



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:02 PM GMT

PDB ID : 4GY5
Title : Crystal structure of the tandem tudor domain and plant homeodomain of UHRF1 with Histone H3K9me3
Authors : Cheng, J.; Yang, Y.; Fang, J.; Xiao, J.; Zhu, T.; Chen, F.; Wang, P.; Xu, Y.
Deposited on : 2012-09-05
Resolution : 2.96 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

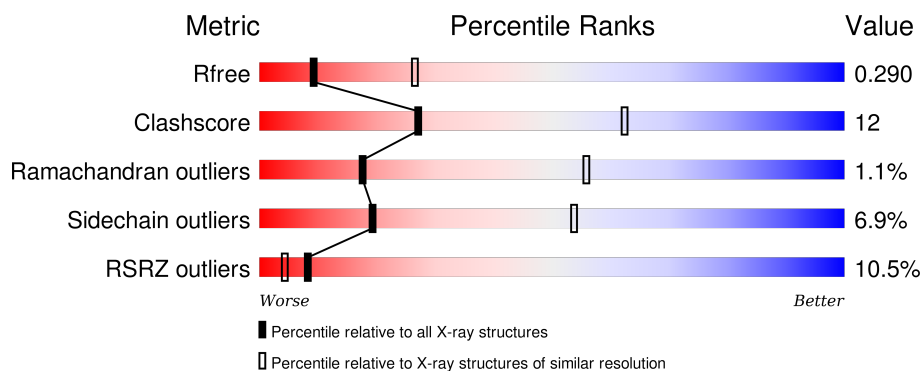
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.96 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	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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	241	<div> <div>8%</div> <div>58%</div> <div>28%</div> <div>11%</div> </div>
1	B	241	<div> <div>15%</div> <div>60%</div> <div>25%</div> <div>13%</div> </div>
1	C	241	<div> <div>2%</div> <div>49%</div> <div>13%</div> <div>36%</div> </div>
1	D	241	<div> <div>5%</div> <div>45%</div> <div>15%</div> <div>38%</div> </div>
2	E	17	<div> <div>6%</div> <div>24%</div> <div>35%</div> <div>41%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	17	<p>29%</p> <p>24%</p> <p>24%</p> <p>6%</p> <p>47%</p>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6138 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 E3 ubiquitin-protein ligase UHRF1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	4	0	0
			1753	1087	315	332	19			
1	B	210	Total	C	N	O	S	0	0	0
			1708	1057	307	325	19			
1	C	154	Total	C	N	O	S	30	0	0
			1267	790	229	241	7			
1	D	150	Total	C	N	O	S	32	0	0
			1235	770	224	235	6			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	126	GLY	-	EXPRESSION TAG	UNP Q96T88
A	127	PRO	-	EXPRESSION TAG	UNP Q96T88
A	128	LEU	-	EXPRESSION TAG	UNP Q96T88
A	129	GLY	-	EXPRESSION TAG	UNP Q96T88
A	130	SER	-	EXPRESSION TAG	UNP Q96T88
A	131	PRO	-	EXPRESSION TAG	UNP Q96T88
A	132	GLU	-	EXPRESSION TAG	UNP Q96T88
A	133	PHE	-	EXPRESSION TAG	UNP Q96T88
B	126	GLY	-	EXPRESSION TAG	UNP Q96T88
B	127	PRO	-	EXPRESSION TAG	UNP Q96T88
B	128	LEU	-	EXPRESSION TAG	UNP Q96T88
B	129	GLY	-	EXPRESSION TAG	UNP Q96T88
B	130	SER	-	EXPRESSION TAG	UNP Q96T88
B	131	PRO	-	EXPRESSION TAG	UNP Q96T88
B	132	GLU	-	EXPRESSION TAG	UNP Q96T88
B	133	PHE	-	EXPRESSION TAG	UNP Q96T88
C	126	GLY	-	EXPRESSION TAG	UNP Q96T88
C	127	PRO	-	EXPRESSION TAG	UNP Q96T88
C	128	LEU	-	EXPRESSION TAG	UNP Q96T88
C	129	GLY	-	EXPRESSION TAG	UNP Q96T88
C	130	SER	-	EXPRESSION TAG	UNP Q96T88

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Chain	Residue	Modelled	Actual	Comment	Reference
C	131	PRO	-	EXPRESSION TAG	UNP Q96T88
C	132	GLU	-	EXPRESSION TAG	UNP Q96T88
C	133	PHE	-	EXPRESSION TAG	UNP Q96T88
D	126	GLY	-	EXPRESSION TAG	UNP Q96T88
D	127	PRO	-	EXPRESSION TAG	UNP Q96T88
D	128	LEU	-	EXPRESSION TAG	UNP Q96T88
D	129	GLY	-	EXPRESSION TAG	UNP Q96T88
D	130	SER	-	EXPRESSION TAG	UNP Q96T88
D	131	PRO	-	EXPRESSION TAG	UNP Q96T88
D	132	GLU	-	EXPRESSION TAG	UNP Q96T88
D	133	PHE	-	EXPRESSION TAG	UNP Q96T88

- Molecule 2 is a protein called Peptide from Histone H3.3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	10	Total	C	N	O	0	0	0
			82	49	19	14			
2	F	9	Total	C	N	O	0	0	0
			76	46	18	12			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Zn	0	0
			3	3		
3	A	3	Total	Zn	0	0
			3	3		
3	C	1	Total	Zn	0	0
			1	1		

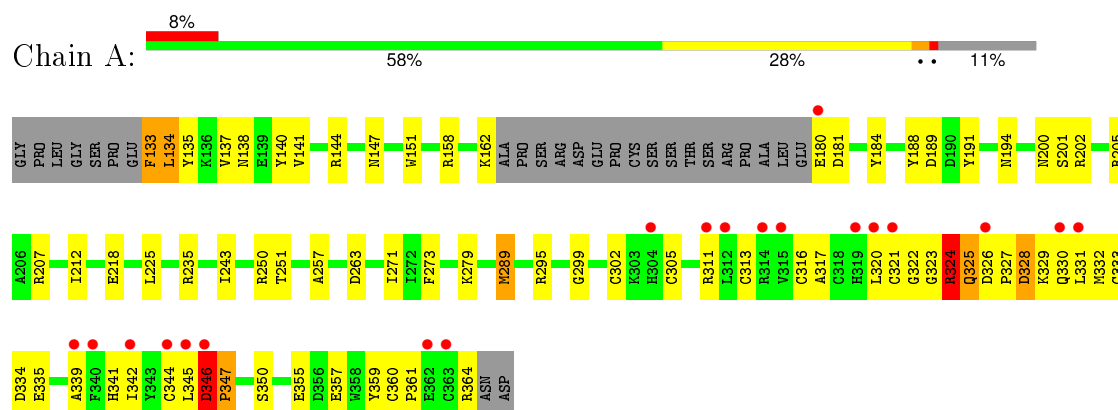
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		
4	B	2	Total	O	0	0
			2	2		
4	C	2	Total	O	0	0
			2	2		
4	D	1	Total	O	0	0
			1	1		

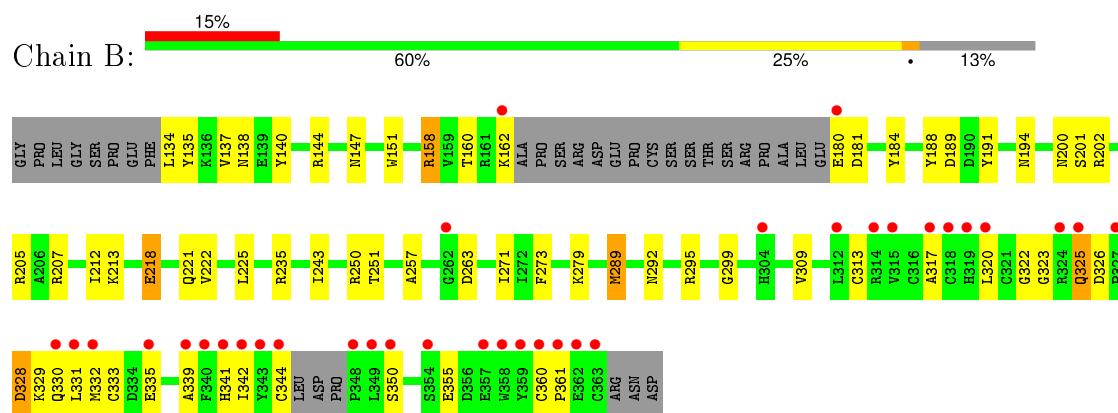
3 Residue-property plots

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.

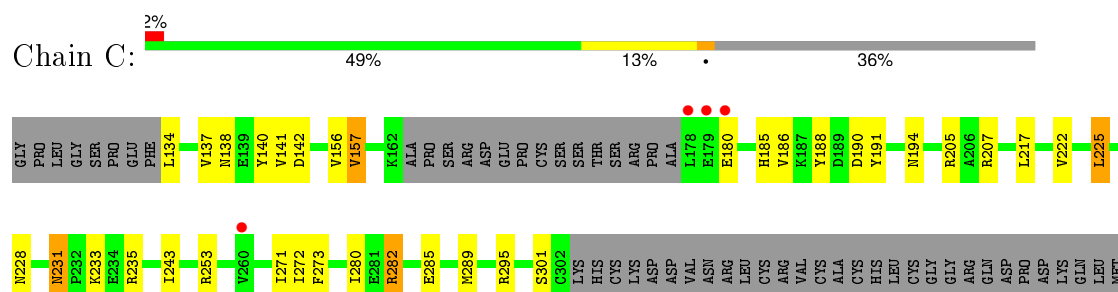
• Molecule 1: E3 ubiquitin-protein ligase UHRF1



• Molecule 1: E3 ubiquitin-protein ligase UHRF1

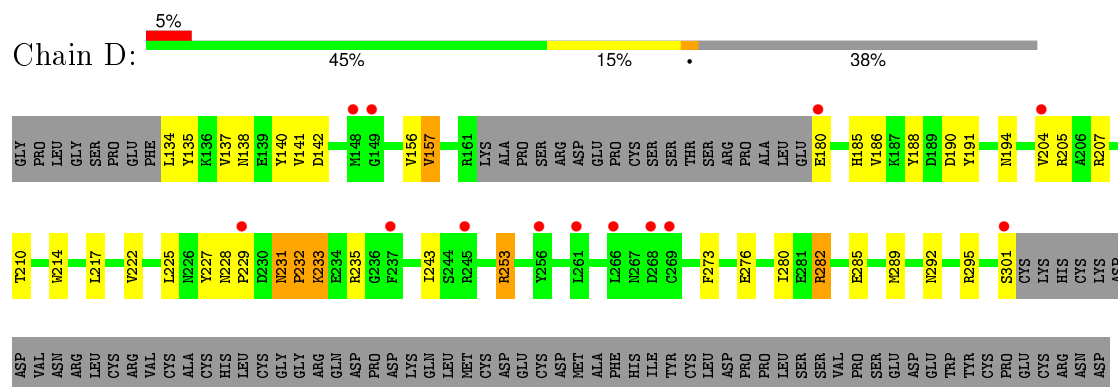


• Molecule 1: E3 ubiquitin-protein ligase UHRF1

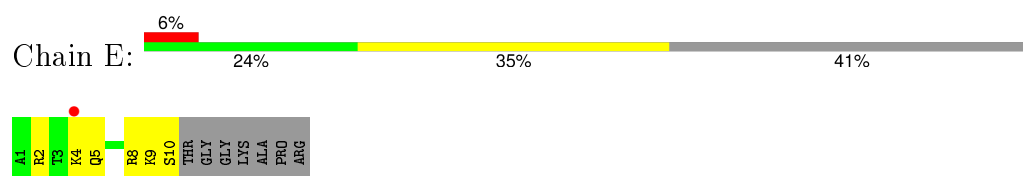


CYS ASP
GLU LEU
CYS ASP
MET MET
ALA PHE
HIS ILE
TYR TYR
CYS LEU
ASP LEU
PRO PRO
PRO LEU
SER SER
SER VAL
PRO VAL
SER SER
GLU GLU
ASP ASP
GLU TRP
TYR TYR
CYS CYS
PRO PRO
GLU GLU
CYS ARG
ASN ASP

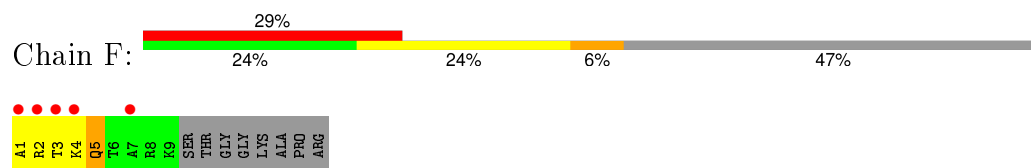
- Molecule 1: E3 ubiquitin-protein ligase UHRF1



- Molecule 2: Peptide from Histone H3.3



- Molecule 2: Peptide from Histone H3.3



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	145.94Å 145.94Å 125.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.38 – 2.96 45.38 – 2.96	Depositor EDS
% Data completeness (in resolution range)	95.9 (45.38-2.96) 99.6 (45.38-2.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_353)	Depositor
R, R_{free}	0.255 , 0.288 0.252 , 0.290	Depositor DCC
R_{free} test set	1471 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	86.6	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 48.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 28928 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6138	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, 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	0.21	0/1791	0.71	9/2421 (0.4%)
1	B	0.25	0/1743	0.65	6/2353 (0.3%)
1	C	0.19	0/1291	0.37	0/1744
1	D	0.24	0/1259	0.39	0/1702
2	E	0.19	0/69	0.41	0/90
2	F	0.19	0/63	0.42	0/82
All	All	0.23	0/6216	0.57	15/8392 (0.2%)

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	2

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	ARG	NE-CZ-NH2	-12.40	114.10	120.30
1	B	207	ARG	NE-CZ-NH1	-12.39	114.10	120.30
1	B	207	ARG	NE-CZ-NH2	12.29	126.45	120.30
1	A	202	ARG	NE-CZ-NH2	-11.94	114.33	120.30
1	B	202	ARG	NE-CZ-NH1	-11.80	114.40	120.30
1	A	207	ARG	NE-CZ-NH1	11.78	126.19	120.30
1	A	202	ARG	NE-CZ-NH1	11.49	126.05	120.30
1	B	202	ARG	NE-CZ-NH2	11.37	125.99	120.30
1	A	346	ASP	CB-CA-C	-9.85	90.71	110.40
1	A	346	ASP	N-CA-C	8.31	133.45	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	207	ARG	CD-NE-CZ	6.29	132.40	123.60
1	A	202	ARG	CD-NE-CZ	5.91	131.87	123.60
1	A	207	ARG	CD-NE-CZ	5.83	131.77	123.60
1	B	202	ARG	CD-NE-CZ	5.79	131.71	123.60
1	A	346	ASP	C-N-CD	-5.25	109.06	120.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	324	ARG	Sidechain
1	A	346	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	1753	0	1665	51	1
1	B	1708	0	1621	42	0
1	C	1267	0	1230	18	0
1	D	1235	0	1195	29	0
2	E	82	0	97	6	0
2	F	76	0	91	6	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	1	0	0	0	0
4	A	5	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
All	All	6138	0	5899	142	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 12.

All (142) 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:D:235:ARG:NH1	1:D:273:PHE:CE2	2.05	1.25
1:B:158:ARG:HH21	1:B:158:ARG:CG	1.57	1.14
1:B:158:ARG:HG3	1:B:158:ARG:NH2	1.43	1.12
1:A:360:CYS:HB2	1:A:361:PRO:HD2	1.69	0.74
1:D:229:PRO:O	1:D:232:PRO:HD3	1.88	0.73
1:A:317:ALA:HB2	1:A:324:ARG:HD3	1.70	0.73
1:D:235:ARG:HH12	1:D:273:PHE:HE2	1.35	0.72
1:C:282:ARG:HG3	1:C:285:GLU:HB2	1.71	0.72
1:D:282:ARG:HG3	1:D:285:GLU:HB2	1.71	0.71
1:A:346:ASP:HB2	1:A:347:PRO:CD	2.21	0.71
1:B:360:CYS:HB2	1:B:361:PRO:HD2	1.71	0.70
1:A:357:GLU:OE1	1:A:359:TYR:OH	2.03	0.70
1:A:188:TYR:HB2	1:A:191:TYR:HB2	1.74	0.70
1:B:158:ARG:HG3	1:B:158:ARG:HH21	0.66	0.70
1:B:188:TYR:HB2	1:B:191:TYR:HB2	1.74	0.69
1:D:235:ARG:NH1	1:D:273:PHE:CZ	2.61	0.67
1:A:311:ARG:O	1:A:324:ARG:NH1	2.26	0.67
1:D:231:ASN:O	1:D:233:LYS:N	2.30	0.65
1:A:345:LEU:H	1:A:345:LEU:HD23	1.61	0.65
1:B:328:ASP:HB3	2:F:5:GLN:CD	2.18	0.63
1:A:133:PHE:N	1:A:133:PHE:CD1	2.66	0.61
1:A:133:PHE:N	1:A:133:PHE:HD1	1.98	0.61
1:D:140:TYR:HB2	1:D:289:MET:HG2	1.82	0.61
1:A:189:ASP:HB3	1:A:295:ARG:HH21	1.66	0.60
1:B:158:ARG:NH2	1:B:158:ARG:CG	2.30	0.60
1:B:189:ASP:HB3	1:B:295:ARG:HH21	1.66	0.60
1:D:188:TYR:HB2	1:D:191:TYR:HB2	1.83	0.60
1:C:140:TYR:HB2	1:C:289:MET:HG2	1.82	0.60
1:C:156:VAL:HA	1:C:186:VAL:HG12	1.83	0.59
1:C:188:TYR:HB2	1:C:191:TYR:HB2	1.83	0.59
1:B:140:TYR:HB2	1:B:289:MET:HG2	1.85	0.59
1:D:156:VAL:HA	1:D:186:VAL:HG12	1.83	0.58
1:A:317:ALA:HB2	1:A:324:ARG:CD	2.33	0.58
1:A:140:TYR:HB2	1:A:289:MET:HG2	1.85	0.58
1:A:313:CYS:O	1:A:317:ALA:HB3	2.05	0.57
1:A:327:PRO:HG2	2:E:5:GLN:NE2	2.20	0.57
1:D:214:TRP:CE2	1:D:253:ARG:HG2	2.40	0.57
1:D:235:ARG:NH2	1:D:276:GLU:OE2	2.34	0.56
1:C:217:LEU:HD22	1:C:243:ILE:HD11	1.87	0.56
1:A:346:ASP:HB2	1:A:347:PRO:HD3	1.86	0.56
1:B:313:CYS:O	1:B:317:ALA:HB3	2.05	0.56
1:B:191:TYR:HB3	1:B:194:ASN:HD22	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:TYR:HB3	1:A:194:ASN:HD22	1.70	0.56
1:D:191:TYR:HB3	1:D:194:ASN:HD22	1.71	0.55
1:A:162:LYS:HD2	1:A:181:ASP:OD1	2.06	0.55
1:B:162:LYS:HD2	1:B:181:ASP:OD1	2.06	0.55
1:C:190:ASP:HB3	1:C:295:ARG:HH22	1.71	0.55
1:D:190:ASP:HB3	1:D:295:ARG:HH22	1.71	0.55
1:C:191:TYR:HB3	1:C:194:ASN:HD22	1.71	0.55
1:D:217:LEU:HD22	1:D:243:ILE:HD11	1.88	0.55
1:A:320:LEU:HD13	1:A:344:CYS:HB3	1.89	0.55
1:A:137:VAL:O	1:A:138:ASN:HB2	2.07	0.55
1:D:235:ARG:NH2	1:D:276:GLU:OE1	2.41	0.54
1:A:191:TYR:HB3	1:A:194:ASN:ND2	2.23	0.54
2:F:3:THR:HG22	2:F:4:LYS:H	1.72	0.54
1:B:158:ARG:NH2	1:B:160:THR:HG23	2.24	0.53
1:B:191:TYR:HB3	1:B:194:ASN:ND2	2.23	0.53
1:A:316:CYS:SG	1:A:324:ARG:NH2	2.81	0.53
1:B:332:MET:HB3	2:F:2:ARG:HH21	1.72	0.53
1:C:233:LYS:HA	1:C:272:ILE:HD11	1.91	0.53
1:B:137:VAL:O	1:B:138:ASN:HB2	2.07	0.52
2:F:3:THR:HG22	2:F:4:LYS:N	2.25	0.52
1:D:141:VAL:HB	1:D:205:ARG:O	2.10	0.51
1:D:228:ASN:O	1:D:232:PRO:N	2.44	0.51
1:C:141:VAL:HB	1:C:205:ARG:O	2.10	0.51
1:A:360:CYS:CB	1:A:361:PRO:HD2	2.41	0.50
1:B:134:LEU:HD12	1:B:180:GLU:CD	2.32	0.50
1:C:222:VAL:HG12	1:C:280:ILE:HD12	1.94	0.50
1:A:325:GLN:H	1:A:325:GLN:CD	2.12	0.49
1:A:330:GLN:HG2	1:A:339:ALA:HB1	1.94	0.49
1:D:222:VAL:HG12	1:D:280:ILE:HD12	1.94	0.49
1:A:134:LEU:HD12	1:A:180:GLU:CD	2.32	0.49
1:B:333:CYS:SG	1:B:335:GLU:HB3	2.53	0.49
1:D:235:ARG:NH1	1:D:273:PHE:HE2	1.89	0.48
1:A:323:GLY:C	1:A:324:ARG:HG2	2.33	0.48
1:C:137:VAL:O	1:C:138:ASN:HB2	2.14	0.48
1:D:137:VAL:O	1:D:138:ASN:HB2	2.14	0.48
1:B:330:GLN:HG2	1:B:339:ALA:HB1	1.95	0.48
1:D:235:ARG:NH1	1:D:273:PHE:CD2	2.75	0.48
1:C:142:ASP:OD1	1:C:207:ARG:HA	2.14	0.47
1:D:235:ARG:NH2	1:D:276:GLU:CD	2.68	0.47
1:A:325:GLN:O	1:A:326:ASP:C	2.53	0.47
1:D:142:ASP:OD1	1:D:207:ARG:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ALA:HB1	1:A:323:GLY:O	2.14	0.47
1:D:227:TYR:OH	1:D:232:PRO:HB3	2.15	0.47
1:B:317:ALA:HB1	1:B:323:GLY:O	2.15	0.46
1:C:235:ARG:HB2	1:C:273:PHE:CZ	2.50	0.46
1:A:333:CYS:SG	1:A:335:GLU:HB3	2.55	0.46
2:E:9:M3L:O	2:E:10:SER:C	2.54	0.46
1:A:235:ARG:HB2	1:A:273:PHE:CZ	2.50	0.46
1:B:218:GLU:O	1:B:221:GLN:HB3	2.15	0.46
1:A:334:ASP:HA	2:E:2:ARG:HH12	1.81	0.45
1:B:235:ARG:HB2	1:B:273:PHE:CZ	2.50	0.45
1:A:135:TYR:OH	1:A:205:ARG:HA	2.17	0.45
1:B:188:TYR:CB	1:B:191:TYR:HB2	2.46	0.44
1:B:313:CYS:O	1:B:322:GLY:HA2	2.18	0.44
1:B:180:GLU:OE1	1:B:201:SER:HB2	2.18	0.44
1:B:330:GLN:OE1	2:F:4:LYS:HD3	2.17	0.44
1:B:328:ASP:N	1:B:328:ASP:OD1	2.47	0.44
1:A:313:CYS:O	1:A:322:GLY:HA2	2.18	0.44
1:A:135:TYR:HB2	1:A:184:TYR:CE1	2.52	0.44
1:C:228:ASN:HB3	1:C:231:ASN:O	2.18	0.44
1:B:329:LYS:HB3	1:B:342:ILE:CG2	2.48	0.43
1:B:135:TYR:HB2	1:B:184:TYR:CE1	2.52	0.43
1:A:355:GLU:H	1:A:355:GLU:CD	2.21	0.43
1:B:320:LEU:HD13	1:B:344:CYS:HB3	1.99	0.43
1:B:360:CYS:CB	1:B:361:PRO:HD2	2.41	0.43
1:A:329:LYS:HB3	1:A:342:ILE:CG2	2.48	0.43
1:A:328:ASP:N	1:A:328:ASP:OD1	2.47	0.43
1:B:144:ARG:HB2	1:B:151:TRP:CD2	2.54	0.43
1:A:250:ARG:NH1	1:A:250:ARG:HB3	2.34	0.43
1:A:180:GLU:OE1	1:A:201:SER:HB2	2.18	0.42
1:A:225:LEU:HD22	1:A:271:ILE:HG21	2.01	0.42
1:A:345:LEU:O	1:A:347:PRO:N	2.52	0.42
1:A:346:ASP:HB2	1:A:347:PRO:HD2	2.01	0.42
1:B:355:GLU:H	1:B:355:GLU:CD	2.21	0.42
1:A:144:ARG:HB2	1:A:151:TRP:CD2	2.54	0.42
1:B:355:GLU:O	2:F:1:ALA:HB2	2.19	0.42
1:B:213:LYS:HE3	1:D:292:ASN:ND2	2.35	0.42
1:B:243:ILE:HA	1:B:257:ALA:HB2	2.02	0.42
1:A:212:ILE:HD11	1:A:279:LYS:HB2	2.02	0.42
1:A:321:CYS:SG	1:A:322:GLY:N	2.93	0.41
1:B:212:ILE:HD11	1:B:279:LYS:HB2	2.02	0.41
1:B:333:CYS:HB2	1:B:360:CYS:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:VAL:HG23	1:C:185:HIS:O	2.20	0.41
1:A:334:ASP:HA	2:E:2:ARG:NH1	2.34	0.41
1:B:225:LEU:HD22	1:B:271:ILE:HG21	2.01	0.41
1:B:250:ARG:NH1	1:B:250:ARG:HB3	2.36	0.41
1:D:188:TYR:CB	1:D:191:TYR:HB2	2.49	0.41
1:C:188:TYR:CB	1:C:191:TYR:HB2	2.49	0.41
1:A:332:MET:SD	2:E:4:LYS:HA	2.60	0.41
1:C:225:LEU:HD22	1:C:271:ILE:HG13	2.03	0.41
1:B:292:ASN:O	1:D:210:THR:HA	2.20	0.41
1:A:141:VAL:HB	1:A:205:ARG:O	2.21	0.41
2:E:4:LYS:O	2:E:8:ARG:HG2	2.21	0.41
1:A:250:ARG:HB3	1:A:250:ARG:HH11	1.86	0.40
1:D:135:TYR:HE2	1:D:204:VAL:O	2.04	0.40
1:D:157:VAL:HG23	1:D:185:HIS:O	2.20	0.40
1:C:190:ASP:HB3	1:C:295:ARG:NH2	2.35	0.40
1:B:325:GLN:O	1:B:326:ASP:C	2.60	0.40
1:A:243:ILE:HA	1:A:257:ALA:HB2	2.02	0.40
1:A:333:CYS:HB2	1:A:360:CYS:HB3	2.03	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)
1:A:158:ARG:NH2	1:A:364:ARG:NH1[7_555]	2.01	0.19

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	211/241 (88%)	186 (88%)	20 (10%)	5 (2%)	7	33
1	B	204/241 (85%)	183 (90%)	19 (9%)	2 (1%)	19	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	150/241 (62%)	136 (91%)	14 (9%)	0	100	100
1	D	146/241 (61%)	131 (90%)	14 (10%)	1 (1%)	26	67
2	E	7/17 (41%)	7 (100%)	0	0	100	100
2	F	7/17 (41%)	6 (86%)	1 (14%)	0	100	100
All	All	725/998 (73%)	649 (90%)	68 (9%)	8 (1%)	17	56

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	LEU
1	A	346	ASP
1	A	347	PRO
1	D	232	PRO
1	A	263	ASP
1	B	263	ASP
1	A	299	GLY
1	B	299	GLY

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	195/217 (90%)	181 (93%)	14 (7%)	18	51
1	B	190/217 (88%)	176 (93%)	14 (7%)	17	49
1	C	138/217 (64%)	130 (94%)	8 (6%)	25	62
1	D	134/217 (62%)	125 (93%)	9 (7%)	20	55
2	E	7/11 (64%)	7 (100%)	0	100	100
2	F	6/11 (54%)	5 (83%)	1 (17%)	3	11
All	All	670/890 (75%)	624 (93%)	46 (7%)	19	54

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	PHE
1	A	147	ASN
1	A	200	ASN
1	A	218	GLU
1	A	251	THR
1	A	289	MET
1	A	302	CYS
1	A	305	CYS
1	A	324	ARG
1	A	325	GLN
1	A	328	ASP
1	A	331	LEU
1	A	341	HIS
1	A	350	SER
1	B	147	ASN
1	B	158	ARG
1	B	200	ASN
1	B	205	ARG
1	B	218	GLU
1	B	222	VAL
1	B	251	THR
1	B	289	MET
1	B	309	VAL
1	B	325	GLN
1	B	328	ASP
1	B	331	LEU
1	B	341	HIS
1	B	350	SER
1	C	134	LEU
1	C	157	VAL
1	C	180	GLU
1	C	225	LEU
1	C	231	ASN
1	C	253	ARG
1	C	282	ARG
1	C	301	SER
1	D	134	LEU
1	D	157	VAL
1	D	180	GLU
1	D	225	LEU
1	D	231	ASN
1	D	233	LYS
1	D	253	ARG

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Mol	Chain	Res	Type
1	D	282	ARG
1	D	301	SER
2	F	5	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	194	ASN
1	A	198	GLN
1	A	231	ASN
1	A	267	ASN
1	B	194	ASN
1	B	198	GLN
1	B	231	ASN
1	B	267	ASN
1	B	325	GLN
1	C	194	ASN
1	C	198	GLN
1	C	267	ASN
1	D	147	ASN
1	D	194	ASN
1	D	198	GLN
1	D	231	ASN
1	D	267	ASN
2	F	5	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	9	2	10,11,12	0.96	0	12,14,16	1.20	2 (16%)
2	M3L	F	9	2	10,11,12	0.99	0	12,14,16	1.23	2 (16%)

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	9	2	-	0/8/10/12	0/0/0/0
2	M3L	F	9	2	-	0/8/10/12	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	9	M3L	O-C-CA	-2.08	120.06	125.49
2	E	9	M3L	O-C-CA	-2.03	120.19	125.49
2	F	9	M3L	CM1-NZ-CE	2.28	118.96	109.90
2	E	9	M3L	CM1-NZ-CE	2.28	118.98	109.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	9	M3L	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	215/241 (89%)	0.72	20 (9%)	11 6	51, 84, 147, 170	1 (0%)
1	B	210/241 (87%)	1.07	35 (16%)	2 1	51, 87, 189, 199	0
1	C	154/241 (63%)	0.36	4 (2%)	59 38	58, 87, 136, 170	7 (4%)
1	D	150/241 (62%)	0.60	13 (8%)	13 6	58, 94, 131, 184	8 (5%)
2	E	9/17 (52%)	0.48	1 (11%)	7 4	87, 90, 114, 120	0
2	F	8/17 (47%)	3.52	5 (62%)	0 0	115, 138, 173, 176	0
All	All	746/998 (74%)	0.75	78 (10%)	8 4	51, 89, 173, 199	16 (2%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	330	GLN	11.7
1	A	320	LEU	8.5
2	F	1	ALA	7.7
1	B	314	ARG	7.6
1	B	320	LEU	7.3
1	B	317	ALA	6.2
2	F	2	ARG	5.9
1	B	340	PHE	5.6
1	D	301	SER	5.3
1	B	319	HIS	5.1
1	B	331	LEU	5.0
1	A	304	HIS	4.9
1	B	324	ARG	4.6
1	B	359	TYR	4.5
1	B	362	GLU	4.5
1	A	180	GLU	4.5
1	A	315	VAL	4.5
1	B	361	PRO	4.5
1	B	339	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	318	CYS	4.4
1	B	344	CYS	4.4
2	F	3	THR	4.3
1	D	245	ARG	4.2
1	A	311	ARG	4.2
1	B	357	GLU	4.2
1	A	312	LEU	4.1
1	B	315	VAL	4.0
1	B	363	CYS	4.0
1	B	180	GLU	4.0
1	A	362	GLU	3.9
1	B	304	HIS	3.8
1	B	343	TYR	3.8
2	F	4	LYS	3.8
1	A	346	ASP	3.7
1	A	340	PHE	3.6
1	D	268	ASP	3.6
1	A	330	GLN	3.5
1	C	180	GLU	3.5
1	A	321	CYS	3.4
1	A	314	ARG	3.4
1	A	363	CYS	3.4
1	A	331	LEU	3.4
1	B	332	MET	3.3
1	B	349	LEU	3.3
1	B	262	GLY	3.2
1	A	345	LEU	3.2
1	D	261	LEU	3.0
2	F	7	ALA	3.0
1	B	354	SER	3.0
1	B	341	HIS	2.9
1	C	179	GLU	2.9
1	D	149	GLY	2.9
1	B	350	SER	2.9
1	A	339	ALA	2.9
1	B	360	CYS	2.8
1	B	358	TRP	2.7
1	B	348	PRO	2.7
1	D	148	MET	2.7
1	B	342	ILE	2.7
1	B	325	GLN	2.7
1	C	178	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	319	HIS	2.6
2	E	4	LYS	2.6
1	A	326	ASP	2.5
1	D	256	TYR	2.5
1	A	342	ILE	2.4
1	D	229	PRO	2.4
1	D	204	VAL	2.4
1	B	162	LYS	2.3
1	D	269	CYS	2.3
1	D	266	LEU	2.3
1	D	180	GLU	2.2
1	A	344	CYS	2.2
1	B	327	PRO	2.2
1	B	335	GLU	2.2
1	D	237	PHE	2.1
1	B	312	LEU	2.1
1	C	260	VAL	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. 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	E	9	12/13	0.96	0.24	-	55,70,111,115	0
2	M3L	F	9	12/13	0.88	0.33	-	60,101,114,115	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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(\AA^2)	Q<0.9
3	ZN	A	401	1/1	0.81	0.15	-0.88	108,108,108,108	0
3	ZN	B	402	1/1	0.92	0.09	-1.15	181,181,181,181	0
3	ZN	A	402	1/1	0.75	0.08	-1.31	143,143,143,143	0
3	ZN	A	403	1/1	0.86	0.12	-1.35	121,121,121,121	0
3	ZN	B	403	1/1	0.95	0.12	-1.62	202,202,202,202	0
3	ZN	B	401	1/1	0.70	0.07	-1.96	190,190,190,190	0
3	ZN	C	401	1/1	0.95	0.18	-	115,115,115,115	0

6.5 Other polymers [i](#)

There are no such residues in this entry.