



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:36 AM UTC

PDB ID : 4OIP / pdb_00004oip
Title : Crystal structure of Thermus thermophilus transcription initiation complex soaked with GE23077, ATP, and CMPcPP
Authors : Zhang, Y.; Ebright, R.H.; Arnold, E.
Deposited on : 2014-01-20
Resolution : 3.40 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

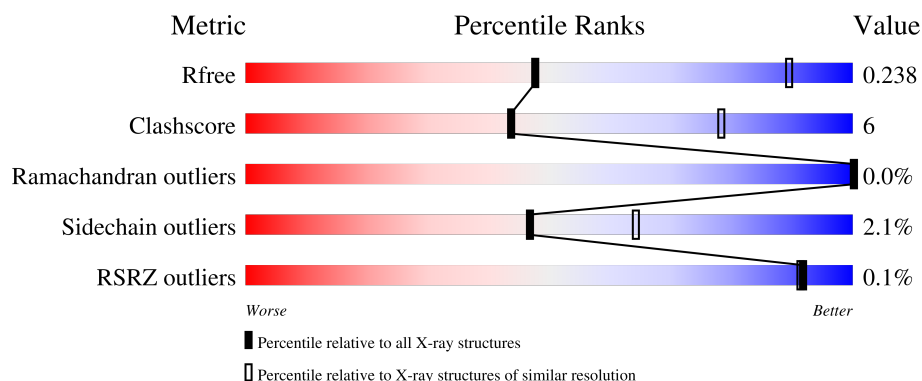
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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.



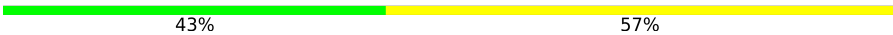
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	60% 12% • 27%
1	B	315	56% 14% • 28%
2	C	1119	82% 16% ••
3	D	1524	79% 18% •
4	E	99	80% 14% • 5%

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Mol	Chain	Length	Quality of chain
5	F	443	 67% 10% 22%
6	G	21	 71% 5% 24%
7	H	27	 44% 44% 11%
8	I	7	 43% 57%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 28603 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1809	1155	315	337	2			
1	B	227	Total	C	N	O	S	0	0	0
			1789	1143	310	334	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1112	Total	C	N	O	S	0	0	0
			8774	5550	1565	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
			11746	7446	2070	2195	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
			758	483	132	139	4			

- Molecule 5 is a protein called DNA directed RNA polymerase sigma factor A.

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 5'-D(*CP*CP*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*GP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	16	Total	C	N	O	P	0	0	0
			331	156	63	96	16			

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

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

- Molecule 8 is a protein called GE23077.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	I	7	Total	C	N	O	0	0	0
			50	26	9	15			

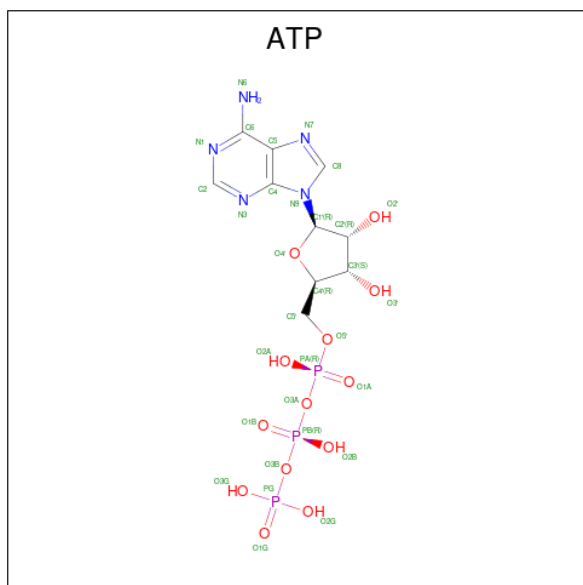
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Mg	0	0
			1	1		
9	D	4	Total	Mg	0	0
			4	4		
9	F	1	Total	Mg	0	0
			1	1		

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

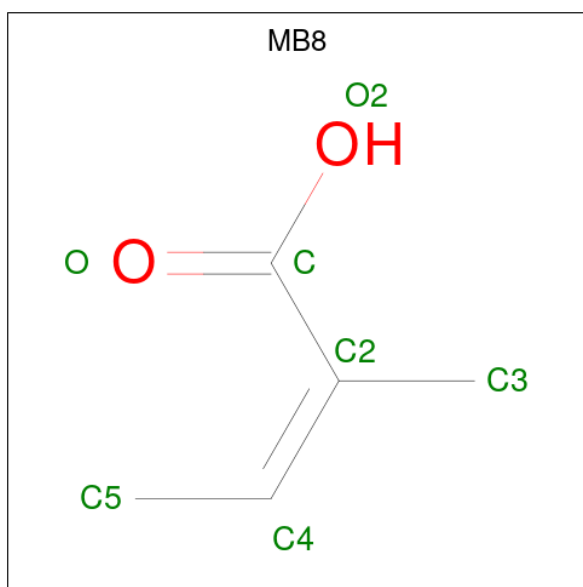
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	2	Total	Zn	0	0
			2	2		

- Molecule 11 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	D	1	Total	C	N	O	P	10	0
			31	10	5	13	3		

- Molecule 12 is (2Z)-2-methylbut-2-enoic acid (CCD ID: MB8) (formula: C₅H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	I	1	Total	C	O	0	0
			2	1	1		

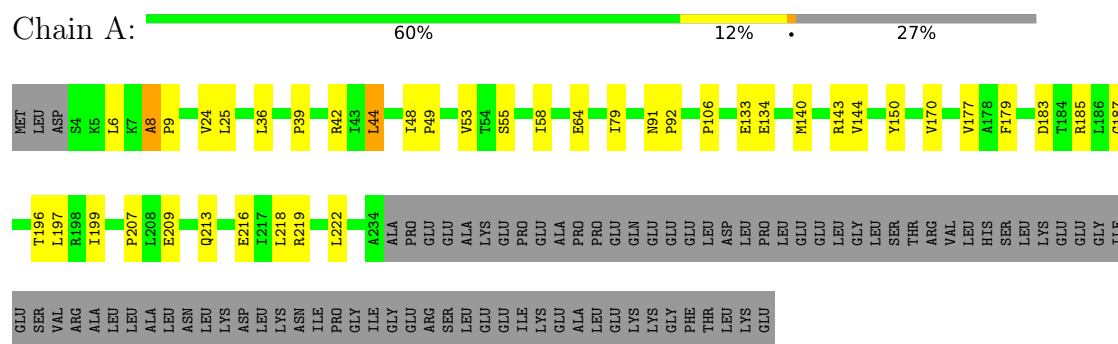
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	D	3	Total	O	0	0
			3	3		

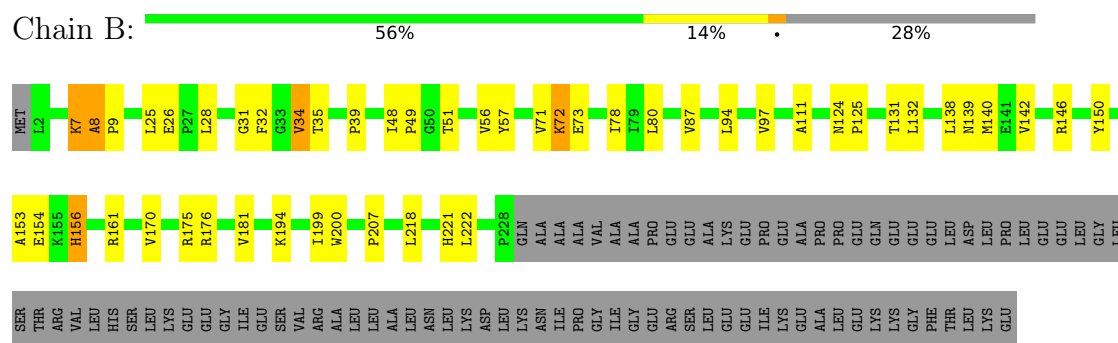
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

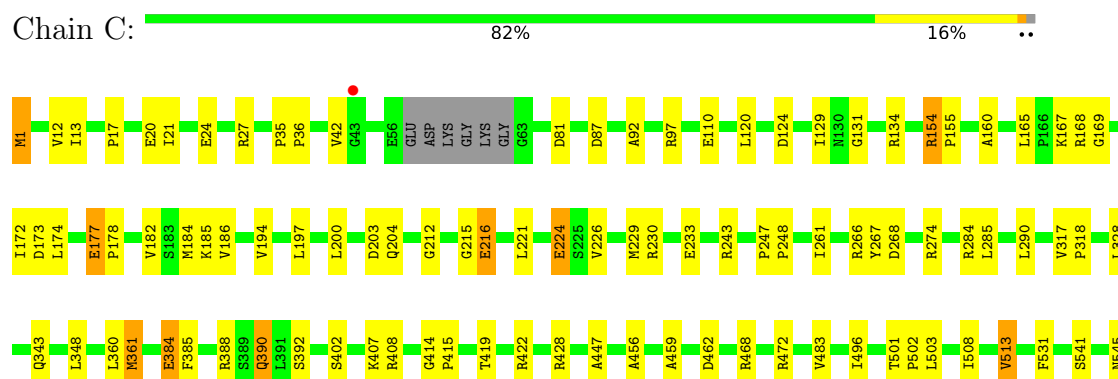
- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha



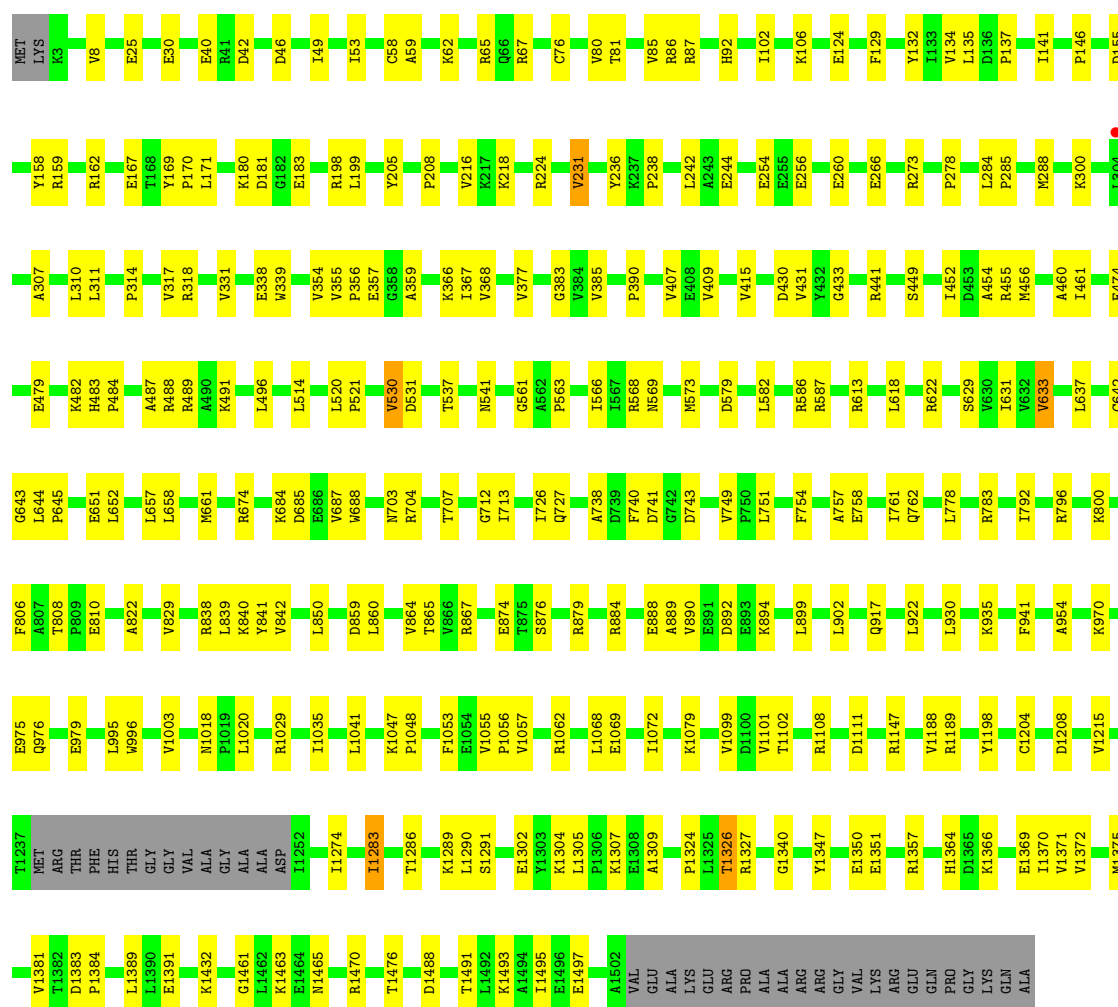
- Molecule 2: DNA-directed RNA polymerase subunit beta





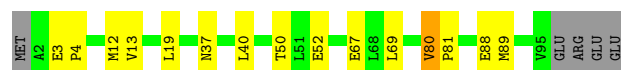
• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D: 79% 18% .



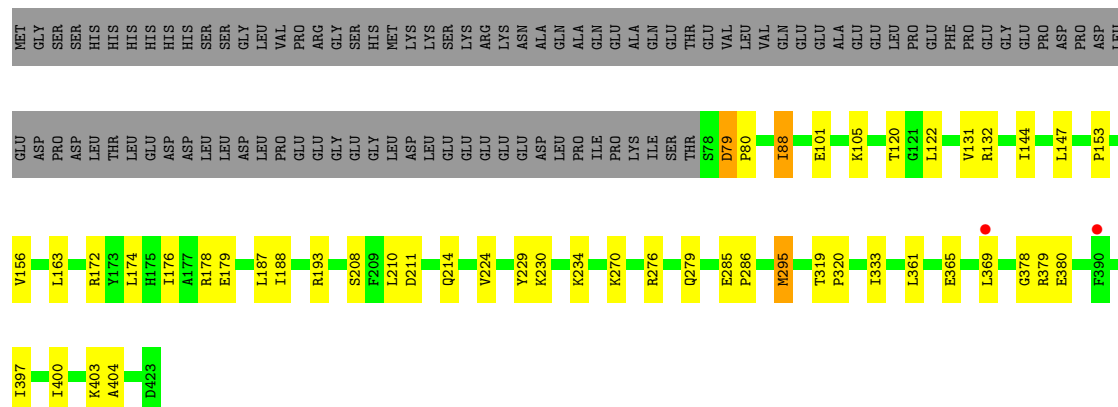
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 80% 14% 5% .



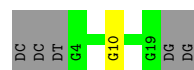
- Molecule 5: DNA directed RNA polymerase sigma factor A

Chain F: 

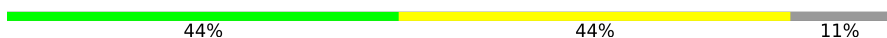


- Molecule 6: 5'-D(*CP*CP*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*A P*GP*GP*G)-3'

Chain G: 



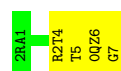
- Molecule 7: 5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP P*GP*GP*AP*TP*GP*CP*AP*GP*G)-3'

Chain H: 



- Molecule 8: GE23077

Chain I: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	182.92Å 104.39Å 294.21Å 90.00° 98.97° 90.00°	Depositor
Resolution (Å)	49.12 – 3.40 49.12 – 3.40	Depositor EDS
% Data completeness (in resolution range)	81.5 (49.12-3.40) 81.5 (49.12-3.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.208 , 0.246 (Not available) , 0.238	Depositor DCC
R_{free} test set	1643 reflections (2.17%)	wwPDB-VP
Wilson B-factor (Å ²)	95.8	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 26.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.018 for $1/2^*h-3/2^*k,-1/2^*h-1/2^*k,-1/2^*h+1/2^*k-l$ 0.014 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	0.93	EDS
Total number of atoms	28603	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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: DSN, 0QZ, R2T, MG, MB8, 2TL, 2RA, DVA, ATP, FGL, 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	0.29	0/1841	0.81	2/2504 (0.1%)
1	B	0.28	0/1821	0.79	0/2476
2	C	0.29	0/8941	0.76	8/12092 (0.1%)
3	D	0.29	0/11955	0.76	6/16163 (0.0%)
4	E	0.29	0/772	0.70	0/1040
5	F	0.27	0/2852	0.75	3/3837 (0.1%)
6	G	0.09	0/371	0.45	0/571
7	H	0.12	0/556	0.59	0/858
All	All	0.28	0/29109	0.76	19/39541 (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
8	I	0	1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1340	GLY	CA-C-N	6.26	126.00	119.05
3	D	1340	GLY	C-N-CA	6.26	126.00	119.05
1	A	8	ALA	CA-C-N	5.91	126.40	120.14
1	A	8	ALA	C-N-CA	5.91	126.40	120.14
2	C	169	GLY	CA-C-N	5.87	125.77	119.85
2	C	169	GLY	C-N-CA	5.87	125.77	119.85
2	C	980	GLY	N-CA-C	-5.37	107.12	114.64
5	F	333	ILE	N-CA-C	5.33	112.83	107.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	433	GLY	N-CA-C	5.33	118.31	110.80
2	C	212	GLY	N-CA-C	5.07	119.01	112.83
3	D	1018	ASN	CA-C-N	5.05	124.49	119.24
3	D	1018	ASN	C-N-CA	5.05	124.49	119.24
2	C	154	ARG	CA-C-N	5.01	124.18	118.97
2	C	154	ARG	C-N-CA	5.01	124.18	118.97
2	C	1081	VAL	CA-C-N	5.01	124.92	119.76
2	C	1081	VAL	C-N-CA	5.01	124.92	119.76
3	D	783	ARG	CB-CA-C	-5.00	110.43	117.23
5	F	79	ASP	CA-C-N	5.00	124.60	119.05
5	F	79	ASP	C-N-CA	5.00	124.60	119.05

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	I	5	2TL	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	28	0
1	B	1789	0	1841	33	0
2	C	8774	0	8877	117	0
3	D	11746	0	11984	159	0
4	E	758	0	770	8	0
5	F	2807	0	2882	31	0
6	G	331	0	180	2	0
7	H	495	0	272	12	0
8	I	50	0	37	0	0
9	B	1	0	0	0	0
9	D	4	0	0	0	0
9	F	1	0	0	0	0
10	D	2	0	0	0	0
11	D	31	0	12	1	0
12	I	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	D	3	0	0	0	0
All	All	28603	0	28718	352	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 6.

All (352) 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:42:ARG:NH2	1:B:31:GLY:O	2.18	0.77
2:C:165:LEU:HB2	2:C:168:ARG:HG3	1.68	0.74
1:A:44:LEU:HA	1:A:48:ILE:HG12	1.70	0.73
3:D:273:ARG:HB3	3:D:278:PRO:HA	1.71	0.72
3:D:65:ARG:NH1	5:F:378:GLY:O	2.23	0.72
1:A:44:LEU:HD13	1:A:177:VAL:HG21	1.72	0.70
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.73	0.70
2:C:674:VAL:HG12	2:C:869:VAL:HB	1.73	0.69
2:C:97:ARG:NH1	2:C:110:GLU:OE1	2.23	0.69
2:C:390:GLN:HG2	2:C:414:GLY:HA2	1.75	0.68
2:C:266:ARG:NH1	7:H:11:DG:O6	2.27	0.68
3:D:106:LYS:O	3:D:586:ARG:NH1	2.27	0.68
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.27	0.68
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.77	0.67
2:C:168:ARG:HD3	2:C:268:ASP:HB3	1.76	0.66
5:F:397:ILE:HD12	5:F:400:ILE:HD11	1.78	0.66
3:D:171:LEU:HD12	3:D:390:PRO:HG2	1.78	0.65
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.78	0.64
3:D:208:PRO:HA	3:D:390:PRO:HA	1.77	0.64
2:C:628:PHE:H	2:C:638:ASP:HB3	1.62	0.64
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.79	0.64
2:C:243:ARG:NH1	7:H:9:DG:O6	2.31	0.64
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.80	0.64
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.31	0.64
3:D:1286:THR:HB	3:D:1289:LYS:H	1.62	0.63
1:A:185:ARG:NH2	1:A:187:GLY:O	2.31	0.63
2:C:428:ARG:NH2	2:C:447:ALA:O	2.32	0.63
2:C:194:VAL:HG22	2:C:221:LEU:HD12	1.80	0.62
3:D:167:GLU:OE2	3:D:198:ARG:NH1	2.32	0.62
3:D:970:LYS:HD3	3:D:995:LEU:HD13	1.80	0.62
3:D:489:ARG:NH1	3:D:1391:GLU:OE2	2.32	0.61
3:D:652:LEU:HB3	3:D:749:VAL:HG21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:197:LEU:HD12	2:C:221:LEU:HD11	1.82	0.61
2:C:17:PRO:HB2	2:C:20:GLU:HB3	1.82	0.61
2:C:709:GLU:OE2	2:C:824:ARG:NH1	2.34	0.61
2:C:24:GLU:OE2	2:C:27:ARG:NH2	2.33	0.61
3:D:1147:ARG:NH2	3:D:1369:GLU:OE1	2.34	0.61
1:B:34:VAL:HG21	2:C:978:ARG:HB3	1.82	0.60
3:D:569:ASN:ND2	5:F:214:GLN:OE1	2.32	0.60
5:F:193:ARG:HB2	7:H:6:DT:H1'	1.84	0.59
3:D:1372:VAL:HA	3:D:1375:MET:HE3	1.84	0.59
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.83	0.59
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.83	0.59
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.84	0.59
1:A:58:ILE:HG12	1:A:140:MET:HG2	1.85	0.58
2:C:768:THR:OG1	2:C:771:GLU:OE1	2.19	0.58
3:D:1003:VAL:HG21	3:D:1041:LEU:HG	1.84	0.58
3:D:657:LEU:HG	3:D:661:MET:HE2	1.85	0.58
3:D:1465:ASN:OD1	3:D:1470:ARG:NH1	2.34	0.58
2:C:419:THR:HB	2:C:422:ARG:HG3	1.86	0.58
2:C:884:GLN:O	2:C:888:THR:OG1	2.22	0.58
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.85	0.58
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.36	0.57
2:C:215:GLY:O	2:C:216:GLU:HB3	2.05	0.57
1:B:8:ALA:HB1	1:B:9:PRO:HA	1.85	0.57
2:C:134:ARG:NH1	2:C:392:SER:OG	2.38	0.57
2:C:630:ARG:NH1	2:C:705:ILE:O	2.37	0.57
3:D:1029:ARG:NH1	11:D:2007:ATP:O1G	2.35	0.57
3:D:180:LYS:NZ	3:D:357:GLU:OE1	2.34	0.57
2:C:129:ILE:HB	2:C:134:ARG:HD2	1.88	0.56
2:C:172:ILE:HG12	2:C:186:VAL:HG22	1.86	0.56
1:B:80:LEU:HD21	3:D:842:VAL:HG12	1.87	0.56
1:A:55:SER:HB3	1:A:143:ARG:HB3	1.86	0.56
5:F:144:ILE:HB	5:F:147:LEU:HD13	1.88	0.56
3:D:704:ARG:HD2	3:D:738:ALA:HB2	1.88	0.56
4:E:37:ASN:HD22	4:E:89:MET:HE1	1.71	0.56
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.88	0.56
2:C:167:LYS:HD3	7:H:12:DC:H6	1.71	0.56
3:D:633:VAL:HB	3:D:740:PHE:CZ	2.41	0.55
3:D:1048:PRO:O	3:D:1079:LYS:NZ	2.36	0.55
2:C:87:ASP:HA	2:C:131:GLY:HA3	1.88	0.55
2:C:1056:LYS:HD3	3:D:751:LEU:HD11	1.89	0.55
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:707:THR:HG23	3:D:712:GLY:HA3	1.89	0.55
3:D:1111:ASP:OD1	3:D:1189:ARG:NH2	2.40	0.55
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.88	0.55
3:D:637:LEU:HD13	3:D:642:CYS:HA	1.88	0.55
1:B:94:LEU:O	1:B:146:ARG:NH2	2.39	0.54
2:C:905:ILE:HD13	2:C:905:ILE:H	1.72	0.54
3:D:644:LEU:HD12	3:D:645:PRO:HD2	1.89	0.54
1:A:183:ASP:HA	2:C:938:LYS:HE3	1.89	0.54
3:D:367:ILE:HG22	3:D:368:VAL:HG23	1.88	0.54
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	1.89	0.54
1:B:80:LEU:HB3	3:D:867:ARG:HH21	1.72	0.54
3:D:758:GLU:OE1	3:D:1476:THR:OG1	2.20	0.54
1:A:48:ILE:HD12	1:A:213:GLN:HG3	1.89	0.54
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.89	0.54
1:A:196:THR:HG21	2:C:934:PHE:HE2	1.73	0.53
2:C:617:ASP:OD1	2:C:617:ASP:N	2.42	0.53
2:C:971:LYS:HG2	2:C:988:VAL:HG22	1.90	0.53
3:D:137:PRO:HA	3:D:452:ILE:HG13	1.91	0.53
1:B:51:THR:OG1	1:B:87:VAL:O	2.21	0.53
5:F:101:GLU:HG2	5:F:105:LYS:HE2	1.90	0.53
2:C:1008:ARG:HH11	2:C:1028:GLY:HA2	1.73	0.53
3:D:838:ARG:NH1	3:D:874:GLU:OE1	2.38	0.53
2:C:1083:GLU:OE2	3:D:87:ARG:NH2	2.42	0.53
2:C:911:GLU:O	2:C:915:LYS:HG2	2.09	0.52
3:D:658:LEU:HA	3:D:661:MET:HE3	1.92	0.52
2:C:939:ARG:HG2	2:C:982:PRO:HD3	1.90	0.52
2:C:1016:ILE:O	3:D:87:ARG:NH1	2.41	0.52
3:D:954:ALA:O	3:D:1062:ARG:NH2	2.42	0.52
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.43	0.52
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.92	0.52
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.92	0.52
1:B:138:LEU:HD11	1:B:140:MET:HE3	1.92	0.51
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.91	0.51
1:B:25:LEU:HD23	1:B:28:LEU:HD11	1.92	0.51
3:D:1198:TYR:OH	3:D:1432:LYS:NZ	2.44	0.51
3:D:141:ILE:HA	3:D:146:PRO:HA	1.93	0.51
6:G:10:DG:O6	7:H:17:DA:N6	2.44	0.51
2:C:758:ARG:HH21	2:C:788:THR:HB	1.75	0.51
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.46	0.51
2:C:847:GLY:HA2	3:D:741:ASP:HA	1.94	0.50
2:C:571:LEU:HD23	2:C:702:SER:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1350:GLU:OE2	3:D:1357:ARG:NH1	2.44	0.50
3:D:134:VAL:HG12	3:D:454:ALA:HB2	1.94	0.50
3:D:629:SER:HB3	3:D:726:ILE:HG13	1.92	0.50
5:F:88:ILE:HG23	5:F:193:ARG:HG2	1.94	0.50
1:A:64:GLU:HG3	1:A:79:ILE:HD12	1.93	0.50
3:D:155:ASP:OD1	3:D:159:ARG:NH1	2.44	0.50
3:D:894:LYS:H	3:D:894:LYS:HD2	1.77	0.50
3:D:899:LEU:HD22	3:D:917:GLN:HB3	1.93	0.50
5:F:188:ILE:HG12	5:F:224:VAL:HG21	1.94	0.50
5:F:79:ASP:OD2	7:H:8:DG:N1	2.39	0.49
2:C:1009:SER:OG	2:C:1010:THR:N	2.45	0.49
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.47	0.49
1:A:53:VAL:HG22	1:A:144:VAL:HG22	1.95	0.49
2:C:402:SER:HA	2:C:566:THR:HG23	1.94	0.49
3:D:1364:HIS:CE1	3:D:1366:LYS:HG3	2.48	0.49
1:B:175:ARG:N	1:B:200:TRP:O	2.44	0.49
2:C:1019:GLN:HG2	2:C:1058:ASP:HB2	1.94	0.49
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.95	0.49
2:C:605:LYS:HB2	2:C:612:VAL:HB	1.93	0.49
2:C:1067:TYR:OH	3:D:674[B]:ARG:NH1	2.46	0.49
2:C:274:ARG:HH22	2:C:284:ARG:HH22	1.60	0.49
2:C:937:ASP:OD1	2:C:938:LYS:N	2.46	0.49
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.13	0.48
1:A:209:GLU:O	1:A:213:GLN:HG2	2.13	0.48
3:D:1101:VAL:HG13	3:D:1102:THR:HG23	1.95	0.48
1:A:199:ILE:HB	1:A:207:PRO:HB3	1.94	0.48
2:C:617:ASP:HB2	2:C:619:ARG:HG2	1.95	0.48
3:D:1020:LEU:HB3	3:D:1035:ILE:HD12	1.95	0.48
2:C:274:ARG:NH2	2:C:285:LEU:O	2.47	0.48
3:D:1208:ASP:HB2	3:D:1215:VAL:HA	1.96	0.48
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.95	0.48
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.95	0.48
5:F:187:LEU:HD23	5:F:224:VAL:HG13	1.95	0.48
2:C:390:GLN:HB3	2:C:415:PRO:HD3	1.96	0.48
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.95	0.48
2:C:1:MET:HG3	2:C:899:GLN:HA	1.95	0.47
3:D:30:GLU:OE1	3:D:40:GLU:HG2	2.14	0.47
2:C:784:ASP:OD1	2:C:784:ASP:N	2.39	0.47
4:E:12:MET:HE1	4:E:69:LEU:HA	1.96	0.47
1:B:71:VAL:HG22	1:B:132:LEU:HG	1.95	0.47
2:C:541:SER:O	2:C:545:ASN:ND2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.49	0.47
2:C:173:ASP:HB2	2:C:185:LYS:HB3	1.97	0.47
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.96	0.47
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.96	0.47
3:D:102:ILE:HD12	3:D:579:ASP:HB3	1.96	0.47
3:D:368:VAL:HB	3:D:377:VAL:HB	1.95	0.47
1:B:199:ILE:HB	1:B:207:PRO:HB3	1.97	0.47
3:D:537:THR:OG1	3:D:541:ASN:ND2	2.47	0.47
3:D:1274:ILE:HG22	3:D:1324:PRO:HA	1.97	0.47
1:B:78:ILE:HG21	1:B:140:MET:HE1	1.96	0.46
2:C:724:ARG:NH2	2:C:734:LEU:O	2.48	0.46
2:C:503:LEU:HD23	2:C:508:ILE:HA	1.97	0.46
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.97	0.46
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.97	0.46
2:C:124:ASP:OD2	2:C:407:LYS:NZ	2.35	0.46
2:C:640:ARG:HE	2:C:642:ARG:HH22	1.63	0.46
2:C:1055:LEU:HD22	2:C:1066:ALA:HB2	1.98	0.46
3:D:840:LYS:HE3	3:D:841:TYR:OH	2.15	0.46
1:B:34:VAL:HG12	1:B:181:VAL:HG21	1.96	0.46
2:C:261:ILE:HG23	2:C:290:LEU:HB2	1.97	0.46
2:C:1095:LEU:HD23	3:D:582:LEU:HD22	1.98	0.46
5:F:163:LEU:HD13	5:F:174:LEU:HD13	1.97	0.46
2:C:760:SER:O	2:C:786:LYS:HG2	2.16	0.46
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.15	0.46
5:F:270:LYS:HG2	5:F:295:MET:HE1	1.97	0.46
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.67	0.46
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.97	0.46
2:C:628:PHE:H	2:C:638:ASP:CB	2.29	0.46
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.98	0.46
3:D:487:ALA:O	3:D:491:LYS:HG2	2.16	0.46
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.97	0.46
3:D:317:VAL:HG23	3:D:339:TRP:HB3	1.97	0.46
1:B:72:LYS:HG2	1:B:131:THR:OG1	2.16	0.45
2:C:501:THR:HG21	2:C:513:VAL:HG23	1.98	0.45
3:D:520:LEU:HD12	3:D:521:PRO:HD2	1.99	0.45
3:D:573:MET:SD	5:F:210:LEU:HB3	2.56	0.45
3:D:864:VAL:HG22	3:D:865:THR:H	1.81	0.45
3:D:890:VAL:HB	3:D:922:LEU:HD13	1.98	0.45
2:C:13:ILE:HD13	2:C:483:VAL:HG11	1.97	0.45
3:D:162:ARG:O	3:D:449:SER:HB2	2.17	0.45
5:F:285:GLU:HA	5:F:286:PRO:HD3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LEU:HD11	1:B:221:HIS:HB3	1.99	0.45
3:D:685:ASP:HA	3:D:688:TRP:HD1	1.82	0.45
3:D:829:VAL:HG21	3:D:839:LEU:HD11	1.99	0.45
3:D:850:LEU:HD12	3:D:884:ARG:NH2	2.32	0.45
3:D:530:VAL:HG12	3:D:531:ASP:H	1.82	0.45
3:D:314:PRO:HB2	3:D:317:VAL:HG12	1.97	0.45
3:D:430:ASP:N	3:D:430:ASP:OD1	2.50	0.45
3:D:890:VAL:HG23	3:D:892:ASP:H	1.82	0.45
2:C:229:MET:HB2	2:C:233:GLU:HB2	1.99	0.45
2:C:571:LEU:HB2	2:C:574:ALA:HB2	1.98	0.45
3:D:561:GLY:HA3	5:F:132:ARG:HD3	1.99	0.45
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.98	0.44
3:D:514:LEU:HD23	3:D:514:LEU:HA	1.85	0.44
3:D:889:ALA:HB1	3:D:930:LEU:HA	1.98	0.44
1:A:91:ASN:HA	1:A:92:PRO:HD3	1.88	0.44
2:C:177:GLU:HG3	2:C:178:PRO:HD2	1.99	0.44
3:D:703:ASN:HB2	3:D:713:ILE:HG12	1.99	0.44
7:H:15:DT:H5'	7:H:15:DT:H6	1.82	0.44
1:A:39:PRO:HG3	1:B:39:PRO:HG3	2.00	0.44
2:C:168:ARG:O	2:C:267:TYR:HA	2.17	0.44
3:D:456:MET:HE1	3:D:568:ARG:NE	2.33	0.44
3:D:684:LYS:O	3:D:687:VAL:HG12	2.17	0.44
1:B:72:LYS:HG3	1:B:73:GLU:N	2.32	0.44
2:C:1031:ARG:HA	3:D:622:ARG:HA	2.00	0.44
5:F:193:ARG:HB3	7:H:7:DG:H5''	1.99	0.44
2:C:154:ARG:HA	2:C:155:PRO:HD3	1.87	0.44
3:D:975:GLU:O	3:D:979:GLU:HG2	2.17	0.44
1:B:153:ALA:HA	1:B:156:HIS:CE1	2.52	0.44
2:C:496:ILE:HG12	2:C:531:PHE:HB2	2.00	0.44
2:C:708:TYR:HB3	2:C:790:LEU:HD21	2.00	0.44
3:D:1057:VAL:HG13	3:D:1069:GLU:CD	2.43	0.44
2:C:408:ARG:NH1	2:C:456:ALA:O	2.51	0.44
2:C:501:THR:HA	2:C:502:PRO:HD3	1.87	0.43
2:C:1115:LEU:HD23	3:D:85:VAL:HG12	1.99	0.43
3:D:563:PRO:HD2	3:D:566:ILE:HD12	2.00	0.43
2:C:172:ILE:HD13	2:C:184:MET:HE3	1.99	0.43
2:C:224:GLU:CD	2:C:224:GLU:H	2.26	0.43
2:C:551:GLU:HG2	2:C:552:HIS:CD2	2.53	0.43
2:C:686:ASP:OD2	2:C:879:ARG:NH1	2.34	0.43
3:D:455:ARG:HB2	3:D:460:ALA:HB2	2.00	0.43
1:B:48:ILE:HA	1:B:49:PRO:HD3	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:53:ILE:HA	3:D:86:ARG:HD2	2.00	0.43
3:D:256:GLU:HG3	3:D:300:LYS:HG3	1.99	0.43
3:D:613:ARG:HG3	3:D:618:LEU:HD23	1.99	0.43
3:D:1371:VAL:HG12	3:D:1375:MET:HE2	1.99	0.43
3:D:1488:ASP:OD1	3:D:1488:ASP:N	2.46	0.43
2:C:328:LEU:HD23	2:C:328:LEU:HA	1.89	0.43
2:C:456:ALA:HB3	2:C:459:ALA:HB2	2.01	0.43
3:D:1305:LEU:HD13	3:D:1309:ALA:HB3	2.00	0.43
1:A:216:GLU:OE2	1:A:219:ARG:NH2	2.51	0.43
2:C:710:ILE:HD12	2:C:790:LEU:HB2	2.00	0.43
3:D:58:CYS:HB2	3:D:76:CYS:SG	2.58	0.43
3:D:840:LYS:HE3	3:D:841:TYR:CZ	2.54	0.43
3:D:1463:LYS:HE2	3:D:1463:LYS:HB3	1.82	0.43
1:B:124:ASN:OD1	1:B:124:ASN:N	2.52	0.43
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.69	0.43
3:D:42:ASP:N	3:D:46:ASP:OD2	2.42	0.43
3:D:800:LYS:HB3	3:D:822:ALA:HB2	2.00	0.43
1:B:32:PHE:HA	1:B:35:THR:HB	2.00	0.43
2:C:226:VAL:HA	2:C:229:MET:HE2	2.00	0.43
1:A:106:PRO:HG3	1:A:134:GLU:HG2	2.01	0.43
1:A:133:GLU:HG2	1:A:134:GLU:H	1.84	0.43
2:C:1009:SER:HB3	3:D:651:GLU:O	2.19	0.43
3:D:244:GLU:HG3	3:D:310:LEU:HG	1.99	0.43
3:D:231:VAL:O	3:D:236:TYR:OH	2.35	0.43
4:E:40:LEU:HG	4:E:67:GLU:HG2	2.00	0.43
2:C:92:ALA:HB2	2:C:120:LEU:HD11	2.01	0.42
2:C:1101:THR:HG22	3:D:8:VAL:HG22	2.00	0.42
3:D:633:VAL:HB	3:D:740:PHE:CE2	2.53	0.42
2:C:35:PRO:HA	2:C:36:PRO:HD3	1.90	0.42
2:C:274:ARG:NH2	2:C:284:ARG:HH22	2.17	0.42
3:D:181:ASP:HB2	3:D:205:TYR:CD1	2.55	0.42
3:D:216:VAL:HG23	3:D:383:GLY:HA2	2.00	0.42
3:D:288:MET:SD	3:D:307:ALA:HB2	2.59	0.42
3:D:796:ARG:NH2	3:D:859:ASP:OD2	2.39	0.42
3:D:1383:ASP:HA	3:D:1384:PRO:HD3	1.87	0.42
3:D:479:GLU:HA	3:D:482:LYS:HE2	2.01	0.42
1:A:39:PRO:CG	1:B:39:PRO:HG3	2.50	0.42
1:B:150:TYR:CE1	1:B:170:VAL:HG22	2.55	0.42
2:C:317:VAL:HA	2:C:318:PRO:HD3	1.91	0.42
2:C:343:GLN:NE2	2:C:384:GLU:OE2	2.53	0.42
2:C:787:ASP:OD2	2:C:791:ARG:NH2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:129:PHE:HD1	3:D:456:MET:HE3	1.85	0.42
1:B:26:GLU:HB3	1:B:194:LYS:HG3	2.02	0.42
3:D:284:LEU:HA	3:D:288:MET:HE2	2.02	0.42
1:B:57:TYR:CD1	1:B:161:ARG:HD2	2.55	0.42
2:C:348:LEU:HD12	2:C:348:LEU:HA	1.93	0.42
3:D:792:ILE:HD13	3:D:941:PHE:CD1	2.55	0.42
3:D:806:PHE:O	3:D:829:VAL:HA	2.20	0.42
5:F:234:LYS:HE2	5:F:234:LYS:HB3	1.94	0.42
7:H:20:DG:H2''	7:H:21:DA:O5'	2.20	0.42
1:B:94:LEU:HD11	1:B:97:VAL:HG22	2.01	0.42
3:D:171:LEU:HD23	3:D:171:LEU:HA	1.82	0.42
3:D:407:VAL:HG22	3:D:409:VAL:H	1.85	0.42
3:D:1326:THR:HG22	3:D:1327:ARG:H	1.85	0.42
2:C:926:PHE:CE2	2:C:930:LYS:HD3	2.55	0.41
3:D:25:GLU:HB2	3:D:92:HIS:CE1	2.55	0.41
5:F:172:ARG:O	5:F:176:ILE:HG12	2.20	0.41
3:D:637:LEU:O	3:D:935:LYS:NZ	2.54	0.41
3:D:1047:LYS:HG2	3:D:1053:PHE:CZ	2.55	0.41
5:F:80:PRO:HB2	5:F:210:LEU:HD11	2.03	0.41
5:F:105:LYS:HD3	5:F:179:GLU:HG2	2.03	0.41
1:A:48:ILE:HA	1:A:49:PRO:HD3	1.86	0.41
1:B:111:ALA:HB3	1:B:125:PRO:HA	2.02	0.41
2:C:937:ASP:OD2	2:C:939:ARG:NH1	2.53	0.41
3:D:67:ARG:HD2	5:F:379:ARG:HB3	2.02	0.41
4:E:13:VAL:HG21	4:E:19:LEU:HB2	2.03	0.41
4:E:52:GLU:OE1	4:E:52:GLU:N	2.45	0.41
2:C:905:ILE:C	2:C:907:ASP:H	2.29	0.41
2:C:1035:MET:HA	2:C:1038:TRP:CE3	2.56	0.41
3:D:59:ALA:HB3	3:D:76:CYS:HB2	2.02	0.41
3:D:285:PRO:HD2	3:D:288:MET:HE2	2.02	0.41
3:D:483:HIS:CG	3:D:484:PRO:HD2	2.55	0.41
5:F:208:SER:HB3	5:F:211:ASP:OD2	2.20	0.41
2:C:134:ARG:HH12	2:C:392:SER:C	2.28	0.41
2:C:944:LEU:HD21	2:C:963:LEU:HD23	2.03	0.41
3:D:224:ARG:NE	3:D:254:GLU:OE2	2.32	0.41
3:D:483:HIS:CE1	3:D:488:ARG:HD3	2.56	0.41
3:D:762:GLN:HE22	3:D:1476:THR:HG23	1.86	0.41
3:D:860:LEU:O	3:D:876:SER:HB2	2.21	0.41
3:D:1291:SER:OG	3:D:1304:LYS:HG2	2.20	0.41
5:F:229:TYR:CZ	5:F:230:LYS:HD3	2.55	0.41
7:H:10:DA:H2''	7:H:11:DG:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:58:CYS:SG	3:D:62:LYS:N	2.93	0.41
3:D:169:TYR:HA	3:D:170:PRO:HD3	1.84	0.41
3:D:1366:LYS:O	3:D:1370:ILE:HG12	2.21	0.41
2:C:124:ASP:HB3	2:C:592:LEU:HD12	2.03	0.41
2:C:578:VAL:HG23	2:C:671:ASN:CG	2.45	0.41
4:E:80:VAL:HG23	4:E:81:PRO:O	2.21	0.41
5:F:276:ARG:O	5:F:279:GLN:HG3	2.20	0.41
1:A:150:TYR:CD1	2:C:696:LYS:HG2	2.56	0.41
1:B:7:LYS:O	1:B:8:ALA:HB3	2.20	0.41
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.79	0.41
3:D:461:ILE:HD13	3:D:461:ILE:HA	1.94	0.41
2:C:612:VAL:HG22	2:C:622:GLU:HG3	2.01	0.40
2:C:1107:ASN:HA	2:C:1108:PRO:HD3	1.95	0.40
3:D:879:ARG:HD3	3:D:902:LEU:O	2.21	0.40
3:D:1283:ILE:H	3:D:1283:ILE:HG13	1.63	0.40
7:H:11:DG:H2"	7:H:12:DC:OP1	2.21	0.40
3:D:1381:VAL:HG21	3:D:1389:LEU:HD23	2.03	0.40
6:G:10:DG:H1	7:H:18:DC:H42	1.68	0.40
1:A:150:TYR:HD1	1:A:170:VAL:HG22	1.86	0.40
2:C:203:ASP:OD2	2:C:204:GLN:N	2.54	0.40
2:C:360:LEU:HB3	2:C:361:MET:HE3	2.03	0.40
3:D:132:TYR:OH	3:D:568:ARG:NH1	2.54	0.40
3:D:631:ILE:HG12	3:D:743:ASP:O	2.21	0.40
3:D:757:ALA:O	3:D:761:ILE:HG12	2.21	0.40
3:D:1290:LEU:HD12	3:D:1291:SER:H	1.87	0.40
3:D:1302:GLU:OE1	3:D:1304:LYS:HE3	2.20	0.40
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.54	0.40
2:C:81:ASP:OD2	2:C:81:ASP:N	2.50	0.40
2:C:771:GLU:O	2:C:775:ARG:HB2	2.21	0.40
3:D:1347:TYR:CZ	3:D:1351:GLU:HG3	2.56	0.40
3:D:1491:THR:O	3:D:1495:ILE:HG13	2.20	0.40
4:E:3:GLU:HA	4:E:4:PRO:HD3	1.95	0.40
5:F:319:THR:HA	5:F:320:PRO:HD3	1.93	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%)	227 (99%)	2 (1%)	0	100	100
1	B	225/315 (71%)	221 (98%)	3 (1%)	1 (0%)	30	59
2	C	1108/1119 (99%)	1088 (98%)	20 (2%)	0	100	100
3	D	1483/1524 (97%)	1463 (99%)	20 (1%)	0	100	100
4	E	92/99 (93%)	91 (99%)	1 (1%)	0	100	100
5	F	344/443 (78%)	339 (98%)	5 (2%)	0	100	100
All	All	3481/3815 (91%)	3429 (98%)	51 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	8	ALA

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%)	197 (98%)	3 (2%)	57	69
1	B	200/273 (73%)	194 (97%)	6 (3%)	36	59
2	C	936/941 (100%)	914 (98%)	22 (2%)	43	62
3	D	1254/1279 (98%)	1230 (98%)	24 (2%)	50	66
4	E	82/88 (93%)	80 (98%)	2 (2%)	43	62
5	F	301/388 (78%)	297 (99%)	4 (1%)	61	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2973/3242 (92%)	2912 (98%)	61 (2%)	47 64

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	25	LEU
1	A	44	LEU
1	B	7	LYS
1	B	34	VAL
1	B	72	LYS
1	B	139	ASN
1	B	154	GLU
1	B	156	HIS
2	C	1	MET
2	C	21	ILE
2	C	42	VAL
2	C	177	GLU
2	C	182	VAL
2	C	200	LEU
2	C	216	GLU
2	C	224	GLU
2	C	230	ARG
2	C	361	MET
2	C	384	GLU
2	C	388	ARG
2	C	390	GLN
2	C	513	VAL
2	C	595	LEU
2	C	617	ASP
2	C	620	LEU
2	C	657	ASP
2	C	715	THR
2	C	848	VAL
2	C	905	ILE
2	C	1057	SER
3	D	49	ILE
3	D	80	VAL
3	D	81	THR
3	D	135	LEU
3	D	183	GLU
3	D	199	LEU

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Mol	Chain	Res	Type
3	D	231	VAL
3	D	331	VAL
3	D	354	VAL
3	D	366	LYS
3	D	415	VAL
3	D	431	VAL
3	D	530	VAL
3	D	633	VAL
3	D	754	PHE
3	D	778	LEU
3	D	808	THR
3	D	810	GLU
3	D	976	GLN
3	D	1055	VAL
3	D	1188	VAL
3	D	1283	ILE
3	D	1307	LYS
3	D	1326	THR
4	E	50	THR
4	E	80	VAL
5	F	88	ILE
5	F	295	MET
5	F	369	LEU
5	F	380	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	188	GLN
1	B	227	ASN
2	C	99	GLN
2	C	117	HIS
2	C	343	GLN
2	C	538	GLN
2	C	834	GLN
3	D	442	ASN
3	D	611	GLN
3	D	724	GLN
3	D	762	GLN
3	D	1014	ASN
3	D	1116	ASN
3	D	1172	HIS

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Mol	Chain	Res	Type
3	D	1442	ASN
5	F	86	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 non-standard protein/DNA/RNA residues are 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	$\# Z > 2$
8	2RA	I	1	8,12	4,5,6	0.56	0	1,5,7	0.28	0
8	2TL	I	5	8	5,6,7	1.06	0	5,7,9	0.93	0
8	0QZ	I	6	8	4,5,6	1.62	1 (25%)	2,5,7	0.55	0
8	FGL	I	7	8	5,6,7	1.47	1 (20%)	1,7,9	1.72	0
8	R2T	I	4	8	8,10,11	1.95	2 (25%)	6,13,15	1.06	0

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
8	2RA	I	1	8,12	-	0/2/4/6	-
8	2TL	I	5	8	-	1/5/6/8	-
8	0QZ	I	6	8	-	2/3/4/6	-
8	FGL	I	7	8	-	0/4/6/8	-
8	R2T	I	4	8	-	2/13/14/16	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	4	R2T	CD-NE2	4.49	1.43	1.32
8	I	6	0QZ	OB-CA	-3.13	1.38	1.43
8	I	4	R2T	OB1-CB	-2.12	1.37	1.43
8	I	7	FGL	OG2-CB	2.08	1.28	1.22

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	4	R2T	OE1-CD-CG-OG1
8	I	4	R2T	NE2-CD-CG-OG1
8	I	5	2TL	O-C-CA-CB
8	I	6	0QZ	N-C1-CA-C
8	I	6	0QZ	N-C1-CA-OB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 8 are 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	$\# Z > 2$
11	ATP	D	2007	9	32,33,33	1.43	5 (15%)	48,52,52	1.80	9 (18%)
12	MB8	I	101	8	0,1,6	-	-	-		

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	ATP	D	2007	9	-	8/22/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	2007	ATP	C5-C4	4.75	1.47	1.39
11	D	2007	ATP	C5-C6	2.78	1.48	1.41
11	D	2007	ATP	C8-N7	2.35	1.36	1.31
11	D	2007	ATP	C5-N7	-2.21	1.35	1.39
11	D	2007	ATP	PB-O3A	2.02	1.61	1.59

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	2007	ATP	C5-C4-N3	-6.02	118.42	126.72
11	D	2007	ATP	N3-C4-N9	4.75	135.24	127.17
11	D	2007	ATP	C2-N3-C4	3.81	121.13	111.83
11	D	2007	ATP	C4-C5-N7	-3.49	106.59	110.58
11	D	2007	ATP	N3-C2-N1	-3.27	123.63	128.58
11	D	2007	ATP	C5-N7-C8	2.57	107.49	103.45
11	D	2007	ATP	C4-N9-C8	2.50	108.36	105.74
11	D	2007	ATP	C3'-C2'-C1'	2.38	105.97	101.46
11	D	2007	ATP	C6-C5-N7	2.08	136.09	132.09

There are no chirality outliers.

All (8) torsion outliers are listed below:

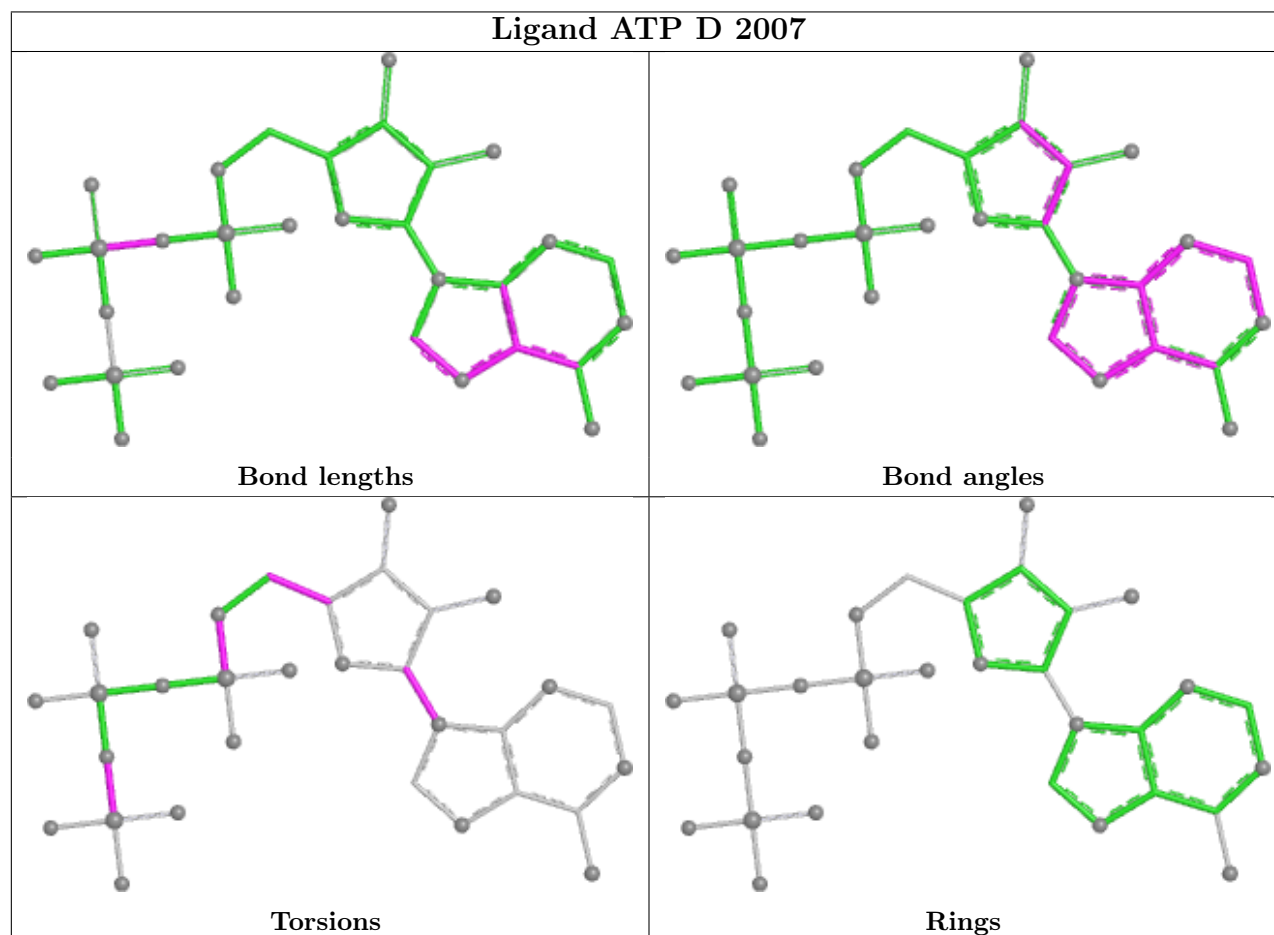
Mol	Chain	Res	Type	Atoms
11	D	2007	ATP	C5'-O5'-PA-O1A
11	D	2007	ATP	C5'-O5'-PA-O2A
11	D	2007	ATP	C5'-O5'-PA-O3A
11	D	2007	ATP	C3'-C4'-C5'-O5'
11	D	2007	ATP	O4'-C1'-N9-C8
11	D	2007	ATP	O4'-C1'-N9-C4
11	D	2007	ATP	O4'-C4'-C5'-O5'
11	D	2007	ATP	PB-O3B-PG-O1G

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	2007	ATP	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	231/315 (73%)	-0.65	0 100 100	38, 57, 83, 133	0
1	B	227/315 (72%)	-0.51	0 100 100	39, 69, 97, 117	0
2	C	1112/1119 (99%)	-0.54	2 (0%) 91 87	19, 52, 116, 143	0
3	D	1486/1524 (97%)	-0.52	1 (0%) 92 91	21, 56, 116, 157	1 (0%)
4	E	94/99 (94%)	-0.61	0 100 100	32, 60, 98, 101	0
5	F	346/443 (78%)	-0.44	2 (0%) 85 75	31, 73, 124, 144	0
6	G	16/21 (76%)	-0.10	0 100 100	65, 94, 203, 205	0
7	H	24/27 (88%)	-0.20	0 100 100	65, 123, 198, 228	0
8	I	0/7	-	-	-	-
All	All	3536/3870 (91%)	-0.53	5 (0%) 92 91	19, 59, 117, 228	1 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	369	LEU	2.5
2	C	43	GLY	2.2
3	D	304	LEU	2.1
5	F	390	PHE	2.1
2	C	998	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
8	FGL	I	7	7/8	0.87	0.08	33,36,38,39	0
8	DVA	I	3	7/8	0.92	0.11	33,36,41,47	0
8	R2T	I	4	11/12	0.92	0.07	34,36,45,46	0
8	2RA	I	1	6/7	0.94	0.05	33,35,41,50	0
8	2TL	I	5	7/8	0.95	0.07	37,41,43,44	0
8	DSN	I	2	6/7	0.96	0.07	34,37,50,56	0
8	0QZ	I	6	6/7	0.96	0.06	33,33,37,38	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

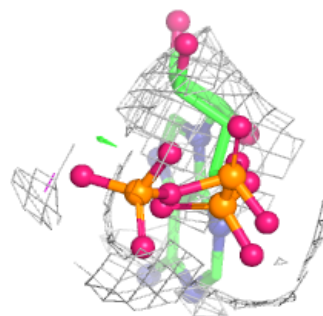
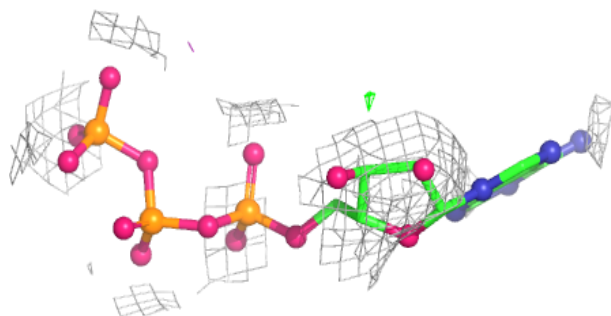
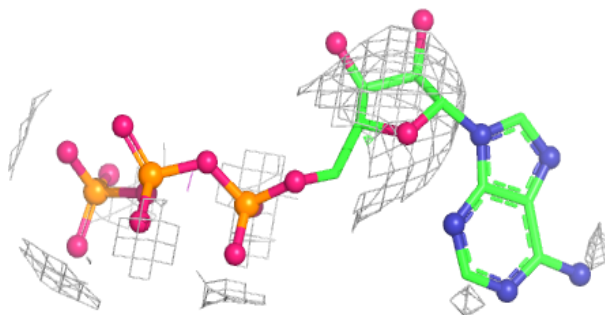
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
9	MG	F	2001	1/1	0.71	0.07	68,68,68,68	0
9	MG	D	2006	1/1	0.80	0.05	50,50,50,50	0
9	MG	B	2001	1/1	0.81	0.07	93,93,93,93	0
9	MG	D	2005	1/1	0.82	0.22	33,33,33,33	0
9	MG	D	2004	1/1	0.91	0.05	69,69,69,69	0
11	ATP	D	2007	31/31	0.91	0.07	53,108,121,122	10
12	MB8	I	101	2/7	0.97	0.05	34,34,34,34	0
10	ZN	D	2002	1/1	0.99	0.02	79,79,79,79	0
10	ZN	D	2001	1/1	1.00	0.01	38,38,38,38	0
9	MG	D	2003	1/1	1.00	0.02	26,26,26,26	0

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

Electron density around ATP D 2007:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.