



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:29 AM UTC

PDB ID : 7LNI / pdb_00007lni
Title : SeMet CamA Adenine Methyltransferase Complexed to Cognate Substrate DNA
Authors : Horton, J.R.; Cheng, X.; Zhou, J.
Deposited on : 2021-02-07
Resolution : 2.68 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
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

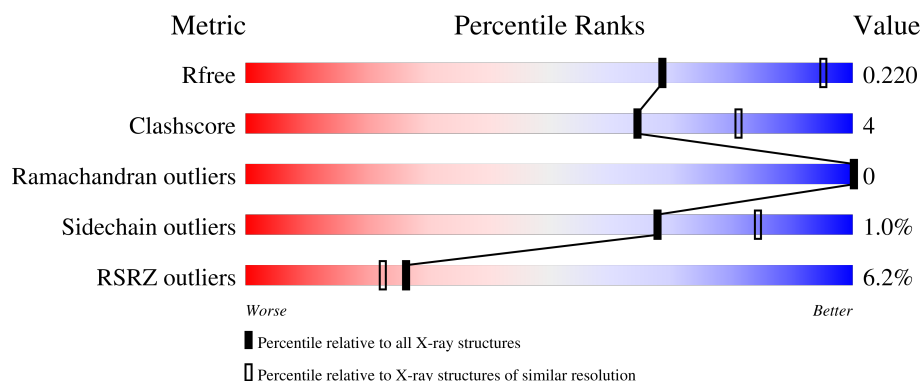
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	578	4% 85% 9% 5%
1	B	578	4% 83% 12% 5%
1	C	578	10% 83% 10% 7%
2	E	14	7% 64% 36%
2	G	14	50% 50%

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Mol	Chain	Length	Quality of chain
2	I	14	7% 64% 36%
3	D	14	7% 86% 14%
3	F	14	86% 14%
3	H	14	100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15353 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 Site-specific DNA-methyltransferase (adenine-specific).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	547	Total	C	N	O	S	Se	0	1	0
			4521	2944	721	839	12	5			
1	B	551	Total	C	N	O	S	Se	0	0	0
			4544	2961	726	840	12	5			
1	C	540	Total	C	N	O	S	Se	0	0	0
			4306	2801	687	801	12	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP Q183J3
B	0	HIS	-	expression tag	UNP Q183J3
C	0	HIS	-	expression tag	UNP Q183J3

- Molecule 2 is a DNA chain called DNA Strand 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	14	Total	C	N	O	P	0	0	0
			287	139	50	85	13			
2	G	14	Total	C	N	O	P	0	0	0
			287	139	50	85	13			
2	I	14	Total	C	N	O	P	0	0	0
			287	139	50	85	13			

- Molecule 3 is a DNA chain called DNA Strand 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	14	Total	C	N	O	P	0	0	0
			281	136	53	79	13			
3	F	14	Total	C	N	O	P	0	0	0
			281	136	53	79	13			
3	H	14	Total	C	N	O	P	0	0	0
			281	136	53	79	13			

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	68	Total	O	0	0
			68	68		
5	B	78	Total	O	0	0
			78	78		
5	C	42	Total	O	0	0
			42	42		
5	E	10	Total	O	0	0
			10	10		
5	D	18	Total	O	0	0
			18	18		
5	F	22	Total	O	0	0
			22	22		
5	G	8	Total	O	0	0
			8	8		
5	H	13	Total	O	0	0
			13	13		

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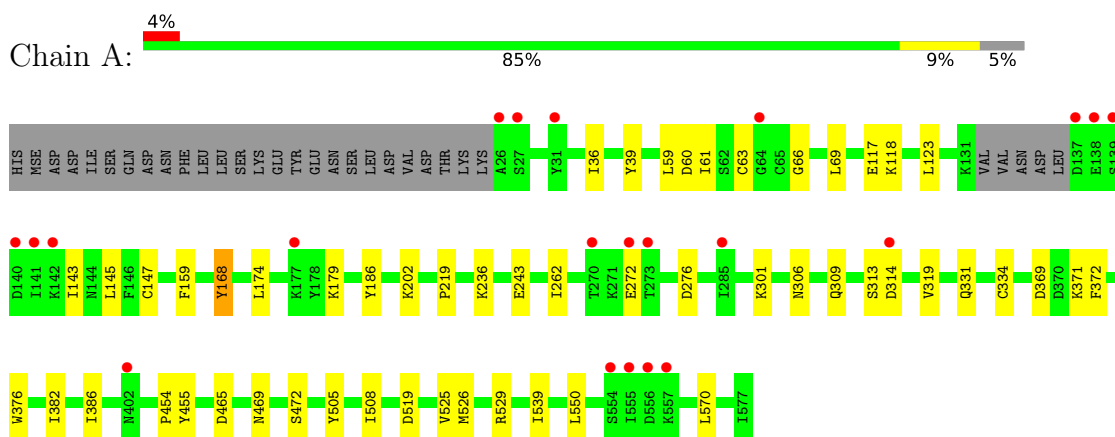
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	7	Total	O	0	0
			7	7		

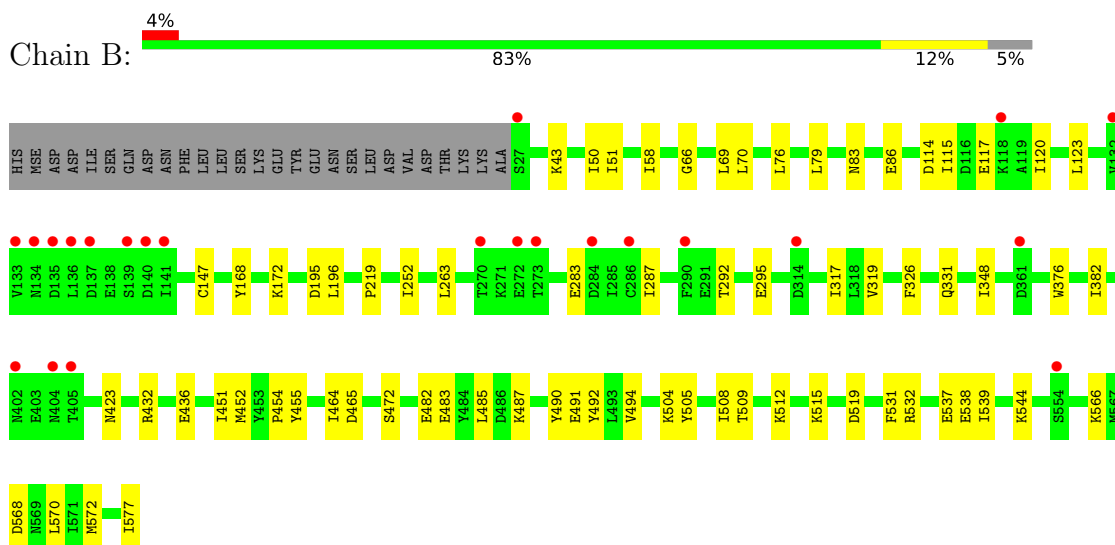
3 Residue-property plots

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 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.

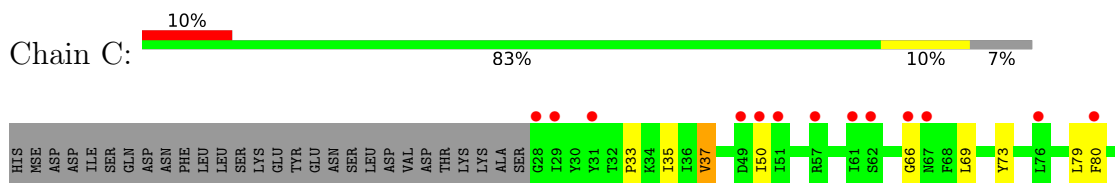
- Molecule 1: Site-specific DNA-methyltransferase (adenine-specific)

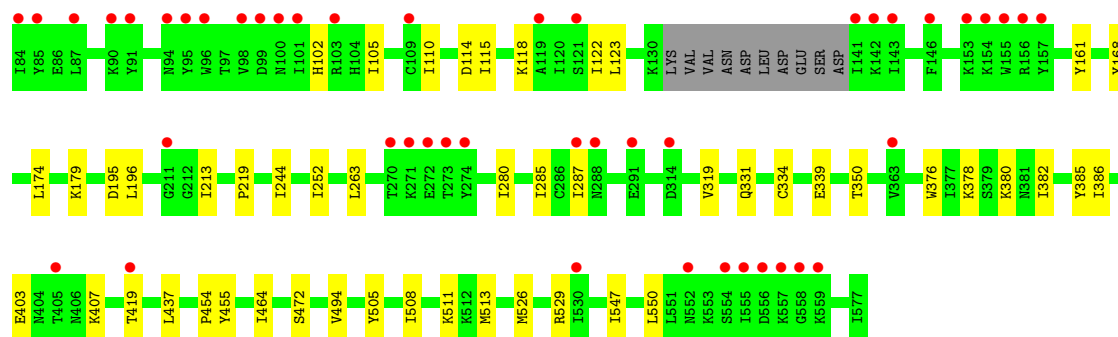


- Molecule 1: Site-specific DNA-methyltransferase (adenine-specific)

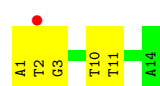


- Molecule 1: Site-specific DNA-methyltransferase (adenine-specific)





- Molecule 2: DNA Strand 2



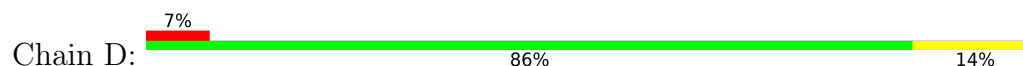
- Molecule 2: DNA Strand 2



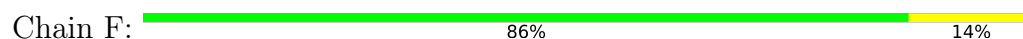
- Molecule 2: DNA Strand 2



- Molecule 3: DNA Strand 1



- Molecule 3: DNA Strand 1



- Molecule 3: DNA Strand 1



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.07Å 160.99Å 231.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.76 – 2.68 40.76 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.2 (40.76-2.68) 90.8 (40.76-2.68)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.92 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.203 , 0.223 0.202 , 0.220	Depositor DCC
R_{free} test set	1999 reflections (2.31%)	wwPDB-VP
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15353	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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: EDO

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	0.09	0/4612	0.25	0/6201
1	B	0.09	0/4633	0.26	0/6230
1	C	0.09	0/4388	0.25	0/5918
2	E	0.19	0/321	0.40	0/495
2	G	0.20	0/321	0.43	0/495
2	I	0.19	0/321	0.40	0/495
3	D	0.15	0/315	0.32	0/483
3	F	0.14	0/315	0.29	0/483
3	H	0.14	0/315	0.28	0/483
All	All	0.10	0/15541	0.27	0/21283

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	4521	0	4484	28	0
1	B	4544	0	4522	41	0
1	C	4306	0	4138	33	0
2	E	287	0	162	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	287	0	162	5	0
2	I	287	0	162	3	0
3	D	281	0	159	1	0
3	F	281	0	159	1	0
3	H	281	0	159	0	0
4	B	4	0	6	0	0
4	F	4	0	6	0	0
4	I	4	0	6	0	0
5	A	68	0	0	0	0
5	B	78	0	0	1	0
5	C	42	0	0	0	0
5	D	18	0	0	0	0
5	E	10	0	0	0	0
5	F	22	0	0	0	0
5	G	8	0	0	0	0
5	H	13	0	0	0	0
5	I	7	0	0	0	0
All	All	15353	0	14125	112	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 4.

All (112) 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:69:LEU:HD12	1:A:123:LEU:HD21	1.75	0.69
1:C:66:GLY:HA3	1:C:123:LEU:HD13	1.75	0.69
1:B:538:GLU:OE2	1:B:566:LYS:NZ	2.25	0.69
2:G:1:DA:H2"	2:G:2:DT:H5"	1.77	0.66
1:C:252:ILE:HD12	1:C:287:ILE:HD12	1.77	0.66
1:C:35:ILE:HD11	1:C:287:ILE:HG12	1.77	0.66
1:B:69:LEU:HD12	1:B:123:LEU:HD21	1.79	0.62
1:C:114:ASP:OD1	1:C:115:ILE:N	2.32	0.62
1:B:66:GLY:HA3	1:B:123:LEU:HD13	1.82	0.61
1:B:51:ILE:HD11	1:B:83:ASN:HB3	1.84	0.59
1:B:452:MSE:HE2	1:B:465:ASP:HB2	1.85	0.58
1:B:252:ILE:HD12	1:B:287:ILE:HD12	1.86	0.58
1:C:174:LEU:O	1:C:179:LYS:NZ	2.38	0.57
1:C:339:GLU:HA	1:C:526:MSE:HE3	1.88	0.56
1:B:168:TYR:CE1	1:B:219:PRO:HD3	2.41	0.55
1:C:168:TYR:CE1	1:C:219:PRO:HD3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:LYS:NZ	2:G:5:DG:OP2	2.39	0.55
1:A:168:TYR:CE1	1:A:219:PRO:HD3	2.42	0.55
1:B:43:LYS:NZ	5:B:704:HOH:O	2.40	0.54
1:A:66:GLY:HA3	1:A:123:LEU:HD13	1.90	0.53
1:C:69:LEU:HD22	1:C:110:ILE:HG23	1.92	0.52
1:C:195:ASP:OD1	1:C:196:LEU:N	2.43	0.52
1:C:73:TYR:HD1	1:C:105:ILE:HG21	1.74	0.52
1:A:117:GLU:HG3	1:A:147:CYS:SG	2.50	0.52
1:C:118:LYS:O	1:C:122:ILE:HG12	2.09	0.52
1:A:369:ASP:OD2	1:A:371:LYS:NZ	2.42	0.51
1:C:376:TRP:HE1	1:C:378:LYS:HE2	1.74	0.51
1:B:58:ILE:HD13	1:B:76:LEU:HD11	1.93	0.50
1:B:491:GLU:HG2	1:B:544:LYS:HG2	1.94	0.50
1:C:50:ILE:HD11	1:C:80:PHE:HE1	1.76	0.50
1:B:86:GLU:N	1:B:86:GLU:OE1	2.41	0.49
1:C:161:TYR:HE1	1:C:213:ILE:HD12	1.77	0.49
1:B:117:GLU:HB3	1:B:147:CYS:SG	2.52	0.49
1:B:331:GLN:OE1	1:B:505:TYR:OH	2.25	0.49
1:B:195:ASP:OD1	1:B:196:LEU:N	2.45	0.48
1:B:504:LYS:O	1:B:508:ILE:HG12	2.13	0.48
1:A:174:LEU:HD23	1:A:179:LYS:HG2	1.93	0.48
2:E:10:DT:H2''	2:E:11:DT:H72	1.95	0.48
1:C:386:ILE:HD13	1:C:550:LEU:HB3	1.94	0.48
1:A:386:ILE:HD13	1:A:550:LEU:HB3	1.95	0.48
1:C:73:TYR:HB2	1:C:110:ILE:HD11	1.95	0.48
1:C:331:GLN:OE1	1:C:505:TYR:OH	2.26	0.48
3:F:13:DC:H2''	3:F:14:DA:C8	2.48	0.48
1:C:73:TYR:OH	1:C:102:HIS:ND1	2.43	0.48
1:C:280:ILE:HD11	1:C:285:ILE:HG12	1.95	0.48
1:B:432:ARG:HG3	1:B:436:GLU:HG3	1.96	0.47
1:C:319:VAL:HG11	1:C:508:ILE:HG23	1.97	0.47
2:G:2:DT:H2''	2:G:3:DG:C8	2.49	0.47
1:B:382:ILE:HG21	1:B:454:PRO:HD3	1.97	0.47
2:I:10:DT:H2''	2:I:11:DT:H72	1.97	0.46
1:B:326:PHE:HE1	1:B:577:ILE:HD13	1.78	0.46
1:A:313:SER:OG	1:A:314:ASP:N	2.48	0.46
1:C:174:LEU:HB3	1:C:179:LYS:HG3	1.98	0.46
1:C:334:CYS:O	1:C:529:ARG:NH1	2.49	0.46
1:C:403:GLU:O	1:C:407:LYS:HG2	2.16	0.46
1:A:276:ASP:OD1	1:A:306:ASN:ND2	2.48	0.46
1:B:283:GLU:OE2	1:B:512:LYS:HE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2:DT:H2"	2:I:3:DG:C8	2.51	0.46
1:A:539:ILE:HG13	1:A:570:LEU:HD23	1.98	0.45
3:D:13:DC:H2"	3:D:14:DA:C8	2.51	0.45
1:A:236:LYS:NZ	1:A:309:GLN:O	2.49	0.45
1:B:539:ILE:HG13	1:B:570:LEU:HD23	1.99	0.45
1:C:376:TRP:CZ2	1:C:472:SER:HB2	2.52	0.45
1:B:50:ILE:HD12	1:B:79:LEU:HD23	1.99	0.44
1:B:508:ILE:HG22	1:B:509:THR:HG23	1.99	0.44
1:B:482:GLU:HA	1:B:485:LEU:HD12	2.00	0.44
1:A:186:TYR:HD2	1:A:202:LYS:HD3	1.82	0.44
1:A:331:GLN:OE1	1:A:505:TYR:OH	2.23	0.44
1:B:117:GLU:HA	1:B:120:ILE:HB	2.00	0.43
2:G:10:DT:H2"	2:G:11:DT:H72	1.99	0.43
1:A:143:ILE:HG22	1:A:145:LEU:HG	2.00	0.43
1:B:114:ASP:O	1:B:147:CYS:HA	2.18	0.43
1:C:376:TRP:HZ2	1:C:472:SER:HB2	1.84	0.43
1:B:492:TYR:OH	1:B:531:PHE:O	2.33	0.43
1:A:36:ILE:HD12	1:A:262:ILE:HD11	2.00	0.43
1:B:172:LYS:NZ	2:G:9:DT:O2	2.52	0.42
1:B:483:GLU:OE1	1:B:483:GLU:N	2.45	0.42
1:C:244:ILE:HG12	1:C:263:LEU:HD13	2.01	0.42
1:B:537:GLU:H	1:B:537:GLU:CD	2.28	0.42
1:B:464:ILE:HG13	1:B:494:VAL:HG11	2.02	0.42
1:A:371:LYS:HE2	1:A:372:PHE:CZ	2.55	0.42
1:B:292:THR:HG23	1:B:295:GLU:H	1.85	0.42
1:C:350:THR:HG22	1:C:437:LEU:HD22	2.02	0.42
1:A:376:TRP:CZ2	1:A:472:SER:HB2	2.55	0.41
1:B:487:LYS:HG3	1:B:532:ARG:HH11	1.85	0.41
1:A:334:CYS:O	1:A:529:ARG:NH1	2.52	0.41
1:B:317:ILE:HG22	1:B:319:VAL:HG22	2.01	0.41
1:B:487:LYS:HE3	1:B:487:LYS:HB2	1.89	0.41
1:B:568:ASP:O	1:B:572:MSE:HG3	2.20	0.41
1:B:114:ASP:OD1	1:B:115:ILE:N	2.53	0.41
1:A:465:ASP:OD1	1:A:469:ASN:ND2	2.46	0.41
1:C:511:LYS:HD3	1:C:513:MSE:SE	2.71	0.41
2:E:1:DA:H2"	2:E:2:DT:H5"	2.03	0.41
1:A:382:ILE:HG21	1:A:454:PRO:HD3	2.03	0.41
1:B:348:ILE:O	1:B:472:SER:HA	2.20	0.41
1:C:380:LYS:HG3	2:I:8:DT:OP2	2.20	0.41
1:B:532:ARG:HE	1:B:532:ARG:HB2	1.54	0.41
1:A:319:VAL:HG11	1:A:508:ILE:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:VAL:HG12	1:A:526:MSE:HE2	2.02	0.40
1:C:464:ILE:HG13	1:C:494:VAL:HG11	2.03	0.40
1:A:39:TYR:OH	1:A:243:GLU:OE2	2.32	0.40
1:A:174:LEU:O	1:A:179:LYS:NZ	2.52	0.40
1:C:33:PRO:O	1:C:37:VAL:HG12	2.21	0.40
1:C:385:TYR:HB3	1:C:547:ILE:HG12	2.02	0.40
1:A:118:LYS:HB3	1:A:118:LYS:HE3	1.71	0.40
1:C:382:ILE:HG21	1:C:454:PRO:HD3	2.01	0.40
1:A:59:LEU:HD22	1:A:159:PHE:CE1	2.56	0.40
1:A:60:ASP:HB3	1:A:63:CYS:HB3	2.04	0.40
1:A:301:LYS:HA	1:A:301:LYS:HD3	1.91	0.40
2:E:2:DT:H2"	2:E:3:DG:C8	2.57	0.40
1:B:376:TRP:CZ2	1:B:472:SER:HB2	2.57	0.40
1:B:451:ILE:HG13	1:B:490:TYR:HD1	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	544/578 (94%)	533 (98%)	11 (2%)	0	100	100
1	B	549/578 (95%)	537 (98%)	12 (2%)	0	100	100
1	C	536/578 (93%)	525 (98%)	11 (2%)	0	100	100
All	All	1629/1734 (94%)	1595 (98%)	34 (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 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	494/542 (91%)	489 (99%)	5 (1%)	68	84
1	B	497/542 (92%)	492 (99%)	5 (1%)	68	84
1	C	449/542 (83%)	445 (99%)	4 (1%)	70	86
All	All	1440/1626 (89%)	1426 (99%)	14 (1%)	68	84

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ILE
1	A	168	TYR
1	A	272	GLU
1	A	455	TYR
1	A	519	ASP
1	B	70	LEU
1	B	263	LEU
1	B	423	ASN
1	B	455	TYR
1	B	519	ASP
1	C	37	VAL
1	C	79	LEU
1	C	419	THR
1	C	455	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	251	ASN
1	B	107	ASN
1	B	306	ASN
1	B	469	ASN
1	C	144	ASN
1	C	251	ASN

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](#)

3 ligands 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	$\# Z > 2$
4	EDO	B	601	-	3,3,3	0.43	0	2,2,2	0.36	0
4	EDO	F	101	-	3,3,3	0.43	0	2,2,2	0.37	0
4	EDO	I	101	-	3,3,3	0.44	0	2,2,2	0.36	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
4	EDO	B	601	-	-	0/1/1/1	-
4	EDO	F	101	-	-	0/1/1/1	-
4	EDO	I	101	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	542/578 (93%)	0.23	21 (3%)	43	38	23, 47, 83, 137	1 (0%)
1	B	546/578 (94%)	0.19	23 (4%)	40	36	27, 46, 83, 193	0
1	C	535/578 (92%)	0.69	59 (11%)	10	8	34, 60, 121, 172	0
2	E	14/14 (100%)	-0.06	1 (7%)	22	18	35, 41, 155, 176	0
2	G	14/14 (100%)	-0.45	0	100	100	32, 38, 64, 69	0
2	I	14/14 (100%)	0.14	1 (7%)	22	18	42, 52, 134, 178	0
3	D	14/14 (100%)	-0.12	1 (7%)	22	18	30, 40, 117, 147	0
3	F	14/14 (100%)	-0.34	0	100	100	29, 36, 74, 75	0
3	H	14/14 (100%)	-0.07	0	100	100	38, 52, 125, 164	0
All	All	1707/1818 (93%)	0.34	106 (6%)	26	22	23, 51, 109, 193	1 (0%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	140	ASP	5.9
1	B	132	VAL	5.7
1	B	402	ASN	5.5
1	C	61	ILE	5.2
1	C	273	THR	5.2
1	A	139	SER	5.1
1	C	272	GLU	4.9
1	C	49	ASP	4.7
1	B	133	VAL	4.7
1	A	140	ASP	4.5
1	C	554	SER	4.5
1	B	134	ASN	4.5
1	C	91	TYR	4.4
1	C	556	ASP	4.3
1	A	554	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	138	GLU	4.1
1	A	273	THR	4.1
1	C	100	ASN	3.9
1	C	28	GLY	3.9
1	C	85	TYR	3.9
1	C	67	ASN	3.9
1	C	270	THR	3.8
1	B	404	ASN	3.8
1	C	95	TYR	3.8
1	B	137	ASP	3.7
1	C	157	TYR	3.6
1	C	557	LYS	3.6
1	C	98	VAL	3.6
2	I	1	DA	3.6
1	C	99	ASP	3.5
1	B	273	THR	3.5
1	C	555	ILE	3.5
1	B	284	ASP	3.4
1	A	272	GLU	3.4
1	C	274	TYR	3.3
1	B	405	THR	3.3
1	A	26	ALA	3.2
1	C	94	ASN	3.2
1	C	119	ALA	3.2
1	C	96	TRP	3.2
1	C	287	ILE	3.2
1	A	137	ASP	3.1
1	B	135	ASP	3.1
1	C	155	TRP	3.0
1	A	556	ASP	2.9
1	B	361	ASP	2.9
1	A	270	THR	2.9
1	C	146	PHE	2.9
1	C	363	VAL	2.9
1	C	141	ILE	2.8
1	C	62	SER	2.8
1	B	136	LEU	2.8
1	C	143	ILE	2.8
1	C	51	ILE	2.7
1	C	405	THR	2.7
1	A	27	SER	2.7
1	C	291	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	50	ILE	2.6
1	B	554	SER	2.6
1	B	314	ASP	2.6
1	A	555	ILE	2.6
1	C	80	PHE	2.6
1	B	272	GLU	2.6
1	B	286	CYS	2.6
1	B	139	SER	2.5
1	C	76	LEU	2.5
1	A	141	ILE	2.5
1	C	153	LYS	2.5
1	A	177	LYS	2.5
1	A	314	ASP	2.5
1	C	31	TYR	2.5
1	A	402	ASN	2.4
1	C	90	LYS	2.4
1	C	142	LYS	2.4
1	C	101	ILE	2.4
1	C	559	LYS	2.4
1	A	285	ILE	2.3
1	B	27	SER	2.3
1	C	271	LYS	2.3
1	C	154	LYS	2.3
1	C	109	CYS	2.3
1	C	84	ILE	2.3
1	A	557	LYS	2.3
1	C	156	ARG	2.3
1	C	288	ASN	2.2
1	B	118	LYS	2.2
1	C	87	LEU	2.2
1	B	270	THR	2.2
1	C	552	ASN	2.2
1	C	211	GLY	2.2
1	C	29	ILE	2.1
1	C	103	ARG	2.1
1	C	419	THR	2.1
1	C	530	ILE	2.1
1	C	314	ASP	2.1
1	C	57	ARG	2.1
1	A	142	LYS	2.1
3	D	14	DA	2.1
1	B	141	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	121	SER	2.0
1	A	64	GLY	2.0
1	C	66	GLY	2.0
1	A	31	TYR	2.0
1	B	290	PHE	2.0
2	E	2	DT	2.0
1	C	558	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	I	101	4/4	0.78	0.22	51,56,61,68	0
4	EDO	B	601	4/4	0.79	0.19	59,72,78,78	0
4	EDO	F	101	4/4	0.88	0.16	33,48,53,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.