



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 28, 2020 – 12:38 PM EDT

PDB ID : 6VIL
Title : Crystal structure of mouse BAHCC1 BAH domain in complex with H3K27me3
Authors : Song, J.; Lu, J.
Deposited on : 2020-01-13
Resolution : 3.30 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 : 2.14.6
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) : 2.14.6

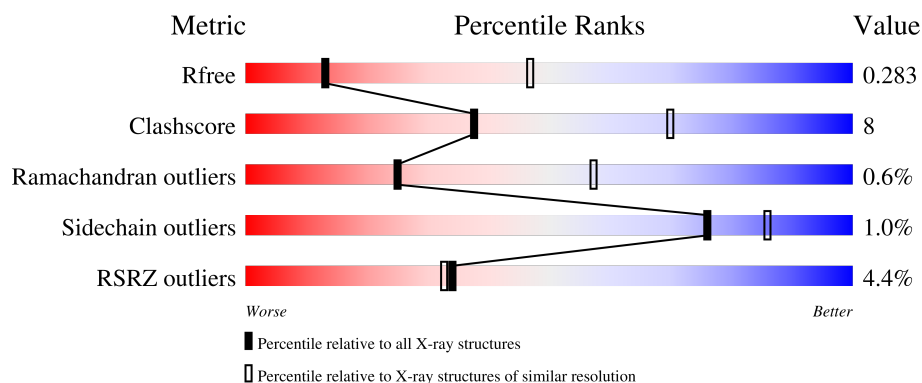
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	160	<div> <div>4%</div> <div>79%</div> <div>18%</div> <div>• •</div> </div>
1	B	160	<div> <div>2%</div> <div>75%</div> <div>19%</div> <div>• 5%</div> </div>
1	C	160	<div> <div>76%</div> <div>18%</div> <div>• 6%</div> </div>
1	D	160	<div> <div>6%</div> <div>81%</div> <div>16%</div> <div>• •</div> </div>
1	E	160	<div> <div>6%</div> <div>71%</div> <div>21%</div> <div>• 7%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	160	<p>3% 74% 17% 8%</p>
1	G	160	<p>8% 82% 14%</p>
1	H	160	<p>4% 81% 11% 8%</p>
2	I	14	<p>7% 43% 43% 14%</p>
2	J	14	<p>7% 57% 29% 14%</p>
2	L	14	<p>29% 7% 64%</p>
2	M	14	<p>7% 29% 71%</p>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9381 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 BAH and coiled-coil domain-containing protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	0	0
			1185	754	205	219	7			
1	B	152	Total	C	N	O	S	0	0	0
			1163	736	201	220	6			
1	D	156	Total	C	N	O	S	0	0	0
			1148	733	194	215	6			
1	E	149	Total	C	N	O	S	0	0	0
			1104	704	186	208	6			
1	F	147	Total	C	N	O	S	0	0	0
			1119	710	193	210	6			
1	G	153	Total	C	N	O	S	0	0	0
			1163	739	197	221	6			
1	H	148	Total	C	N	O	S	0	0	0
			1121	713	188	214	6			
1	C	151	Total	C	N	O	S	0	0	0
			1151	727	197	221	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2484	SER	-	expression tag	UNP Q3UHR0
B	2484	SER	-	expression tag	UNP Q3UHR0
D	2484	SER	-	expression tag	UNP Q3UHR0
E	2484	SER	-	expression tag	UNP Q3UHR0
F	2484	SER	-	expression tag	UNP Q3UHR0
G	2484	SER	-	expression tag	UNP Q3UHR0
H	2484	SER	-	expression tag	UNP Q3UHR0
C	2484	SER	-	expression tag	UNP Q3UHR0

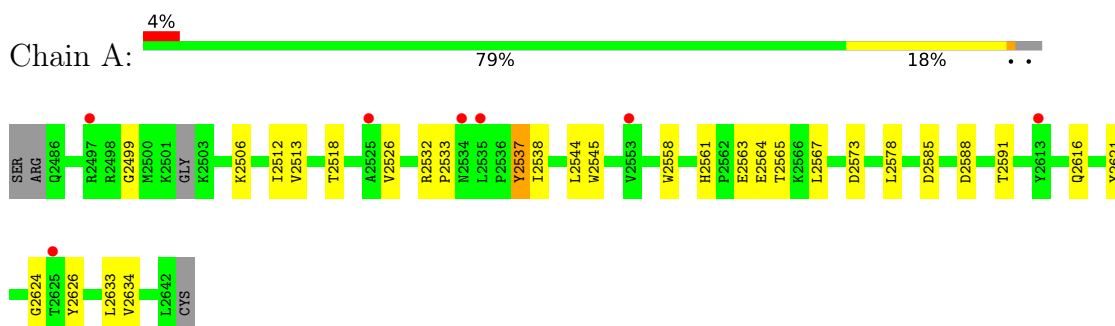
- Molecule 2 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	12	Total	C	N	O	0	0	0
			83	51	17	15			
2	J	12	Total	C	N	O	0	0	0
			83	51	17	15			
2	L	5	Total	C	N	O	0	0	0
			33	21	6	6			
2	M	4	Total	C	N	O	0	0	0
			28	18	5	5			

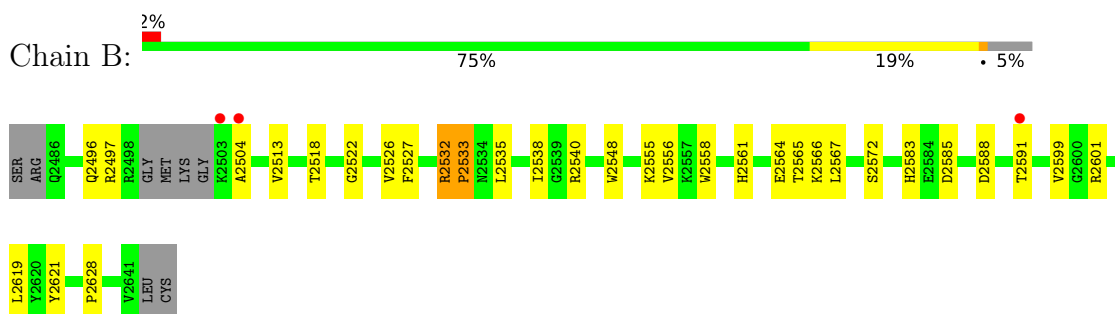
3 Residue-property plots [i](#)

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.

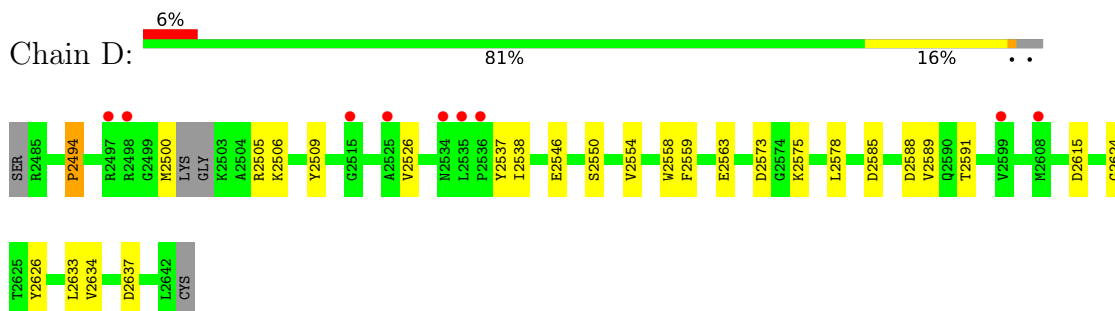
- Molecule 1: BAH and coiled-coil domain-containing protein 1



- Molecule 1: BAH and coiled-coil domain-containing protein 1

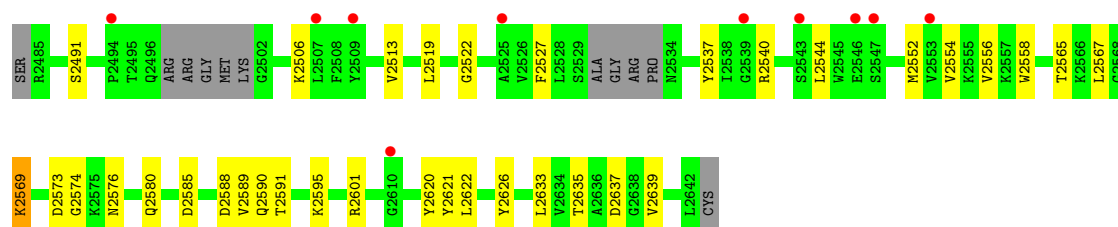


- Molecule 1: BAH and coiled-coil domain-containing protein 1

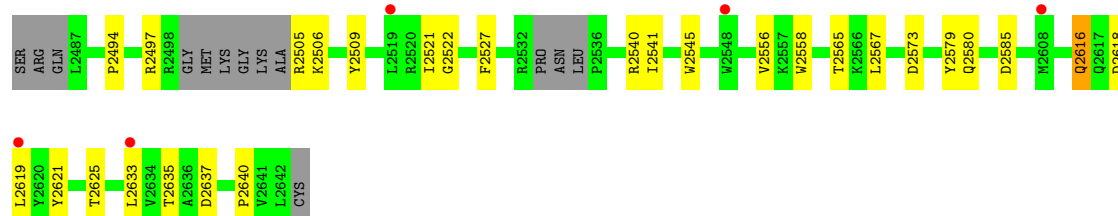
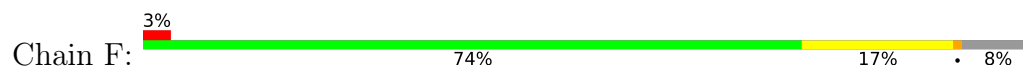


- Molecule 1: BAH and coiled-coil domain-containing protein 1

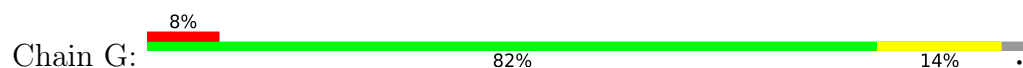




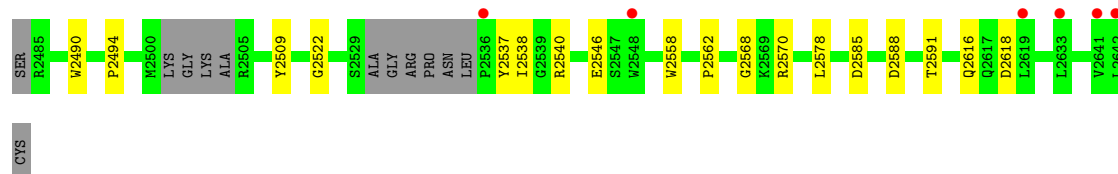
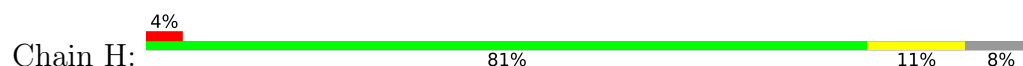
- Molecule 1: BAH and coiled-coil domain-containing protein 1



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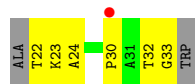
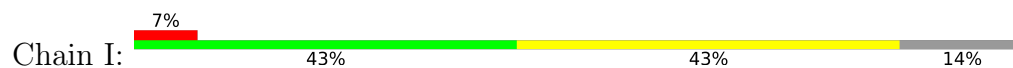
- Molecule 1: BAH and coiled-coil domain-containing protein 1



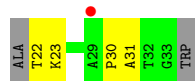
- Molecule 1: BAH and coiled-coil domain-containing protein 1



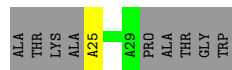
● Molecule 2: Histone H3.1



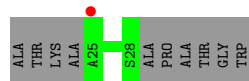
● Molecule 2: Histone H3.1



● Molecule 2: Histone H3.1



● Molecule 2: Histone H3.1



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	184.18Å 184.18Å 70.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.04 – 3.30 46.04 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.04-3.30) 99.8 (46.04-3.30)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 3.32Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.248 , 0.283 0.248 , 0.283	Depositor DCC
R_{free} test set	2016 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	87.4	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 62.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.428 for -h,-k,l 0.045 for h,-h-k,-l 0.043 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	9381	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: M3L

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	0/1214	0.45	0/1651
1	B	0.24	0/1192	0.44	0/1623
1	C	0.24	0/1180	0.43	0/1608
1	D	0.24	0/1177	0.45	0/1606
1	E	0.24	0/1131	0.44	0/1542
1	F	0.24	0/1146	0.44	0/1559
1	G	0.24	0/1192	0.45	0/1626
1	H	0.23	0/1148	0.44	0/1563
2	I	0.25	0/71	0.43	0/95
2	J	0.24	0/71	0.47	0/95
2	L	0.17	0/20	0.38	0/26
2	M	0.17	0/15	0.38	0/19
All	All	0.24	0/9557	0.44	0/13013

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	1185	0	1082	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1163	0	1047	23	0
1	C	1151	0	1016	22	0
1	D	1148	0	1002	16	0
1	E	1104	0	963	21	0
1	F	1119	0	1006	17	0
1	G	1163	0	1046	15	0
1	H	1121	0	998	8	0
2	I	83	0	92	5	0
2	J	83	0	92	3	0
2	L	33	0	34	1	0
2	M	28	0	29	0	0
All	All	9381	0	8407	137	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 8.

All (137) 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:2616:GLN:HE22	1:F:2619:LEU:HB3	1.42	0.85
1:A:2499:GLY:O	1:A:2506:LYS:NZ	2.14	0.80
1:G:2635:THR:HG23	1:G:2637:ASP:H	1.47	0.79
1:C:2573:ASP:O	1:C:2621:TYR:OH	2.06	0.74
1:E:2635:THR:HG22	1:E:2639:VAL:H	1.52	0.74
1:A:2526:VAL:HG22	1:A:2538:ILE:HG12	1.70	0.72
1:D:2526:VAL:HG22	1:D:2538:ILE:HG12	1.72	0.72
1:C:2616:GLN:OE1	1:C:2618:ASP:N	2.24	0.69
1:H:2616:GLN:HG3	1:H:2618:ASP:H	1.57	0.69
1:F:2497:ARG:O	1:F:2505:ARG:N	2.27	0.68
1:B:2532:ARG:HH22	1:B:2535:LEU:HB2	1.58	0.68
1:D:2624:GLY:HA3	1:D:2634:VAL:O	1.95	0.66
1:F:2573:ASP:O	1:F:2621:TYR:OH	2.12	0.66
1:E:2635:THR:HG23	1:E:2637:ASP:H	1.64	0.63
1:B:2558:TRP:NE1	1:B:2585:ASP:OD1	2.31	0.62
1:A:2513:VAL:HG12	1:A:2518:THR:HG22	1.80	0.62
1:A:2573:ASP:O	1:A:2621:TYR:OH	2.17	0.62
1:B:2513:VAL:HG12	1:B:2518:THR:HG22	1.80	0.61
1:A:2532:ARG:HG3	1:A:2533:PRO:HD3	1.81	0.61
1:B:2526:VAL:HG22	1:B:2538:ILE:HG12	1.83	0.61
1:C:2526:VAL:HG22	1:C:2538:ILE:HG12	1.82	0.61
1:A:2626:TYR:HD1	1:A:2633:LEU:HB3	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:22:THR:OG1	2:I:23:LYS:N	2.33	0.61
1:F:2635:THR:HG23	1:F:2637:ASP:H	1.66	0.60
1:G:2616:GLN:NE2	1:G:2619:LEU:O	2.34	0.60
1:F:2558:TRP:NE1	1:F:2585:ASP:OD1	2.34	0.60
1:F:2522:GLY:O	1:F:2540:ARG:NH1	2.36	0.59
1:F:2616:GLN:OE1	1:F:2618:ASP:N	2.30	0.58
1:G:2616:GLN:HE21	1:G:2619:LEU:H	1.52	0.58
1:B:2527:PHE:CZ	1:B:2556:VAL:HG21	2.39	0.57
1:C:2588:ASP:HB3	1:C:2591:THR:HG23	1.86	0.57
1:D:2558:TRP:NE1	1:D:2585:ASP:OD1	2.38	0.57
1:A:2563:GLU:OE1	1:A:2563:GLU:N	2.38	0.56
1:E:2580:GLN:HB2	1:E:2622:LEU:HD11	1.87	0.55
1:C:2522:GLY:O	1:C:2540:ARG:NH1	2.40	0.55
1:B:2522:GLY:O	1:B:2540:ARG:NH1	2.41	0.54
2:I:24:ALA:HB1	1:C:2530:ALA:HB2	1.88	0.54
1:G:2616:GLN:HG2	1:G:2618:ASP:H	1.72	0.54
1:E:2527:PHE:HB2	1:E:2537:TYR:HB2	1.91	0.53
1:A:2565:THR:OG1	1:A:2567:LEU:O	2.27	0.52
1:C:2558:TRP:HE1	1:C:2585:ASP:HB2	1.75	0.52
1:D:2575:LYS:NZ	1:D:2615:ASP:OD1	2.38	0.52
1:D:2563:GLU:OE1	1:D:2563:GLU:N	2.43	0.52
1:E:2591:THR:HG1	2:L:25:ALA:N	2.08	0.52
1:C:2576:ASN:HB3	1:C:2620:TYR:CD2	2.46	0.51
2:J:22:THR:OG1	2:J:23:LYS:N	2.43	0.51
1:H:2522:GLY:O	1:H:2540:ARG:NH1	2.44	0.51
1:E:2558:TRP:NE1	1:E:2585:ASP:OD1	2.44	0.51
1:E:2573:ASP:O	1:E:2621:TYR:OH	2.24	0.51
1:A:2616:GLN:HA	1:C:2616:GLN:HA	1.93	0.51
1:F:2521:ILE:HD13	1:F:2541:ILE:HG22	1.94	0.50
1:G:2576:ASN:HB2	1:G:2620:TYR:CD2	2.47	0.50
1:A:2506:LYS:HD3	1:A:2545:TRP:CD1	2.47	0.49
1:E:2552:MET:SD	1:E:2590:GLN:NE2	2.85	0.49
1:G:2535:LEU:O	1:G:2535:LEU:HD12	2.12	0.49
1:H:2558:TRP:NE1	1:H:2585:ASP:OD1	2.44	0.49
1:B:2532:ARG:NH2	1:B:2535:LEU:HB2	2.27	0.49
1:B:2527:PHE:HD2	1:B:2591:THR:HG23	1.76	0.49
1:D:2500:MET:H	1:D:2506:LYS:NZ	2.11	0.49
1:H:2562:PRO:O	1:H:2568:GLY:HA2	2.13	0.49
1:E:2544:LEU:CD2	1:E:2554:VAL:HG23	2.43	0.48
1:H:2490:TRP:NE1	1:H:2546:GLU:OE1	2.43	0.48
1:B:2588:ASP:O	1:B:2591:THR:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2637:ASP:HA	1:F:2521:ILE:HG21	1.94	0.48
1:E:2544:LEU:HD23	1:E:2554:VAL:HG23	1.96	0.48
1:E:2576:ASN:HB3	1:E:2620:TYR:CD2	2.49	0.48
1:B:2527:PHE:HZ	1:B:2556:VAL:HG21	1.78	0.48
2:I:32:THR:HB	1:C:2583:HIS:HA	1.96	0.48
1:A:2558:TRP:NE1	1:A:2585:ASP:OD1	2.47	0.48
1:E:2554:VAL:HB	1:E:2589:VAL:HG22	1.96	0.48
1:E:2588:ASP:O	1:E:2591:THR:HG22	2.14	0.48
1:B:2504:ALA:N	1:D:2546:GLU:OE2	2.48	0.47
1:B:2561:HIS:N	1:B:2564:GLU:OE1	2.46	0.47
1:E:2626:TYR:HD1	1:E:2633:LEU:HB3	1.80	0.47
1:H:2494:PRO:HB3	1:H:2509:TYR:CZ	2.49	0.47
1:D:2559:PHE:HB3	1:D:2578:LEU:HD22	1.97	0.47
1:G:2532:ARG:HH11	1:G:2537:TYR:HE1	1.63	0.47
1:A:2512:ILE:HG23	1:A:2544:LEU:HD13	1.97	0.46
1:E:2569:LYS:NZ	1:E:2574:GLY:O	2.45	0.46
1:A:2533:PRO:HG2	1:A:2537:TYR:HE2	1.81	0.46
1:E:2491:SER:HB2	1:E:2513:VAL:HG22	1.98	0.46
1:B:2532:ARG:NH1	1:B:2564:GLU:OE2	2.38	0.46
1:C:2616:GLN:OE1	1:C:2618:ASP:HB2	2.16	0.45
1:F:2565:THR:OG1	1:F:2567:LEU:O	2.34	0.45
1:G:2634:VAL:HA	1:G:2640:PRO:HA	1.98	0.45
1:A:2538:ILE:HD12	1:A:2578:LEU:HD21	1.97	0.45
1:B:2565:THR:OG1	1:B:2567:LEU:O	2.34	0.45
1:B:2583:HIS:CD2	2:J:31:ALA:H	2.34	0.45
1:A:2588:ASP:HB3	1:A:2591:THR:HG23	1.98	0.45
1:B:2566:LYS:HE2	1:B:2566:LYS:HB3	1.82	0.45
1:E:2527:PHE:CZ	1:E:2556:VAL:HG11	2.50	0.45
1:F:2580:GLN:O	1:F:2625:THR:HA	2.16	0.45
1:D:2626:TYR:HD1	1:D:2633:LEU:HG	1.82	0.45
1:F:2616:GLN:NE2	1:F:2619:LEU:HB3	2.21	0.45
1:G:2526:VAL:HG13	1:G:2536:PRO:HB2	1.99	0.45
1:D:2500:MET:H	1:D:2506:LYS:HZ1	1.65	0.44
1:D:2554:VAL:HB	1:D:2589:VAL:HG22	2.00	0.43
1:H:2538:ILE:HD12	1:H:2578:LEU:HD11	2.00	0.43
2:I:30:PRO:HB3	1:C:2628:PRO:HB2	2.00	0.43
1:D:2588:ASP:HB3	1:D:2591:THR:HG23	1.99	0.43
1:G:2616:GLN:O	1:G:2618:ASP:N	2.51	0.43
1:B:2599:VAL:O	1:B:2621:TYR:HA	2.18	0.43
1:D:2494:PRO:HB3	1:D:2509:TYR:CZ	2.54	0.43
1:F:2494:PRO:HB3	1:F:2509:TYR:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2588:ASP:O	1:G:2591:THR:HG22	2.18	0.42
1:F:2616:GLN:H	1:F:2616:GLN:HG3	1.64	0.42
1:B:2572:SER:O	1:B:2601:ARG:NH2	2.47	0.42
1:C:2599:VAL:O	1:C:2621:TYR:HA	2.20	0.42
1:F:2527:PHE:CZ	1:F:2556:VAL:HG11	2.54	0.42
1:C:2497:ARG:HD3	1:C:2497:ARG:HA	1.89	0.42
1:C:2541:ILE:HG23	1:C:2554:VAL:HG23	2.01	0.42
1:D:2550:SER:OG	1:D:2550:SER:O	2.32	0.42
1:E:2519:LEU:HD21	1:E:2595:LYS:HB2	2.01	0.42
1:B:2585:ASP:OD1	1:B:2585:ASP:N	2.53	0.42
1:E:2522:GLY:O	1:E:2540:ARG:NH1	2.52	0.42
1:C:2527:PHE:CZ	1:C:2556:VAL:HG21	2.55	0.42
1:B:2628:PRO:HB2	2:J:30:PRO:HB3	2.02	0.41
1:C:2603:GLN:O	1:C:2607:MET:HG2	2.20	0.41
1:G:2521:ILE:HD13	1:G:2541:ILE:HG22	2.00	0.41
1:C:2558:TRP:NE1	1:C:2585:ASP:HB2	2.35	0.41
1:B:2548:TRP:HE1	1:D:2505:ARG:HB2	1.85	0.41
1:A:2624:GLY:HA3	1:A:2634:VAL:O	2.21	0.41
1:C:2556:VAL:O	1:C:2584:GLU:HA	2.20	0.41
1:G:2490:TRP:HA	1:G:2512:ILE:HG22	2.00	0.41
1:H:2588:ASP:O	1:H:2591:THR:HG22	2.21	0.41
1:F:2506:LYS:HD3	1:F:2545:TRP:CD1	2.56	0.41
1:F:2579:TYR:CZ	1:F:2633:LEU:HD21	2.56	0.41
1:G:2536:PRO:HG3	1:G:2617:GLN:HE21	1.85	0.41
1:B:2497:ARG:HG3	1:G:2639:VAL:HG13	2.02	0.41
1:A:2561:HIS:N	1:A:2564:GLU:OE1	2.47	0.41
1:C:2554:VAL:HG22	1:C:2556:VAL:HG22	2.03	0.41
1:E:2565:THR:OG1	1:E:2567:LEU:O	2.37	0.41
1:C:2625:THR:HB	1:C:2634:VAL:HG22	2.02	0.41
1:E:2601:ARG:NH1	1:E:2621:TYR:OH	2.54	0.40
2:I:32:THR:OG1	2:I:33:GLY:N	2.53	0.40
1:B:2532:ARG:HA	1:B:2533:PRO:HD3	1.96	0.40
1:C:2600:GLY:O	1:C:2604:TYR:N	2.46	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	152/160 (95%)	144 (95%)	8 (5%)	0	100	100
1	B	148/160 (92%)	134 (90%)	13 (9%)	1 (1%)	22	54
1	C	147/160 (92%)	133 (90%)	14 (10%)	0	100	100
1	D	152/160 (95%)	141 (93%)	9 (6%)	2 (1%)	12	40
1	E	143/160 (89%)	132 (92%)	9 (6%)	2 (1%)	11	38
1	F	141/160 (88%)	130 (92%)	10 (7%)	1 (1%)	22	54
1	G	149/160 (93%)	136 (91%)	13 (9%)	0	100	100
1	H	142/160 (89%)	136 (96%)	5 (4%)	1 (1%)	22	54
2	I	9/14 (64%)	8 (89%)	1 (11%)	0	100	100
2	J	9/14 (64%)	9 (100%)	0	0	100	100
2	L	2/14 (14%)	2 (100%)	0	0	100	100
2	M	1/14 (7%)	1 (100%)	0	0	100	100
All	All	1195/1336 (89%)	1106 (93%)	82 (7%)	7 (1%)	25	57

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2533	PRO
1	D	2573	ASP
1	E	2569	LYS
1	H	2570	ARG
1	E	2506	LYS
1	F	2640	PRO
1	D	2494	PRO

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	113/138 (82%)	112 (99%)	1 (1%)	78	87
1	B	112/138 (81%)	108 (96%)	4 (4%)	35	63
1	C	110/138 (80%)	109 (99%)	1 (1%)	78	87
1	D	102/138 (74%)	101 (99%)	1 (1%)	76	86
1	E	101/138 (73%)	101 (100%)	0	100	100
1	F	108/138 (78%)	107 (99%)	1 (1%)	78	87
1	G	112/138 (81%)	112 (100%)	0	100	100
1	H	108/138 (78%)	107 (99%)	1 (1%)	78	87
2	I	6/7 (86%)	6 (100%)	0	100	100
2	J	6/7 (86%)	6 (100%)	0	100	100
2	L	1/7 (14%)	1 (100%)	0	100	100
2	M	1/7 (14%)	1 (100%)	0	100	100
All	All	880/1132 (78%)	871 (99%)	9 (1%)	76	86

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

Mol	Chain	Res	Type
1	A	2537	TYR
1	B	2496	GLN
1	B	2532	ARG
1	B	2555	LYS
1	B	2619	LEU
1	D	2537	TYR
1	F	2616	GLN
1	H	2537	TYR
1	C	2616	GLN

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

Mol	Chain	Res	Type
1	G	2617	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	$\# Z > 2$
2	M3L	M	27	2	10,11,12	0.51	0	9,14,16	0.53	0
2	M3L	L	27	2	10,11,12	0.50	0	9,14,16	0.45	0
2	M3L	J	27	2	10,11,12	0.52	0	9,14,16	0.47	0
2	M3L	I	27	2	10,11,12	0.51	0	9,14,16	0.45	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
2	M3L	M	27	2	-	5/9/10/12	-
2	M3L	L	27	2	-	3/9/10/12	-
2	M3L	J	27	2	-	3/9/10/12	-
2	M3L	I	27	2	-	0/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	M	27	M3L	C-CA-CB-CG
2	L	27	M3L	C-CA-CB-CG
2	J	27	M3L	N-CA-CB-CG
2	J	27	M3L	C-CA-CB-CG
2	L	27	M3L	CG-CD-CE-NZ
2	J	27	M3L	CG-CD-CE-NZ
2	M	27	M3L	CG-CD-CE-NZ
2	M	27	M3L	CD-CE-NZ-CM3
2	M	27	M3L	CD-CE-NZ-CM1
2	M	27	M3L	CD-CE-NZ-CM2
2	L	27	M3L	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	156/160 (97%)	0.53	7 (4%) 33 32	58, 85, 133, 160	0
1	B	152/160 (95%)	0.45	3 (1%) 65 64	49, 76, 126, 149	0
1	C	151/160 (94%)	0.41	0 100 100	46, 72, 121, 142	0
1	D	156/160 (97%)	0.68	9 (5%) 23 22	55, 86, 134, 166	0
1	E	149/160 (93%)	0.61	10 (6%) 17 17	56, 97, 141, 167	0
1	F	147/160 (91%)	0.53	5 (3%) 45 43	68, 107, 145, 185	0
1	G	153/160 (95%)	0.65	12 (7%) 13 12	54, 99, 144, 169	0
1	H	148/160 (92%)	0.58	6 (4%) 37 35	66, 105, 136, 172	0
2	I	11/14 (78%)	0.43	1 (9%) 9 9	76, 100, 117, 119	0
2	J	11/14 (78%)	0.79	1 (9%) 9 9	81, 103, 119, 127	0
2	L	4/14 (28%)	-0.03	0 100 100	107, 118, 121, 122	0
2	M	3/14 (21%)	1.32	1 (33%) 0 0	121, 121, 122, 131	0
All	All	1241/1336 (92%)	0.56	55 (4%) 34 33	46, 93, 137, 185	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2498	ARG	4.9
1	D	2535	LEU	4.6
1	D	2534	ASN	4.2
1	A	2534	ASN	4.1
1	F	2619	LEU	3.9
1	H	2548	TRP	3.6
2	M	25	ALA	3.6
1	F	2519	LEU	3.4
1	F	2548	TRP	3.3
1	E	2507	LEU	3.3
1	E	2610	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	2494	PRO	3.2
1	G	2494	PRO	3.2
1	G	2587	ASN	3.1
1	H	2536	PRO	3.1
1	B	2504	ALA	2.9
1	A	2535	LEU	2.8
1	B	2503	LYS	2.8
2	I	30	PRO	2.7
1	G	2519	LEU	2.7
1	G	2548	TRP	2.7
1	H	2619	LEU	2.6
1	G	2553	VAL	2.6
1	D	2525	ALA	2.5
1	D	2515	GLY	2.5
1	B	2591	THR	2.4
1	F	2608	MET	2.3
1	G	2530	ALA	2.3
1	E	2547	SER	2.3
1	D	2608	MET	2.3
1	A	2553	VAL	2.3
1	G	2491	SER	2.3
2	J	29	ALA	2.2
1	G	2556	VAL	2.2
1	H	2641	VAL	2.2
1	E	2525	ALA	2.2
1	E	2509	TYR	2.2
1	D	2599	VAL	2.2
1	A	2525	ALA	2.2
1	G	2504	ALA	2.2
1	H	2642	LEU	2.2
1	E	2539	GLY	2.1
1	E	2553	VAL	2.1
1	E	2546	GLU	2.1
1	A	2613	TYR	2.1
1	G	2558	TRP	2.1
1	H	2633	LEU	2.1
1	E	2543	SER	2.1
1	A	2625	THR	2.0
1	A	2497	ARG	2.0
1	G	2621	TYR	2.0
1	D	2497	ARG	2.0
1	D	2536	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	2633	LEU	2.0
1	G	2509	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	M3L	L	27	12/13	0.93	0.44	69,103,117,118	0
2	M3L	M	27	12/13	0.94	0.38	58,113,125,132	0
2	M3L	I	27	12/13	0.95	0.33	44,68,101,113	0
2	M3L	J	27	12/13	0.97	0.33	56,99,107,111	0

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.