



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:58 PM UTC

PDB ID : 5Y5W / pdb_00005y5w
Title : Crystal structure of human Spindlin1 in complex with a histone H4K20(me3) peptide
Authors : Wang, C.; Zang, J.
Deposited on : 2017-08-10
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

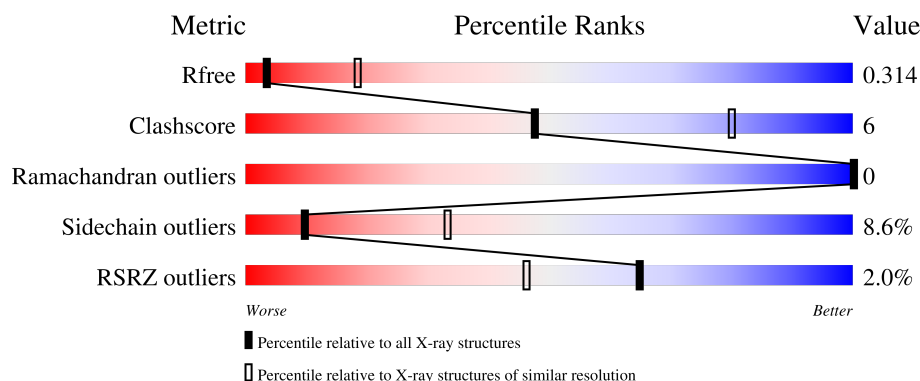
1 Overall quality at a glance i

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.



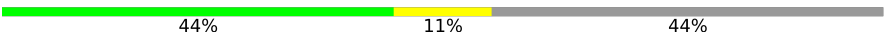
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	235	% 65% 23% • 10%
1	B	235	2% 62% 20% • 17%
1	C	235	% 68% 17% • 14%
1	D	235	3% 73% 9% • 15%
2	E	9	 44% 11% 44%

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Mol	Chain	Length	Quality of chain
2	F	9	 33% 11% 56%
2	G	9	 44% 11% 44%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6354 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 Spindlin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1664	1064	281	311	8			
1	B	195	Total	C	N	O	S	0	0	0
			1511	972	249	282	8			
1	C	201	Total	C	N	O	S	0	0	0
			1577	1014	255	300	8			
1	D	200	Total	C	N	O	S	0	1	0
			1482	959	240	275	8			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	MET	-	initiating methionine	UNP Q9Y657
A	29	SER	-	expression tag	UNP Q9Y657
A	30	SER	-	expression tag	UNP Q9Y657
A	31	GLY	-	expression tag	UNP Q9Y657
A	32	HIS	-	expression tag	UNP Q9Y657
A	33	HIS	-	expression tag	UNP Q9Y657
A	34	HIS	-	expression tag	UNP Q9Y657
A	35	HIS	-	expression tag	UNP Q9Y657
A	36	HIS	-	expression tag	UNP Q9Y657
A	37	HIS	-	expression tag	UNP Q9Y657
A	38	HIS	-	expression tag	UNP Q9Y657
A	39	HIS	-	expression tag	UNP Q9Y657
A	40	GLY	-	expression tag	UNP Q9Y657
A	41	SER	-	expression tag	UNP Q9Y657
A	42	SER	-	expression tag	UNP Q9Y657
A	43	GLU	-	expression tag	UNP Q9Y657
A	44	ASN	-	expression tag	UNP Q9Y657
A	45	LEU	-	expression tag	UNP Q9Y657
A	46	TYR	-	expression tag	UNP Q9Y657
A	47	PHE	-	expression tag	UNP Q9Y657
A	48	GLN	-	expression tag	UNP Q9Y657

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Chain	Residue	Modelled	Actual	Comment	Reference
A	49	GLY	-	expression tag	UNP Q9Y657
A	50	SER	-	expression tag	UNP Q9Y657
B	28	MET	-	initiating methionine	UNP Q9Y657
B	29	SER	-	expression tag	UNP Q9Y657
B	30	SER	-	expression tag	UNP Q9Y657
B	31	GLY	-	expression tag	UNP Q9Y657
B	32	HIS	-	expression tag	UNP Q9Y657
B	33	HIS	-	expression tag	UNP Q9Y657
B	34	HIS	-	expression tag	UNP Q9Y657
B	35	HIS	-	expression tag	UNP Q9Y657
B	36	HIS	-	expression tag	UNP Q9Y657
B	37	HIS	-	expression tag	UNP Q9Y657
B	38	HIS	-	expression tag	UNP Q9Y657
B	39	HIS	-	expression tag	UNP Q9Y657
B	40	GLY	-	expression tag	UNP Q9Y657
B	41	SER	-	expression tag	UNP Q9Y657
B	42	SER	-	expression tag	UNP Q9Y657
B	43	GLU	-	expression tag	UNP Q9Y657
B	44	ASN	-	expression tag	UNP Q9Y657
B	45	LEU	-	expression tag	UNP Q9Y657
B	46	TYR	-	expression tag	UNP Q9Y657
B	47	PHE	-	expression tag	UNP Q9Y657
B	48	GLN	-	expression tag	UNP Q9Y657
B	49	GLY	-	expression tag	UNP Q9Y657
B	50	SER	-	expression tag	UNP Q9Y657
C	28	MET	-	initiating methionine	UNP Q9Y657
C	29	SER	-	expression tag	UNP Q9Y657
C	30	SER	-	expression tag	UNP Q9Y657
C	31	GLY	-	expression tag	UNP Q9Y657
C	32	HIS	-	expression tag	UNP Q9Y657
C	33	HIS	-	expression tag	UNP Q9Y657
C	34	HIS	-	expression tag	UNP Q9Y657
C	35	HIS	-	expression tag	UNP Q9Y657
C	36	HIS	-	expression tag	UNP Q9Y657
C	37	HIS	-	expression tag	UNP Q9Y657
C	38	HIS	-	expression tag	UNP Q9Y657
C	39	HIS	-	expression tag	UNP Q9Y657
C	40	GLY	-	expression tag	UNP Q9Y657
C	41	SER	-	expression tag	UNP Q9Y657
C	42	SER	-	expression tag	UNP Q9Y657
C	43	GLU	-	expression tag	UNP Q9Y657
C	44	ASN	-	expression tag	UNP Q9Y657

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Chain	Residue	Modelled	Actual	Comment	Reference
C	45	LEU	-	expression tag	UNP Q9Y657
C	46	TYR	-	expression tag	UNP Q9Y657
C	47	PHE	-	expression tag	UNP Q9Y657
C	48	GLN	-	expression tag	UNP Q9Y657
C	49	GLY	-	expression tag	UNP Q9Y657
C	50	SER	-	expression tag	UNP Q9Y657
D	28	MET	-	initiating methionine	UNP Q9Y657
D	29	SER	-	expression tag	UNP Q9Y657
D	30	SER	-	expression tag	UNP Q9Y657
D	31	GLY	-	expression tag	UNP Q9Y657
D	32	HIS	-	expression tag	UNP Q9Y657
D	33	HIS	-	expression tag	UNP Q9Y657
D	34	HIS	-	expression tag	UNP Q9Y657
D	35	HIS	-	expression tag	UNP Q9Y657
D	36	HIS	-	expression tag	UNP Q9Y657
D	37	HIS	-	expression tag	UNP Q9Y657
D	38	HIS	-	expression tag	UNP Q9Y657
D	39	HIS	-	expression tag	UNP Q9Y657
D	40	GLY	-	expression tag	UNP Q9Y657
D	41	SER	-	expression tag	UNP Q9Y657
D	42	SER	-	expression tag	UNP Q9Y657
D	43	GLU	-	expression tag	UNP Q9Y657
D	44	ASN	-	expression tag	UNP Q9Y657
D	45	LEU	-	expression tag	UNP Q9Y657
D	46	TYR	-	expression tag	UNP Q9Y657
D	47	PHE	-	expression tag	UNP Q9Y657
D	48	GLN	-	expression tag	UNP Q9Y657
D	49	GLY	-	expression tag	UNP Q9Y657
D	50	SER	-	expression tag	UNP Q9Y657

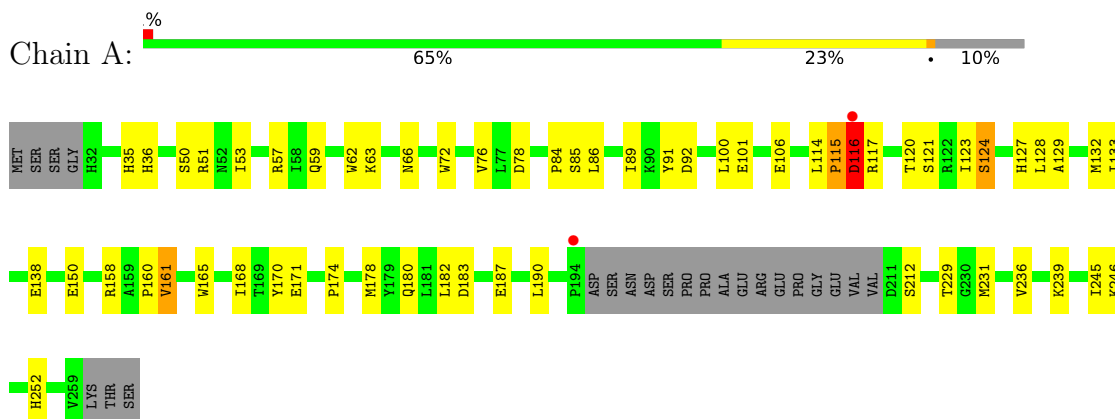
- Molecule 2 is a protein called Histone peptide H4K20(me3).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	5	Total	C	N	O	0	0	0
			51	32	14	5			
2	F	4	Total	C	N	O	0	0	0
			32	21	7	4			
2	G	5	Total	C	N	O	0	0	0
			37	24	8	5			

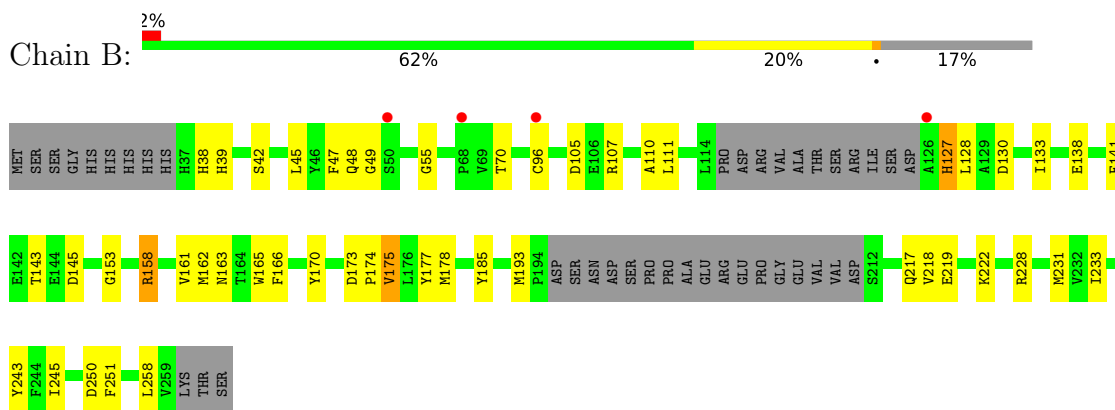
3 Residue-property plots [i](#)

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.

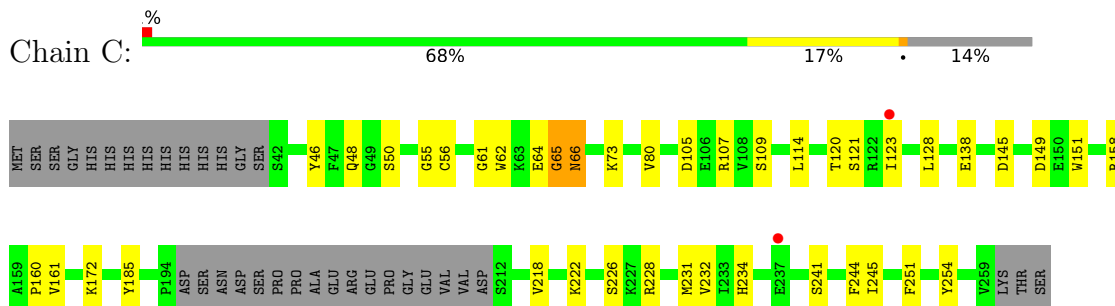
• Molecule 1: Spindlin-1



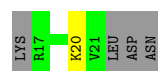
• Molecule 1: Spindlin-1



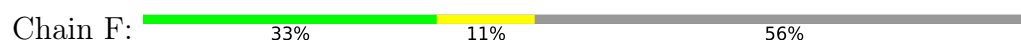
• Molecule 1: Spindlin-1



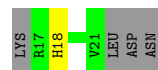
Chain D: 3% 73% 9% 15%



- Molecule 2: Histone peptide H4K20(me3)



- Molecule 2: Histone peptide H4K20(me3)



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	88.77Å 148.50Å 169.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.61 – 3.30 84.61 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (84.61-3.30) 99.7 (84.61-3.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.04 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.219 , 0.308 0.231 , 0.314	Depositor DCC
R_{free} test set	903 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å ²)	65.2	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.032 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6354	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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	1.37	8/1710 (0.5%)	1.32	16/2328 (0.7%)
1	B	0.99	0/1550	1.14	6/2111 (0.3%)
1	C	0.99	0/1616	1.09	7/2199 (0.3%)
1	D	0.86	0/1523	1.00	3/2088 (0.1%)
2	E	0.68	0/39	0.61	0/50
2	F	0.74	0/20	0.72	0/26
2	G	0.73	0/25	0.77	0/33
All	All	1.08	8/6483 (0.1%)	1.14	32/8835 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	PRO	N-CD	8.39	1.59	1.47
1	A	116	ASP	CA-C	8.21	1.62	1.52
1	A	180	GLN	CA-C	-6.79	1.45	1.53
1	A	62	TRP	C-O	6.38	1.31	1.23
1	A	63	LYS	C-O	6.08	1.30	1.23
1	A	114	LEU	C-N	5.63	1.40	1.33
1	A	76	VAL	C-O	-5.58	1.17	1.23
1	A	84	PRO	CA-C	-5.23	1.47	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	ASP	N-CA-CB	12.86	133.14	111.66
1	B	111	LEU	N-CA-C	8.61	122.93	110.10
1	B	49	GLY	N-CA-C	-8.45	98.38	111.64
1	A	161	VAL	CB-CA-C	7.25	118.33	111.44
1	A	124	SER	N-CA-C	7.21	118.78	111.07
1	A	114	LEU	CA-C-N	-6.47	113.28	120.14
1	A	114	LEU	C-N-CA	-6.47	113.28	120.14
1	C	66	ASN	N-CA-C	6.47	120.09	112.72
1	A	160	PRO	CA-C-N	-6.32	116.70	123.08
1	A	160	PRO	C-N-CA	-6.32	116.70	123.08
1	C	160	PRO	CA-C-N	-5.94	117.08	123.08
1	C	160	PRO	C-N-CA	-5.94	117.08	123.08
1	C	114	LEU	CA-C-N	5.73	125.75	119.90
1	C	114	LEU	C-N-CA	5.73	125.75	119.90
1	B	133	ILE	N-CA-C	5.70	115.89	110.42
1	A	92	ASP	N-CA-C	-5.70	101.21	109.59
1	A	252	HIS	N-CA-C	5.66	118.22	110.24
1	A	127	HIS	N-CA-C	-5.59	105.10	111.14
1	A	53	ILE	N-CA-C	5.58	116.87	111.91
1	A	174	PRO	CB-CA-C	5.58	116.24	110.00
1	A	174	PRO	N-CA-C	5.56	121.54	114.92
1	A	115	PRO	CA-N-CD	-5.51	104.28	112.00
1	A	116	ASP	N-CA-C	-5.47	100.75	109.07
1	A	120	THR	N-CA-C	-5.46	102.40	110.48
1	D	48	GLN	N-CA-C	-5.46	102.56	110.64
1	B	233	ILE	CB-CA-C	-5.46	104.92	110.93
1	D	48	GLN	CB-CA-C	5.40	116.45	109.80
1	C	80	VAL	N-CA-CB	5.40	116.01	110.23
1	D	192	ILE	N-CA-C	5.29	115.51	108.11
1	B	175	VAL	N-CA-CB	5.24	119.88	111.23
1	C	65	GLY	N-CA-C	-5.17	100.93	113.18
1	B	110	ALA	N-CA-C	5.05	121.55	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	ASP	Peptide

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	1664	0	1532	16	0
1	B	1511	0	1384	25	0
1	C	1577	0	1479	19	0
1	D	1482	0	1307	14	0
2	E	51	0	60	1	0
2	F	32	0	28	1	0
2	G	37	0	31	0	0
All	All	6354	0	5821	68	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 6.

All (68) 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:C:62:TRP:CH2	1:C:107:ARG:HD2	2.26	0.70
1:C:105:ASP:OD2	1:C:107:ARG:NH1	2.26	0.68
1:B:47:PHE:HB3	1:C:218:VAL:HG12	1.75	0.67
1:B:143:THR:OG1	1:B:145:ASP:OD1	2.11	0.65
1:B:96:CYS:SG	1:B:177:TYR:CE1	2.93	0.59
1:B:128:LEU:HD21	1:B:185:TYR:CD1	2.38	0.58
1:D:193:MET:SD	1:D:193:MET:N	2.77	0.58
1:B:39:HIS:HB3	1:C:254:TYR:HE2	1.70	0.56
1:B:47:PHE:HA	1:C:218:VAL:HA	1.89	0.55
1:C:120:THR:OG1	1:C:121:SER:N	2.40	0.54
1:A:170:TYR:CE2	2:E:20:M3L:HM31	2.42	0.54
1:D:115:PRO:O	1:D:116:ASP:OD1	2.25	0.54
1:D:137:VAL:HG21	1:D:190:LEU:HD11	1.91	0.53
1:A:59:GLN:HA	1:A:72:TRP:O	2.09	0.53
1:D:158:ARG:HD2	1:D:163:ASN:O	2.09	0.53
1:B:166:PHE:O	1:B:178:MET:HA	2.10	0.52
1:B:105:ASP:OD2	1:B:107:ARG:NH2	2.42	0.52
1:B:162:MET:HB3	1:B:165:TRP:CD1	2.44	0.51
1:B:141:PHE:CZ	2:F:20:M3L:HM23	2.46	0.51
1:A:183:ASP:O	1:A:187:GLU:HG3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:MET:HG2	1:C:232:VAL:N	2.27	0.49
1:C:55:GLY:HA2	1:C:161:VAL:HG21	1.94	0.49
1:B:174:PRO:O	1:B:175:VAL:HG13	2.12	0.49
1:B:39:HIS:HB3	1:C:254:TYR:CE2	2.47	0.49
1:C:151:TRP:CZ3	1:C:172:LYS:HB2	2.48	0.48
1:A:85:SER:HB3	1:A:101:GLU:HG2	1.94	0.48
1:A:86:LEU:HD21	1:A:246:LYS:HG2	1.95	0.48
1:B:158:ARG:HG2	1:B:163:ASN:O	2.14	0.48
1:A:35:HIS:ND1	1:A:36:HIS:O	2.47	0.48
1:A:129:ALA:HB2	1:A:182:LEU:HD11	1.96	0.47
1:B:158:ARG:CG	1:B:163:ASN:O	2.62	0.47
1:B:250:ASP:OD1	1:B:251:PHE:N	2.48	0.47
1:C:61:GLY:N	1:C:109:SER:O	2.44	0.46
1:B:48:GLN:O	1:B:48:GLN:HG3	2.15	0.46
1:C:149:ASP:OD2	1:C:151:TRP:NE1	2.45	0.46
1:C:234:HIS:HB3	1:C:244:PHE:HB2	1.98	0.46
1:A:57:ARG:HG3	1:A:116:ASP:OD2	2.15	0.45
1:B:55:GLY:HA2	1:B:161:VAL:HG11	1.98	0.45
1:C:123:ILE:HG21	1:C:158:ARG:HH12	1.81	0.45
1:B:153:GLY:HA2	1:B:170:TYR:HA	1.98	0.45
1:D:138:GLU:HB2	1:D:193:MET:HE1	1.97	0.45
1:D:153:GLY:HA2	1:D:170:TYR:HA	1.97	0.45
1:D:235:GLN:HG3	1:D:243:TYR:CZ	2.52	0.45
1:A:165:TRP:HB2	1:A:178:MET:HE3	1.99	0.45
1:A:50:SER:OG	1:A:51:ARG:N	2.49	0.45
1:C:222:LYS:HD3	1:C:226:SER:HB2	1.98	0.45
1:D:85:SER:HB2	1:D:101:GLU:HG2	2.00	0.44
1:D:220:TYR:C	1:D:220:TYR:HD1	2.26	0.44
1:C:128:LEU:HD21	1:C:185:TYR:CD2	2.53	0.44
1:C:64:GLU:O	1:C:65:GLY:C	2.61	0.43
1:D:220:TYR:C	1:D:220:TYR:CD1	2.96	0.43
1:A:117:ARG:HG2	1:C:46:TYR:CE2	2.53	0.43
1:D:241:SER:HB2	1:D:259:VAL:HG23	2.01	0.43
1:B:174:PRO:O	1:B:175:VAL:CG1	2.66	0.43
1:A:57:ARG:HG3	1:A:116:ASP:HB2	2.00	0.43
1:A:57:ARG:HG3	1:A:116:ASP:CB	2.49	0.42
1:D:184:ASP:OD1	1:D:184:ASP:N	2.52	0.42
1:D:128:LEU:O	1:D:131:THR:OG1	2.36	0.42
1:A:89:ILE:HG21	1:A:91:TYR:CZ	2.54	0.42
1:B:217:GLN:O	1:B:218:VAL:HG13	2.19	0.42
1:D:255:VAL:O	1:D:256:TYR:HD1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:TYR:CD1	1:B:258:LEU:HD12	2.55	0.41
1:B:96:CYS:SG	1:B:177:TYR:HE1	2.41	0.41
1:B:219:GLU:OE2	1:C:48:GLN:HB2	2.21	0.41
1:A:132:MET:O	1:A:133:ILE:C	2.64	0.41
1:B:173:ASP:OD1	1:B:173:ASP:C	2.64	0.40
1:A:236:VAL:HG12	1:A:239:LYS:H	1.86	0.40
1:B:127:HIS:O	1:B:130:ASP:OD2	2.39	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	208/235 (88%)	193 (93%)	15 (7%)	0	100	100
1	B	189/235 (80%)	172 (91%)	17 (9%)	0	100	100
1	C	197/235 (84%)	186 (94%)	11 (6%)	0	100	100
1	D	197/235 (84%)	176 (89%)	21 (11%)	0	100	100
2	E	2/9 (22%)	2 (100%)	0	0	100	100
2	F	1/9 (11%)	1 (100%)	0	0	100	100
2	G	2/9 (22%)	2 (100%)	0	0	100	100
All	All	796/967 (82%)	732 (92%)	64 (8%)	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	171/207 (83%)	151 (88%)	20 (12%)	5	20
1	B	152/207 (73%)	140 (92%)	12 (8%)	11	36
1	C	164/207 (79%)	154 (94%)	10 (6%)	17	45
1	D	137/207 (66%)	125 (91%)	12 (9%)	9	32
2	E	4/8 (50%)	4 (100%)	0	100	100
2	F	1/8 (12%)	1 (100%)	0	100	100
2	G	1/8 (12%)	0	1 (100%)	0	0
All	All	630/852 (74%)	575 (91%)	55 (9%)	10	32

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	78	ASP
1	A	100	LEU
1	A	106	GLU
1	A	115	PRO
1	A	121	SER
1	A	123	ILE
1	A	124	SER
1	A	128	LEU
1	A	138	GLU
1	A	150	GLU
1	A	158	ARG
1	A	161	VAL
1	A	168	ILE
1	A	171	GLU
1	A	190	LEU
1	A	212	SER
1	A	229	THR
1	A	231	MET
1	A	245	ILE
1	B	38	HIS
1	B	42	SER
1	B	45	LEU
1	B	70	THR
1	B	127	HIS
1	B	138	GLU

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Mol	Chain	Res	Type
1	B	158	ARG
1	B	193	MET
1	B	222	LYS
1	B	228	ARG
1	B	231	MET
1	B	245	ILE
1	C	50	SER
1	C	56	CYS
1	C	66	ASN
1	C	73	LYS
1	C	138	GLU
1	C	145	ASP
1	C	228	ARG
1	C	241	SER
1	C	245	ILE
1	C	251	PHE
1	D	45	LEU
1	D	85	SER
1	D	96[A]	CYS
1	D	96[B]	CYS
1	D	128	LEU
1	D	138	GLU
1	D	173	ASP
1	D	184	ASP
1	D	193	MET
1	D	220	TYR
1	D	245	ILE
1	D	259	VAL
2	G	18	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	235	GLN
1	B	37	HIS
1	B	52	ASN
1	C	52	ASN
1	C	66	ASN
1	C	252	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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	E	20	2	10,11,12	0.98	0	9,14,16	0.66	0
2	M3L	G	20	2	10,11,12	0.75	0	9,14,16	0.49	0
2	M3L	F	20	2	10,11,12	0.74	0	9,14,16	0.63	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	E	20	2	-	5/9/10/12	-
2	M3L	G	20	2	-	3/9/10/12	-
2	M3L	F	20	2	-	7/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	20	M3L	O-C-CA-CB
2	F	20	M3L	C-CA-CB-CG
2	G	20	M3L	O-C-CA-CB
2	F	20	M3L	CG-CD-CE-NZ

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Mol	Chain	Res	Type	Atoms
2	E	20	M3L	CG-CD-CE-NZ
2	G	20	M3L	CG-CD-CE-NZ
2	G	20	M3L	CA-CB-CG-CD
2	E	20	M3L	CE-CD-CG-CB
2	E	20	M3L	CA-CB-CG-CD
2	F	20	M3L	N-CA-CB-CG
2	F	20	M3L	CD-CE-NZ-CM1
2	F	20	M3L	CD-CE-NZ-CM2
2	F	20	M3L	CD-CE-NZ-CM3
2	F	20	M3L	CE-CD-CG-CB
2	E	20	M3L	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	20	M3L	1	0
2	F	20	M3L	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	212/235 (90%)	-0.12	2 (0%) 81 65	21, 45, 90, 115	0
1	B	195/235 (82%)	0.06	4 (2%) 63 44	29, 58, 112, 141	0
1	C	201/235 (85%)	-0.11	2 (0%) 79 63	26, 56, 104, 124	0
1	D	200/235 (85%)	0.47	8 (4%) 42 28	47, 80, 139, 170	1 (0%)
2	E	4/9 (44%)	0.78	0 100 100	66, 92, 97, 109	0
2	F	3/9 (33%)	0.78	0 100 100	98, 98, 100, 116	0
2	G	4/9 (44%)	0.75	0 100 100	82, 90, 106, 117	0
All	All	819/967 (84%)	0.08	16 (1%) 65 46	21, 61, 118, 170	1 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	116	ASP	4.8
1	D	124	SER	3.1
1	A	116	ASP	2.6
1	A	194	PRO	2.5
1	B	126	ALA	2.5
1	D	122	ARG	2.4
1	D	224	ASP	2.4
1	D	112	GLU	2.4
1	B	96	CYS	2.3
1	D	119	ALA	2.3
1	D	111	LEU	2.2
1	C	123	ILE	2.2
1	B	68	PRO	2.2
1	C	237	GLU	2.1
1	B	50	SER	2.0
1	D	123	ILE	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($\text{\AA}^2$)	Q<0.9
2	M3L	F	20	12/13	0.87	0.22	99,108,120,121	0
2	M3L	G	20	12/13	0.94	0.13	75,91,99,109	0
2	M3L	E	20	12/13	0.96	0.13	53,61,81,83	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.