



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 10:59 PM EDT

PDB ID : 7LNJ
Title : 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 : 4.02b-467
Xtrriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

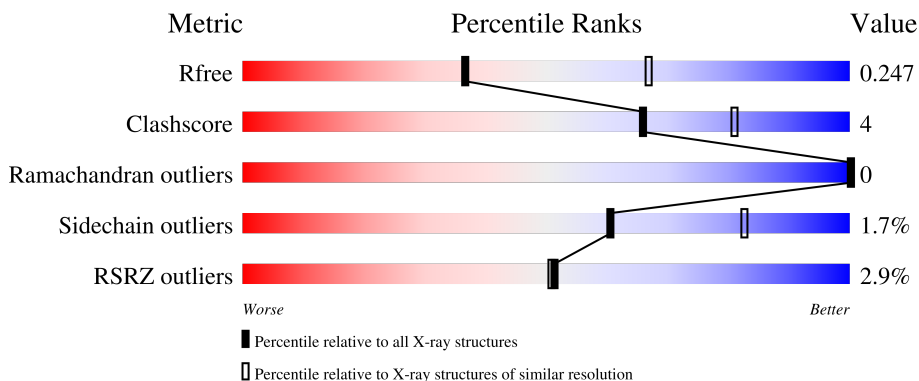
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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.



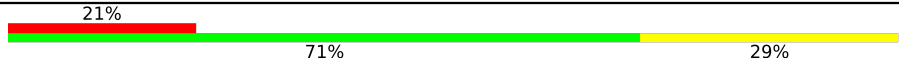
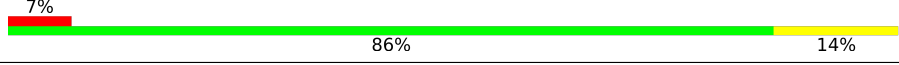
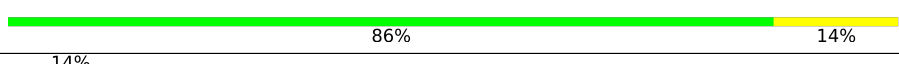

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">81% 12% 6%</p>
1	B	578	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 84%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">84% 10% 5%</p>
1	C	578	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">81% 12% 7%</p>
2	E	14	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">79% 14% 7%</p>
2	G	14	<div style="display: flex; align-items: center;"> <div style="width: 71%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 29%; height: 10px; background-color: yellow;"></div> </div> <p style="text-align: center;">71% 29%</p>

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Mol	Chain	Length	Quality of chain
2	I	14	
3	D	14	
3	F	14	
3	H	14	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15057 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
			Total	C	N	O	S			
1	A	543	Total 4465	C 2908	N 714	O 827	S 16	0	1	0
1	B	550	Total 4502	C 2932	N 720	O 834	S 16	0	0	0
1	C	539	Total 4280	C 2791	N 681	O 791	S 17	0	0	0

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.

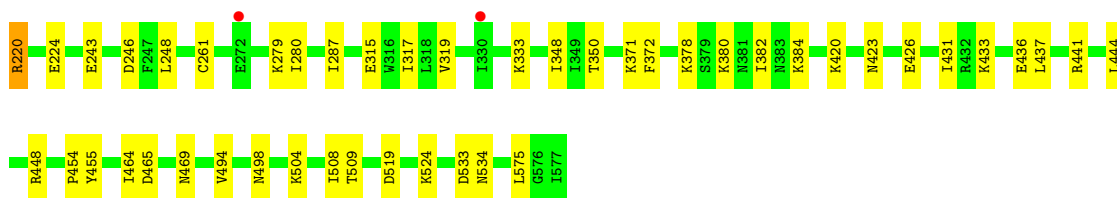
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	E	13	Total 269	C 129	N 45	O 82	P 13	0	0	0
2	G	14	Total 287	C 139	N 50	O 85	P 13	0	0	0
2	I	14	Total 287	C 139	N 50	O 85	P 13	0	0	0

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

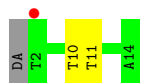
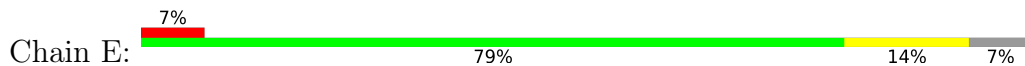
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	D	14	Total 281	C 136	N 53	O 79	P 13	0	0	0
3	F	14	Total 281	C 136	N 53	O 79	P 13	0	0	0
3	H	14	Total 281	C 136	N 53	O 79	P 13	0	0	0

- Molecule 4 is water.

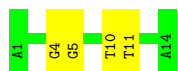
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	29	Total O 29 29	0	0
4	B	40	Total O 40 40	0	0
4	C	14	Total O 14 14	0	0
4	E	3	Total O 3 3	0	0
4	D	10	Total O 10 10	0	0
4	F	11	Total O 11 11	0	0
4	G	4	Total O 4 4	0	0
4	H	11	Total O 11 11	0	0
4	I	2	Total O 2 2	0	0



• Molecule 2: DNA Strand 2



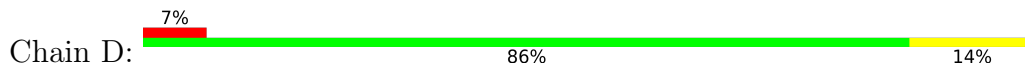
• Molecule 2: DNA Strand 2



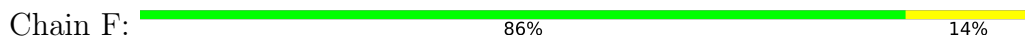
• Molecule 2: DNA Strand 2



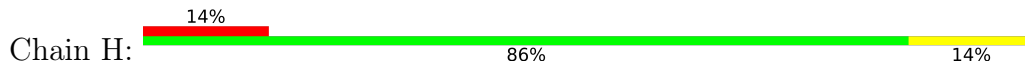
• Molecule 3: DNA Strand 1



• Molecule 3: DNA Strand 1



• Molecule 3: DNA Strand 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.25Å 161.36Å 230.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.35 – 2.68 44.35 – 2.68	Depositor EDS
% Data completeness (in resolution range)	87.3 (44.35-2.68) 87.3 (44.35-2.68)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.69Å)	Xtrriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.210 , 0.251 0.208 , 0.247	Depositor DCC
R_{free} test set	3871 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	56.9	Xtrriage
Anisotropy	0.520	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15057	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.24	0/4560	0.43	0/6144
1	B	0.24	0/4596	0.43	0/6197
1	C	0.24	0/4368	0.43	0/5904
2	E	0.52	0/300	1.01	0/462
2	G	0.54	0/321	1.00	0/495
2	I	0.52	0/321	0.98	0/495
3	D	0.46	0/315	0.84	0/483
3	F	0.45	0/315	0.83	0/483
3	H	0.45	0/315	0.82	0/483
All	All	0.29	0/15411	0.53	0/21146

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 [i](#)

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	4465	0	4412	40	0
1	B	4502	0	4431	31	0
1	C	4280	0	4104	37	0
2	E	269	0	150	1	0
2	G	287	0	162	2	0
2	I	287	0	162	3	0
3	D	281	0	159	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	281	0	159	1	0
3	H	281	0	159	1	0
4	A	29	0	0	0	0
4	B	40	0	0	0	0
4	C	14	0	0	0	0
4	D	10	0	0	0	0
4	E	3	0	0	0	0
4	F	11	0	0	0	0
4	G	4	0	0	0	0
4	H	11	0	0	0	0
4	I	2	0	0	0	0
All	All	15057	0	13898	115	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 (115) 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:349:ILE:HB	1:A:439:TRP:HB2	1.77	0.66
1:A:69:LEU:HD12	1:A:123:LEU:HD21	1.78	0.65
1:A:369:ASP:OD2	1:A:371:LYS:NZ	2.28	0.64
1:C:220:ARG:HB3	1:C:261:CYS:HB3	1.80	0.64
1:B:66:GLY:HA3	1:B:123:LEU:HD13	1.78	0.64
1:A:425:ARG:HA	1:A:428:LYS:HE2	1.81	0.63
1:A:66:GLY:HA3	1:A:123:LEU:HD13	1.80	0.62
1:B:58:ILE:HD13	1:B:76:LEU:HD11	1.85	0.59
1:A:168:TYR:CE1	1:A:219:PRO:HD3	2.39	0.57
1:B:280:ILE:HD11	1:B:285:ILE:HG12	1.87	0.57
1:C:168:TYR:CE1	1:C:219:PRO:HD3	2.40	0.56
1:B:168:TYR:CE1	1:B:219:PRO:HD3	2.42	0.55
1:A:86:GLU:N	1:A:86:GLU:OE1	2.38	0.55
1:B:44:THR:HG21	1:B:163:VAL:HG12	1.87	0.54
1:B:69:LEU:HD12	1:B:123:LEU:HD21	1.89	0.54
1:C:465:ASP:OD1	1:C:469:ASN:ND2	2.41	0.54
1:A:195:ASP:OD1	1:A:196:LEU:N	2.40	0.54
1:C:378:LYS:NZ	2:I:9:DT:OP2	2.40	0.54
1:A:482:GLU:HA	1:A:485:LEU:HD23	1.90	0.53
1:A:337:SER:OG	1:A:340:ASP:OD1	2.21	0.53
1:B:464:ILE:HG13	1:B:494:VAL:HG11	1.91	0.53
1:A:252:ILE:HD12	1:A:287:ILE:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:ASN:OD1	1:A:545:GLN:NE2	2.39	0.52
1:B:220:ARG:HB3	1:B:261:CYS:HB3	1.92	0.52
1:A:383:ASN:ND2	1:A:388:ASP:OD1	2.43	0.52
1:C:66:GLY:HA3	1:C:123:LEU:HD13	1.90	0.52
1:B:426:GLU:HG3	1:B:431:ILE:HD11	1.92	0.51
1:C:195:ASP:OD1	1:C:196:LEU:N	2.43	0.51
1:C:426:GLU:HG3	1:C:431:ILE:HD11	1.93	0.51
1:C:220:ARG:NH2	1:C:224:GLU:OE1	2.44	0.51
1:C:382:ILE:HG21	1:C:454:PRO:HD3	1.91	0.51
1:B:382:ILE:HG21	1:B:454:PRO:HD3	1.93	0.50
1:A:358:LEU:HB2	1:A:365:LEU:HD21	1.94	0.49
1:B:51:ILE:HD11	1:B:83:ASN:HB3	1.94	0.49
1:B:441:ARG:HB2	1:B:446:PHE:HE2	1.77	0.49
3:F:13:DC:H2"	3:F:14:DA:C8	2.47	0.49
1:A:143:ILE:HG22	1:A:145:LEU:HG	1.95	0.49
1:C:315:GLU:OE2	1:C:524:LYS:NZ	2.46	0.48
1:B:401:ASP:OD1	1:B:401:ASP:N	2.40	0.48
1:B:428:LYS:O	1:B:429:SER:OG	2.27	0.48
1:C:36:ILE:HG21	1:C:217:ILE:HD12	1.93	0.48
1:B:540:GLU:HG2	1:B:544:LYS:HE2	1.96	0.48
3:D:13:DC:H2"	3:D:14:DA:C8	2.49	0.48
1:C:348:ILE:HD13	1:C:441:ARG:HG2	1.95	0.48
1:C:120:ILE:HG13	1:C:145:LEU:HD13	1.95	0.47
1:B:195:ASP:OD1	1:B:196:LEU:N	2.47	0.47
1:C:248:LEU:HB2	1:C:280:ILE:HG22	1.96	0.47
1:C:533:ASP:OD1	1:C:534:ASN:N	2.43	0.47
2:E:10:DT:H2"	2:E:11:DT:H72	1.96	0.47
1:C:106:LEU:HD21	1:C:127:LEU:HD22	1.96	0.46
1:C:333:LYS:HG2	1:C:575:LEU:HA	1.97	0.46
1:A:378:LYS:HD3	1:A:378:LYS:HA	1.80	0.46
1:A:319:VAL:HG11	1:A:508:ILE:HG23	1.96	0.46
1:C:319:VAL:HG11	1:C:508:ILE:HG23	1.96	0.46
1:A:339:GLU:HG3	1:A:526:MET:HB3	1.97	0.46
1:A:464:ILE:HG13	1:A:494:VAL:HG11	1.98	0.46
1:B:192:ASP:OD1	1:B:193:LYS:NZ	2.37	0.45
1:A:382:ILE:HG21	1:A:454:PRO:HD3	1.99	0.45
1:A:39:TYR:OH	1:A:243:GLU:OE2	2.26	0.45
2:G:4:DG:H2"	2:G:5:DG:C8	2.52	0.45
1:A:297:LEU:HD13	1:A:297:LEU:HA	1.81	0.45
1:A:329:LYS:HE3	1:A:577:ILE:HG22	1.99	0.45
1:C:464:ILE:HG13	1:C:494:VAL:HG11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ARG:HH21	1:B:512:LYS:HB3	1.83	0.44
1:A:546:ILE:HG23	1:A:560:VAL:HG13	1.99	0.44
1:B:504:LYS:O	1:B:508:ILE:HG12	2.18	0.44
1:A:348:ILE:HD13	1:A:441:ARG:HG2	2.00	0.44
1:B:143:ILE:HG22	1:B:145:LEU:HG	1.99	0.44
1:C:317:ILE:HD12	1:C:509:THR:HG22	1.99	0.44
1:C:39:TYR:OH	1:C:243:GLU:OE2	2.29	0.43
1:A:389:LYS:HE3	1:A:389:LYS:HB2	1.86	0.43
1:B:485:LEU:HD23	1:B:485:LEU:HA	1.87	0.43
1:C:384:LYS:O	1:C:498:ASN:ND2	2.51	0.43
1:A:117:GLU:HG3	1:A:147:CYS:SG	2.59	0.43
1:B:114:ASP:OD1	1:B:115:ILE:N	2.52	0.43
1:B:566:LYS:HE3	1:B:566:LYS:HB2	1.87	0.43
1:C:371:LYS:HE3	1:C:372:PHE:CZ	2.53	0.43
1:C:119:ALA:O	1:C:122:ILE:HG22	2.19	0.43
1:A:319:VAL:HB	1:A:323:ASP:HB2	2.00	0.42
1:A:441:ARG:HB2	1:A:446:PHE:HE2	1.85	0.42
1:A:59:LEU:HD22	1:A:159:PHE:CE1	2.54	0.42
1:B:418:LYS:HG3	1:B:434:TRP:CE3	2.53	0.42
1:C:350:THR:HG22	1:C:437:LEU:HD22	2.01	0.42
1:B:338:LEU:HD23	1:B:338:LEU:HA	1.93	0.42
1:C:444:LEU:O	1:C:448:ARG:HD2	2.20	0.42
1:B:197:TYR:HA	1:B:200:PHE:HB2	2.00	0.42
1:B:348:ILE:HD13	1:B:441:ARG:HG2	2.01	0.42
1:C:380:LYS:HG3	2:I:7:DC:H3'	2.02	0.42
2:I:10:DT:H2''	2:I:11:DT:H72	2.02	0.42
1:B:36:ILE:HD12	1:B:262:ILE:HD11	2.02	0.42
3:H:13:DC:H2''	3:H:14:DA:C8	2.55	0.42
1:A:35:ILE:HD12	1:A:35:ILE:H	1.84	0.42
1:A:36:ILE:HD12	1:A:262:ILE:HD11	2.01	0.42
1:C:59:LEU:HA	1:C:111:TYR:O	2.21	0.41
1:C:59:LEU:HD22	1:C:159:PHE:CE1	2.55	0.41
1:C:433:LYS:HB2	1:C:436:GLU:HG3	2.03	0.41
1:A:168:TYR:CZ	1:A:219:PRO:HD3	2.54	0.41
2:G:10:DT:H2''	2:G:11:DT:H72	2.02	0.41
1:A:58:ILE:HD13	1:A:76:LEU:HD11	2.03	0.41
1:A:203:LYS:O	1:A:207:ILE:HG12	2.20	0.41
1:A:244:ILE:HG12	1:A:263:LEU:HD12	2.02	0.41
1:A:433:LYS:HB2	1:A:436:GLU:HG3	2.03	0.41
1:C:201:TYR:CE2	1:C:218:THR:HG21	2.56	0.41
1:C:420:LYS:HE2	1:C:420:LYS:HB2	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:TYR:HD1	1:C:105:ILE:HG21	1.85	0.41
1:C:143:ILE:HD12	1:C:143:ILE:H	1.86	0.41
1:C:287:ILE:H	1:C:287:ILE:HG13	1.62	0.41
1:A:192:ASP:OD1	1:A:193:LYS:NZ	2.44	0.40
1:A:369:ASP:OD1	1:A:370:ASP:N	2.54	0.40
1:A:512:LYS:HD3	1:A:518:TYR:CE2	2.56	0.40
1:B:201:TYR:CE2	1:B:218:THR:HG21	2.56	0.40
1:B:376:TRP:CZ2	1:B:472:SER:HB2	2.56	0.40
1:C:504:LYS:O	1:C:508:ILE:HG13	2.21	0.40
1:B:546:ILE:HG23	1:B:560:VAL:HG13	2.03	0.40
1:C:246:ASP:HB3	1:C:279:LYS:HD3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	540/578 (93%)	526 (97%)	14 (3%)	0	100	100
1	B	548/578 (95%)	535 (98%)	13 (2%)	0	100	100
1	C	535/578 (93%)	522 (98%)	13 (2%)	0	100	100
All	All	1623/1734 (94%)	1583 (98%)	40 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	484/548 (88%)	477 (99%)	7 (1%)	67	85
1	B	486/548 (89%)	477 (98%)	9 (2%)	57	80
1	C	443/548 (81%)	435 (98%)	8 (2%)	59	81
All	All	1413/1644 (86%)	1389 (98%)	24 (2%)	60	82

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	TYR
1	A	297	LEU
1	A	314	ASP
1	A	408	ARG
1	A	455	TYR
1	A	485	LEU
1	A	519	ASP
1	B	54	PRO
1	B	97	THR
1	B	168	TYR
1	B	220	ARG
1	B	273	THR
1	B	411	ASP
1	B	412	GLU
1	B	455	TYR
1	B	519	ASP
1	C	77	TYR
1	C	127	LEU
1	C	168	TYR
1	C	178	TYR
1	C	220	ARG
1	C	423	ASN
1	C	455	TYR
1	C	519	ASP

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

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	543/578 (93%)	-0.18	4 (0%) 87 88	30, 52, 84, 145	0
1	B	550/578 (95%)	-0.08	8 (1%) 73 74	32, 53, 87, 178	0
1	C	539/578 (93%)	0.22	31 (5%) 23 21	44, 70, 125, 158	0
2	E	13/14 (92%)	-0.32	1 (7%) 13 11	43, 45, 123, 159	0
2	G	14/14 (100%)	-0.60	0 100 100	41, 48, 66, 67	0
2	I	14/14 (100%)	0.55	3 (21%) 0 0	53, 57, 155, 159	0
3	D	14/14 (100%)	-0.15	1 (7%) 16 13	36, 45, 128, 153	0
3	F	14/14 (100%)	-0.17	0 100 100	36, 42, 77, 84	0
3	H	14/14 (100%)	0.36	2 (14%) 2 1	52, 62, 124, 158	0
All	All	1715/1818 (94%)	-0.02	50 (2%) 51 51	30, 58, 111, 178	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	14	DA	6.5
1	C	91	TYR	6.0
2	I	1	DA	5.6
1	C	87	LEU	4.8
1	C	95	TYR	4.8
1	C	94	ASN	4.8
1	C	113	ALA	4.6
1	C	108	TYR	4.3
1	C	55	TYR	4.0
1	C	121	SER	3.9
1	B	135	ASP	3.7
1	C	76	LEU	3.6
1	C	99	ASP	3.5
1	C	155	TRP	3.2
1	C	31	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	139	SER	3.1
3	D	14	DA	3.1
1	B	290	PHE	3.0
1	B	137	ASP	3.0
1	C	92	ASP	2.9
1	C	143	ILE	2.9
2	I	2	DT	2.8
1	C	103	ARG	2.7
1	C	96	TRP	2.6
1	C	97	THR	2.5
1	B	136	LEU	2.5
3	H	13	DC	2.5
1	C	73	TYR	2.5
1	A	409	ILE	2.5
1	C	100	ASN	2.5
1	A	284	ASP	2.5
1	B	404	ASN	2.4
1	C	118	LYS	2.4
1	C	89	LYS	2.3
1	C	77	TYR	2.3
1	C	80	PHE	2.3
1	C	106	LEU	2.2
2	I	3	DG	2.2
1	C	49	ASP	2.2
1	C	330	ILE	2.2
1	C	104	HIS	2.1
1	C	93	GLU	2.1
1	C	272	GLU	2.1
1	B	411	ASP	2.1
2	E	2	DT	2.1
1	A	372	PHE	2.0
1	A	289	LYS	2.0
1	C	90	LYS	2.0
1	C	119	ALA	2.0
1	B	123	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.