



Full wwPDB EM Validation Report ⓘ

Feb 19, 2025 – 06:12 am GMT

PDB ID : 8RAP
EMDB ID : EMD-19022
Title : Structure of Sen1-ADP.BeF3 bound RNA Polymerase II pre-termination complex
Authors : Rengachari, S.; Lidscreiber, M.; Cramer, P.
Deposited on : 2023-12-01
Resolution : 4.30 Å (reported)
Based on initial models : 2XZO, 7NKX, ., 6I59

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

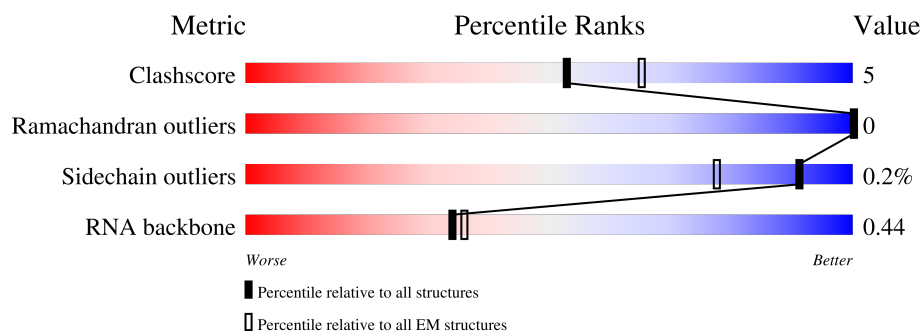
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.















Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	A	1733	68% (green), 13% (yellow), 19% (grey)
2	B	1224	78% (green), 13% (yellow), 9% (grey)
3	C	318	73% (green), 10% (yellow), 17% (grey)
4	D	221	63% (green), 9% (yellow), 28% (grey)
5	E	215	85% (green), 15% (yellow)
6	F	155	49% (green), 6% (yellow), 45% (grey)
7	G	171	88% (green), 12% (yellow)

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Mol	Chain	Length	Quality of chain
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	M	145	
14	N	58	
15	O	2231	
16	P	35	
17	T	58	
18	Y	102	
19	Z	1063	

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
23	BEF	O	3003	-	-	X	-

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 42924 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1400	Total	C	N	O	S	0	0
			11020	6948	1929	2081	62		

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1113	Total	C	N	O	S	0	0
			8839	5596	1553	1635	55		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	264	Total	C	N	O	S	0	0
			2078	1308	346	411	13		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	159	Total	C	N	O	S	0	0
			1270	788	223	257	2		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1752	1111	309	321	11		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	85	Total	C	N	O	S	0	0
			688	439	116	130	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	133	Total	C	N	O	S	0	0
			1068	673	180	211	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	118	Total	C	N	O	S	0	0
			964	592	178	184	10		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	65	Total	C	N	O	S	0	0
			532	339	93	94	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	1
			920	590	157	171	2		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	43	Total	C	N	O	S	0	0
			343	211	69	59	4		

- Molecule 13 is a protein called Transcription elongation factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	65	Total	C	N	O	S	0	0
			504	311	87	101	5		

- Molecule 14 is a DNA chain called Non-template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	27	Total	C	N	O	P	0	0
			547	262	98	160	27		

- Molecule 15 is a protein called Helicase SEN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	694	Total	C	N	O	S	0	0
			5557	3509	973	1044	31		

- Molecule 16 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	25	Total	C	N	O	P	0	0
			540	240	101	174	25		

- Molecule 17 is a DNA chain called Template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	38	Total	C	N	O	P	0	0
			786	374	142	232	38		

- Molecule 18 is a protein called Transcription elongation factor SPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	100	Total	C	N	O	S	0	0
			760	474	129	147	10		

- Molecule 19 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	426	Total	C	N	O	S	0	0
			3374	2136	599	630	9		

- Molecule 20 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
20	A	2	Total	Zn	0
			2	2	
20	B	1	Total	Zn	0
			1	1	

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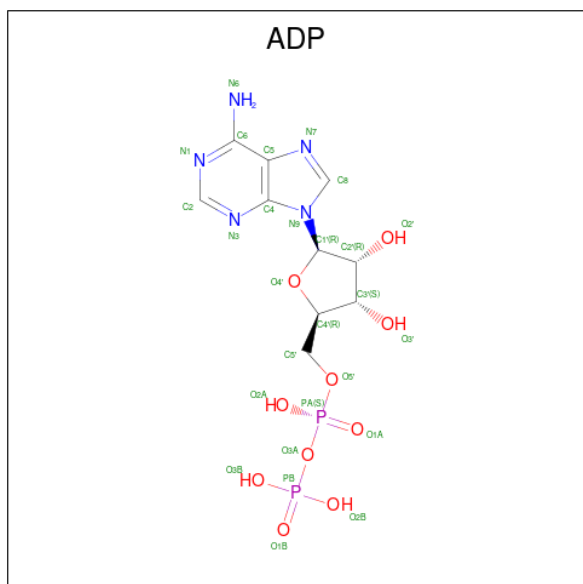
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Mol	Chain	Residues	Atoms		AltConf
20	C	1	Total	Zn	0
			1	1	
20	I	2	Total	Zn	0
			2	2	
20	J	1	Total	Zn	0
			1	1	
20	L	1	Total	Zn	0
			1	1	
20	M	1	Total	Zn	0
			1	1	

- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

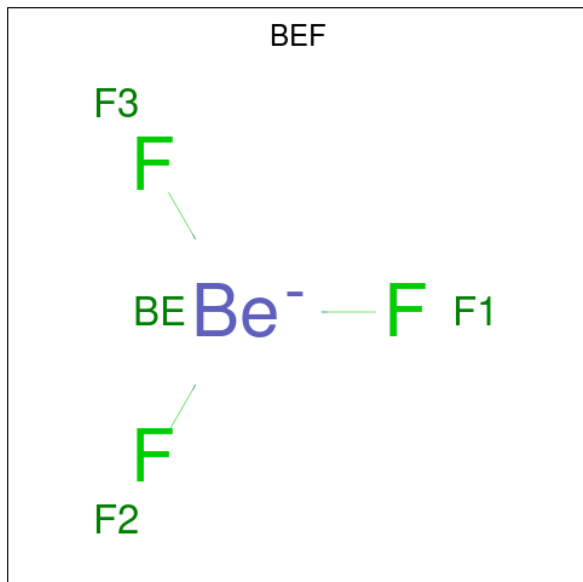
Mol	Chain	Residues	Atoms		AltConf
21	A	1	Total	Mg	0
			1	1	
21	O	1	Total	Mg	0
			1	1	

- Molecule 22 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
22	O	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 23 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).

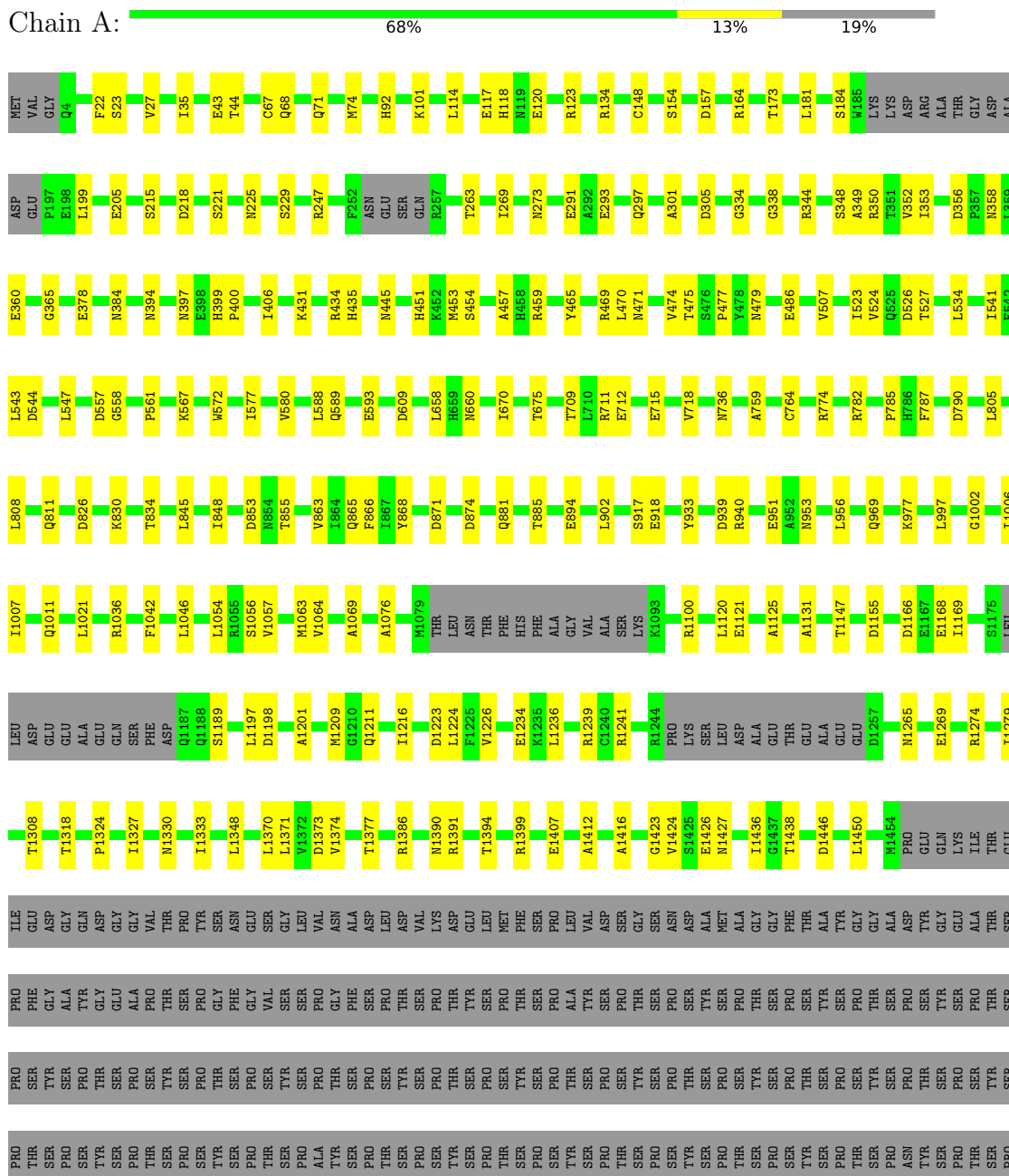


Mol	Chain	Residues	Atoms			AltConf
			Total	Be	F	
23	O	1	4	1	3	0


3 Residue-property plots

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. 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. 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 II subunit RPB1



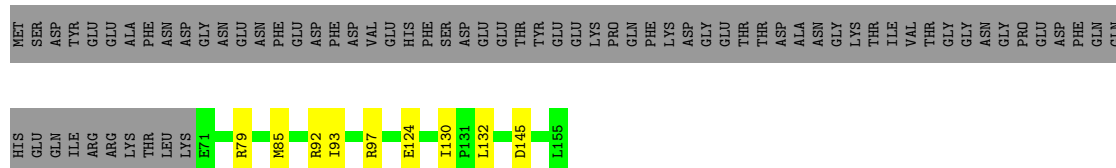
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:  85% 15%



- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:  49% 6% 45%




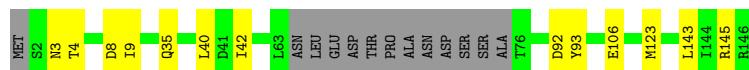
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G:  88% 12%




- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:  82% 9% 9%




- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:  87% 10% 3%




- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:  83% 10% 7%



- Molecule 11: DNA-directed RNA polymerase II subunit RPB11

Chain K:  78% 18% 4%



GLY	HIS	TRP	GLN	GLY	ASN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9095	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.02	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ZN, BEF, 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	0.23	0/11217	0.39	0/15166
2	B	0.24	0/9011	0.40	0/12149
3	C	0.23	0/2116	0.39	0/2868
4	D	0.24	0/1279	0.38	0/1716
5	E	0.24	0/1788	0.37	0/2406
6	F	0.23	0/700	0.38	0/945
7	G	0.25	0/1368	0.42	0/1844
8	H	0.24	0/1086	0.43	0/1470
9	I	0.24	0/982	0.42	0/1321
10	J	0.24	0/541	0.37	0/727
11	K	0.24	0/938	0.38	0/1267
12	L	0.22	0/345	0.42	0/457
13	M	0.23	0/512	0.39	0/689
14	N	0.51	0/611	0.89	0/936
15	O	0.24	0/5659	0.37	0/7624
16	P	0.11	0/603	0.65	0/937
17	T	0.52	0/881	0.94	0/1360
18	Y	0.24	0/776	0.39	0/1050
19	Z	0.23	0/3419	0.40	0/4599
All	All	0.25	0/43832	0.43	0/59531

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	11020	0	11104	152	0
2	B	8839	0	8896	118	0
3	C	2078	0	2041	26	0
4	D	1270	0	1287	13	0
5	E	1752	0	1776	22	0
6	F	688	0	707	5	0
7	G	1340	0	1357	13	0
8	H	1068	0	1040	10	0
9	I	964	0	922	9	0
10	J	532	0	542	6	0
11	K	920	0	929	18	0
12	L	343	0	363	3	0
13	M	504	0	480	4	0
14	N	547	0	306	3	0
15	O	5557	0	5587	44	0
16	P	540	0	272	3	0
17	T	786	0	431	8	0
18	Y	760	0	741	3	0
19	Z	3374	0	3478	36	0
20	A	2	0	0	0	0
20	B	1	0	0	0	0
20	C	1	0	0	0	0
20	I	2	0	0	0	0
20	J	1	0	0	0	0
20	L	1	0	0	0	0
20	M	1	0	0	0	0
21	A	1	0	0	0	0
21	O	1	0	0	0	0
22	O	27	0	12	0	0
23	O	4	0	0	3	0
All	All	42924	0	42271	430	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 5.

All (430) 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:B:1177:HIS:CD2	19:Z:645:LEU:HD22	1.57	1.38
2:B:1177:HIS:CD2	19:Z:645:LEU:CD2	2.21	1.22
2:B:1177:HIS:NE2	19:Z:645:LEU:HD22	1.58	1.18
2:B:1177:HIS:HD2	19:Z:645:LEU:CD2	1.78	0.96
1:A:956:LEU:HD13	1:A:1021:LEU:HD22	1.53	0.89
1:A:853:ASP:OD1	1:A:855:THR:OG1	1.94	0.85
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.58	0.85
2:B:1177:HIS:CD2	19:Z:645:LEU:HD23	2.11	0.83
19:Z:849:ASN:ND2	19:Z:869:PRO:O	2.15	0.80
2:B:1177:HIS:NE2	19:Z:645:LEU:CD2	2.33	0.80
10:J:21:TYR:OH	10:J:32:GLU:OE1	2.00	0.80
1:A:344:ARG:NH1	17:T:27:DT:OP1	2.15	0.79
4:D:22:GLU:OE1	4:D:28:GLN:NE2	2.15	0.79
1:A:811:GLN:NE2	2:B:705:MET:SD	2.56	0.78
1:A:885:THR:O	1:A:940:ARG:NH1	2.17	0.78
1:A:350:ARG:NH1	1:A:486:GLU:OE1	2.17	0.78
15:O:1654:GLN:NE2	15:O:1676:ASP:OD1	2.16	0.78
2:B:287:ARG:NH1	2:B:292:ILE:O	2.16	0.78
15:O:1191:VAL:O	15:O:1266:ARG:NH2	2.17	0.78
1:A:134:ARG:NH1	1:A:221:SER:O	2.17	0.77
15:O:1125:TYR:O	15:O:1173:ARG:NH1	2.18	0.77
2:B:906:SER:OG	19:Z:830:GLU:OE1	2.03	0.77
2:B:822:ASN:O	10:J:48:ARG:NH1	2.18	0.76
11:K:11:LEU:O	11:K:37:LYS:NZ	2.18	0.76
7:G:97:HIS:NE2	19:Z:622:GLU:OE2	2.19	0.75
6:F:97:ARG:NE	6:F:124:GLU:OE1	2.21	0.74
13:M:37:THR:OG1	13:M:46:THR:OG1	2.05	0.74
2:B:315:LYS:NZ	2:B:319:GLU:OE2	2.19	0.74
7:G:25:TYR:O	7:G:28:THR:OG1	2.05	0.74
1:A:215:SER:OG	1:A:218:ASP:OD1	2.05	0.74
1:A:567:LYS:NZ	8:H:93:TYR:O	2.21	0.73
2:B:101:MET:O	2:B:169:ARG:NH2	2.20	0.73
2:B:39:ARG:NH2	2:B:665:GLU:OE1	2.21	0.73
7:G:129:SER:OG	7:G:137:ILE:O	2.07	0.73
2:B:26:THR:OG1	2:B:29:ASP:OD1	2.06	0.72
19:Z:626:THR:OG1	19:Z:629:ASN:OD1	2.07	0.72
1:A:782:ARG:NH2	1:A:785:PRO:O	2.22	0.72
1:A:1446:ASP:OD1	7:G:58:ARG:NH1	2.23	0.72
2:B:604:ARG:NH2	2:B:691:GLU:OE2	2.23	0.71
1:A:1100:ARG:NH2	1:A:1330:ASN:OD1	2.24	0.71
1:A:148:CYS:SG	1:A:164:ARG:NH2	2.64	0.70
1:A:360:GLU:OE1	1:A:459:ARG:NH2	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1394:THR:O	1:A:1399:ARG:NH1	2.25	0.70
8:H:8:ASP:OD1	8:H:9:ILE:N	2.24	0.70
2:B:857:ARG:NH1	2:B:858:SER:O	2.25	0.70
2:B:98:THR:O	2:B:126:SER:OG	2.05	0.69
18:Y:75:LYS:NZ	18:Y:77:ASP:OD1	2.25	0.69
9:I:19:ASP:O	9:I:23:ASN:N	2.24	0.69
1:A:291:GLU:N	1:A:291:GLU:OE1	2.25	0.69
1:A:711:ARG:NH1	9:I:95:THR:O	2.26	0.69
1:A:291:GLU:OE2	19:Z:61:ARG:NH2	2.26	0.69
2:B:53:GLN:NE2	2:B:547:VAL:O	2.26	0.69
2:B:341:LEU:HD22	19:Z:73:GLU:OE1	1.93	0.69
1:A:1386:ARG:O	1:A:1391:ARG:NH1	2.26	0.68
1:A:378:GLU:OE2	1:A:384:ASN:ND2	2.27	0.68
2:B:1065:GLN:OE1	2:B:1067:ARG:N	2.27	0.68
4:D:139:LYS:O	4:D:143:ASN:ND2	2.27	0.68
4:D:153:ARG:NH2	4:D:182:SER:O	2.26	0.68
1:A:378:GLU:OE1	1:A:434:ARG:NE	2.27	0.67
17:T:41:DT:OP2	19:Z:216:ARG:NH1	2.28	0.67
2:B:1177:HIS:NE2	19:Z:645:LEU:HB2	2.09	0.67
1:A:881:GLN:HB2	1:A:956:LEU:HD12	1.77	0.67
2:B:649:LYS:NZ	2:B:737:THR:O	2.27	0.67
5:E:24:LYS:NZ	5:E:32:GLN:OE1	2.27	0.67
1:A:951:GLU:OE1	1:A:953:ASN:N	2.28	0.66
1:A:358:ASN:OD1	2:B:833:TYR:OH	2.13	0.66
1:A:114:LEU:O	1:A:164:ARG:NH1	2.29	0.66
1:A:865:GLN:NE2	1:A:1373:ASP:OD2	2.29	0.66
2:B:971:THR:OG1	3:C:61:GLU:OE1	2.03	0.66
3:C:226:ASP:OD1	3:C:227:THR:N	2.28	0.66
7:G:85:GLU:N	7:G:85:GLU:OE1	2.28	0.65
15:O:1668:GLU:O	15:O:1671:GLN:NE2	2.30	0.65
2:B:328:GLU:N	2:B:328:GLU:OE1	2.30	0.65
8:H:3:ASN:OD1	8:H:4:THR:N	2.30	0.65
2:B:496:ARG:NH2	2:B:540:SER:O	2.29	0.64
15:O:1246:LYS:NZ	15:O:1292:GLU:OE2	2.20	0.64
2:B:711:GLU:N	2:B:711:GLU:OE1	2.29	0.64
1:A:997:LEU:O	1:A:1011:GLN:NE2	2.30	0.64
1:A:1155:ASP:OD2	1:A:1239:ARG:NH2	2.31	0.64
15:O:1293:ARG:NH1	15:O:1570:SER:O	2.30	0.63
19:Z:28:ILE:CD1	19:Z:52:ILE:HG22	2.29	0.63
2:B:862:GLN:OE1	2:B:957:ASN:ND2	2.31	0.63
2:B:28:GLU:OE2	2:B:807:ARG:NH1	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1390:ASN:OD1	1:A:1391:ARG:NH2	2.32	0.63
2:B:287:ARG:NE	2:B:324:ILE:O	2.31	0.63
3:C:4:GLU:OE2	11:K:104:ASN:ND2	2.31	0.62
2:B:995:ARG:NH2	11:K:39:ASP:OD2	2.32	0.62
2:B:125:SER:O	2:B:169:ARG:NH2	2.33	0.62
2:B:776:GLN:OE1	16:P:33:A:O2'	2.15	0.62
2:B:1177:HIS:HD2	19:Z:645:LEU:HD23	1.51	0.62
9:I:90:GLN:OE1	9:I:92:ARG:NH1	2.33	0.61
2:B:908:GLU:N	2:B:908:GLU:OE1	2.33	0.61
2:B:639:ILE:HD12	2:B:688:GLY:O	2.00	0.61
1:A:154:SER:OG	1:A:157:ASP:O	2.18	0.61
19:Z:854:GLU:N	19:Z:854:GLU:OE1	2.33	0.61
2:B:310:MET:HG3	2:B:386:LEU:HD13	1.83	0.61
2:B:1084:GLN:OE1	2:B:1084:GLN:N	2.34	0.61
1:A:1318:THR:HG23	5:E:141:VAL:HG11	1.83	0.61
2:B:816:GLU:N	2:B:816:GLU:OE1	2.34	0.60
4:D:41:GLN:OE1	4:D:41:GLN:N	2.34	0.60
15:O:1127:ARG:NE	15:O:1129:SER:OG	2.34	0.60
1:A:1168:GLU:N	1:A:1168:GLU:OE1	2.35	0.60
2:B:499:ASN:OD1	2:B:500:THR:N	2.35	0.59
19:Z:860:GLU:N	19:Z:860:GLU:OE1	2.34	0.59
1:A:1426:GLU:OE1	1:A:1426:GLU:N	2.36	0.59
2:B:904:ARG:NH1	2:B:905:VAL:O	2.35	0.59
15:O:1699:PHE:O	15:O:1854:ALA:N	2.35	0.59
1:A:22:PHE:CE2	1:A:27:VAL:HG22	2.38	0.59
2:B:733:HIS:O	2:B:733:HIS:ND1	2.35	0.59
1:A:1166:ASP:O	1:A:1169:ILE:HG22	2.02	0.59
4:D:150:ASN:OD1	4:D:151:PHE:N	2.36	0.59
2:B:399:ASP:OD2	2:B:510:LYS:NZ	2.35	0.58
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.85	0.58
2:B:805:THR:OG1	2:B:1041:GLU:OE2	2.12	0.58
2:B:262:GLU:OE1	2:B:267:ARG:NH2	2.36	0.58
1:A:1423:GLY:O	1:A:1427:ASN:ND2	2.34	0.58
3:C:90:ASP:OD1	19:Z:848:TYR:OH	2.22	0.58
1:A:173:THR:OG1	1:A:184:SER:OG	2.22	0.58
2:B:314:LEU:HD21	2:B:386:LEU:HD11	1.84	0.58
1:A:269:ILE:O	1:A:273:ASN:ND2	2.36	0.58
19:Z:870:GLN:OE1	19:Z:870:GLN:N	2.36	0.58
5:E:36:GLU:OE1	5:E:36:GLU:N	2.37	0.58
1:A:547:LEU:HD22	11:K:58:PHE:CD1	2.40	0.57
1:A:871:ASP:OD1	5:E:204:THR:OG1	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:567:GLU:N	2:B:567:GLU:OE1	2.38	0.57
1:A:43:GLU:OE1	1:A:43:GLU:N	2.36	0.57
1:A:68:GLN:N	1:A:68:GLN:OE1	2.38	0.57
2:B:851:PHE:O	2:B:1094:ARG:NH1	2.37	0.57
2:B:570:VAL:O	2:B:570:VAL:HG13	2.04	0.57
15:O:1770:MET:N	15:O:1770:MET:SD	2.78	0.57
1:A:293:GLU:OE2	1:A:297:GLN:NE2	2.39	0.56
1:A:808:LEU:O	2:B:728:ARG:NH2	2.39	0.56
2:B:1129:ARG:NE	17:T:26:DG:OP1	2.35	0.56
5:E:33:GLU:N	5:E:33:GLU:OE1	2.38	0.56
11:K:36:GLU:OE1	11:K:70:ARG:NE	2.38	0.56
2:B:984:HIS:NE2	2:B:1028:GLU:OE1	2.38	0.56
1:A:205:GLU:N	1:A:205:GLU:OE1	2.38	0.56
7:G:117:GLN:N	7:G:117:GLN:OE1	2.39	0.56
4:D:199:ASN:OD1	4:D:200:ASN:N	2.35	0.56
1:A:588:LEU:HD23	1:A:589:GLN:N	2.21	0.56
1:A:917:SER:OG	1:A:918:GLU:OE1	2.21	0.56
13:M:39:ASP:O	13:M:43:SER:N	2.39	0.56
5:E:85:GLU:N	5:E:85:GLU:OE1	2.38	0.56
1:A:365:GLY:N	1:A:469:ARG:O	2.34	0.56
1:A:660:ASN:O	2:B:1082:MET:N	2.39	0.56
15:O:1591:GLU:OE2	23:O:3003:BEF:F1	2.14	0.56
1:A:1169:ILE:HG21	1:A:1239:ARG:HD3	1.87	0.56
11:K:64:GLU:OE1	11:K:64:GLU:N	2.39	0.55
1:A:43:GLU:O	1:A:44:THR:OG1	2.14	0.55
1:A:1407:GLU:N	1:A:1407:GLU:OE1	2.36	0.55
15:O:1837:SER:HG	15:O:1840:TRP:HD1	1.51	0.55
2:B:357:GLN:NE2	2:B:368:GLU:OE1	2.39	0.55
1:A:451:HIS:NE2	1:A:477:PRO:O	2.36	0.55
1:A:1120:LEU:HD21	1:A:1131:ALA:HA	1.87	0.55
2:B:468:GLU:N	2:B:468:GLU:OE1	2.38	0.55
11:K:79:GLU:OE1	11:K:79:GLU:N	2.38	0.55
2:B:1177:HIS:NE2	19:Z:645:LEU:CB	2.69	0.55
15:O:1253:THR:HG22	15:O:1254:LYS:H	1.71	0.55
1:A:67:CYS:O	1:A:71:GLN:N	2.39	0.55
2:B:868:MET:O	2:B:869:SER:OG	2.17	0.55
4:D:157:GLN:N	4:D:157:GLN:OE1	2.40	0.54
1:A:344:ARG:NE	2:B:1120:GLU:OE1	2.40	0.54
2:B:25:ILE:HD11	2:B:658:ILE:HG13	1.88	0.54
2:B:872:GLU:N	2:B:872:GLU:OE1	2.38	0.54
2:B:996:ARG:CZ	3:C:38:ILE:HD11	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:LEU:HD21	1:A:1374:VAL:HG11	1.89	0.54
2:B:610:ASN:O	2:B:613:VAL:HG12	2.08	0.54
3:C:215:GLU:OE1	3:C:215:GLU:N	2.40	0.54
1:A:1265:ASN:ND2	1:A:1269:GLU:OE2	2.40	0.54
7:G:22:MET:SD	7:G:23:LYS:N	2.81	0.54
1:A:1064:VAL:HG12	1:A:1370:LEU:HD22	1.89	0.53
2:B:828:ALA:HB2	2:B:1085:ILE:HG23	1.90	0.53
5:E:185:ALA:O	5:E:189:GLY:N	2.40	0.53
18:Y:99:VAL:HG12	18:Y:99:VAL:O	2.09	0.53
11:K:38:GLU:OE1	11:K:42:LEU:HD12	2.08	0.53
15:O:1431:GLN:OE1	15:O:1431:GLN:N	2.39	0.53
1:A:577:ILE:O	1:A:580:VAL:HG22	2.08	0.53
18:Y:83:GLU:OE1	18:Y:83:GLU:N	2.39	0.53
19:Z:24:GLU:OE1	19:Z:24:GLU:N	2.40	0.53
15:O:1776:ASP:OD1	15:O:1777:PHE:N	2.41	0.53
1:A:22:PHE:CD2	1:A:27:VAL:HG22	2.44	0.53
5:E:40:GLU:OE1	5:E:43:LYS:NZ	2.35	0.53
15:O:1191:VAL:HG23	15:O:1194:PHE:HB2	1.90	0.53
1:A:593:GLU:OE1	1:A:593:GLU:N	2.41	0.53
8:H:106:GLU:OE1	8:H:106:GLU:N	2.41	0.53
1:A:348:SER:HB2	2:B:1128:LEU:HD22	1.91	0.52
1:A:675:THR:OG1	1:A:736:ASN:OD1	2.25	0.52
2:B:760:ASP:OD1	2:B:761:HIS:ND1	2.42	0.52
3:C:11:ARG:NH1	3:C:12:GLU:OE2	2.42	0.52
2:B:322:PHE:O	2:B:325:GLN:NE2	2.40	0.52
1:A:1189:SER:O	1:A:1241:ARG:NH1	2.41	0.52
3:C:259:LEU:HD21	11:K:91:CYS:HB2	1.91	0.52
5:E:90:VAL:HG23	14:N:51:DA:OP1	2.08	0.52
2:B:564:GLU:N	2:B:564:GLU:OE1	2.40	0.52
15:O:1707:GLN:N	15:O:1707:GLN:OE1	2.42	0.52
2:B:762:ASN:OD1	2:B:763:GLN:N	2.42	0.52
5:E:168:TYR:HB3	5:E:170:LEU:HD13	1.91	0.52
15:O:1820:ARG:NH2	23:O:3003:BEF:F3	2.32	0.52
1:A:863:VAL:O	1:A:863:VAL:HG23	2.10	0.52
3:C:58:LEU:HD11	10:J:2:ILE:HD11	1.92	0.52
2:B:259:TYR:OH	2:B:279:ASP:OD2	2.27	0.52
10:J:48:ARG:O	10:J:52:THR:OG1	2.15	0.52
1:A:1211:GLN:OE1	1:A:1274:ARG:NH1	2.41	0.51
7:G:11:ILE:HD11	7:G:29:LYS:HD3	1.92	0.51
2:B:1174:LYS:O	2:B:1178:ASN:N	2.43	0.51
5:E:138:ALA:O	5:E:141:VAL:HG12	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:790:ASP:OD2	9:I:87:GLN:N	2.43	0.51
1:A:1412:ALA:O	1:A:1416:ALA:N	2.44	0.51
3:C:111:THR:HG23	15:O:1266:ARG:HH22	1.76	0.51
3:C:75:MET:O	3:C:246:ARG:NH2	2.42	0.51
15:O:1619:GLN:NE2	23:O:3003:BEF:F3	2.34	0.51
3:C:47:ASP:OD1	12:L:70:ARG:NH1	2.44	0.51
1:A:394:ASN:ND2	1:A:400:PRO:O	2.41	0.50
2:B:640:VAL:HG22	2:B:651:LEU:CD2	2.42	0.50
5:E:48:ASP:OD1	5:E:51:GLY:N	2.44	0.50
3:C:17:ASN:OD1	3:C:231:ASN:ND2	2.42	0.50
19:Z:801:LEU:HD23	19:Z:802:GLY:N	2.26	0.50
1:A:874:ASP:N	1:A:1056:SER:O	2.38	0.50
1:A:101:LYS:NZ	14:N:43:DC:OP1	2.37	0.50
1:A:526:ASP:OD2	2:B:835:GLN:NE2	2.44	0.50
2:B:786:ASN:O	2:B:967:ARG:NH2	2.45	0.50
1:A:406:ILE:N	1:A:431:LYS:O	2.45	0.50
19:Z:24:GLU:OE2	19:Z:60:GLY:N	2.39	0.50
1:A:845:LEU:HD23	1:A:848:ILE:HD12	1.94	0.50
1:A:1324:PRO:O	1:A:1327:ILE:HG22	2.12	0.50
7:G:11:ILE:HD13	7:G:26:LEU:HG	1.94	0.50
14:N:45:DT:O2	17:T:16:DG:N2	2.45	0.50
2:B:120:ARG:NH2	2:B:956:THR:O	2.45	0.50
2:B:1035:ALA:O	2:B:1039:GLY:N	2.44	0.50
15:O:1183:ILE:HG22	15:O:1201:VAL:HG22	1.94	0.50
2:B:766:ARG:NH2	2:B:985:GLY:O	2.45	0.49
9:I:60:GLN:OE1	9:I:60:GLN:N	2.41	0.49
15:O:1332:SER:OG	15:O:1430:LYS:O	2.16	0.49
1:A:1223:ASP:C	1:A:1224:LEU:HD12	2.33	0.49
2:B:488:TYR:CE2	2:B:492:LEU:HD11	2.47	0.49
8:H:40:LEU:HD13	8:H:123:MET:HB2	1.93	0.49
1:A:544:ASP:O	11:K:47:ARG:NH2	2.45	0.49
2:B:1104:HIS:NE2	2:B:1126:GLY:O	2.44	0.49
15:O:1441:ARG:NH1	15:O:1442:VAL:O	2.45	0.49
8:H:92:ASP:O	8:H:145:ARG:NH2	2.45	0.49
19:Z:732:PHE:CD1	19:Z:746:VAL:HG22	2.48	0.49
4:D:34:GLN:N	4:D:34:GLN:OE1	2.46	0.49
1:A:1063:MET:SD	1:A:1436:ILE:HG23	2.53	0.49
15:O:1127:ARG:NH2	15:O:1134:ASP:OD1	2.40	0.49
1:A:120:GLU:OE1	1:A:123:ARG:NH2	2.43	0.49
1:A:977:LYS:O	1:A:1036:ARG:NH2	2.45	0.49
3:C:258:ILE:HD11	11:K:42:LEU:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:68:LEU:O	9:I:70:ARG:NH1	2.45	0.49
1:A:23:SER:O	1:A:27:VAL:HG23	2.12	0.49
1:A:1042:PHE:CE1	1:A:1046:LEU:HD11	2.48	0.49
1:A:782:ARG:NE	1:A:787:PHE:O	2.42	0.48
17:T:35:DA:H2'	17:T:35:DA:N3	2.28	0.48
2:B:481:GLN:NE2	16:P:32:C:OP1	2.47	0.48
1:A:349:ALA:O	2:B:1128:LEU:HD21	2.13	0.48
2:B:364:ILE:CD1	2:B:365:THR:HG22	2.44	0.48
1:A:74:MET:O	2:B:1116:ARG:NH1	2.47	0.48
1:A:334:GLY:O	1:A:338:GLY:N	2.46	0.48
15:O:1702:ILE:O	15:O:1830:HIS:ND1	2.45	0.48
1:A:1216:ILE:HG21	1:A:1226:VAL:HG21	1.96	0.48
2:B:618:ASP:O	2:B:622:LYS:N	2.47	0.48
2:B:1176:ASN:OD1	2:B:1177:HIS:CD2	2.67	0.48
6:F:85:MET:CE	6:F:93:ILE:HD12	2.44	0.48
2:B:824:ILE:N	2:B:824:ILE:HD12	2.28	0.48
1:A:1279:ILE:HG23	1:A:1308:THR:CG2	2.43	0.48
2:B:566:LEU:HD22	2:B:586:TRP:O	2.14	0.48
19:Z:28:ILE:HD13	19:Z:52:ILE:HG22	1.95	0.47
2:B:234:ILE:HD13	2:B:257:LYS:HD3	1.97	0.47
15:O:1339:GLN:NE2	15:O:1361:THR:O	2.46	0.47
1:A:670:ILE:HG12	1:A:805:LEU:HD21	1.95	0.47
1:A:1209:MET:HE3	1:A:1236:LEU:HD13	1.97	0.47
11:K:37:LYS:N	11:K:69:ALA:O	2.46	0.47
15:O:1408:ILE:HD12	15:O:1408:ILE:N	2.30	0.47
1:A:894:GLU:OE2	1:A:933:TYR:OH	2.30	0.47
3:C:38:ILE:HB	3:C:176:ILE:HD12	1.97	0.47
1:A:475:THR:O	1:A:479:ASN:N	2.47	0.47
1:A:1198:ASP:OD2	1:A:1201:ALA:N	2.45	0.47
2:B:301:ILE:HD13	2:B:379:GLY:HA2	1.97	0.47
15:O:1731:TYR:OH	15:O:1735:LYS:NZ	2.32	0.47
3:C:248:ILE:HG21	11:K:102:LYS:HB2	1.96	0.47
1:A:1438:THR:HG23	6:F:92:ARG:HB2	1.97	0.47
3:C:33:LEU:HD13	3:C:248:ILE:HD13	1.96	0.47
1:A:247:ARG:NH2	1:A:263:THR:OG1	2.43	0.46
1:A:557:ASP:OD1	1:A:558:GLY:N	2.46	0.46
2:B:640:VAL:HG12	2:B:649:LYS:HG3	1.96	0.46
15:O:1362:GLY:O	15:O:1366:THR:N	2.43	0.46
19:Z:699:ASP:OD1	19:Z:703:ASN:N	2.49	0.46
1:A:1234:GLU:OE1	1:A:1234:GLU:N	2.40	0.46
2:B:364:ILE:HD12	2:B:365:THR:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:806:THR:HG23	2:B:1045:SER:HA	1.96	0.46
8:H:40:LEU:HD21	8:H:42:ILE:HD11	1.97	0.46
4:D:133:THR:O	4:D:134:THR:OG1	2.30	0.46
15:O:1641:ARG:O	15:O:1645:ASN:ND2	2.43	0.46
15:O:1749:ILE:HD11	15:O:1793:ILE:HG12	1.96	0.46
6:F:79:ARG:NH1	6:F:145:ASP:O	2.49	0.46
19:Z:711:ILE:HD12	19:Z:711:ILE:C	2.36	0.46
1:A:356:ASP:OD1	11:K:65:HIS:NE2	2.47	0.46
1:A:68:GLN:O	1:A:71:GLN:NE2	2.49	0.46
1:A:1054:LEU:O	1:A:1057:VAL:HG12	2.16	0.46
19:Z:860:GLU:O	19:Z:864:ARG:N	2.45	0.46
3:C:101:LEU:HD23	3:C:102:GLN:N	2.31	0.45
1:A:830:LYS:O	1:A:834:THR:HG23	2.17	0.45
5:E:163:GLU:OE2	5:E:167:ARG:NE	2.46	0.45
9:I:21:GLU:OE1	9:I:21:GLU:N	2.45	0.45
1:A:457:ALA:O	1:A:507:VAL:HG23	2.17	0.45
1:A:1424:VAL:CG2	1:A:1436:ILE:HD11	2.38	0.45
15:O:1309:GLN:O	15:O:1313:ALA:N	2.50	0.45
1:A:1436:ILE:HD13	2:B:1139:ILE:HG23	1.99	0.45
1:A:453:MET:SD	1:A:453:MET:N	2.90	0.45
1:A:709:THR:HG23	1:A:712:GLU:H	1.82	0.45
2:B:773:MET:SD	2:B:987:LYS:NZ	2.81	0.45
3:C:234:SER:OG	3:C:238:ILE:O	2.12	0.45
7:G:39:THR:O	7:G:43:GLY:N	2.50	0.45
1:A:1450:LEU:HD23	1:A:1450:LEU:O	2.17	0.45
2:B:120:ARG:HE	2:B:122:LEU:HD11	1.81	0.45
2:B:326:ASP:OD1	2:B:327:ARG:N	2.50	0.45
2:B:337:ARG:NH1	13:M:65:GLN:OE1	2.50	0.45
1:A:1147:THR:HG22	1:A:1197:LEU:CD2	2.47	0.45
1:A:1318:THR:CG2	5:E:141:VAL:HG11	2.47	0.44
2:B:22:SER:O	2:B:654:ARG:NH1	2.50	0.44
3:C:111:THR:HG23	15:O:1266:ARG:NH2	2.32	0.44
15:O:1354:LEU:HD21	15:O:1642:MET:HB2	1.99	0.44
1:A:445:ASN:ND2	1:A:454:SER:O	2.51	0.44
4:D:45:GLU:OE1	4:D:45:GLU:N	2.49	0.44
5:E:136:ASN:OD1	5:E:137:GLU:N	2.50	0.44
15:O:1167:GLN:NE2	16:P:2:G:O6	2.50	0.44
1:A:868:TYR:HE1	1:A:1064:VAL:HG13	1.82	0.44
1:A:1386:ARG:NH2	17:T:21:DA:N3	2.65	0.44
12:L:40:LEU:HD21	12:L:56:LEU:HD21	1.98	0.44
2:B:619:ILE:N	2:B:619:ILE:HD12	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:143:LEU:N	8:H:143:LEU:HD12	2.32	0.44
19:Z:616:SER:O	19:Z:620:SER:N	2.49	0.44
11:K:60:ALA:O	11:K:73:LEU:HD12	2.17	0.44
2:B:310:MET:CG	2:B:386:LEU:HD13	2.48	0.44
3:C:36:VAL:HG13	11:K:41:THR:HG21	1.99	0.44
15:O:1137:ILE:N	15:O:1137:ILE:HD12	2.33	0.44
15:O:1733:PHE:O	15:O:1737:ASP:N	2.51	0.44
1:A:1333:ILE:HD12	1:A:1333:ILE:H	1.82	0.44
3:C:37:MET:SD	3:C:244:VAL:HG12	2.57	0.44
1:A:526:ASP:OD1	1:A:527:THR:N	2.50	0.44
2:B:228:LYS:O	2:B:261:ARG:NH1	2.51	0.44
15:O:1686:ARG:NE	15:O:1789:GLU:OE2	2.45	0.44
2:B:255:GLN:N	2:B:255:GLN:OE1	2.50	0.44
3:C:121:VAL:HA	15:O:1276:LEU:HD12	1.99	0.44
1:A:471:ASN:O	1:A:474:VAL:HG22	2.18	0.43
2:B:183:GLU:N	2:B:183:GLU:OE1	2.51	0.43
2:B:785:TYR:O	2:B:967:ARG:NH1	2.50	0.43
1:A:118:HIS:O	1:A:123:ARG:NH1	2.51	0.43
1:A:352:VAL:HG12	1:A:353:ILE:N	2.33	0.43
1:A:834:THR:HG21	1:A:1076:ALA:O	2.18	0.43
15:O:1779:THR:O	15:O:1783:PHE:N	2.50	0.43
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	2.00	0.43
13:M:34:VAL:HG13	13:M:47:LEU:HD21	2.00	0.43
17:T:9:DT:H2'	17:T:10:DT:H71	2.01	0.43
8:H:40:LEU:CD2	8:H:42:ILE:HD11	2.48	0.43
11:K:49:GLU:OE2	11:K:93:SER:OG	2.35	0.43
12:L:66:GLN:HE21	19:Z:816:LEU:HG	1.84	0.43
1:A:718:VAL:HG11	1:A:774:ARG:NH1	2.33	0.43
1:A:465:TYR:HB3	2:B:976:ILE:HD11	2.00	0.43
1:A:523:ILE:HG22	1:A:524:VAL:N	2.34	0.43
1:A:1169:ILE:HG21	1:A:1239:ARG:CD	2.49	0.43
2:B:983:ARG:NH2	2:B:1028:GLU:OE2	2.43	0.43
2:B:581:PHE:O	2:B:626:ILE:N	2.45	0.43
2:B:327:ARG:O	2:B:331:LEU:HD23	2.18	0.42
19:Z:625:ILE:HG22	19:Z:626:THR:N	2.35	0.42
1:A:225:ASN:O	1:A:229:SER:OG	2.33	0.42
1:A:715:GLU:OE1	1:A:774:ARG:NE	2.51	0.42
1:A:759:ALA:O	1:A:764:CYS:N	2.41	0.42
5:E:43:LYS:HZ2	5:E:43:LYS:HB2	1.84	0.42
10:J:21:TYR:CE2	10:J:25:LEU:HD11	2.54	0.42
1:A:117:GLU:O	1:A:123:ARG:NH1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:301:ILE:HD12	2:B:382:ILE:HG21	2.00	0.42
1:A:301:ALA:O	1:A:305:ASP:N	2.41	0.42
1:A:609:ASP:OD2	1:A:969:GLN:NE2	2.52	0.42
3:C:35:ARG:NE	11:K:41:THR:OG1	2.42	0.42
4:D:192:LYS:NZ	4:D:199:ASN:O	2.50	0.42
8:H:35:GLN:OE1	8:H:35:GLN:N	2.41	0.42
15:O:1815:ASN:O	15:O:1819:THR:HG23	2.20	0.42
2:B:1103:ILE:O	2:B:1122:ARG:NH2	2.47	0.42
4:D:130:LEU:O	4:D:130:LEU:HD23	2.19	0.42
7:G:12:THR:OG1	7:G:69:GLU:OE1	2.20	0.42
19:Z:79:VAL:HG11	19:Z:82:ILE:HD12	2.01	0.42
1:A:543:LEU:HD13	1:A:572:TRP:CH2	2.54	0.42
9:I:54:GLU:OE2	9:I:118:ARG:NH2	2.52	0.42
1:A:1318:THR:HG22	1:A:1318:THR:O	2.20	0.42
1:A:199:LEU:N	1:A:199:LEU:HD12	2.35	0.42
1:A:1279:ILE:HG23	1:A:1308:THR:HG21	2.01	0.42
6:F:130:ILE:HG22	6:F:132:LEU:H	1.85	0.42
3:C:260:LEU:HD23	3:C:260:LEU:O	2.20	0.41
5:E:165:LEU:O	5:E:169:ARG:N	2.52	0.41
1:A:181:LEU:HD12	1:A:181:LEU:O	2.20	0.41
7:G:119:LEU:HD23	7:G:120:THR:N	2.35	0.41
1:A:658:LEU:HD23	1:A:658:LEU:O	2.19	0.41
1:A:1373:ASP:O	1:A:1377:THR:N	2.54	0.41
2:B:90:ILE:N	2:B:90:ILE:HD12	2.36	0.41
2:B:1037:LEU:O	10:J:47:ARG:NH2	2.54	0.41
15:O:1187:ASN:OD1	15:O:1188:ARG:N	2.54	0.41
17:T:34:DC:H4'	17:T:35:DA:H5'	2.02	0.41
1:A:35:ILE:HD12	1:A:35:ILE:N	2.35	0.41
1:A:225:ASN:O	1:A:229:SER:N	2.53	0.41
1:A:826:ASP:O	1:A:830:LYS:HG2	2.21	0.41
2:B:269:ILE:HD12	2:B:269:ILE:N	2.35	0.41
2:B:845:SER:HB3	2:B:850:LEU:HD22	2.03	0.41
1:A:534:LEU:HD11	1:A:541:ILE:HD11	2.02	0.41
1:A:561:PRO:O	1:A:572:TRP:NE1	2.42	0.41
1:A:1121:GLU:O	1:A:1125:ALA:N	2.54	0.41
2:B:952:VAL:HG23	2:B:966:VAL:HG22	2.02	0.41
5:E:68:SER:O	5:E:72:PHE:N	2.45	0.41
5:E:50:MET:SD	5:E:52:ARG:NH2	2.91	0.41
7:G:103:VAL:O	7:G:103:VAL:HG13	2.19	0.41
1:A:902:LEU:HD23	1:A:902:LEU:O	2.21	0.41
1:A:1371:LEU:O	1:A:1374:VAL:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:27:LEU:N	4:D:27:LEU:HD22	2.36	0.41
9:I:19:ASP:O	9:I:23:ASN:CA	2.69	0.41
2:B:861:ASP:OD1	2:B:862:GLN:N	2.53	0.41
5:E:77:SER:HG	5:E:105:PHE:HD2	1.69	0.41
5:E:128:PRO:N	5:E:129:PRO:HD2	2.35	0.41
15:O:1216:LEU:HD12	15:O:1245:ALA:O	2.21	0.41
15:O:1574:HIS:ND1	15:O:1576:VAL:HG12	2.35	0.41
1:A:866:PHE:N	5:E:208:TYR:OH	2.53	0.40
1:A:1006:ILE:N	1:A:1006:ILE:HD12	2.36	0.40
1:A:1348:LEU:O	1:A:1348:LEU:HD23	2.21	0.40
2:B:1168:LEU:HD11	2:B:1208:MET:SD	2.61	0.40
3:C:33:LEU:HD13	3:C:248:ILE:CD1	2.50	0.40
19:Z:711:ILE:HD13	19:Z:752:VAL:CG1	2.51	0.40
1:A:399:HIS:O	1:A:435:HIS:ND1	2.53	0.40
1:A:397:ASN:HB3	19:Z:839:THR:HG21	2.02	0.40
2:B:1013:ASN:OD1	2:B:1015:HIS:ND1	2.44	0.40
19:Z:806:ARG:CZ	19:Z:816:LEU:HD21	2.51	0.40
1:A:1002:GLY:N	1:A:1007:ILE:HG21	2.37	0.40
15:O:1253:THR:HG22	15:O:1254:LYS:N	2.34	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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1388/1733 (80%)	1345 (97%)	43 (3%)	0	100	100
2	B	1099/1224 (90%)	1077 (98%)	22 (2%)	0	100	100
3	C	262/318 (82%)	251 (96%)	11 (4%)	0	100	100
4	D	155/221 (70%)	153 (99%)	2 (1%)	0	100	100
5	E	212/215 (99%)	210 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	83/155 (54%)	82 (99%)	1 (1%)	0	100	100
7	G	169/171 (99%)	169 (100%)	0	0	100	100
8	H	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
9	I	116/122 (95%)	113 (97%)	3 (3%)	0	100	100
10	J	63/70 (90%)	63 (100%)	0	0	100	100
11	K	113/120 (94%)	113 (100%)	0	0	100	100
12	L	41/70 (59%)	41 (100%)	0	0	100	100
13	M	63/145 (43%)	63 (100%)	0	0	100	100
15	O	688/2231 (31%)	675 (98%)	13 (2%)	0	100	100
18	Y	98/102 (96%)	98 (100%)	0	0	100	100
19	Z	412/1063 (39%)	406 (98%)	6 (2%)	0	100	100
All	All	5091/8106 (63%)	4981 (98%)	110 (2%)	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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1225/1520 (81%)	1222 (100%)	3 (0%)	92	93
2	B	964/1061 (91%)	961 (100%)	3 (0%)	91	92
3	C	232/274 (85%)	231 (100%)	1 (0%)	89	91
4	D	141/200 (70%)	140 (99%)	1 (1%)	81	87
5	E	196/197 (100%)	196 (100%)	0	100	100
6	F	75/137 (55%)	75 (100%)	0	100	100
7	G	152/152 (100%)	151 (99%)	1 (1%)	81	87
8	H	117/128 (91%)	117 (100%)	0	100	100
9	I	112/116 (97%)	112 (100%)	0	100	100
10	J	60/65 (92%)	60 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	99/102 (97%)	99 (100%)	0	100	100
12	L	38/57 (67%)	38 (100%)	0	100	100
13	M	60/131 (46%)	60 (100%)	0	100	100
15	O	618/2010 (31%)	618 (100%)	0	100	100
18	Y	85/87 (98%)	85 (100%)	0	100	100
19	Z	374/876 (43%)	374 (100%)	0	100	100
All	All	4548/7113 (64%)	4539 (100%)	9 (0%)	91	93

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	A	470	LEU
1	A	939	ASP
2	B	61	ASP
2	B	429	PHE
2	B	961	LEU
3	C	249	ASP
4	D	127	ASP
7	G	164	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	23/35 (65%)	8 (34%)	0

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	P	3	U
16	P	4	C
16	P	5	G
16	P	6	U
16	P	9	G
16	P	21	G

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Mol	Chain	Res	Type
16	P	23	G
16	P	25	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 11 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	$\# Z > 2$
23	BEF	O	3003	-	0,3,3	-	-	-		
22	ADP	O	3001	21	24,29,29	0.97	1 (4%)	29,45,45	1.57	5 (17%)

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
22	ADP	O	3001	21	-	2/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	O	3001	ADP	C5-C4	2.51	1.47	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	O	3001	ADP	PA-O3A-PB	-3.89	119.48	132.83
22	O	3001	ADP	N3-C2-N1	-3.63	123.00	128.68
22	O	3001	ADP	C3'-C2'-C1'	3.52	106.28	100.98
22	O	3001	ADP	C4-C5-N7	-2.89	106.39	109.40
22	O	3001	ADP	C2-N1-C6	2.03	122.22	118.75

There are no chirality outliers.

All (2) torsion outliers are listed below:

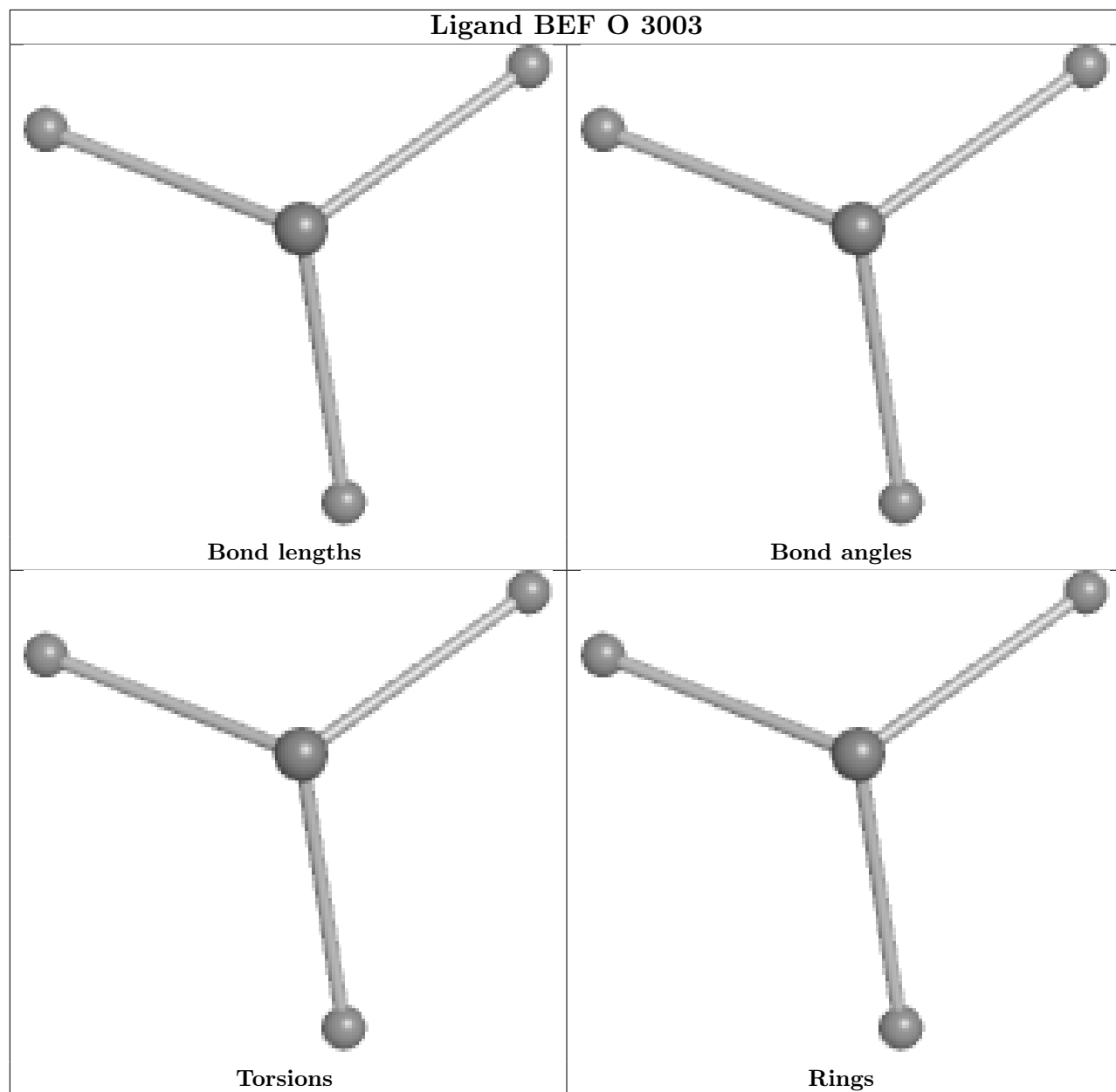
Mol	Chain	Res	Type	Atoms
22	O	3001	ADP	O4'-C4'-C5'-O5'
22	O	3001	ADP	C3'-C4'-C5'-O5'

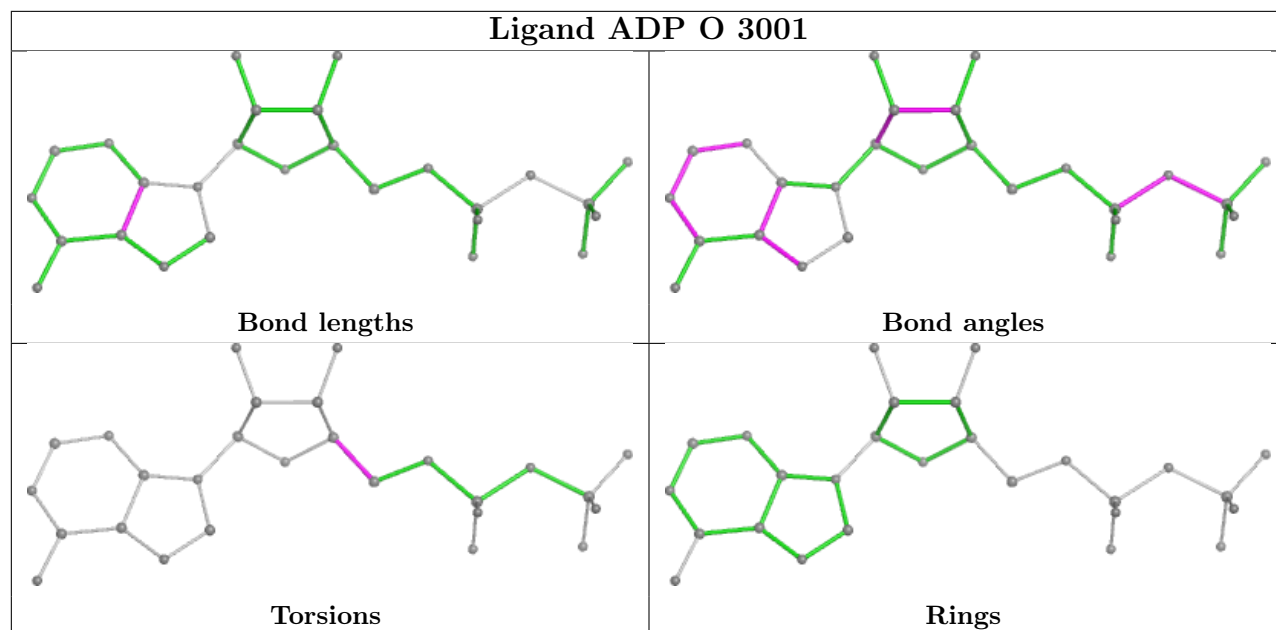
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	O	3003	BEF	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.