MG, ZN

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	0.21	0/1841	0.45	0/2504
1	B	0.22	0/1795	0.48	3/2442 (0.1%)
2	C	0.22	0/8935	0.43	0/12085
3	D	0.22	0/11935	0.44	0/16140
4	E	0.20	0/775	0.40	0/1045
5	F	0.20	0/2852	0.38	0/3837
6	G	0.28	0/580	0.47	0/895
7	H	0.28	0/392	0.44	0/604
8	I	0.20	0/43	0.34	0/65
All	All	0.22	0/29148	0.43	3/39617 (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 (3) 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
1	B	8	ALA	CA-C-N	5.92	141.22	127.00
1	B	8	ALA	C-N-CA	5.92	141.22	127.00

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

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	31	0
1	B	1763	0	1810	38	0
2	C	8768	0	8866	131	0
3	D	11726	0	11947	189	0
4	E	761	0	778	11	0
5	F	2807	0	2882	43	0
6	G	516	0	283	17	0
7	H	349	0	193	7	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	418	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 (418) 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
2:C:360:LEU:HB3	2:C:361:MET:HE3	1.64	0.80
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.66	0.77
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
3:D:657:LEU:HG	3:D:661:MET:HE2	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:1372:VAL:HA	3:D:1375:MET:HE3	1.72	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
1:B:58:ILE:HG12	1:B:140:MET:HE2	1.79	0.64
3:D:566:ILE:HD11	5:F:192:LEU:HD21	1.80	0.64
3:D:658:LEU:HA	3:D:661:MET:HE3	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
2:C:224:GLU:CD	2:C:224:GLU:H	2.06	0.62
4:E:45:ARG:NH1	4:E:56:ASP:OD2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:124:ASP:OD2	2:C:407:LYS:NZ	2.31	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: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: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
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
1:A:154:GLU:CD	1:A:154:GLU:H	2.11	0.57
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
2:C:704:HIS:CE1	2:C:1000:MET:HE1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:C:615:TYR:OH	2:C:623:TYR:OH	2.22	0.54
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.92	0.52
3:D:456:MET:HE1	3:D:568:ARG:NE	2.25	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
3:D:1371:VAL:HG12	3:D:1375:MET:HE2	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:D:1168:MET:HE3	3:D:1171:VAL:HB	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:420:ARG:C	2:C:422:ARG:H	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:818:ARG:HE	3:D:820:GLU:CD	2.21	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
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:758:GLU:OE1	3:D:1476:THR:OG1	2.30	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
3:D:1422:MET:HE2	3:D:1422:MET:HB3	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:924:MET:HB3	3:D:924:MET:HE2	1.78	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:610:LYS:NZ	7:H:14:DG:OP1	2.28	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
1:A:4:SER:C	1:A:189:ARG:HH22	2.24	0.43
3:D:689:ASP:CG	4:E:51:LEU:HD11	2.43	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
5:F:270:LYS:HG2	5:F:295:MET:HE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:313:MET:HE3	3:D:313:MET:HB3	1.83	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
1:B:216:GLU:CD	1:B:219:ARG:HH21	2.25	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
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
2:C:929:ARG:HH22	2:C:940:GLU:CD	2.29	0.41
3:D:229:ALA:HB1	3:D:245:LEU:HD12	2.01	0.41
3:D:288:MET:HE2	3:D:288:MET:HB3	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

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%)	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 [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%)	192 (96%)	8 (4%)	28	63
1	B	196/273 (72%)	189 (96%)	7 (4%)	31	66
2	C	935/941 (99%)	896 (96%)	39 (4%)	26	61
3	D	1250/1279 (98%)	1215 (97%)	35 (3%)	38	73
4	E	83/88 (94%)	81 (98%)	2 (2%)	43	77
5	F	301/388 (78%)	289 (96%)	12 (4%)	28	63
All	All	2965/3242 (92%)	2862 (96%)	103 (4%)	32	67

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	96	THR
1	A	134	GLU
1	A	170	VAL
1	A	205	VAL
1	A	213	GLN
1	A	223	THR
1	A	229	GLN
1	B	6	LEU
1	B	34	VAL
1	B	55	SER
1	B	93	SER
1	B	96	THR
1	B	129	ILE
1	B	154	GLU
2	C	1	MET
2	C	11	GLU
2	C	33	ASP
2	C	100	LEU
2	C	174	LEU
2	C	182	VAL
2	C	186	VAL
2	C	200	LEU
2	C	206	THR
2	C	257	VAL
2	C	261	ILE
2	C	276	LYS
2	C	317	VAL

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Mol	Chain	Res	Type
2	C	321	GLU
2	C	322	VAL
2	C	336	VAL
2	C	342	ASP
2	C	348	LEU
2	C	360	LEU
2	C	361	MET
2	C	402	SER
2	C	421	GLU
2	C	427	VAL
2	C	430	VAL
2	C	441	VAL
2	C	454	SER
2	C	524	VAL
2	C	590	ASP
2	C	595	LEU
2	C	620	LEU
2	C	670	GLN
2	C	674	VAL
2	C	715	THR
2	C	722	ILE
2	C	815	LEU
2	C	819	VAL
2	C	848	VAL
2	C	869	VAL
2	C	939	ARG
3	D	40	GLU
3	D	80	VAL
3	D	81	THR
3	D	145	VAL
3	D	153	LEU
3	D	175	VAL
3	D	216	VAL
3	D	354	VAL
3	D	427	VAL
3	D	623	VAL
3	D	632	VAL
3	D	633	VAL
3	D	687	VAL
3	D	709	HIS
3	D	754	PHE
3	D	783	ARG

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Mol	Chain	Res	Type
3	D	810	GLU
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	1188	VAL
3	D	1200	VAL
3	D	1221	VAL
3	D	1305	LEU
3	D	1418	LYS
3	D	1424	VAL
3	D	1433	SER
3	D	1441	GLN
3	D	1486	VAL
3	D	1488	ASP
3	D	1493	LYS
4	E	37	ASN
4	E	93	TYR
5	F	88	ILE
5	F	98	GLU
5	F	120	THR
5	F	205	ARG
5	F	257	THR
5	F	279	GLN
5	F	310	ILE
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 (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	HIS
1	B	188	GLN
2	C	130	ASN
2	C	187	ASN
2	C	663	ASN

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Mol	Chain	Res	Type
3	D	703	ASN
3	D	709	HIS
3	D	737	ASN
3	D	1046	GLN
3	D	1124	GLN
3	D	1227	GLN
5	F	83	GLN

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 oligosaccharides 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	-	26,30,30	3.71	15 (57%)	39,47,47	1.09	2 (5%)

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	-	-	3/19/38/38	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	2006	2TM	C2-N3	7.63	1.51	1.36
11	D	2006	2TM	C2'-C3'	-6.72	1.35	1.53
11	D	2006	2TM	C6-C5	6.45	1.50	1.35
11	D	2006	2TM	O4'-C4'	5.96	1.58	1.45
11	D	2006	2TM	C4-N3	4.93	1.44	1.34
11	D	2006	2TM	O4'-C1'	-4.74	1.31	1.42
11	D	2006	2TM	C4-N4	4.47	1.44	1.33
11	D	2006	2TM	C2-N1	4.35	1.49	1.40
11	D	2006	2TM	PB-O3B	3.81	1.62	1.58
11	D	2006	2TM	C5'-C4'	-3.68	1.40	1.51
11	D	2006	2TM	C6-N1	3.68	1.46	1.38
11	D	2006	2TM	C2'-C1'	3.34	1.64	1.53
11	D	2006	2TM	C5-C4	3.18	1.50	1.42
11	D	2006	2TM	O2-C2	-3.13	1.17	1.23
11	D	2006	2TM	O3'-C3'	2.98	1.50	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	2006	2TM	C3'-C2'-C1'	3.56	108.20	101.46
11	D	2006	2TM	C2'-C3'-C4'	2.67	107.77	102.61

There are no chirality outliers.

All (3) torsion outliers are listed below:

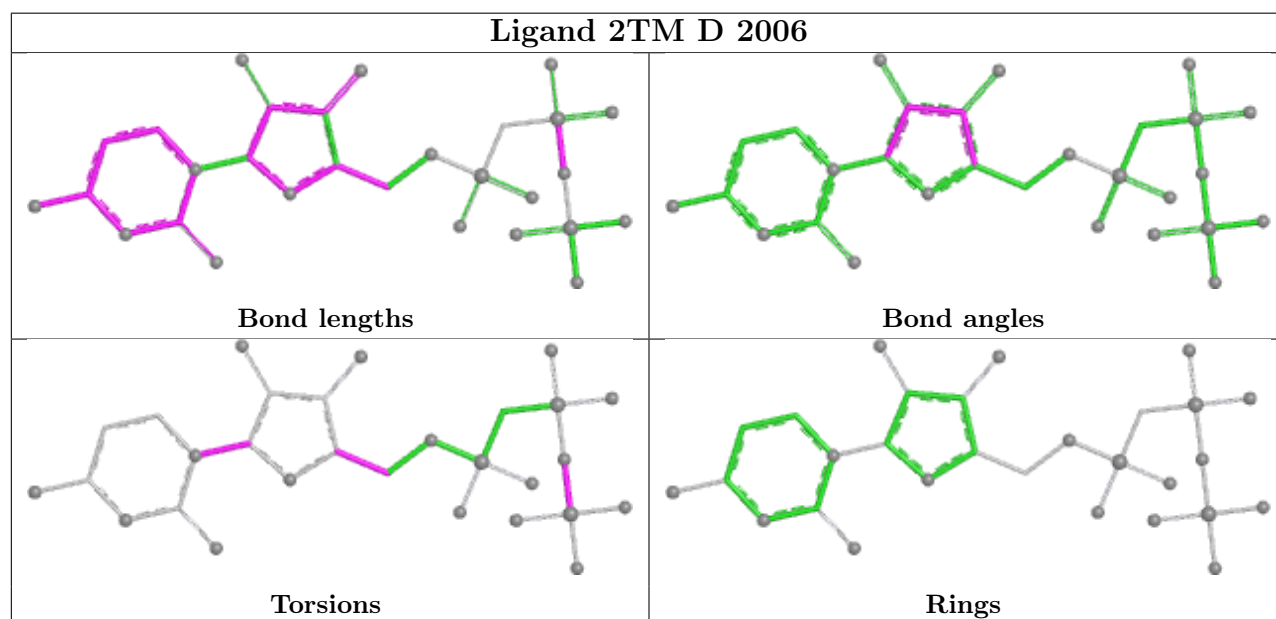
Mol	Chain	Res	Type	Atoms
11	D	2006	2TM	PB-O3B-PG-O1G
11	D	2006	2TM	O4'-C4'-C5'-O5'
11	D	2006	2TM	C2'-C1'-N1-C2

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%)	-0.07	2 (0%) 81 74	48, 64, 90, 139	0
1	B	224/315 (71%)	0.12	2 (0%) 81 74	49, 73, 100, 114	0
2	C	1112/1119 (99%)	-0.12	8 (0%) 84 77	32, 60, 118, 143	0
3	D	1486/1524 (97%)	0.07	41 (2%) 55 45	27, 62, 123, 151	1 (0%)
4	E	94/99 (94%)	-0.05	1 (1%) 78 70	40, 63, 96, 104	0
5	F	346/443 (78%)	0.35	11 (3%) 50 40	41, 80, 121, 143	0
6	G	25/27 (92%)	0.47	0 100 100	75, 114, 164, 170	0
7	H	17/19 (89%)	0.48	2 (11%) 9 7	70, 89, 162, 167	0
8	I	2/2 (100%)	2.90	2 (100%) 0 0	61, 61, 61, 62	2 (100%)
All	All	3537/3863 (91%)	0.04	69 (1%) 65 56	27, 65, 121, 170	3 (0%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	203	ALA	5.2
3	D	420	VAL	4.7
1	B	229	GLN	3.6
5	F	139	ALA	3.5
3	D	1252	ILE	3.5
3	D	431	VAL	3.4
3	D	290	PRO	3.4
8	I	1	U	3.4
3	D	202	VAL	3.1
1	B	6	LEU	3.1
3	D	445	ARG	3.0
3	D	161	LEU	2.9
3	D	434	ARG	2.9
2	C	275	TYR	2.9
3	D	436	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
3	D	415	VAL	2.8
3	D	353	VAL	2.8
4	E	95	VAL	2.8
3	D	409	VAL	2.8
3	D	182	GLY	2.8
2	C	767	PRO	2.8
5	F	422	LEU	2.7
3	D	352	ASN	2.7
3	D	402	PRO	2.7
5	F	138	SER	2.7
3	D	142	LEU	2.6
3	D	1502	ALA	2.6
2	C	41	ASN	2.6
3	D	449	SER	2.5
3	D	201	GLY	2.5
1	A	233	VAL	2.5
5	F	78	SER	2.5
3	D	447	VAL	2.5
3	D	393	ILE	2.4
5	F	146	GLY	2.4
8	I	2	A	2.4
5	F	324	GLU	2.4
3	D	170	PRO	2.4
2	C	207	LEU	2.4
5	F	325	LYS	2.3
3	D	1283	ILE	2.3
7	H	19	DG	2.3
5	F	141	VAL	2.3
3	D	490	ALA	2.3
1	A	232	ALA	2.2
3	D	289	THR	2.2
5	F	91	VAL	2.2
2	C	188	LYS	2.2
3	D	310	LEU	2.2
3	D	394	LEU	2.2
3	D	416	ALA	2.2
3	D	298	VAL	2.2
5	F	92	PRO	2.2
3	D	421	LEU	2.2
7	H	3	DT	2.2
3	D	177	ALA	2.2
3	D	560	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
3	D	292	VAL	2.1
2	C	311	PHE	2.1
2	C	251	ASP	2.1
3	D	141	ILE	2.1
3	D	369	ALA	2.1
2	C	254	VAL	2.0
3	D	172	PRO	2.0
3	D	1130	ARG	2.0
3	D	422	ALA	2.0
3	D	400	VAL	2.0
5	F	219	GLY	2.0
3	D	235	ALA	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 oligosaccharides in this entry.

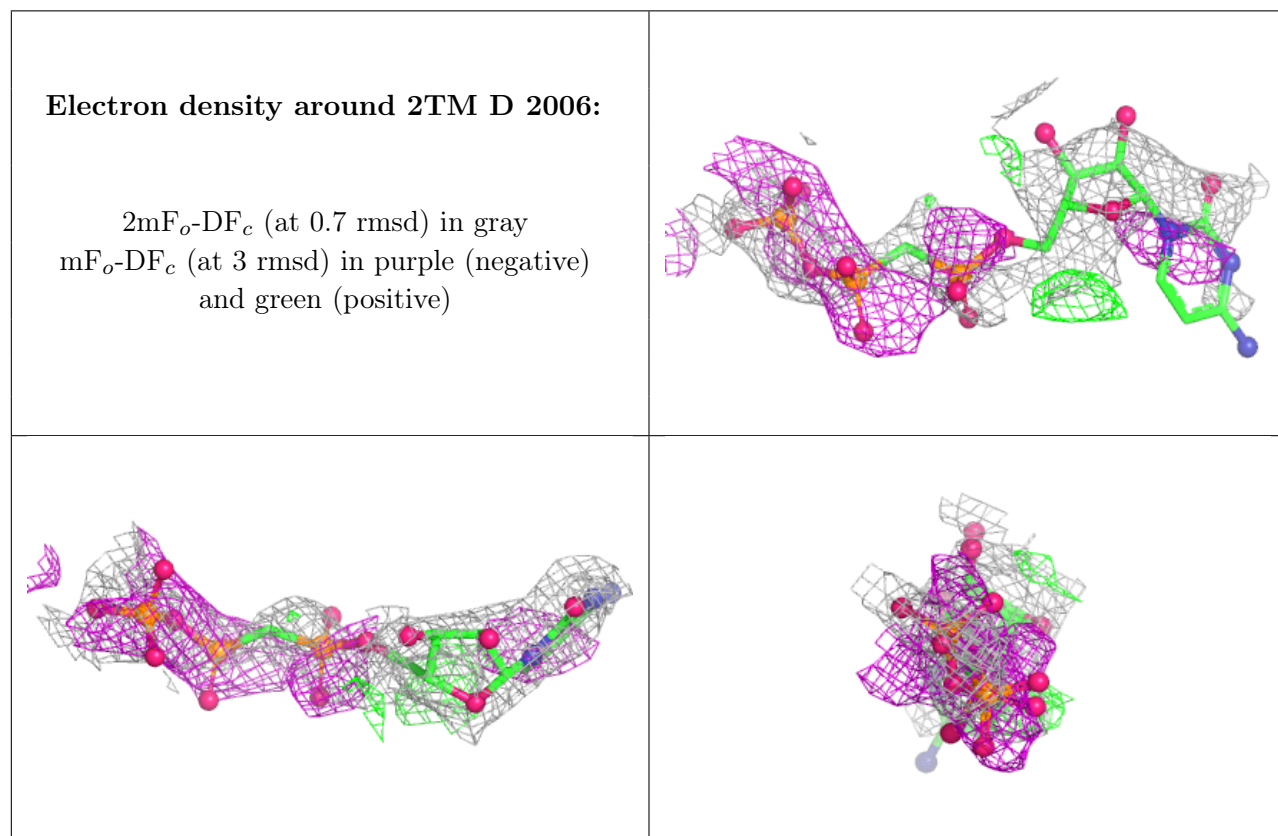
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
11	2TM	D	2006	29/29	0.54	0.19	63,80,103,108	29
9	MG	D	2005	1/1	0.81	0.13	65,65,65,65	0
9	MG	F	2001	1/1	0.91	0.06	69,69,69,69	0
9	MG	D	2004	1/1	0.91	0.28	59,59,59,59	0
9	MG	B	2001	1/1	0.94	0.10	77,77,77,77	0
9	MG	D	2003	1/1	0.96	0.09	40,40,40,40	0
10	ZN	D	2002	1/1	1.00	0.01	92,92,92,92	0
10	ZN	D	2001	1/1	1.00	0.03	49,49,49,49	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 ⓘ

There are no such residues in this entry.