



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2020 – 10:13 AM BST

PDB ID : 3K4G
Title : Crystal structure of E. coli RNA polymerase alpha subunit C-terminal domain
Authors : Lara-Gonzalez, S.; Birktoft, J.; Lawson, C.L.
Deposited on : 2009-10-05
Resolution : 2.05 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

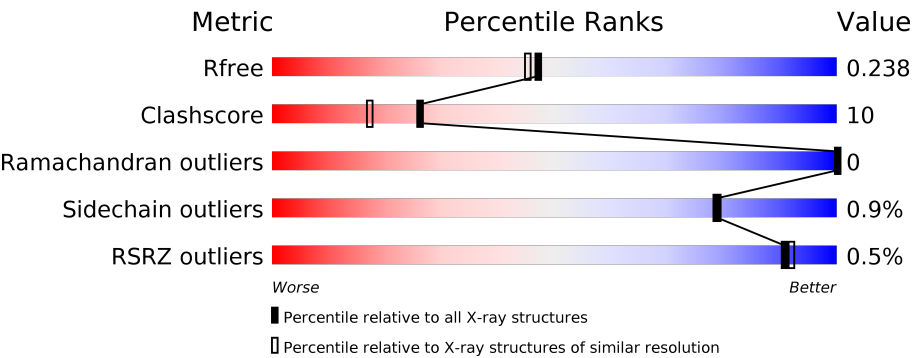
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

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 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 on 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	86	<div><div></div><div>78%19%..</div></div>
1	B	86	<div><div></div><div>74%21%..</div></div>
1	C	86	<div><div>2%</div><div></div><div>73%23%..</div></div>
1	D	86	<div><div></div><div>77%20%. </div></div>
1	E	86	<div><div></div><div>83%14%. </div></div>
1	F	86	<div><div></div><div>70%27%..</div></div>

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Mol	Chain	Length	Quality of chain
1	G	86	<div><div></div><div>77%</div><div>21%</div><div></div><div>.</div></div>
1	H	86	<div>%<div><div></div><div>81%</div><div>14%</div><div></div><div>..</div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5585 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	84	Total	C	N	O	S	0	1	0
			668	427	114	125	2			
1	B	83	Total	C	N	O	S	0	1	0
			654	422	111	119	2			
1	C	84	Total	C	N	O	S	0	1	0
			668	427	113	126	2			
1	D	83	Total	C	N	O	S	0	1	0
			657	421	113	121	2			
1	E	83	Total	C	N	O	S	0	1	0
			648	415	112	119	2			
1	F	84	Total	C	N	O	S	0	0	0
			663	423	111	127	2			
1	G	84	Total	C	N	O	S	0	1	0
			659	420	110	127	2			
1	H	83	Total	C	N	O	S	0	0	0
			647	415	107	123	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	244	MET	-	EXPRESSION TAG	UNP P0A7Z4
B	244	MET	-	EXPRESSION TAG	UNP P0A7Z4
C	244	MET	-	EXPRESSION TAG	UNP P0A7Z4
D	244	MET	-	EXPRESSION TAG	UNP P0A7Z4
E	244	MET	-	EXPRESSION TAG	UNP P0A7Z4
F	244	MET	-	EXPRESSION TAG	UNP P0A7Z4
G	244	MET	-	EXPRESSION TAG	UNP P0A7Z4
H	244	MET	-	EXPRESSION TAG	UNP P0A7Z4

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Na 1 1	0	0
2	A	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0
2	E	1	Total Na 1 1	0	0


- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	46	Total O 46 46	0	0
3	B	37	Total O 37 37	0	0
3	C	43	Total O 43 43	0	0
3	D	38	Total O 38 38	0	0
3	E	38	Total O 38 38	0	0
3	F	41	Total O 41 41	0	0
3	G	40	Total O 40 40	0	0
3	H	34	Total O 34 34	0	0

3 Residue-property plots [i](#)

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

- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A: 



- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B: 



- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain C: 




- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain D: 



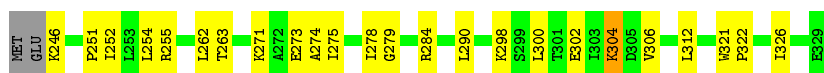
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain E: 

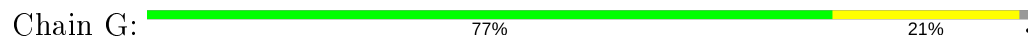


- Molecule 1: DNA-directed RNA polymerase subunit alpha

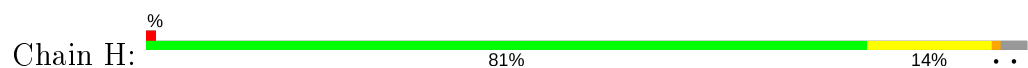
Chain F: 



- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.34Å 67.61Å 116.55Å 90.00° 90.12° 90.00°	Depositor
Resolution (Å)	47.02 – 2.05 47.02 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.02-2.05) 99.3 (47.02-2.05)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.5 _2	Depositor
R, R_{free}	0.193 , 0.236 0.194 , 0.238	Depositor DCC
R_{free} test set	1997 reflections (3.98%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 30.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.429 for h,-k,-l	Xtriage
Reported twinning fraction	0.437 for h,-k,-l	Depositor
Outliers	4 of 50220 reflections (0.008%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5585	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.36 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0677e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, MLY

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	0.22	0/622	0.43	0/850
1	B	0.21	0/602	0.44	0/826
1	C	0.21	0/622	0.42	0/850
1	D	0.22	0/611	0.43	0/837
1	E	0.21	0/608	0.42	0/833
1	F	0.22	0/614	0.41	0/840
1	G	0.22	0/619	0.42	0/847
1	H	0.22	0/598	0.45	0/821
All	All	0.22	0/4896	0.43	0/6704

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	668	0	697	14	0
1	B	654	0	690	17	0
1	C	668	0	695	19	0
1	D	657	0	689	14	0
1	E	648	0	673	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	663	0	686	18	0
1	G	659	0	674	16	0
1	H	647	0	669	12	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	E	1	0	0	0	0
2	G	1	0	0	0	0
3	A	46	0	0	1	0
3	B	37	0	0	0	0
3	C	43	0	0	1	0
3	D	38	0	0	0	0
3	E	38	0	0	0	0
3	F	41	0	0	0	0
3	G	40	0	0	2	0
3	H	34	0	0	0	0
All	All	5585	0	5473	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 10.

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:F:255:ARG:HB2	1:F:278:ILE:HD12	1.77	0.65
1:A:262:LEU:HD21	1:A:306:VAL:HG11	1.82	0.62
1:C:254:LEU:O	1:C:254:LEU:HD23	1.99	0.62
1:C:321:TRP:CD2	1:C:322:PRO:HA	2.36	0.61
1:E:252:ILE:HD13	1:E:312:LEU:HD11	1.83	0.60
1:B:262:LEU:HD13	1:B:306:VAL:HG21	1.84	0.59
1:E:279:GLY:HA3	1:E:321:TRP:CZ3	2.37	0.59
1:C:262:LEU:HD23	1:C:306:VAL:HG21	1.85	0.59
1:C:321:TRP:CZ3	1:C:323:PRO:HD3	2.39	0.58
1:D:286:GLU:HG3	1:D:300:LEU:HD12	1.85	0.58
1:C:265:ARG:HD2	1:F:326:ILE:HG21	1.86	0.57
1:A:285:THR:HG23	1:A:288:GLU:H	1.70	0.57
1:E:254:LEU:O	1:E:254:LEU:HD23	2.05	0.57
1:F:302:GLU:O	1:F:306:VAL:HG23	2.06	0.56
1:D:321:TRP:CD2	1:D:322:PRO:HA	2.42	0.55
1:A:279:GLY:HA3	1:A:321:TRP:CH2	2.41	0.55
1:E:279:GLY:HA3	1:E:321:TRP:CH2	2.41	0.55
1:F:263:THR:HG23	1:F:302:GLU:OE2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ARG:HB2	1:A:278:ILE:HD12	1.89	0.54
1:H:321:TRP:CD2	1:H:322:PRO:HA	2.43	0.53
1:F:321:TRP:CD2	1:F:322:PRO:HA	2.44	0.53
1:F:321:TRP:CG	1:F:322:PRO:HA	2.44	0.52
1:G:321:TRP:CD2	1:G:322:PRO:HA	2.44	0.52
1:G:310:ARG:HD2	3:G:333:HOH:O	2.10	0.52
1:G:279:GLY:O	1:G:283:GLN:HG3	2.10	0.52
1:B:321:TRP:CG	1:B:322:PRO:HA	2.45	0.51
1:C:301:THR:HA	1:C:304:MLY:HH23	1.93	0.51
1:H:288:GLU:OE1	1:H:291:MLY:HH23	2.11	0.51
1:A:321:TRP:CG	1:A:322:PRO:HA	2.45	0.51
1:D:302:GLU:O	1:D:306:VAL:HG23	2.11	0.50
1:D:321:TRP:CG	1:D:322:PRO:HA	2.46	0.50
1:F:262:LEU:HD23	1:F:306:VAL:HG21	1.94	0.50
1:A:321:TRP:CD2	1:A:322:PRO:HA	2.46	0.50
1:C:252:ILE:HG13	1:C:255:ARG:HH11	1.76	0.50
1:H:321:TRP:CG	1:H:322:PRO:HA	2.47	0.50
1:C:249:PHE:CZ	1:D:323:PRO:HD2	2.47	0.50
1:G:302:GLU:O	1:G:306:VAL:HG23	2.13	0.49
1:B:299:SER:O	1:B:303:ILE:HG13	2.12	0.49
1:C:321:TRP:CE3	1:C:323:PRO:HD3	2.48	0.48
1:F:279:GLY:HA3	1:F:321:TRP:CH2	2.49	0.48
1:G:321:TRP:CE3	1:G:323:PRO:HD3	2.47	0.48
1:A:321:TRP:CE3	1:A:323:PRO:HD3	2.49	0.48
1:B:279:GLY:HA3	1:B:321:TRP:CZ3	2.49	0.48
1:B:286:GLU:HG3	1:B:300:LEU:HD12	1.95	0.47
1:G:321:TRP:CG	1:G:322:PRO:HA	2.48	0.47
1:C:263:THR:HG23	1:C:302:GLU:OE2	2.14	0.47
1:C:321:TRP:CG	1:C:322:PRO:HA	2.50	0.47
1:H:321:TRP:CZ3	1:H:323:PRO:HD3	2.49	0.47
1:A:321:TRP:CZ3	1:A:323:PRO:HD3	2.49	0.47
1:G:262:LEU:HD23	1:G:306:VAL:HG21	1.97	0.47
1:G:246:MLY:HB3	1:H:276:HIS:CD2	2.51	0.46
1:F:275:ILE:HD11	1:F:284:ARG:HG3	1.98	0.46
1:G:279:GLY:HA3	1:G:321:TRP:CH2	2.51	0.46
1:H:283:GLN:CG	1:H:318:LEU:HD22	2.45	0.46
1:B:265:ARG:HH11	1:B:265:ARG:HG3	1.80	0.46
1:A:300:LEU:O	1:A:304:MLY:HG2	2.16	0.46
1:G:321:TRP:CZ3	1:G:323:PRO:HD3	2.51	0.46
1:C:295:LEU:HA	3:C:337:HOH:O	2.15	0.46
1:E:249:PHE:CE2	1:F:322:PRO:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:TRP:CD2	1:B:322:PRO:HA	2.51	0.45
1:H:321:TRP:CE3	1:H:323:PRO:HD3	2.51	0.45
1:A:254:LEU:HD21	1:B:254:LEU:HD21	1.99	0.45
1:C:290:LEU:HG	1:C:300:LEU:HG	1.97	0.45
1:A:271:MLY:HD2	1:A:271:MLY:HH13	1.73	0.45
1:B:321:TRP:CE3	1:B:323:PRO:HD3	2.52	0.45
1:E:265:ARG:HG3	1:E:265:ARG:HH11	1.81	0.45
1:D:271:MLY:HD3	1:D:271:MLY:HH22	1.51	0.44
1:B:265:ARG:NH1	1:B:265:ARG:HG3	2.31	0.44
1:D:252:ILE:HD11	1:D:310:ARG:HH11	1.82	0.44
1:F:252:ILE:HD13	1:F:312:LEU:HD11	2.00	0.44
1:C:255:ARG:HB2	1:C:278:ILE:HD12	2.00	0.44
1:B:252:ILE:HD13	1:B:312:LEU:HD11	2.00	0.44
1:G:249:PHE:CZ	1:H:323:PRO:HD2	2.53	0.44
1:F:273:GLU:O	1:F:274:ALA:HB3	2.18	0.44
1:G:269:CYS:SG	1:G:294:ASN:HB2	2.59	0.43
1:A:310:ARG:HD2	3:A:330:HOH:O	2.17	0.43
1:A:276:HIS:CG	1:B:246:MLY:HB3	2.53	0.43
1:E:321:TRP:CG	1:E:322:PRO:HA	2.53	0.43
1:E:262:LEU:HD23	1:E:306:VAL:HG21	2.01	0.43
1:F:251:PRO:O	1:F:254:LEU:HG	2.19	0.43
1:H:290:LEU:HG	1:H:300:LEU:HG	2.01	0.42
1:B:290:LEU:HG	1:B:300:LEU:HG	2.01	0.42
1:E:265:ARG:HG3	1:E:265:ARG:NH1	2.34	0.42
1:F:304:MLY:HH23	1:F:304:MLY:HD2	1.87	0.42
1:H:286:GLU:HG3	1:H:300:LEU:HD12	2.01	0.42
1:C:246:MLY:HD2	1:C:246:MLY:HH13	1.86	0.42
1:E:279:GLY:O	1:E:283:GLN:HG3	2.19	0.42
1:F:246:MLY:HH22	1:F:246:MLY:HD2	1.69	0.42
1:G:279:GLY:HA3	1:G:321:TRP:CZ3	2.54	0.42
1:B:279:GLY:HA3	1:B:321:TRP:CH2	2.55	0.42
1:C:276:HIS:CG	1:D:246:MLY:HB3	2.54	0.42
1:D:269:CYS:SG	1:D:294:ASN:HB2	2.61	0.41
1:G:246:MLY:HA	1:G:247:PRO:HD3	1.87	0.41
1:D:279:GLY:HA3	1:D:321:TRP:CH2	2.56	0.41
1:F:271:MLY:HH22	1:F:271:MLY:HD3	1.81	0.41
1:F:298:MLY:HD3	1:F:298:MLY:HH12	1.84	0.41
1:C:249:PHE:CE1	1:D:323:PRO:HD2	2.56	0.41
1:B:260:LEU:HB2	1:B:262:LEU:HD22	2.03	0.41
1:F:290:LEU:HG	1:F:300:LEU:HG	2.01	0.41
1:H:246:MLY:HD2	1:H:246:MLY:HH13	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:MLY:HD3	1:A:246:MLY:HH22	1.78	0.41
1:D:262:LEU:HD23	1:D:306:VAL:HG21	2.03	0.41
1:E:283:GLN:NE2	1:E:318:LEU:HD12	2.36	0.41
1:C:302:GLU:O	1:C:306:VAL:HG23	2.21	0.41
1:B:271:MLY:HH22	1:B:271:MLY:HD3	1.73	0.41
1:D:279:GLY:HA3	1:D:321:TRP:CZ3	2.56	0.41
1:C:297:MLY:HD2	1:C:297:MLY:HH22	1.81	0.41
1:G:271:MLY:HH13	1:G:271:MLY:HD2	1.85	0.40
1:D:255:ARG:HH21	1:D:259:ASP:HB3	1.86	0.40
1:G:292:THR:O	3:G:330:HOH:O	2.22	0.40
1:B:304:MLY:HH12	1:B:304:MLY:HD3	1.66	0.40
1:H:271:MLY:HH22	1:H:271:MLY:HD3	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	78/86 (91%)	76 (97%)	2 (3%)	0	100	100
1	B	77/86 (90%)	75 (97%)	2 (3%)	0	100	100
1	C	78/86 (91%)	76 (97%)	2 (3%)	0	100	100
1	D	77/86 (90%)	77 (100%)	0	0	100	100
1	E	77/86 (90%)	76 (99%)	1 (1%)	0	100	100
1	F	77/86 (90%)	77 (100%)	0	0	100	100
1	G	78/86 (91%)	76 (97%)	2 (3%)	0	100	100
1	H	76/86 (88%)	76 (100%)	0	0	100	100
All	All	618/688 (90%)	609 (98%)	9 (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	68/70 (97%)	67 (98%)	1 (2%)	65	63
1	B	65/70 (93%)	64 (98%)	1 (2%)	65	63
1	C	68/70 (97%)	68 (100%)	0	100	100
1	D	67/70 (96%)	67 (100%)	0	100	100
1	E	66/70 (94%)	66 (100%)	0	100	100
1	F	68/70 (97%)	68 (100%)	0	100	100
1	G	68/70 (97%)	66 (97%)	2 (3%)	42	35
1	H	66/70 (94%)	65 (98%)	1 (2%)	65	63
All	All	536/560 (96%)	531 (99%)	5 (1%)	78	79

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	254	LEU
1	B	254	LEU
1	G	254	LEU
1	G	265	ARG
1	H	318	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	294	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

48 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	MLY	F	291	1	9,10,11	0.37	0	6,11,13	1.07	0
1	MLY	B	304	1	9,10,11	0.32	0	6,11,13	1.15	0
1	MLY	C	304	1	9,10,11	0.31	0	6,11,13	1.28	1 (16%)
1	MLY	F	246	1	9,10,11	0.37	0	6,11,13	1.13	0
1	MLY	F	304	1	9,10,11	0.31	0	6,11,13	1.27	1 (16%)
1	MLY	H	271	1	9,10,11	0.41	0	6,11,13	0.83	0
1	MLY	D	297	1	9,10,11	0.32	0	6,11,13	1.08	0
1	MLY	B	271	1	9,10,11	0.37	0	6,11,13	0.86	0
1	MLY	H	297	1	3,4,11	0.27	0	2,4,13	0.94	0
1	MLY	B	291	1	9,10,11	0.34	0	6,11,13	1.14	0
1	MLY	B	246	1	9,10,11	0.33	0	6,11,13	1.24	0
1	MLY	A	291	1	3,4,11	0.35	0	2,4,13	0.97	0
1	MLY	G	246	1	9,10,11	0.33	0	6,11,13	1.13	0
1	MLY	B	298	1	9,10,11	0.36	0	6,11,13	1.18	0
1	MLY	A	271	1	9,10,11	0.36	0	6,11,13	0.99	0
1	MLY	G	297	1	3,4,11	0.27	0	2,4,13	0.86	0
1	MLY	F	271	1	9,10,11	0.36	0	6,11,13	0.86	0
1	MLY	D	246	1	9,10,11	0.33	0	6,11,13	1.37	0
1	MLY	H	246	1	9,10,11	0.35	0	6,11,13	1.22	0
1	MLY	D	298	1	3,4,11	0.28	0	2,4,13	0.81	0
1	MLY	G	298	1	9,10,11	0.33	0	6,11,13	1.13	0
1	MLY	E	246	1	9,10,11	0.32	0	6,11,13	1.25	0
1	MLY	A	298	1	9,10,11	0.33	0	6,11,13	1.23	0
1	MLY	C	297	1	9,10,11	0.39	0	6,11,13	1.04	0
1	MLY	H	291	1	9,10,11	0.35	0	6,11,13	1.08	0
1	MLY	A	304	1	9,10,11	0.34	0	6,11,13	1.20	0
1	MLY	A	246	1	9,10,11	0.36	0	6,11,13	0.99	0
1	MLY	B	297	1	9,10,11	0.35	0	6,11,13	1.21	0
1	MLY	F	298	1	9,10,11	0.35	0	6,11,13	1.17	0
1	MLY	C	291	1	3,4,11	0.37	0	2,4,13	1.05	0
1	MLY	F	297	1	3,4,11	0.31	0	2,4,13	0.91	0
1	MLY	C	298	1	9,10,11	0.37	0	6,11,13	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	G	291	1	3,4,11	0.33	0	2,4,13	1.00	0
1	MLY	D	271	1	9,10,11	0.34	0	6,11,13	1.27	0
1	MLY	D	291	1	9,10,11	0.32	0	6,11,13	1.28	0
1	MLY	E	297	1	3,4,11	0.26	0	2,4,13	0.84	0
1	MLY	G	304	1	9,10,11	0.32	0	6,11,13	1.21	0
1	MLY	C	246	1	9,10,11	0.35	0	6,11,13	1.26	0
1	MLY	E	304	1	9,10,11	0.32	0	6,11,13	1.04	0
1	MLY	D	304	1	9,10,11	0.30	0	6,11,13	1.22	0
1	MLY	C	271	1	9,10,11	0.35	0	6,11,13	1.03	0
1	MLY	G	271	1	9,10,11	0.34	0	6,11,13	1.13	0
1	MLY	H	304	1	9,10,11	0.35	0	6,11,13	1.10	0
1	MLY	E	291	1	3,4,11	0.35	0	2,4,13	1.02	0
1	MLY	E	271	1	9,10,11	0.36	0	6,11,13	0.87	0
1	MLY	H	298	1	9,10,11	0.33	0	6,11,13	1.18	0
1	MLY	E	298	1	9,10,11	0.38	0	6,11,13	1.01	0
1	MLY	A	297	1	9,10,11	0.40	0	6,11,13	0.85	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
1	MLY	F	291	1	-	2/8/9/11	-
1	MLY	B	304	1	-	0/8/9/11	-
1	MLY	C	304	1	-	2/8/9/11	-
1	MLY	F	246	1	-	3/8/9/11	-
1	MLY	F	304	1	-	0/8/9/11	-
1	MLY	H	271	1	-	0/8/9/11	-
1	MLY	D	297	1	-	1/8/9/11	-
1	MLY	B	271	1	-	1/8/9/11	-
1	MLY	H	297	1	-	0/0/2/11	-
1	MLY	B	291	1	-	6/8/9/11	-
1	MLY	B	246	1	-	1/8/9/11	-
1	MLY	A	291	1	-	0/0/2/11	-
1	MLY	G	246	1	-	3/8/9/11	-
1	MLY	B	298	1	-	0/8/9/11	-
1	MLY	A	271	1	-	0/8/9/11	-
1	MLY	G	297	1	-	0/0/2/11	-
1	MLY	F	271	1	-	0/8/9/11	-
1	MLY	D	246	1	-	3/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	H	246	1	-	2/8/9/11	-
1	MLY	D	298	1	-	0/0/2/11	-
1	MLY	G	298	1	-	2/8/9/11	-
1	MLY	E	246	1	-	5/8/9/11	-
1	MLY	A	298	1	-	3/8/9/11	-
1	MLY	C	297	1	-	3/8/9/11	-
1	MLY	H	291	1	-	2/8/9/11	-
1	MLY	A	304	1	-	0/8/9/11	-
1	MLY	A	246	1	-	1/8/9/11	-
1	MLY	B	297	1	-	1/8/9/11	-
1	MLY	F	298	1	-	4/8/9/11	-
1	MLY	C	291	1	-	0/0/2/11	-
1	MLY	F	297	1	-	0/0/2/11	-
1	MLY	C	298	1	-	4/8/9/11	-
1	MLY	G	291	1	-	0/0/2/11	-
1	MLY	D	271	1	-	1/8/9/11	-
1	MLY	D	291	1	-	0/8/9/11	-
1	MLY	E	297	1	-	0/0/2/11	-
1	MLY	G	304	1	-	0/8/9/11	-
1	MLY	C	246	1	-	0/8/9/11	-
1	MLY	E	304	1	-	0/8/9/11	-
1	MLY	D	304	1	-	0/8/9/11	-
1	MLY	C	271	1	-	1/8/9/11	-
1	MLY	G	271	1	-	0/8/9/11	-
1	MLY	H	304	1	-	0/8/9/11	-
1	MLY	E	291	1	-	0/0/2/11	-
1	MLY	E	271	1	-	0/8/9/11	-
1	MLY	H	298	1	-	0/8/9/11	-
1	MLY	E	298	1	-	3/8/9/11	-
1	MLY	A	297	1	-	2/8/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	304	MLY	CD-CE-NZ	-2.34	107.45	113.79
1	C	304	MLY	CD-CE-NZ	-2.09	108.12	113.79

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	291	MLY	N-CA-CB-CG
1	B	291	MLY	C-CA-CB-CG
1	H	246	MLY	O-C-CA-CB
1	G	298	MLY	N-CA-CB-CG
1	G	298	MLY	C-CA-CB-CG
1	E	246	MLY	C-CA-CB-CG
1	A	298	MLY	C-CA-CB-CG
1	F	298	MLY	N-CA-CB-CG
1	F	298	MLY	C-CA-CB-CG
1	C	298	MLY	C-CA-CB-CG
1	B	291	MLY	CD-CE-NZ-CH1
1	B	291	MLY	CD-CE-NZ-CH2
1	D	246	MLY	CD-CE-NZ-CH1
1	D	246	MLY	CD-CE-NZ-CH2
1	E	298	MLY	CD-CE-NZ-CH1
1	B	291	MLY	CG-CD-CE-NZ
1	F	246	MLY	CG-CD-CE-NZ
1	H	291	MLY	CD-CE-NZ-CH2
1	A	297	MLY	CD-CE-NZ-CH2
1	B	291	MLY	CA-CB-CG-CD
1	C	298	MLY	CD-CE-NZ-CH2
1	B	297	MLY	CG-CD-CE-NZ
1	E	298	MLY	CD-CE-NZ-CH2
1	E	246	MLY	CG-CD-CE-NZ
1	C	298	MLY	CE-CD-CG-CB
1	A	298	MLY	CD-CE-NZ-CH1
1	G	246	MLY	C-CA-CB-CG
1	D	246	MLY	C-CA-CB-CG
1	B	246	MLY	C-CA-CB-CG
1	C	297	MLY	CG-CD-CE-NZ
1	E	246	MLY	CA-CB-CG-CD
1	H	291	MLY	CE-CD-CG-CB
1	C	297	MLY	CA-CB-CG-CD
1	G	246	MLY	CD-CE-NZ-CH2
1	E	298	MLY	CE-CD-CG-CB
1	C	304	MLY	CA-CB-CG-CD
1	E	246	MLY	CE-CD-CG-CB
1	F	298	MLY	CE-CD-CG-CB
1	A	297	MLY	CE-CD-CG-CB
1	F	298	MLY	CD-CE-NZ-CH2
1	G	246	MLY	N-CA-CB-CG
1	E	246	MLY	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	C	297	MLY	CE-CD-CG-CB
1	C	304	MLY	C-CA-CB-CG
1	H	246	MLY	C-CA-CB-CG
1	D	271	MLY	CD-CE-NZ-CH2
1	D	297	MLY	CE-CD-CG-CB
1	F	291	MLY	CD-CE-NZ-CH1
1	F	291	MLY	C-CA-CB-CG
1	A	298	MLY	CE-CD-CG-CB
1	F	246	MLY	CE-CD-CG-CB
1	F	246	MLY	CD-CE-NZ-CH2
1	B	271	MLY	CD-CE-NZ-CH2
1	A	246	MLY	CD-CE-NZ-CH2
1	C	271	MLY	CD-CE-NZ-CH2
1	C	298	MLY	N-CA-CB-CG

There are no ring outliers.

20 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	304	MLY	1	0
1	C	304	MLY	1	0
1	F	246	MLY	1	0
1	F	304	MLY	1	0
1	H	271	MLY	1	0
1	B	271	MLY	1	0
1	B	246	MLY	1	0
1	G	246	MLY	2	0
1	A	271	MLY	1	0
1	F	271	MLY	1	0
1	D	246	MLY	1	0
1	H	246	MLY	1	0
1	C	297	MLY	1	0
1	H	291	MLY	1	0
1	A	304	MLY	1	0
1	A	246	MLY	1	0
1	F	298	MLY	1	0
1	D	271	MLY	1	0
1	C	246	MLY	1	0
1	G	271	MLY	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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 [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	78/86 (90%)	0.10	0 100 100	23, 30, 40, 43	0
1	B	77/86 (89%)	0.03	0 100 100	23, 30, 39, 40	0
1	C	78/86 (90%)	0.20	2 (2%) 56 60	22, 30, 41, 42	0
1	D	77/86 (89%)	0.03	0 100 100	22, 31, 39, 43	0
1	E	77/86 (89%)	0.17	0 100 100	23, 30, 38, 40	0
1	F	78/86 (90%)	0.07	0 100 100	23, 31, 41, 45	0
1	G	78/86 (90%)	0.06	0 100 100	23, 31, 40, 41	0
1	H	77/86 (89%)	0.10	1 (1%) 77 79	22, 30, 39, 43	0
All	All	620/688 (90%)	0.09	3 (0%) 91 92	22, 30, 40, 45	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	293	PRO	2.7
1	H	328	ASP	2.4
1	C	295	LEU	2.0

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

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(Å ²)	Q<0.9
1	MLY	F	291	11/12	0.86	0.21	38,41,44,46	0
1	MLY	G	291	5/12	0.86	0.19	39,40,42,46	0
1	MLY	E	298	11/12	0.86	0.17	34,37,41,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	MLY	G	246	11/12	0.87	0.16	29,32,40,44	0
1	MLY	C	297	11/12	0.87	0.16	30,36,37,38	0
1	MLY	A	297	11/12	0.87	0.23	37,41,47,48	0
1	MLY	C	246	11/12	0.88	0.15	30,33,36,40	0
1	MLY	A	291	5/12	0.88	0.16	39,40,43,46	0
1	MLY	D	291	11/12	0.88	0.20	39,43,46,47	0
1	MLY	C	291	5/12	0.89	0.21	40,40,43,47	0
1	MLY	B	271	11/12	0.89	0.18	28,30,39,41	0
1	MLY	A	271	11/12	0.90	0.17	27,30,40,42	0
1	MLY	G	298	11/12	0.90	0.21	27,34,38,38	0
1	MLY	F	246	11/12	0.90	0.14	28,31,35,39	0
1	MLY	C	304	11/12	0.91	0.15	33,33,44,44	0
1	MLY	A	298	11/12	0.91	0.17	28,34,37,38	0
1	MLY	B	298	11/12	0.91	0.13	30,34,38,38	0
1	MLY	B	297	11/12	0.91	0.16	37,38,42,43	0
1	MLY	D	297	11/12	0.91	0.15	36,39,43,44	0
1	MLY	G	304	11/12	0.92	0.16	31,34,42,42	0
1	MLY	H	291	11/12	0.92	0.14	35,39,42,45	0
1	MLY	B	246	11/12	0.92	0.14	30,33,37,39	0
1	MLY	E	291	5/12	0.92	0.14	40,40,41,45	0
1	MLY	A	246	11/12	0.92	0.12	29,33,41,45	0
1	MLY	B	291	11/12	0.92	0.15	40,42,44,46	0
1	MLY	D	246	11/12	0.93	0.13	29,33,38,39	0
1	MLY	H	297	5/12	0.93	0.13	37,37,39,40	0
1	MLY	E	246	11/12	0.93	0.12	28,31,33,34	0
1	MLY	F	304	11/12	0.93	0.16	32,34,42,47	0
1	MLY	F	297	5/12	0.93	0.12	37,37,38,40	0
1	MLY	C	298	11/12	0.93	0.13	34,37,43,43	0
1	MLY	G	297	5/12	0.93	0.10	37,37,37,38	0
1	MLY	H	246	11/12	0.94	0.11	26,31,32,33	0
1	MLY	F	271	11/12	0.94	0.13	27,30,39,41	0
1	MLY	D	271	11/12	0.94	0.14	28,31,36,36	0
1	MLY	H	298	11/12	0.94	0.16	33,37,38,39	0
1	MLY	E	304	11/12	0.94	0.15	31,33,39,40	0
1	MLY	A	304	11/12	0.94	0.14	33,34,40,41	0
1	MLY	C	271	11/12	0.95	0.11	28,29,35,35	0
1	MLY	G	271	11/12	0.95	0.13	27,30,36,36	0
1	MLY	H	304	11/12	0.95	0.16	31,33,41,41	0
1	MLY	H	271	11/12	0.95	0.11	28,30,35,35	0
1	MLY	B	304	11/12	0.95	0.12	32,33,40,40	0
1	MLY	F	298	11/12	0.95	0.11	33,37,39,42	0
1	MLY	D	298	5/12	0.95	0.08	34,36,37,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	MLY	E	297	5/12	0.96	0.09	37,37,38,38	0
1	MLY	D	304	11/12	0.96	0.12	32,34,38,39	0
1	MLY	E	271	11/12	0.96	0.10	28,31,35,35	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(\AA^2)	Q<0.9
2	NA	G	1	1/1	0.88	0.15	27,27,27,27	0
2	NA	E	3	1/1	0.90	0.11	24,24,24,24	0
2	NA	C	4	1/1	0.92	0.14	25,25,25,25	0
2	NA	A	2	1/1	0.99	0.12	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.