



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 29, 2016 – 03:00 PM EST

PDB ID : 5D6Y
Title : Crystal structure of double tudor domain of human lysine demethylase KDM4A complexed with histone H3K23me3
Authors : Wang, F.; Su, Z.; Miller, M.D.; Denu, J.M.; Phillips Jr., G.N.; Enzyme Discovery for Natural Product Biosynthesis (NatPro)
Deposited on : 2015-08-13
Resolution : 2.29 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

<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028320
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028320

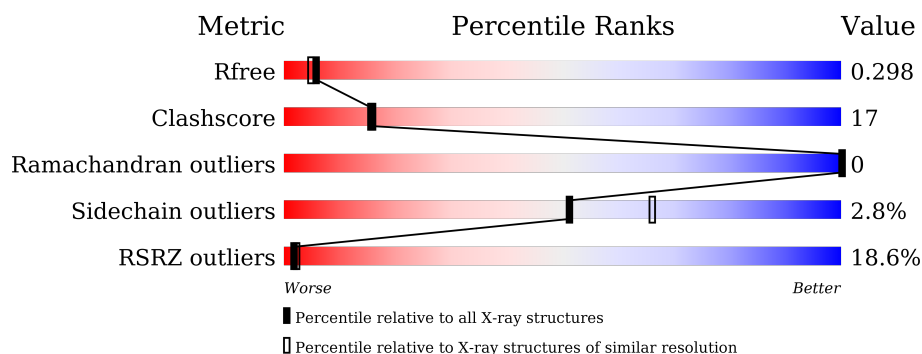
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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}	91344	5193 (2.30-2.26)
Clashscore	102246	5929 (2.30-2.26)
Ramachandran outliers	100387	5851 (2.30-2.26)
Sidechain outliers	100360	5850 (2.30-2.26)
RSRZ outliers	91569	5204 (2.30-2.26)

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. 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	121	<div> <div>72%</div> <div>17%</div> <div>11%</div> </div>
1	B	121	<div> <div>68%</div> <div>21%</div> <div>11%</div> </div>
1	C	121	<div> <div>2%</div> <div>63%</div> <div>21%</div> <div>14%</div> </div>
1	D	121	<div> <div>2%</div> <div>63%</div> <div>21%</div> <div>14%</div> </div>
1	E	121	<div> <div>46%</div> <div>55%</div> <div>31%</div> <div>12%</div> </div>
1	F	121	<div> <div>52%</div> <div>55%</div> <div>31%</div> <div>11%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	a	10	 90%10%
2	b	10	 90%10%
2	c	10	 70%30%
2	d	10	 70%30%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5533 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 Lysine-specific demethylase 4A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	108	Total	C	N	O	S	0	0	0
			867	549	142	173	3			
1	B	108	Total	C	N	O	S	0	0	0
			867	549	142	173	3			
1	C	104	Total	C	N	O	S	0	0	0
			831	527	138	163	3			
1	D	104	Total	C	N	O	S	0	0	0
			831	527	138	163	3			
1	E	107	Total	C	N	O	S	0	0	0
			836	532	134	167	3			
1	F	108	Total	C	N	O	S	0	0	0
			837	535	134	165	3			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	891	GLY	-	expression tag	UNP O75164
A	892	SER	-	expression tag	UNP O75164
A	893	HIS	-	expression tag	UNP O75164
A	894	MET	-	expression tag	UNP O75164
B	891	GLY	-	expression tag	UNP O75164
B	892	SER	-	expression tag	UNP O75164
B	893	HIS	-	expression tag	UNP O75164
B	894	MET	-	expression tag	UNP O75164
C	891	GLY	-	expression tag	UNP O75164
C	892	SER	-	expression tag	UNP O75164
C	893	HIS	-	expression tag	UNP O75164
C	894	MET	-	expression tag	UNP O75164
D	891	GLY	-	expression tag	UNP O75164
D	892	SER	-	expression tag	UNP O75164
D	893	HIS	-	expression tag	UNP O75164
D	894	MET	-	expression tag	UNP O75164
E	891	GLY	-	expression tag	UNP O75164

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	892	SER	-	expression tag	UNP O75164
E	893	HIS	-	expression tag	UNP O75164
E	894	MET	-	expression tag	UNP O75164
F	891	GLY	-	expression tag	UNP O75164
F	892	SER	-	expression tag	UNP O75164
F	893	HIS	-	expression tag	UNP O75164
F	894	MET	-	expression tag	UNP O75164

- Molecule 2 is a protein called peptide H3K23me3 (19-28).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	a	9	Total	C	N	O	0	0	0
			71	45	15	11			
2	b	9	Total	C	N	O	0	0	0
			71	45	15	11			
2	c	7	Total	C	N	O	0	0	0
			53	34	11	8			
2	d	7	Total	C	N	O	0	0	0
			53	34	11	8			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	25	Total	O	0	0
			25	25		
3	a	1	Total	O	0	0
			1	1		
3	B	28	Total	O	0	0
			28	28		
3	b	5	Total	O	0	0
			5	5		
3	C	28	Total	O	0	0
			28	28		
3	c	4	Total	O	0	0
			4	4		
3	D	35	Total	O	0	0
			35	35		
3	d	4	Total	O	0	0
			4	4		
3	E	42	Total	O	0	0
			42	42		
3	F	44	Total	O	0	0
			44	44		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

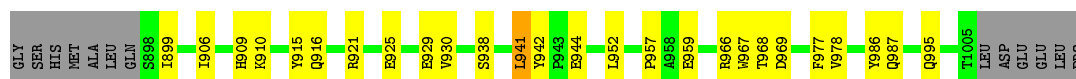
- Molecule 1: Lysine-specific demethylase 4A

Chain A: 



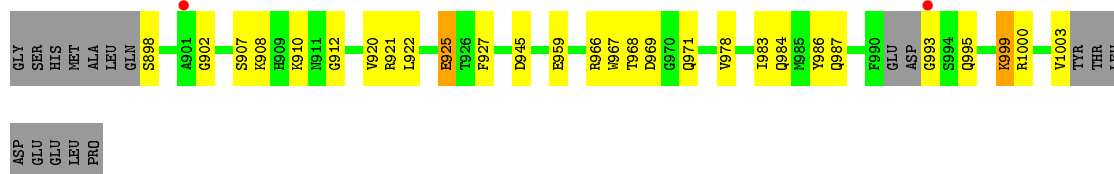
- Molecule 1: Lysine-specific demethylase 4A

Chain B: 



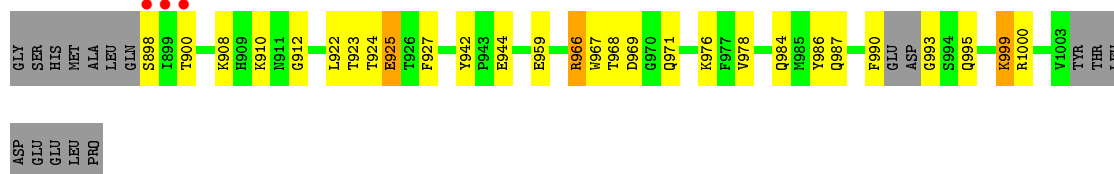
- Molecule 1: Lysine-specific demethylase 4A

Chain C: 



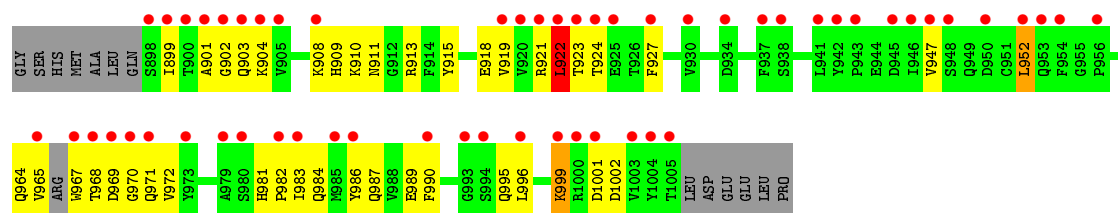
- Molecule 1: Lysine-specific demethylase 4A

Chain D: 

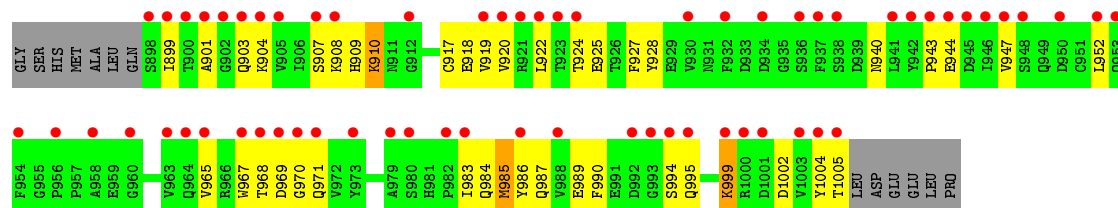


- Molecule 1: Lysine-specific demethylase 4A

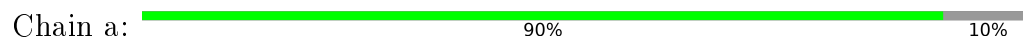
Chain E: 



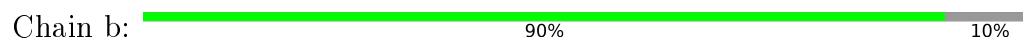
- Molecule 1: Lysine-specific demethylase 4A



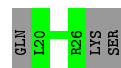
- Molecule 2: peptide H3K23me3 (19-28)



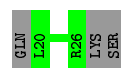
- Molecule 2: peptide H3K23me3 (19-28)



- Molecule 2: peptide H3K23me3 (19-28)



- Molecule 2: peptide H3K23me3 (19-28)



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	106.16 Å 106.16 Å 79.21 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.58 – 2.29 28.58 – 2.29	Depositor EDS
% Data completeness (in resolution range)	91.4 (28.58-2.29) 83.0 (28.58-2.29)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.29 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.264 , 0.295 0.265 , 0.298	Depositor DCC
R_{free} test set	1716 reflections (4.47%)	DCC
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l 0.480 for h,-h-k,-l 0.034 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5533	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.82% 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: 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	0.64	0/887	0.72	0/1203
1	B	0.65	0/887	0.71	1/1203 (0.1%)
1	C	0.63	0/849	0.70	0/1149
1	D	0.62	0/849	0.69	0/1149
1	E	0.49	0/855	0.74	2/1161 (0.2%)
1	F	0.45	0/857	0.70	0/1166
2	a	0.43	0/58	0.66	0/76
2	b	0.40	0/58	0.54	0/76
2	c	0.58	0/40	0.63	0/53
2	d	0.64	0/40	0.68	0/53
All	All	0.58	0/5380	0.71	3/7289 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	922	LEU	CA-CB-CG	5.86	128.78	115.30
1	E	952	LEU	CB-CG-CD1	-5.14	102.26	111.00
1	B	941	LEU	CB-CG-CD1	-5.01	102.48	111.00

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	867	0	813	15	0
1	B	867	0	813	17	0
1	C	831	0	786	29	0
1	D	831	0	786	32	0
1	E	836	0	767	48	0
1	F	837	0	771	52	0
2	a	71	0	84	0	0
2	b	71	0	84	0	0
2	c	53	0	63	0	0
2	d	53	0	63	0	0
3	A	25	0	0	2	0
3	B	28	0	0	2	0
3	C	28	0	0	11	0
3	D	35	0	0	18	1
3	E	42	0	0	15	0
3	F	44	0	0	33	0
3	a	1	0	0	0	0
3	b	5	0	0	0	0
3	c	4	0	0	0	0
3	d	4	0	0	0	1
All	All	5533	0	5030	172	1

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 17.

All (172) 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:E:903:GLN:HB2	3:E:1108:HOH:O	1.35	1.22
1:B:910:LYS:HG2	3:B:1112:HOH:O	1.37	1.21
1:F:901:ALA:HB1	3:F:1114:HOH:O	1.35	1.21
1:E:910:LYS:HE3	3:E:1109:HOH:O	1.37	1.20
1:E:968:THR:HA	3:E:1107:HOH:O	1.38	1.18
1:D:984:GLN:HB3	3:D:1106:HOH:O	1.46	1.14
1:F:919:VAL:HG21	3:F:1106:HOH:O	1.47	1.11
1:A:910:LYS:HG2	3:A:1113:HOH:O	1.48	1.09
1:F:925:GLU:HB2	3:F:1118:HOH:O	1.56	1.04
1:E:908:LYS:HD2	3:E:1120:HOH:O	1.57	1.02
1:F:968:THR:HA	3:F:1110:HOH:O	1.58	1.02
1:F:899:ILE:HG23	3:F:1106:HOH:O	1.60	1.02
1:C:910:LYS:HE2	3:C:1117:HOH:O	1.60	1.00
1:C:984:GLN:HB3	3:C:1119:HOH:O	1.63	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:902:GLY:HA2	3:C:1105:HOH:O	1.66	0.94
1:F:903:GLN:HB3	3:F:1106:HOH:O	1.68	0.94
1:D:944:GLU:OE1	3:D:1101:HOH:O	1.85	0.93
1:F:910:LYS:HA	3:F:1107:HOH:O	1.70	0.92
1:C:999:LYS:HD2	1:C:999:LYS:H	1.34	0.91
1:E:995:GLN:CB	3:F:1110:HOH:O	2.17	0.91
1:E:947:VAL:CG1	3:F:1114:HOH:O	2.17	0.91
1:E:947:VAL:HG12	3:F:1114:HOH:O	1.69	0.90
1:F:899:ILE:CG2	3:F:1106:HOH:O	2.16	0.90
1:F:908:LYS:HB2	3:F:1116:HOH:O	1.73	0.89
1:C:908:LYS:HE3	1:C:912:GLY:HA2	1.54	0.89
1:D:908:LYS:HE3	1:D:912:GLY:HA2	1.54	0.88
1:E:947:VAL:HB	3:F:1114:HOH:O	1.75	0.86
1:D:976:LYS:HD2	3:D:1124:HOH:O	1.74	0.86
1:E:947:VAL:CB	3:F:1114:HOH:O	2.24	0.85
1:E:902:GLY:O	3:E:1101:HOH:O	1.92	0.85
1:D:923:THR:HA	3:D:1110:HOH:O	1.76	0.85
1:F:999:LYS:HG2	3:F:1120:HOH:O	1.76	0.84
1:D:898:SER:HA	1:D:1000:ARG:HH21	1.40	0.84
1:F:985:MET:HB2	3:F:1118:HOH:O	1.76	0.83
1:C:925:GLU:HG3	3:C:1122:HOH:O	1.76	0.83
1:C:898:SER:HA	1:C:1000:ARG:HH21	1.41	0.83
1:C:984:GLN:O	3:C:1101:HOH:O	1.98	0.81
1:C:921:ARG:NE	3:C:1102:HOH:O	2.03	0.81
1:D:944:GLU:OE2	3:D:1102:HOH:O	1.99	0.80
1:E:986:TYR:OH	3:E:1102:HOH:O	2.02	0.78
1:D:925:GLU:OE2	3:D:1103:HOH:O	2.04	0.76
1:D:925:GLU:HG3	3:D:1120:HOH:O	1.85	0.75
1:D:984:GLN:CG	3:D:1106:HOH:O	2.34	0.74
1:E:901:ALA:O	3:E:1103:HOH:O	2.06	0.74
1:D:942:TYR:HB3	3:D:1101:HOH:O	1.87	0.73
1:E:971:GLN:NE2	3:E:1104:HOH:O	2.22	0.73
1:E:904:LYS:NZ	1:E:918:GLU:OE1	2.22	0.72
1:C:999:LYS:HD2	1:C:999:LYS:N	2.04	0.72
1:C:999:LYS:H	1:C:999:LYS:CD	2.04	0.70
1:F:904:LYS:NZ	1:F:918:GLU:OE1	2.25	0.68
1:F:925:GLU:CB	3:F:1118:HOH:O	2.25	0.68
1:D:990:PHE:O	3:D:1104:HOH:O	2.11	0.68
1:F:968:THR:CA	3:F:1110:HOH:O	2.25	0.66
1:E:908:LYS:CG	3:E:1120:HOH:O	2.44	0.66
1:E:923:THR:HG23	1:F:944:GLU:OE1	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:971:GLN:NE2	3:F:1104:HOH:O	2.26	0.65
1:F:901:ALA:CB	3:F:1114:HOH:O	2.10	0.65
1:E:968:THR:O	1:F:994:SER:N	2.29	0.65
1:F:986:TYR:OH	3:F:1101:HOH:O	2.12	0.64
1:E:908:LYS:CD	3:E:1120:HOH:O	2.27	0.64
1:E:921:ARG:CB	1:F:944:GLU:HG2	2.28	0.64
1:E:923:THR:HG23	1:F:944:GLU:CD	2.18	0.63
1:C:987:GLN:NE2	1:C:995:GLN:OE1	2.28	0.63
1:F:999:LYS:HG3	3:F:1129:HOH:O	1.99	0.62
1:D:987:GLN:NE2	1:D:995:GLN:OE1	2.30	0.62
1:C:925:GLU:HG2	1:C:927:PHE:CZ	2.36	0.61
1:F:999:LYS:HB2	3:F:1102:HOH:O	2.01	0.61
1:C:945:ASP:OD1	1:C:966:ARG:NH1	2.32	0.61
1:D:925:GLU:HG2	1:D:927:PHE:CZ	2.36	0.60
1:D:969:ASP:OD1	1:D:971:GLN:HB3	2.00	0.60
1:B:966:ARG:HH22	1:C:925:GLU:CD	2.05	0.60
1:D:923:THR:CA	3:D:1110:HOH:O	2.40	0.59
1:D:999:LYS:HD2	1:D:999:LYS:H	1.67	0.59
1:A:966:ARG:HH22	1:D:925:GLU:CD	2.06	0.59
1:E:952:LEU:HD11	1:F:924:THR:N	2.18	0.57
1:B:925:GLU:CD	1:C:966:ARG:HH22	2.08	0.57
1:D:898:SER:O	3:D:1105:HOH:O	2.17	0.57
1:A:959:GLU:HG3	1:A:978:VAL:O	2.04	0.56
1:E:967:TRP:CG	1:E:968:THR:N	2.73	0.56
1:E:999:LYS:NZ	1:E:1002:ASP:OD2	2.37	0.56
1:A:984:GLN:NE2	3:A:1101:HOH:O	2.28	0.56
1:E:969:ASP:HA	1:F:990:PHE:O	2.05	0.55
1:A:925:GLU:CD	1:D:966:ARG:HH22	2.10	0.55
1:F:999:LYS:NZ	1:F:1002:ASP:OD2	2.34	0.55
1:E:910:LYS:CE	3:E:1109:HOH:O	2.18	0.55
1:D:898:SER:HB2	3:D:1115:HOH:O	2.06	0.55
1:C:920:VAL:HG12	3:C:1123:HOH:O	2.05	0.55
1:C:993:GLY:N	3:C:1104:HOH:O	2.40	0.55
1:D:900:THR:HG23	3:D:1105:HOH:O	2.08	0.54
1:F:999:LYS:CG	3:F:1120:HOH:O	2.46	0.54
1:C:910:LYS:CE	3:C:1117:HOH:O	2.38	0.53
1:C:927:PHE:HD1	1:C:983:ILE:HD12	1.74	0.53
1:A:969:ASP:O	1:D:910:LYS:HD2	2.09	0.53
1:E:989:GLU:CB	1:F:970:GLY:H	2.22	0.53
1:E:921:ARG:CB	1:E:987:GLN:HB3	2.39	0.52
1:B:969:ASP:O	1:C:910:LYS:HD2	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:990:PHE:O	1:F:969:ASP:HA	2.10	0.52
1:B:959:GLU:HG3	1:B:978:VAL:O	2.09	0.52
1:F:967:TRP:CG	1:F:968:THR:N	2.77	0.52
1:C:969:ASP:OD1	1:C:971:GLN:HB3	2.11	0.51
1:F:910:LYS:CA	3:F:1107:HOH:O	2.42	0.50
1:D:984:GLN:CB	3:D:1106:HOH:O	2.18	0.50
1:C:922:LEU:HD23	1:C:984:GLN:CD	2.32	0.50
1:B:987:GLN:NE2	1:B:995:GLN:OE1	2.45	0.49
1:E:924:THR:N	1:F:952:LEU:HD11	2.27	0.49
1:E:908:LYS:N	3:E:1106:HOH:O	2.43	0.49
1:B:942:TYR:HB3	1:B:944:GLU:OE1	2.11	0.49
1:A:909:HIS:HB2	1:A:915:TYR:CD1	2.48	0.48
1:A:942:TYR:HB3	1:A:944:GLU:OE1	2.14	0.48
1:D:986:TYR:OH	1:D:1000:ARG:HD3	2.14	0.48
1:C:907:SER:HB3	1:C:1003:VAL:HG22	1.95	0.48
1:E:902:GLY:N	1:E:919:VAL:O	2.47	0.48
1:E:947:VAL:HG12	1:F:901:ALA:HB1	1.95	0.47
1:E:921:ARG:HA	1:F:944:GLU:O	2.14	0.47
1:A:904:LYS:NZ	1:A:918:GLU:OE1	2.47	0.47
1:C:986:TYR:OH	1:C:1000:ARG:HD3	2.15	0.47
1:B:967:TRP:CG	1:B:968:THR:N	2.83	0.47
1:F:968:THR:HG22	3:F:1110:HOH:O	2.14	0.47
1:C:902:GLY:CA	3:C:1105:HOH:O	2.42	0.46
1:D:923:THR:CB	3:D:1110:HOH:O	2.62	0.46
1:B:909:HIS:HB2	1:B:915:TYR:CD1	2.51	0.46
1:E:922:LEU:HD22	1:E:986:TYR:CD2	2.51	0.46
1:D:922:LEU:HD23	1:D:984:GLN:CD	2.36	0.46
1:F:907:SER:HG	1:F:917:CYS:HG	1.63	0.46
1:E:924:THR:H	1:F:952:LEU:HD11	1.82	0.45
1:F:927:PHE:HD1	1:F:983:ILE:HD12	1.80	0.45
1:A:909:HIS:HB2	1:A:915:TYR:HD1	1.82	0.45
1:A:967:TRP:CG	1:A:968:THR:N	2.84	0.45
1:F:940:ASN:ND2	3:F:1111:HOH:O	2.49	0.45
1:E:927:PHE:HD1	1:E:983:ILE:HD12	1.81	0.45
1:F:968:THR:CG2	3:F:1110:HOH:O	2.64	0.45
1:D:959:GLU:HG3	1:D:978:VAL:O	2.17	0.44
1:D:993:GLY:N	3:D:1108:HOH:O	2.50	0.44
1:E:952:LEU:HD11	1:F:924:THR:H	1.82	0.44
1:D:898:SER:CB	3:D:1115:HOH:O	2.62	0.44
1:E:969:ASP:OD1	1:E:971:GLN:HB3	2.18	0.44
1:F:1004:TYR:HB3	3:F:1113:HOH:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:899:ILE:HB	1:B:986:TYR:CE2	2.52	0.44
1:B:957:PRO:HD2	1:B:977:PHE:CE1	2.53	0.43
1:F:944:GLU:N	1:F:944:GLU:OE1	2.38	0.43
1:E:910:LYS:HG2	1:E:996:LEU:HD21	2.00	0.43
1:E:964:GLN:HB3	1:E:972:VAL:CG1	2.48	0.43
1:C:920:VAL:CG1	3:C:1123:HOH:O	2.66	0.43
1:B:952:LEU:HA	1:B:952:LEU:HD23	1.85	0.43
1:B:921:ARG:NH2	3:B:1105:HOH:O	2.50	0.43
1:E:984:GLN:HG2	3:E:1102:HOH:O	2.18	0.43
1:E:969:ASP:C	1:E:971:GLN:H	2.22	0.43
1:E:899:ILE:HB	1:E:986:TYR:CE2	2.53	0.42
1:F:967:TRP:C	3:F:1110:HOH:O	2.58	0.42
1:F:920:VAL:HG22	1:F:987:GLN:O	2.18	0.42
1:E:970:GLY:H	1:F:989:GLU:CB	2.32	0.42
1:F:928:TYR:CD1	1:F:943:PRO:HA	2.54	0.42
1:B:909:HIS:HB2	1:B:915:TYR:HD1	1.85	0.42
1:B:930:VAL:HG22	1:B:941:LEU:HD11	2.01	0.42
3:E:1107:HOH:O	1:F:995:GLN:CB	2.68	0.42
1:E:968:THR:CA	3:E:1107:HOH:O	2.23	0.42
1:F:984:GLN:O	3:F:1102:HOH:O	2.21	0.41
1:C:959:GLU:HG3	1:C:978:VAL:O	2.20	0.41
1:C:967:TRP:CG	1:C:968:THR:N	2.88	0.41
1:F:968:THR:N	3:F:1110:HOH:O	2.47	0.41
1:D:967:TRP:CG	1:D:968:THR:N	2.89	0.41
1:A:925:GLU:OE1	1:D:966:ARG:NH2	2.52	0.41
1:A:930:VAL:HG22	1:A:941:LEU:HD11	2.03	0.41
1:A:899:ILE:HB	1:A:986:TYR:CE2	2.55	0.41
1:E:981:HIS:HA	1:E:982:PRO:HD2	1.96	0.41
1:F:1005:THR:N	3:F:1113:HOH:O	2.53	0.40
1:E:909:HIS:HB3	1:E:911:ASN:OD1	2.21	0.40
1:A:957:PRO:HD2	1:A:977:PHE:CE1	2.56	0.40
1:E:913:ARG:HB2	1:E:915:TYR:CE1	2.56	0.40
1:F:909:HIS:HD2	1:F:990:PHE:CG	2.40	0.40
1:B:906:ILE:HD13	1:B:916:GLN:HA	2.04	0.40
1:B:929:GLU:HA	1:B:938:SER:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1108:HOH:O	3:d:104:HOH:O[2_544]	2.15	0.05

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	106/121 (88%)	106 (100%)	0	0	100	100
1	B	106/121 (88%)	106 (100%)	0	0	100	100
1	C	100/121 (83%)	100 (100%)	0	0	100	100
1	D	100/121 (83%)	100 (100%)	0	0	100	100
1	E	103/121 (85%)	102 (99%)	1 (1%)	0	100	100
1	F	106/121 (88%)	104 (98%)	2 (2%)	0	100	100
2	a	6/10 (60%)	5 (83%)	1 (17%)	0	100	100
2	b	6/10 (60%)	5 (83%)	1 (17%)	0	100	100
2	c	4/10 (40%)	4 (100%)	0	0	100	100
2	d	4/10 (40%)	4 (100%)	0	0	100	100
All	All	641/766 (84%)	636 (99%)	5 (1%)	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	96/107 (90%)	96 (100%)	0	100	100
1	B	96/107 (90%)	96 (100%)	0	100	100
1	C	92/107 (86%)	90 (98%)	2 (2%)	60	75
1	D	92/107 (86%)	88 (96%)	4 (4%)	35	46

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	90/107 (84%)	86 (96%)	4 (4%)	35	45
1	F	89/107 (83%)	83 (93%)	6 (7%)	20	24
2	a	5/6 (83%)	5 (100%)	0	100	100
2	b	5/6 (83%)	5 (100%)	0	100	100
2	c	3/6 (50%)	3 (100%)	0	100	100
2	d	3/6 (50%)	3 (100%)	0	100	100
All	All	571/666 (86%)	555 (97%)	16 (3%)	51	66

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	925	GLU
1	C	999	LYS
1	D	924	THR
1	D	925	GLU
1	D	966	ARG
1	D	999	LYS
1	E	922	LEU
1	E	965	VAL
1	E	999	LYS
1	E	1001	ASP
1	F	910	LYS
1	F	922	LEU
1	F	947	VAL
1	F	965	VAL
1	F	985	MET
1	F	999	LYS

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

Mol	Chain	Res	Type
2	b	19	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	a	23	2	9,11,12	0.28	0	12,14,16	1.21	2 (16%)
2	M3L	b	23	2	9,11,12	0.35	0	12,14,16	1.15	2 (16%)
2	M3L	c	23	2	9,11,12	0.41	0	12,14,16	0.84	0
2	M3L	d	23	2	9,11,12	0.29	0	12,14,16	0.94	1 (8%)

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	a	23	2	-	0/8/10/12	0/0/0/0
2	M3L	b	23	2	-	0/8/10/12	0/0/0/0
2	M3L	c	23	2	-	0/8/10/12	0/0/0/0
2	M3L	d	23	2	-	0/8/10/12	0/0/0/0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	a	23	M3L	CD-CG-CB	-2.87	103.49	113.67
2	b	23	M3L	CD-CG-CB	-2.70	104.11	113.67
2	d	23	M3L	CD-CG-CB	-2.34	105.39	113.67
2	b	23	M3L	CB-CA-N	2.70	118.12	110.54
2	a	23	M3L	CB-CA-N	2.86	118.60	110.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	108/121 (89%)	-0.06	0 100 100	25, 38, 57, 81	0
1	B	108/121 (89%)	-0.11	0 100 100	28, 39, 57, 81	0
1	C	104/121 (85%)	0.09	2 (1%) 70 76	26, 39, 67, 83	0
1	D	104/121 (85%)	0.09	3 (2%) 55 63	26, 40, 67, 88	0
1	E	107/121 (88%)	2.49	56 (52%) 0 0	74, 92, 130, 148	0
1	F	108/121 (89%)	2.75	63 (58%) 0 0	71, 95, 142, 164	0
2	a	8/10 (80%)	0.06	0 100 100	41, 47, 65, 76	0
2	b	8/10 (80%)	-0.10	0 100 100	40, 54, 67, 76	0
2	c	6/10 (60%)	0.31	0 100 100	26, 37, 51, 57	0
2	d	6/10 (60%)	0.20	0 100 100	28, 35, 52, 56	0
All	All	667/766 (87%)	0.85	124 (18%) 2 2	25, 48, 115, 164	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	902	GLY	15.4
1	F	902	GLY	13.5
1	E	924	THR	10.6
1	E	920	VAL	8.8
1	F	994	SER	7.5
1	E	968	THR	7.5
1	E	942	TYR	7.2
1	E	967	TRP	6.9
1	F	924	THR	6.8
1	F	968	THR	6.6
1	F	943	PRO	6.2
1	F	971	GLN	6.2
1	E	898	SER	6.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	1000	ARG	6.0
1	F	1005	THR	5.9
1	E	919	VAL	5.8
1	F	945	ASP	5.7
1	E	938	SER	5.5
1	F	901	ALA	5.4
1	F	903	GLN	5.4
1	F	969	ASP	5.3
1	E	901	ALA	5.3
1	E	993	GLY	5.3
1	F	905	VAL	5.1
1	F	919	VAL	5.0
1	F	947	VAL	5.0
1	F	967	TRP	5.0
1	F	986	TYR	4.9
1	F	950	ASP	4.8
1	F	979	ALA	4.8
1	E	921	ARG	4.6
1	F	908	LYS	4.6
1	E	937	PHE	4.4
1	F	1004	TYR	4.4
1	F	898	SER	4.4
1	E	994	SER	4.4
1	E	986	TYR	4.3
1	F	980	SER	4.3
1	E	1004	TYR	4.3
1	E	943	PRO	4.2
1	F	934	ASP	4.1
1	E	903	GLN	4.1
1	F	944	GLU	4.0
1	E	930	VAL	4.0
1	E	1003	VAL	4.0
1	F	937	PHE	4.0
1	F	942	TYR	3.9
1	F	920	VAL	3.9
1	E	1005	THR	3.8
1	E	934	ASP	3.7
1	E	908	LYS	3.7
1	F	983	ILE	3.6
1	E	965	VAL	3.5
1	E	1000	ARG	3.5
1	F	930	VAL	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	932	PHE	3.4
1	E	922	LEU	3.4
1	E	983	ILE	3.4
1	F	946	ILE	3.4
1	E	980	SER	3.4
1	E	996	LEU	3.3
1	F	988	VAL	3.3
1	F	923	THR	3.3
1	F	912	GLY	3.2
1	F	904	LYS	3.2
1	E	971	GLN	3.2
1	F	900	THR	3.1
1	E	969	ASP	3.1
1	C	901	ALA	3.1
1	F	956	PRO	3.1
1	E	999	LYS	3.1
1	E	952	LEU	3.1
1	F	1001	ASP	3.1
1	F	954	PHE	3.1
1	E	904	LYS	3.0
1	E	925	GLU	3.0
1	F	1003	VAL	3.0
1	F	993	GLY	2.9
1	E	946	ILE	2.9
1	E	979	ALA	2.9
1	F	970	GLY	2.9
1	F	982	PRO	2.9
1	F	922	LEU	2.8
1	E	941	LEU	2.8
1	F	907	SER	2.8
1	F	938	SER	2.7
1	F	964	GLN	2.7
1	E	905	VAL	2.7
1	E	947	VAL	2.7
1	F	921	ARG	2.7
1	E	990	PHE	2.7
1	E	923	THR	2.6
1	F	936	SER	2.6
1	D	898	SER	2.6
1	F	999	LYS	2.6
1	E	956	PRO	2.6
1	F	963	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	985	MET	2.4
1	F	958	ALA	2.4
1	E	950	ASP	2.4
1	E	900	THR	2.4
1	F	995	GLN	2.4
1	E	973	TYR	2.4
1	F	899	ILE	2.4
1	E	1001	ASP	2.4
1	F	965	VAL	2.4
1	F	992	ASP	2.4
1	F	960	GLY	2.4
1	E	953	GLN	2.3
1	E	982	PRO	2.3
1	E	945	ASP	2.3
1	F	948	SER	2.3
1	F	953	GLN	2.3
1	C	993	GLY	2.3
1	F	952	LEU	2.3
1	F	941	LEU	2.2
1	E	899	ILE	2.2
1	E	954	PHE	2.2
1	E	927	PHE	2.2
1	E	970	GLY	2.1
1	E	948	SER	2.1
1	F	973	TYR	2.1
1	D	899	ILE	2.0
1	D	900	THR	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	M3L	a	23	12/13	0.95	0.18	-	36,38,42,42	0
2	M3L	b	23	12/13	0.94	0.15	-	36,43,49,54	0
2	M3L	c	23	12/13	0.98	0.14	-	20,22,30,31	0
2	M3L	d	23	12/13	0.98	0.14	-	22,24,35,35	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.