



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 08:20 PM UTC

PDB ID : 9CQ3 / pdb_00009cq3
EMDB ID : EMD-45807
Title : The gap-filling complex with Pol mu engaged in the NHEJ pathway
Authors : Li, J.; Liu, L.; Gellert, M.; Yang, W.
Deposited on : 2024-07-19
Resolution : 2.80 Å(reported)

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 : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

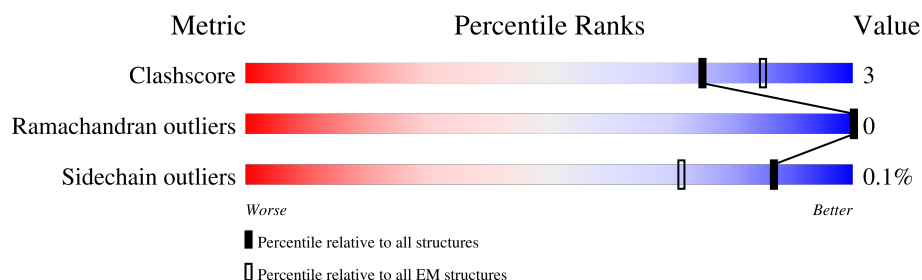
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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.



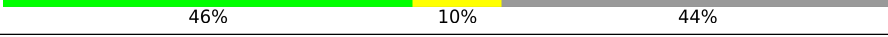
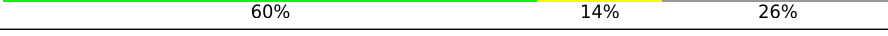
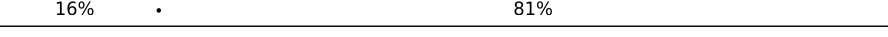
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	612	77% 7% 16%
1	a	612	76% 6% 17%
2	B	732	67% 5% 28%
2	b	732	68% 28%
3	C	302	72% 5% 24%
3	c	302	70% 5% 25%
4	D	336	56% 40%
4	E	336	56% 40%
4	d	336	54% 5% 40%

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Mol	Chain	Length	Quality of chain
4	e	336	
5	F	914	
5	f	914	
6	G	218	
6	H	218	
7	I	68	
8	J	68	
9	K	51	
10	L	50	
11	M	512	
11	m	512	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 43972 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 X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	516	Total	C	N	O	S	1	0
			4188	2678	708	783	19		
1	a	505	Total	C	N	O	S	0	0
			4081	2610	691	762	18		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P12956
A	-1	PRO	-	expression tag	UNP P12956
A	0	VAL	-	expression tag	UNP P12956
a	-2	GLY	-	expression tag	UNP P12956
a	-1	PRO	-	expression tag	UNP P12956
a	0	VAL	-	expression tag	UNP P12956

- Molecule 2 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	526	Total	C	N	O	S	0	0
			4211	2697	707	784	23		
2	b	525	Total	C	N	O	S	0	0
			4204	2692	706	783	23		

- Molecule 3 is a protein called Non-homologous end-joining factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	231	Total	C	N	O	S	0	0
			1831	1170	306	340	15		
3	c	228	Total	C	N	O	S	0	0
			1813	1158	303	337	15		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP Q9H9Q4
C	-1	PRO	-	expression tag	UNP Q9H9Q4
C	0	VAL	-	expression tag	UNP Q9H9Q4
c	-2	GLY	-	expression tag	UNP Q9H9Q4
c	-1	PRO	-	expression tag	UNP Q9H9Q4
c	0	VAL	-	expression tag	UNP Q9H9Q4

- Molecule 4 is a protein called DNA repair protein XRCC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	202	Total	C	N	O	S	0	0
			1633	1034	279	313	7		
4	E	201	Total	C	N	O	S	0	0
			1628	1031	278	312	7		
4	d	200	Total	C	N	O	S	0	0
			1623	1028	277	311	7		
4	e	200	Total	C	N	O	S	0	0
			1623	1028	277	311	7		

- Molecule 5 is a protein called DNA ligase 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	679	Total	C	N	O	S	0	0
			5503	3504	945	1021	33		
5	f	255	Total	C	N	O	S	0	0
			2069	1315	349	392	13		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP P49917
F	-1	PRO	-	expression tag	UNP P49917
F	0	VAL	-	expression tag	UNP P49917
f	-2	GLY	-	expression tag	UNP P49917
f	-1	PRO	-	expression tag	UNP P49917
f	0	VAL	-	expression tag	UNP P49917

- Molecule 6 is a protein called Protein PAXX.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	164	Total	C	N	O	S	0	0
			1219	767	210	236	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	149	Total	C	N	O	S	0	0
			1114	710	192	206	6		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-13	MET	-	expression tag	UNP Q9BUH6
G	-12	GLY	-	expression tag	UNP Q9BUH6
G	-11	SER	-	expression tag	UNP Q9BUH6
G	-10	SER	-	expression tag	UNP Q9BUH6
G	-9	HIS	-	expression tag	UNP Q9BUH6
G	-8	HIS	-	expression tag	UNP Q9BUH6
G	-7	HIS	-	expression tag	UNP Q9BUH6
G	-6	HIS	-	expression tag	UNP Q9BUH6
G	-5	HIS	-	expression tag	UNP Q9BUH6
G	-4	HIS	-	expression tag	UNP Q9BUH6
G	-3	SER	-	expression tag	UNP Q9BUH6
G	-2	GLN	-	expression tag	UNP Q9BUH6
G	-1	ASP	-	expression tag	UNP Q9BUH6
G	0	PRO	-	expression tag	UNP Q9BUH6
H	-13	MET	-	expression tag	UNP Q9BUH6
H	-12	GLY	-	expression tag	UNP Q9BUH6
H	-11	SER	-	expression tag	UNP Q9BUH6
H	-10	SER	-	expression tag	UNP Q9BUH6
H	-9	HIS	-	expression tag	UNP Q9BUH6
H	-8	HIS	-	expression tag	UNP Q9BUH6
H	-7	HIS	-	expression tag	UNP Q9BUH6
H	-6	HIS	-	expression tag	UNP Q9BUH6
H	-5	HIS	-	expression tag	UNP Q9BUH6
H	-4	HIS	-	expression tag	UNP Q9BUH6
H	-3	SER	-	expression tag	UNP Q9BUH6
H	-2	GLN	-	expression tag	UNP Q9BUH6
H	-1	ASP	-	expression tag	UNP Q9BUH6
H	0	PRO	-	expression tag	UNP Q9BUH6

- Molecule 7 is a DNA chain called DNA (38-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	38	Total	C	N	O	P	0	0
			771	370	131	232	38		

- Molecule 8 is a DNA chain called DNA (42-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	42	Total	C	N	O	P	0	0
			857	410	154	251	42		

- Molecule 9 is a DNA chain called DNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	34	Total	C	N	O	P	0	0
			702	335	136	198	33		

- Molecule 10 is a DNA chain called DNA (37-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	37	Total	C	N	O	P	0	0
			763	364	137	225	37		

- Molecule 11 is a protein called DNA-directed DNA/RNA polymerase mu.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	426	Total	C	N	O	S	0	0
			3375	2129	620	612	14		
11	m	96	Total	C	N	O	S	0	0
			732	457	135	134	6		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-17	HIS	-	expression tag	UNP Q9NP87
M	-16	HIS	-	expression tag	UNP Q9NP87
M	-15	HIS	-	expression tag	UNP Q9NP87
M	-14	HIS	-	expression tag	UNP Q9NP87
M	-13	HIS	-	expression tag	UNP Q9NP87
M	-12	HIS	-	expression tag	UNP Q9NP87
M	-11	SER	-	expression tag	UNP Q9NP87
M	-10	SER	-	expression tag	UNP Q9NP87
M	-9	GLY	-	expression tag	UNP Q9NP87
M	-8	LEU	-	expression tag	UNP Q9NP87
M	-7	GLU	-	expression tag	UNP Q9NP87
M	-6	VAL	-	expression tag	UNP Q9NP87
M	-5	LEU	-	expression tag	UNP Q9NP87
M	-4	PHE	-	expression tag	UNP Q9NP87
M	-3	GLN	-	expression tag	UNP Q9NP87
M	-2	GLY	-	expression tag	UNP Q9NP87
M	-1	PRO	-	expression tag	UNP Q9NP87

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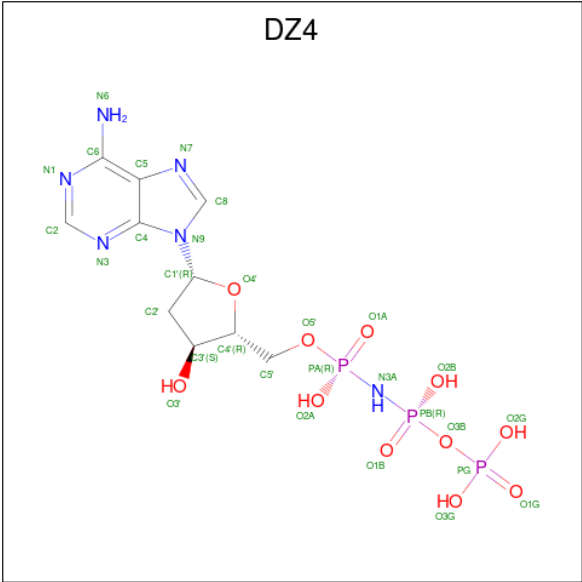
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Chain	Residue	Modelled	Actual	Comment	Reference
M	0	HIS	-	expression tag	UNP Q9NP87
m	-17	HIS	-	expression tag	UNP Q9NP87
m	-16	HIS	-	expression tag	UNP Q9NP87
m	-15	HIS	-	expression tag	UNP Q9NP87
m	-14	HIS	-	expression tag	UNP Q9NP87
m	-13	HIS	-	expression tag	UNP Q9NP87
m	-12	HIS	-	expression tag	UNP Q9NP87
m	-11	SER	-	expression tag	UNP Q9NP87
m	-10	SER	-	expression tag	UNP Q9NP87
m	-9	GLY	-	expression tag	UNP Q9NP87
m	-8	LEU	-	expression tag	UNP Q9NP87
m	-7	GLU	-	expression tag	UNP Q9NP87
m	-6	VAL	-	expression tag	UNP Q9NP87
m	-5	LEU	-	expression tag	UNP Q9NP87
m	-4	PHE	-	expression tag	UNP Q9NP87
m	-3	GLN	-	expression tag	UNP Q9NP87
m	-2	GLY	-	expression tag	UNP Q9NP87
m	-1	PRO	-	expression tag	UNP Q9NP87
m	0	HIS	-	expression tag	UNP Q9NP87

- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
12	M	2	Total Mg 2 2	0

- Molecule 13 is 2'-deoxy-5'-O-[(R)-hydroxy{[(R)-hydroxy(phosphonooxy)phosphoryl]amino}phosphoryl]adenosine (CCD ID: DZ4) (formula: C₁₀H₁₇N₆O₁₁P₃) (labeled as "Ligand of Interest" by depositor).

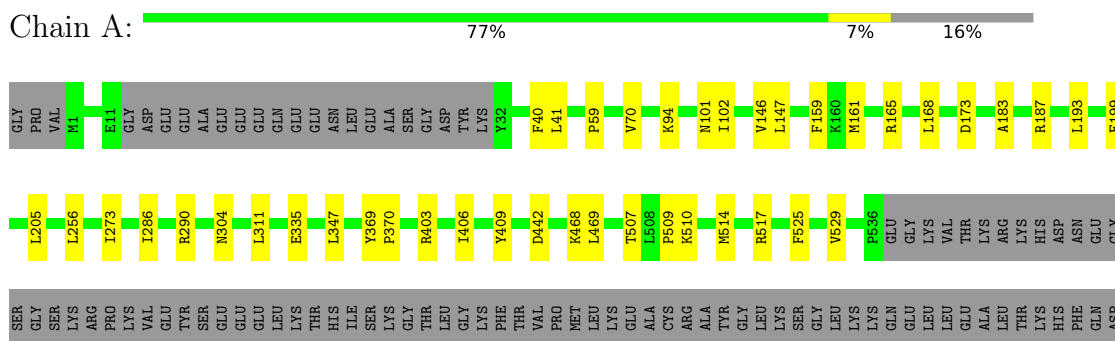


Mol	Chain	Residues	Atoms					AltConf
13	M	1	Total	C	N	O	P	0
			30	10	6	11	3	

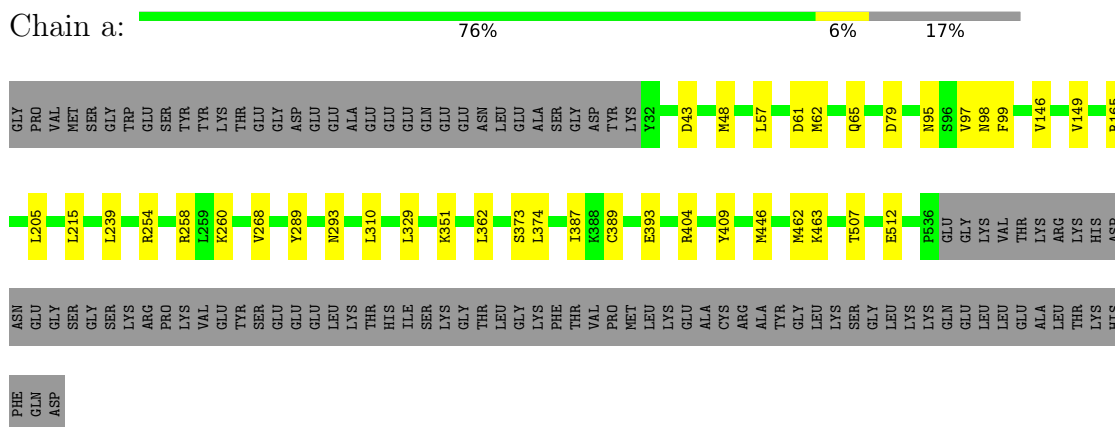
3 Residue-property plots

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.

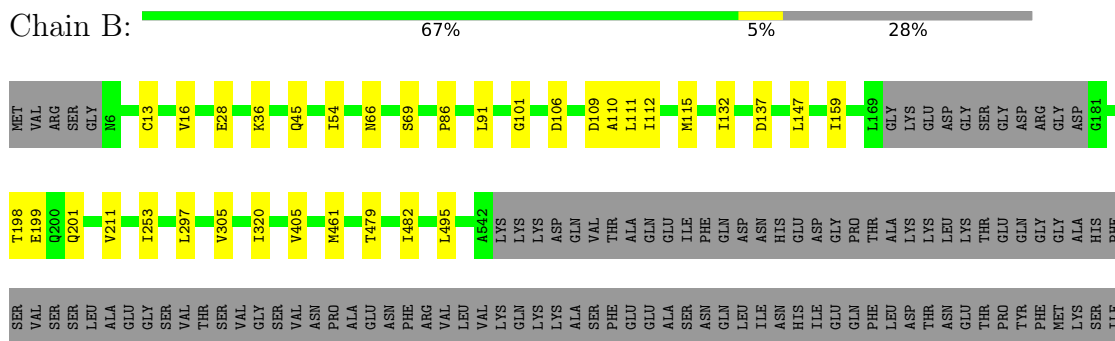
- Molecule 1: X-ray repair cross-complementing protein 6

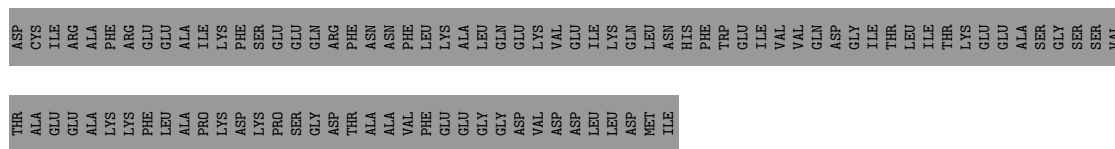


- Molecule 1: X-ray repair cross-complementing protein 6

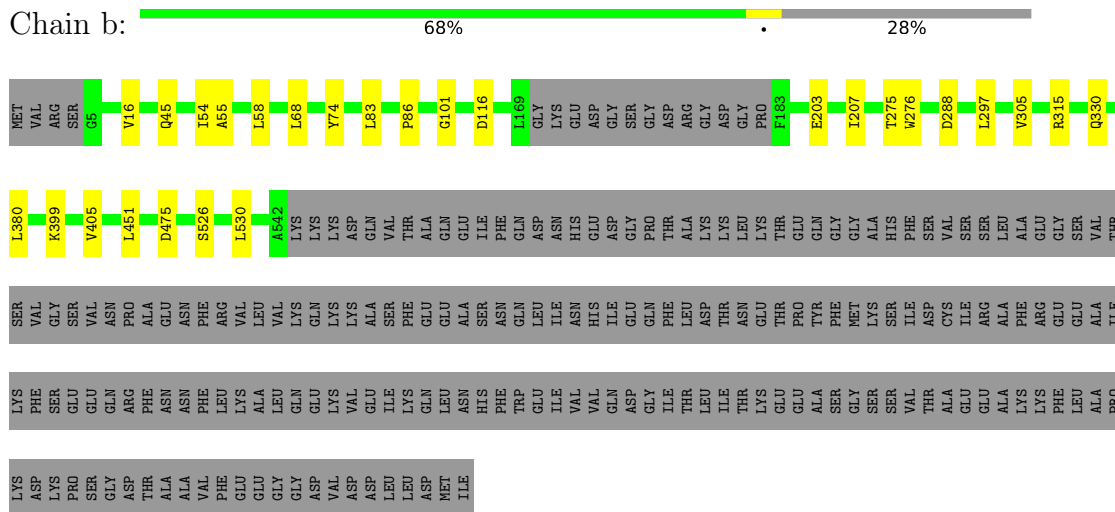


- Molecule 2: X-ray repair cross-complementing protein 5

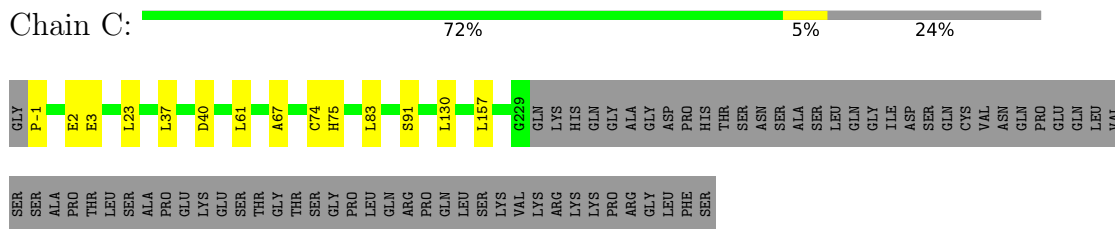




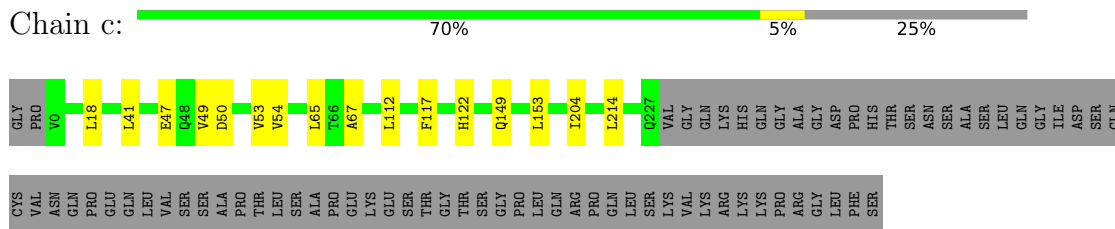
- Molecule 2: X-ray repair cross-complementing protein 5



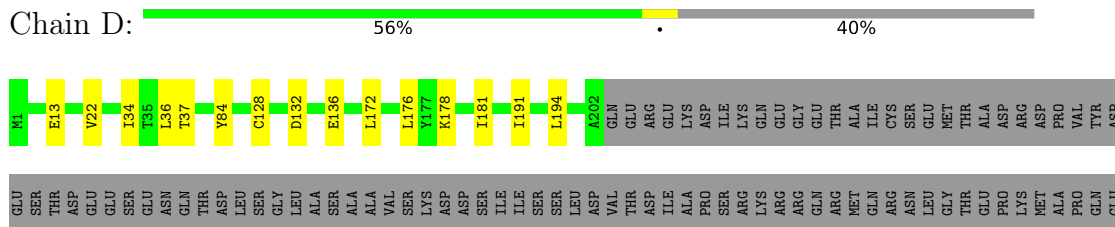
- Molecule 3: Non-homologous end-joining factor 1

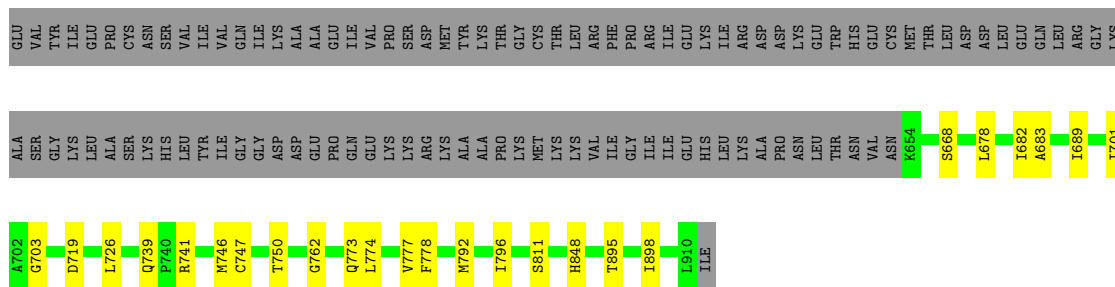


- Molecule 3: Non-homologous end-joining factor 1

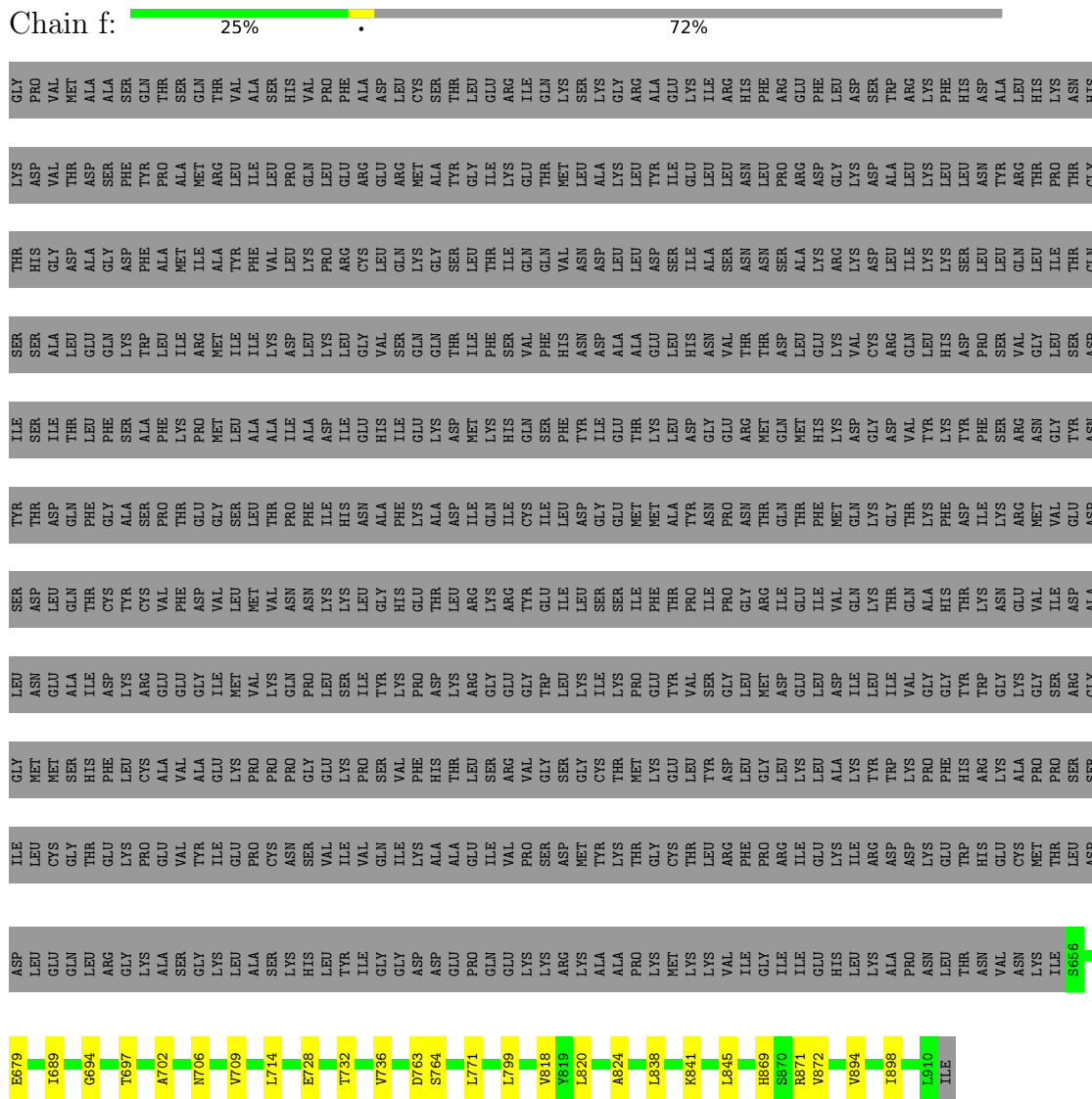


- Molecule 4: DNA repair protein XRCC4

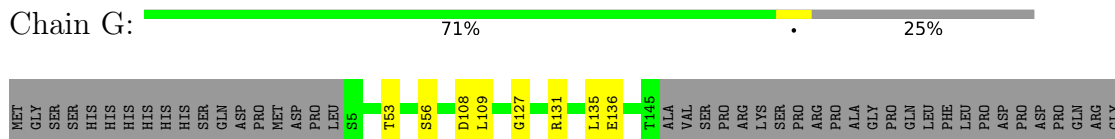


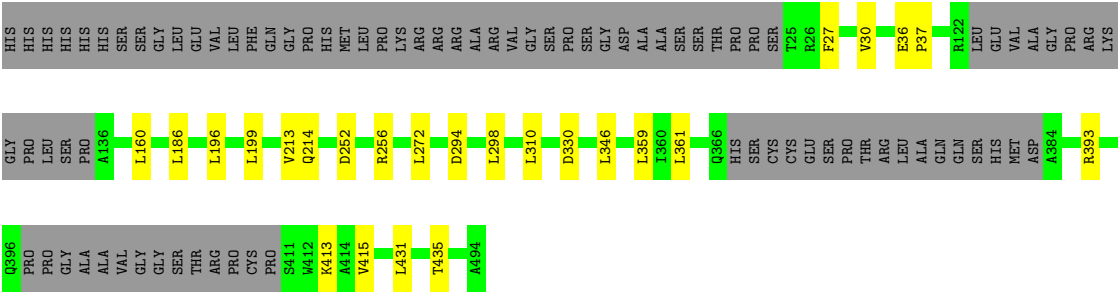


- Molecule 5: DNA ligase 4

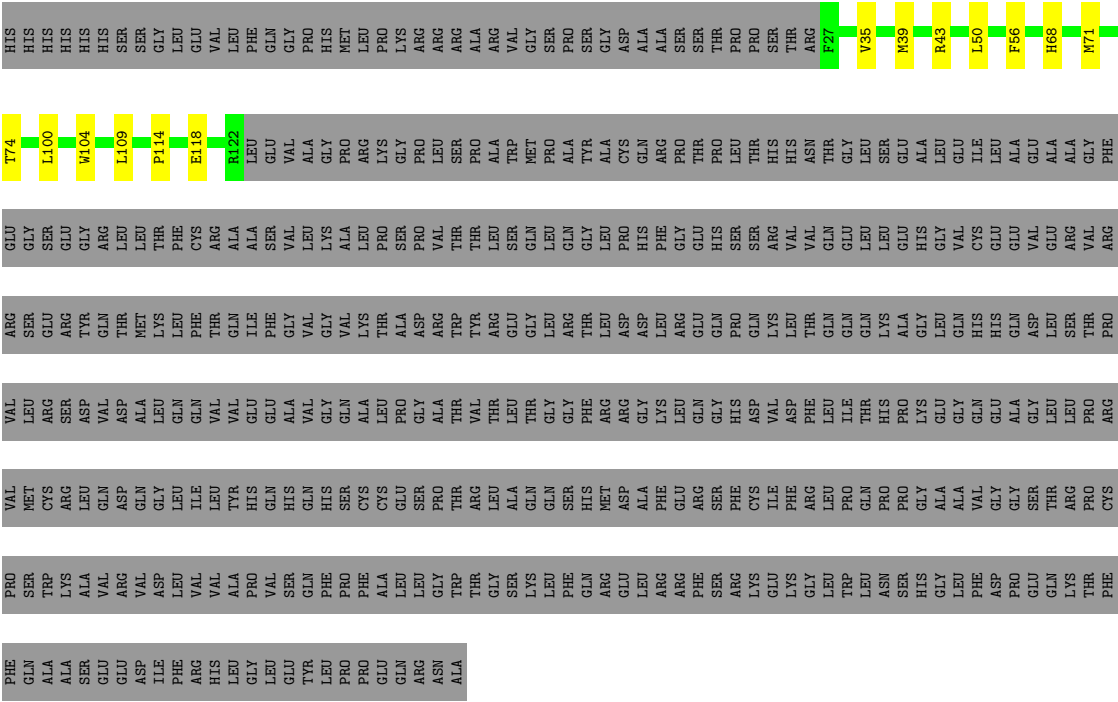


- Molecule 6: Protein PAXX





● Molecule 11: DNA-directed DNA/RNA polymerase mu



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	891208	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	54.4	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DZ4, 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	0.10	0/4272	0.24	0/5755
1	a	0.09	0/4162	0.23	0/5609
2	B	0.09	0/4298	0.22	0/5800
2	b	0.08	0/4290	0.22	0/5788
3	C	0.08	0/1869	0.24	0/2536
3	c	0.09	0/1850	0.24	0/2510
4	D	0.10	0/1662	0.22	0/2235
4	E	0.10	0/1657	0.24	0/2228
4	d	0.10	0/1652	0.24	0/2221
4	e	0.10	0/1652	0.21	0/2221
5	F	0.09	0/5617	0.24	0/7568
5	f	0.09	0/2118	0.23	0/2862
6	G	0.07	0/1247	0.21	0/1695
6	H	0.10	0/1140	0.25	0/1549
7	I	0.21	0/861	0.47	0/1325
8	J	0.18	0/960	0.44	0/1478
9	K	0.21	0/790	0.43	0/1219
10	L	0.18	0/855	0.43	0/1317
11	M	0.10	0/3452	0.23	0/4671
11	m	0.10	0/749	0.26	0/1017
All	All	0.10	0/45153	0.26	0/61604

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	4188	0	4248	32	0
1	a	4081	0	4152	33	0
2	B	4211	0	4252	22	0
2	b	4204	0	4245	22	0
3	C	1831	0	1841	8	0
3	c	1813	0	1822	15	0
4	D	1633	0	1625	13	0
4	E	1628	0	1620	9	0
4	d	1623	0	1615	14	0
4	e	1623	0	1615	6	0
5	F	5503	0	5504	34	0
5	f	2069	0	2011	19	0
6	G	1219	0	1197	7	0
6	H	1114	0	1112	19	0
7	I	771	0	431	6	0
8	J	857	0	475	0	0
9	K	702	0	384	5	0
10	L	763	0	420	4	0
11	M	3375	0	3345	20	0
11	m	732	0	726	14	0
12	M	2	0	0	0	0
13	M	30	0	13	0	0
All	All	43972	0	42653	268	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 3.

All (268) 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)
11:m:50:LEU:HD23	11:m:109:LEU:HD23	1.26	1.09
5:f:679:GLU:HG3	5:f:689:ILE:HG12	1.40	1.04
11:m:50:LEU:HD23	11:m:109:LEU:CD2	1.94	0.97
11:m:50:LEU:CD2	11:m:109:LEU:HD23	1.96	0.95
3:c:50:ASP:O	3:c:54:VAL:HG23	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:199:LEU:HD11	11:M:213:VAL:HG11	1.66	0.76
11:m:100:LEU:HD13	11:m:104:TRP:CZ3	2.21	0.75
5:F:773:GLN:O	5:F:777:VAL:HG23	1.86	0.75
1:a:462:MET:HE2	2:b:380:LEU:HD13	1.73	0.71
7:I:50:DG:H21	1:a:254:ARG:HH21	1.40	0.70
4:d:22:VAL:HG12	4:d:34:ILE:HG22	1.74	0.69
5:F:762:GLY:O	5:F:777:VAL:HG22	1.96	0.66
11:m:68:HIS:CG	11:m:104:TRP:HH2	2.14	0.66
7:I:59:DC:H2''	7:I:60:DT:H71	1.78	0.66
11:M:431:LEU:O	11:M:435:THR:HG22	1.96	0.65
4:d:59:MET:HE1	4:d:66:TYR:CD1	2.33	0.64
5:F:381:THR:HG22	5:F:437:ILE:CG2	2.28	0.64
4:d:180:PHE:HE2	5:f:799:LEU:HD21	1.62	0.64
1:A:102:ILE:HD12	1:A:146:VAL:HG22	1.80	0.63
5:F:381:THR:HG22	5:F:437:ILE:HG22	1.80	0.63
4:D:22:VAL:HG12	4:D:34:ILE:HG22	1.80	0.63
11:M:298:LEU:HD11	11:M:415:VAL:HG21	1.81	0.63
1:A:41:LEU:HD21	1:A:146:VAL:CG1	2.29	0.62
1:a:205:LEU:HD23	1:a:239:LEU:HD21	1.81	0.62
7:I:50:DG:H21	1:a:254:ARG:NH2	1.97	0.62
5:f:820:LEU:HB3	5:f:838:LEU:HD11	1.81	0.61
4:d:180:PHE:CE2	5:f:799:LEU:HD21	2.36	0.61
6:H:47:LEU:HD13	6:H:117:ALA:CB	2.31	0.61
1:A:147:LEU:HD12	1:A:193:LEU:CD1	2.31	0.61
1:A:41:LEU:HD23	1:A:168:LEU:HD13	1.83	0.60
4:d:59:MET:HE3	4:d:61:MET:HB3	1.84	0.60
2:B:297:LEU:HD21	2:B:305:VAL:HG11	1.82	0.60
2:B:66:ASN:OD1	2:B:69:SER:HB3	2.02	0.60
5:F:683:ALA:HB2	5:F:689:ILE:HD11	1.83	0.59
5:F:263:MET:HE3	5:F:263:MET:H	1.67	0.58
6:H:75:ARG:HE	6:H:98:LEU:HD13	1.68	0.58
6:H:79:ALA:O	6:H:83:GLN:N	2.37	0.58
1:A:286:ILE:HD11	2:B:320:ILE:HD12	1.85	0.57
2:b:54:ILE:HD12	2:b:86:PRO:HG3	1.87	0.57
5:F:302:PHE:O	5:F:312:THR:OG1	2.20	0.57
4:E:176:LEU:HD22	4:E:180:PHE:CZ	2.40	0.56
3:C:37:LEU:HD13	3:C:130:LEU:HD21	1.88	0.56
2:b:16:VAL:O	2:b:16:VAL:HG12	2.05	0.56
11:M:196:LEU:HD11	11:M:214:GLN:HG2	1.88	0.56
5:f:728:GLU:O	5:f:732:THR:HG22	2.06	0.56
6:H:47:LEU:HD21	6:H:121:LEU:HG	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:62:MET:HE3	1:a:205:LEU:HD22	1.88	0.55
1:a:310:LEU:HD21	11:m:43:ARG:HH12	1.72	0.54
3:c:49:VAL:HG13	3:c:53:VAL:HG13	1.88	0.54
4:D:191:ILE:HD13	4:E:191:ILE:HD12	1.89	0.54
3:C:67:ALA:HB1	4:E:104:VAL:HG12	1.90	0.54
4:D:172:LEU:HD12	4:D:176:LEU:HD23	1.89	0.54
5:F:746:MET:HE2	5:F:750:THR:HG22	1.89	0.54
6:H:38:ASN:OD1	6:H:52:PHE:N	2.41	0.54
5:F:678:LEU:O	5:F:682:ILE:HG23	2.07	0.53
6:H:23:TYR:OH	6:H:124:LEU:HD22	2.09	0.53
7:I:59:DC:C2'	7:I:60:DT:H71	2.37	0.53
4:D:194:LEU:HD23	4:D:194:LEU:O	2.09	0.53
10:L:33:DT:H2'	10:L:34:DT:H72	1.89	0.53
2:b:526:SER:O	2:b:530:LEU:HD12	2.09	0.53
6:H:403:LEU:O	1:a:165:ARG:NH1	2.39	0.52
5:F:299:THR:O	5:F:303:GLY:N	2.42	0.52
1:a:95:ASN:ND2	1:a:99:PHE:O	2.43	0.52
6:H:47:LEU:HD13	6:H:117:ALA:HB1	1.91	0.52
5:f:841:LYS:HE2	5:f:841:LYS:HA	1.92	0.51
5:f:838:LEU:O	5:f:838:LEU:HD12	2.10	0.51
6:H:96:LEU:HD23	6:H:109:LEU:CD1	2.41	0.51
1:A:183:ALA:O	1:A:187:ARG:HG3	2.10	0.51
5:F:792:MET:O	5:F:796:ILE:HG12	2.11	0.51
4:e:181:ILE:HD11	5:f:771:LEU:HA	1.92	0.51
5:F:383:ARG:HH11	5:F:383:ARG:HG3	1.75	0.50
5:f:824:ALA:O	5:f:871:ARG:NH1	2.45	0.50
5:F:219:THR:HG22	5:F:219:THR:O	2.11	0.50
6:H:117:ALA:O	6:H:121:LEU:HD12	2.12	0.50
1:A:41:LEU:HD21	1:A:146:VAL:HG12	1.94	0.50
1:a:61:ASP:O	1:a:65:GLN:HG2	2.12	0.49
1:a:43:ASP:HB3	1:a:48:MET:SD	2.52	0.49
1:a:310:LEU:HD21	11:m:43:ARG:NH1	2.27	0.49
4:D:132:ASP:O	4:D:136:GLU:HG3	2.13	0.49
1:A:41:LEU:HD21	1:A:146:VAL:HG11	1.93	0.49
1:A:165:ARG:NH1	6:G:403:LEU:O	2.46	0.49
6:G:135:LEU:CD1	6:H:135:LEU:HD13	2.43	0.49
3:C:157:LEU:HD12	3:c:153:LEU:CD1	2.43	0.49
3:c:112:LEU:HD22	3:c:117:PHE:HB2	1.95	0.49
4:d:89:SER:O	4:d:93:CYS:N	2.46	0.49
1:A:347:LEU:CD2	2:B:461:MET:HE1	2.43	0.48
4:E:170:GLU:CD	4:E:170:GLU:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:747:CYS:HG	5:F:750:THR:HG1	1.56	0.48
5:F:668:SER:O	5:F:703:GLY:N	2.46	0.48
4:d:65:LYS:O	4:d:69:GLU:HG2	2.13	0.48
6:H:112:VAL:HG22	6:H:113:PRO:HD2	1.96	0.48
3:c:18:LEU:O	3:c:18:LEU:HD12	2.14	0.48
11:M:298:LEU:HD11	11:M:415:VAL:CG2	2.44	0.47
6:G:127:GLY:O	6:G:131:ARG:HG3	2.14	0.47
4:E:184:LEU:HD12	5:F:774:LEU:HD13	1.96	0.47
2:b:16:VAL:HG21	2:b:58:LEU:HD23	1.97	0.47
6:G:135:LEU:HD11	6:H:135:LEU:HD13	1.97	0.47
2:b:16:VAL:HG12	2:b:101:GLY:H	1.79	0.47
2:B:91:LEU:HD13	2:B:495:LEU:HD13	1.97	0.47
11:M:160:LEU:HD12	11:M:186:LEU:HD12	1.95	0.47
2:B:147:LEU:HD11	2:B:211:VAL:HG22	1.96	0.47
10:L:30:DG:H2'	10:L:31:DT:H71	1.95	0.47
1:A:525:PHE:O	1:A:529:VAL:HG22	2.15	0.47
5:F:701:ILE:HD13	5:F:726:LEU:HD11	1.96	0.46
6:G:135:LEU:HD12	6:G:136:GLU:N	2.31	0.46
2:b:55:ALA:HB2	2:b:83:LEU:HD12	1.96	0.46
11:m:71:MET:HE1	11:m:74:THR:HG21	1.97	0.46
4:D:178:LYS:HA	4:D:181:ILE:HG22	1.97	0.46
2:B:109:ASP:HA	2:B:112:ILE:HD12	1.97	0.46
11:M:196:LEU:HD11	11:M:214:GLN:HE21	1.81	0.46
1:a:373:SER:C	1:a:374:LEU:HD12	2.39	0.46
4:d:185:ASN:O	4:d:189:THR:HG23	2.14	0.46
1:A:409:TYR:OH	1:A:442:ASP:OD2	2.32	0.46
9:K:5:DA:H2'	9:K:6:DG:C8	2.51	0.46
1:a:362:LEU:HD22	1:a:409:TYR:OH	2.16	0.46
4:e:89:SER:O	4:e:93:CYS:N	2.49	0.46
1:a:446:MET:HA	1:a:446:MET:HE2	1.98	0.46
4:d:23:SER:OG	4:d:33:VAL:HG12	2.16	0.46
1:A:304:ASN:HB2	1:A:311:LEU:HD11	1.97	0.46
2:b:45:GLN:HG3	2:b:54:ILE:HD11	1.98	0.46
3:c:112:LEU:HD23	3:c:112:LEU:H	1.81	0.46
5:F:385:ARG:O	5:F:389:LEU:HD13	2.16	0.45
5:f:702:ALA:HB1	5:f:709:VAL:HG21	1.98	0.45
1:A:173:ASP:N	1:A:173:ASP:OD1	2.48	0.45
4:d:172:LEU:C	4:d:172:LEU:HD23	2.42	0.45
2:B:16:VAL:O	2:B:101:GLY:N	2.41	0.45
2:B:199:GLU:H	2:B:199:GLU:CD	2.25	0.45
11:M:310:LEU:HD13	11:M:346:LEU:HD21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:330:GLN:NE2	5:f:714:LEU:HD13	2.32	0.45
1:A:94:LYS:O	1:A:94:LYS:HG3	2.17	0.45
5:f:694:GLY:O	5:f:697:THR:HG22	2.17	0.45
1:A:159:PHE:O	1:A:161:MET:HE2	2.18	0.44
1:a:462:MET:HE2	2:b:380:LEU:CD1	2.45	0.44
6:H:39:LEU:HD21	6:H:96:LEU:HG	1.97	0.44
3:c:49:VAL:CG1	3:c:53:VAL:HG13	2.48	0.44
1:A:507:THR:HG23	2:B:405:VAL:CG2	2.47	0.44
5:F:103:GLY:O	5:F:107:LEU:HD22	2.17	0.44
4:d:8:ILE:HD11	4:d:86:PHE:CG	2.52	0.44
4:d:163:GLU:OE1	4:d:163:GLU:HA	2.18	0.44
1:a:48:MET:HE3	1:a:205:LEU:CD1	2.48	0.44
6:H:73:THR:HG22	6:H:77:ARG:HH12	1.83	0.44
1:a:507:THR:HG23	2:b:405:VAL:CG2	2.48	0.44
2:B:111:LEU:HG	2:B:115:MET:HE2	1.99	0.44
5:F:24:GLU:OE1	5:F:184:LYS:NZ	2.49	0.44
11:M:361:LEU:HD21	11:M:393:ARG:NE	2.32	0.44
1:a:97:VAL:O	1:a:98:ASN:HB2	2.18	0.44
3:c:41:LEU:HD13	3:c:204:ILE:HD12	2.00	0.44
1:a:97:VAL:O	1:a:97:VAL:CG1	2.65	0.43
1:A:41:LEU:HD23	1:A:168:LEU:CD1	2.47	0.43
3:C:83:LEU:HD11	3:C:91:SER:HB2	2.01	0.43
9:K:4:DT:H2''	9:K:5:DA:C8	2.53	0.43
1:a:389:CYS:O	1:a:393:GLU:N	2.51	0.43
1:A:199:PHE:CD1	1:A:199:PHE:C	2.96	0.43
2:B:54:ILE:HD12	2:B:86:PRO:HG3	2.00	0.43
5:f:898:ILE:N	5:f:898:ILE:HD13	2.33	0.43
3:c:49:VAL:HG13	3:c:53:VAL:CG1	2.47	0.43
5:F:719:ASP:OD1	5:F:719:ASP:N	2.52	0.43
6:H:80:CYS:SG	6:H:81:GLU:N	2.92	0.43
9:K:33:DT:H2'	9:K:34:DT:H72	2.01	0.43
4:d:86:PHE:CD1	4:d:86:PHE:N	2.87	0.43
5:f:818:VAL:HG21	5:f:845:LEU:HD21	2.00	0.43
11:m:100:LEU:HD13	11:m:104:TRP:HZ3	1.79	0.43
1:A:369:TYR:CG	1:A:370:PRO:HD2	2.54	0.43
4:E:117:GLU:OE1	4:E:117:GLU:HA	2.19	0.43
1:A:40:PHE:HZ	1:A:70:VAL:HG11	1.83	0.43
5:F:250:LEU:N	5:F:250:LEU:HD23	2.34	0.43
5:F:260:GLU:HA	5:F:263:MET:HE1	2.00	0.43
6:H:117:ALA:O	6:H:120:ARG:N	2.52	0.43
1:a:289:TYR:O	1:a:293:ASN:N	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:CYS:SG	2:B:110:ALA:HB1	2.59	0.43
2:b:68:LEU:HD23	2:b:74:TYR:CE2	2.53	0.43
11:m:39:MET:HE2	11:m:39:MET:HB3	1.96	0.42
11:M:36:GLU:N	11:M:37:PRO:CD	2.83	0.42
11:m:68:HIS:CG	11:m:104:TRP:CH2	3.03	0.42
4:D:36:LEU:HD23	4:D:37:THR:N	2.34	0.42
9:K:32:DT:H2'	9:K:33:DT:H72	2.00	0.42
11:M:272:LEU:HD12	11:M:272:LEU:N	2.33	0.42
1:a:146:VAL:HA	1:a:149:VAL:HG22	2.01	0.42
4:E:89:SER:O	4:E:93:CYS:N	2.52	0.42
9:K:21:DA:OP2	2:b:275:THR:HG22	2.19	0.42
1:a:329:LEU:HD12	2:b:276:TRP:CH2	2.55	0.42
11:m:118:GLU:N	11:m:118:GLU:OE1	2.52	0.42
4:D:84:TYR:N	4:D:84:TYR:CD1	2.88	0.42
11:M:27:PHE:CB	11:M:30:VAL:HG12	2.50	0.42
11:M:199:LEU:HD11	11:M:213:VAL:CG1	2.44	0.42
1:a:387:ILE:HD11	2:b:451:LEU:HD22	2.02	0.42
3:c:149:GLN:O	3:c:153:LEU:HD23	2.19	0.42
4:d:7:ARG:NH1	4:e:132:ASP:OD1	2.51	0.42
2:B:137:ASP:OD1	2:B:201:GLN:NE2	2.53	0.42
5:F:383:ARG:HG3	5:F:383:ARG:NH1	2.35	0.42
5:F:811:SER:N	5:F:848:HIS:O	2.47	0.42
11:M:359:LEU:O	11:M:393:ARG:N	2.52	0.42
2:B:45:GLN:HG3	2:B:54:ILE:HD11	2.01	0.42
2:B:132:ILE:HD12	2:B:159:ILE:HG21	2.02	0.42
3:C:74:CYS:SG	3:C:75:HIS:N	2.93	0.42
4:D:13:GLU:N	4:D:13:GLU:OE1	2.53	0.42
4:D:128:CYS:SG	4:E:7:ARG:NH1	2.90	0.42
4:D:178:LYS:HD3	5:F:792:MET:HE1	2.01	0.42
10:L:12:DG:H2''	10:L:13:DA:C8	2.55	0.42
5:f:894:VAL:O	5:f:898:ILE:HG12	2.20	0.42
7:I:62:DG:H2''	7:I:63:DT:H71	2.02	0.41
1:a:215:LEU:C	1:a:215:LEU:HD23	2.45	0.41
1:a:463:LYS:HB3	1:a:463:LYS:NZ	2.35	0.41
5:F:214:LEU:HD23	5:F:214:LEU:O	2.19	0.41
5:F:321:ALA:O	5:F:324:GLN:NE2	2.54	0.41
5:F:774:LEU:HD11	5:F:778:PHE:HE1	1.84	0.41
11:M:27:PHE:HB3	11:M:30:VAL:HG12	2.01	0.41
3:c:47:GLU:OE1	3:c:122:HIS:N	2.53	0.41
2:B:28:GLU:OE2	2:B:36:LYS:NZ	2.53	0.41
3:C:2:GLU:OE1	3:C:2:GLU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:194:LEU:HD23	4:D:194:LEU:C	2.45	0.41
7:I:48:DC:H2'	7:I:49:DT:H71	2.01	0.41
5:f:869:HIS:O	5:f:872:VAL:HG22	2.20	0.41
1:A:101:ASN:C	1:A:102:ILE:HD13	2.44	0.41
1:A:335:GLU:OE2	1:A:335:GLU:HA	2.20	0.41
3:C:23:LEU:CD2	3:C:40:ASP:HB3	2.50	0.41
4:D:176:LEU:HD11	4:E:177:TYR:CZ	2.54	0.41
11:M:36:GLU:O	11:M:37:PRO:C	2.64	0.41
1:a:258:ARG:HH21	1:a:374:LEU:HD11	1.86	0.41
11:m:35:VAL:O	11:m:39:MET:HE3	2.21	0.41
1:A:59:PRO:HB3	1:A:205:LEU:HD13	2.02	0.41
1:A:509:PRO:O	1:A:510:LYS:HG2	2.21	0.41
2:B:253:ILE:O	2:B:253:ILE:HG22	2.20	0.41
2:b:288:ASP:N	2:b:288:ASP:OD1	2.53	0.41
1:A:256:LEU:N	1:A:273:ILE:O	2.50	0.41
2:B:479:THR:HA	2:B:482:ILE:HD12	2.02	0.41
5:F:739:GLN:OE1	5:F:741:ARG:NH2	2.52	0.41
11:M:330:ASP:OD1	11:M:330:ASP:C	2.64	0.41
3:c:65:LEU:HD13	4:e:106:PHE:CZ	2.56	0.41
6:G:108:ASP:O	6:G:109:LEU:HD12	2.21	0.41
10:L:34:DT:H2'	10:L:35:DT:H72	2.01	0.41
2:b:68:LEU:HD11	2:b:116:ASP:CG	2.46	0.41
3:c:67:ALA:CB	4:e:104:VAL:HG12	2.51	0.41
1:A:469:LEU:HD22	1:A:514:MET:HG2	2.02	0.41
5:F:449:LYS:HD2	5:F:449:LYS:C	2.46	0.41
5:F:895:THR:O	5:F:898:ILE:HG22	2.21	0.41
6:G:53:THR:H	6:G:56:SER:HG	1.66	0.41
2:b:297:LEU:HD21	2:b:305:VAL:HG11	2.03	0.41
3:c:67:ALA:HB1	4:e:104:VAL:HG12	2.03	0.41
3:c:214:LEU:HD23	3:c:214:LEU:H	1.84	0.41
5:f:706:ASN:OD1	5:f:709:VAL:HG23	2.21	0.41
5:f:728:GLU:OE2	5:f:736:VAL:HG21	2.21	0.41
5:f:763:ASP:OD1	5:f:764:SER:N	2.54	0.41
1:A:147:LEU:HB3	1:A:193:LEU:HD11	2.02	0.41
1:A:507:THR:HG22	1:A:507:THR:O	2.21	0.41
2:B:106:ASP:C	2:B:106:ASP:OD1	2.62	0.41
6:H:23:TYR:O	6:H:39:LEU:HD12	2.20	0.41
1:A:403:ARG:O	1:A:406:ILE:HG22	2.21	0.40
5:F:449:LYS:HD2	5:F:450:ILE:N	2.36	0.40
1:a:404:ARG:NH1	1:a:404:ARG:HB3	2.36	0.40
11:M:252:ASP:OD1	11:M:256:ARG:NH1	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:294:ASP:OD2	11:M:413:LYS:NZ	2.38	0.40
1:a:260:LYS:HG2	1:a:268:VAL:HG13	2.04	0.40
2:b:203:GLU:O	2:b:207:ILE:HG12	2.20	0.40
2:B:198:THR:HG22	2:B:199:GLU:N	2.37	0.40
1:a:79:ASP:OD2	2:b:315:ARG:NH1	2.49	0.40
1:a:512:GLU:OE1	1:a:512:GLU:C	2.65	0.40
1:A:290:ARG:HG2	1:A:290:ARG:NH1	2.36	0.40
1:A:468:LYS:O	1:A:517:ARG:NH2	2.49	0.40
2:B:199:GLU:CD	2:B:199:GLU:N	2.80	0.40
6:H:95:SER:C	6:H:96:LEU:HD22	2.46	0.40
1:a:351:LYS:NZ	2:b:475:ASP:OD2	2.49	0.40
2:b:399:LYS:HB3	2:b:399:LYS:NZ	2.37	0.40
3:C:-1:PRO:O	3:C:3:GLU:HG3	2.22	0.40
5:F:429:ILE:HG22	5:F:430:MET:N	2.37	0.40
11:M:196:LEU:HD11	11:M:214:GLN:CG	2.50	0.40
1:a:57:LEU:H	1:a:57:LEU:HD23	1.85	0.40
11:m:56:PHE:CZ	11:m:114:PRO:HG3	2.56	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	513/612 (84%)	506 (99%)	7 (1%)	0	100	100
1	a	503/612 (82%)	490 (97%)	13 (3%)	0	100	100
2	B	522/732 (71%)	509 (98%)	13 (2%)	0	100	100
2	b	521/732 (71%)	510 (98%)	11 (2%)	0	100	100
3	C	229/302 (76%)	223 (97%)	6 (3%)	0	100	100
3	c	226/302 (75%)	221 (98%)	5 (2%)	0	100	100
4	D	200/336 (60%)	194 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	199/336 (59%)	196 (98%)	3 (2%)	0	100	100
4	d	198/336 (59%)	197 (100%)	1 (0%)	0	100	100
4	e	198/336 (59%)	196 (99%)	2 (1%)	0	100	100
5	F	671/914 (73%)	656 (98%)	15 (2%)	0	100	100
5	f	253/914 (28%)	244 (96%)	9 (4%)	0	100	100
6	G	160/218 (73%)	159 (99%)	1 (1%)	0	100	100
6	H	141/218 (65%)	139 (99%)	2 (1%)	0	100	100
11	M	418/512 (82%)	409 (98%)	9 (2%)	0	100	100
11	m	94/512 (18%)	93 (99%)	1 (1%)	0	100	100
All	All	5046/7924 (64%)	4942 (98%)	104 (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	470/550 (86%)	470 (100%)	0	100	100
1	a	459/550 (84%)	459 (100%)	0	100	100
2	B	474/649 (73%)	474 (100%)	0	100	100
2	b	473/649 (73%)	473 (100%)	0	100	100
3	C	204/264 (77%)	203 (100%)	1 (0%)	81	93
3	c	202/264 (76%)	202 (100%)	0	100	100
4	D	180/303 (59%)	180 (100%)	0	100	100
4	E	180/303 (59%)	178 (99%)	2 (1%)	65	87
4	d	180/303 (59%)	179 (99%)	1 (1%)	78	92
4	e	180/303 (59%)	179 (99%)	1 (1%)	78	92
5	F	611/810 (75%)	611 (100%)	0	100	100
5	f	231/810 (28%)	231 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	G	127/173 (73%)	127 (100%)	0	100	100
6	H	117/173 (68%)	116 (99%)	1 (1%)	70	89
11	M	358/428 (84%)	358 (100%)	0	100	100
11	m	77/428 (18%)	77 (100%)	0	100	100
All	All	4523/6960 (65%)	4517 (100%)	6 (0%)	87	97

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	61	LEU
4	E	70	LEU
4	E	146	LYS
6	H	37	PHE
4	d	172	LEU
4	e	98	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	GLN
1	A	204	HIS
3	C	6	GLN
3	C	46	HIS
3	C	147	GLN
3	C	149	GLN
4	D	112	ASN
4	D	148	ASN
4	E	159	GLN
5	F	13	HIS
5	F	177	GLN
5	F	227	GLN
5	F	816	HIS
11	M	365	HIS
11	M	459	HIS
1	a	128	GLN
1	a	416	GLN
2	b	82	HIS
2	b	120	HIS
3	c	6	GLN
3	c	21	ASN

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Mol	Chain	Res	Type
3	c	224	GLN
4	d	9	HIS
4	d	54	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 3 ligands modelled in this entry, 2 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	$\# Z > 2$
13	DZ4	M	503	12	31,32,32	3.37	15 (48%)	44,50,50	1.93	11 (25%)

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
13	DZ4	M	503	12	-	8/19/34/34	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	503	DZ4	C2'-C3'	-8.42	1.31	1.52
13	M	503	DZ4	O4'-C4'	-6.88	1.29	1.45
13	M	503	DZ4	O4'-C1'	6.62	1.57	1.42
13	M	503	DZ4	C1'-N9	-6.06	1.34	1.46
13	M	503	DZ4	PB-O3B	5.77	1.66	1.59
13	M	503	DZ4	C6-N6	4.85	1.46	1.34
13	M	503	DZ4	C3'-C4'	3.69	1.62	1.53
13	M	503	DZ4	PB-N3A	3.43	1.72	1.63
13	M	503	DZ4	PA-N3A	3.20	1.71	1.63
13	M	503	DZ4	PA-O1A	3.10	1.50	1.46
13	M	503	DZ4	PB-O1B	2.83	1.50	1.46
13	M	503	DZ4	C5-C4	-2.65	1.34	1.39
13	M	503	DZ4	C5-N7	-2.33	1.34	1.39
13	M	503	DZ4	PB-O2B	-2.13	1.51	1.56
13	M	503	DZ4	PA-O2A	-2.09	1.51	1.56

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	503	DZ4	N3-C2-N1	-5.59	120.12	128.58
13	M	503	DZ4	C5-C4-N3	-4.91	119.95	126.72
13	M	503	DZ4	N9-C8-N7	-4.25	107.90	113.94
13	M	503	DZ4	C2-N3-C4	3.32	119.95	111.83
13	M	503	DZ4	O1A-PA-N3A	-3.24	107.00	111.77
13	M	503	DZ4	N3-C4-N9	3.05	132.35	127.17
13	M	503	DZ4	C5-N7-C8	2.85	107.94	103.45
13	M	503	DZ4	C4-N9-C8	2.37	108.22	105.74
13	M	503	DZ4	N6-C6-N1	-2.31	113.23	118.38
13	M	503	DZ4	C4-C5-N7	-2.05	108.24	110.58
13	M	503	DZ4	O5'-PA-O1A	-2.02	108.28	114.27

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	M	503	DZ4	PB-N3A-PA-O5'
13	M	503	DZ4	PG-O3B-PB-O1B
13	M	503	DZ4	PG-O3B-PB-O2B
13	M	503	DZ4	O4'-C4'-C5'-O5'
13	M	503	DZ4	C3'-C4'-C5'-O5'
13	M	503	DZ4	O4'-C1'-N9-C4

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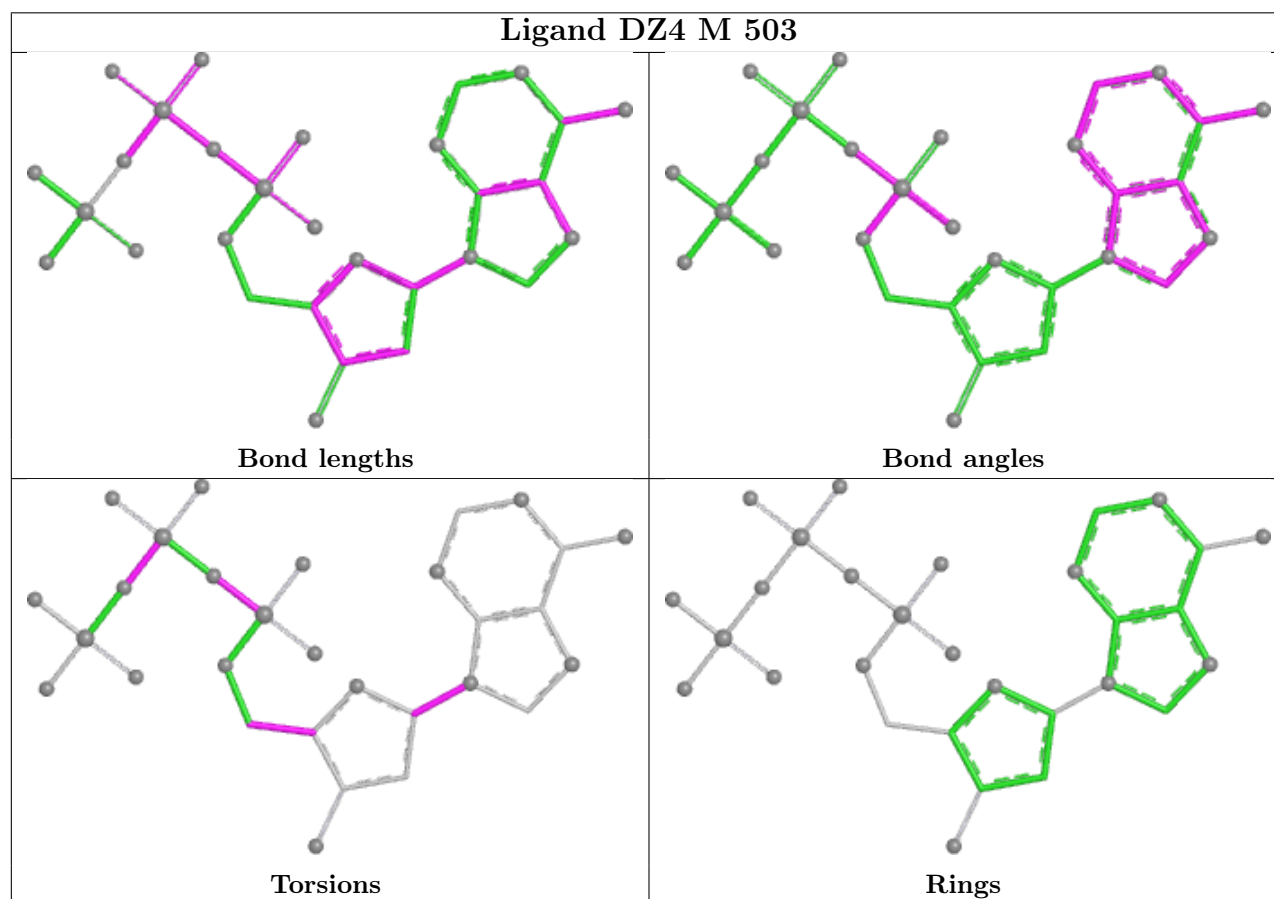
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Mol	Chain	Res	Type	Atoms
13	M	503	DZ4	O4'-C1'-N9-C8
13	M	503	DZ4	C2'-C1'-N9-C4

There are no ring outliers.

No monomer is involved in short contacts.

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 Map visualisation

This section contains visualisations of the EMDB entry EMD-45807. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.