



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:26 AM GMT

PDB ID : 3ASK  
Title : Structure of UHRF1 in complex with histone tail  
Authors : Arita, K.; Sugita, K.; Unoki, M.; Hamamoto, R.; Sekiyama, N.; Tochio, H.;  
Ariyoshi, M.; Shirakawa, M.  
Deposited on : 2010-12-16  
Resolution : 2.90 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](mailto: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.

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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

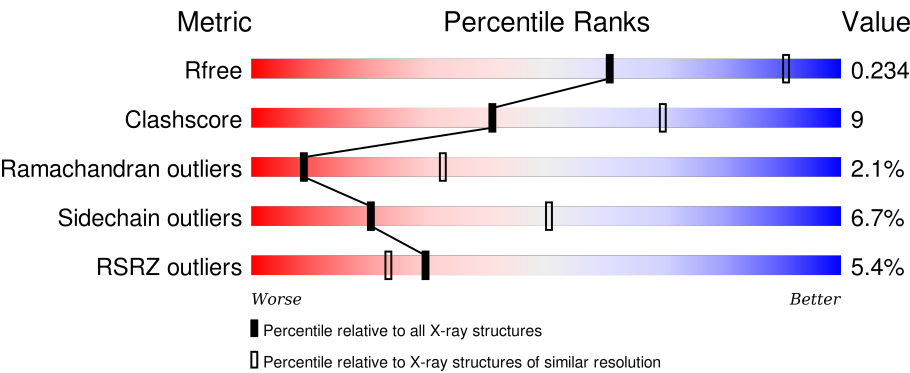
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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 <sub>free</sub>	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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  $\geq 3$ , 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	226	<div><div>6%</div><div><div></div><div></div><div></div><div></div></div><div>66%21%6%6%</div></div>
1	B	226	<div><div>6%</div><div><div></div><div></div><div></div><div></div></div><div>75%16%•7%</div></div>
1	C	226	<div><div>•</div><div><div></div><div></div><div></div><div></div></div><div>58%8%•32%</div></div>
1	D	226	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>55%11%•33%</div></div>
2	P	13	<div><div>8%</div><div><div></div><div></div><div></div><div></div></div><div>31%46%23%</div></div>

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Mol	Chain	Length	Quality of chain
2	Q	13	<div><div><div></div><div></div><div></div><div></div></div><div>31%62%8%31%</div></div>
2	R	13	<div><div><div></div><div></div></div><div>8%92%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6141 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	213	Total	C	N	O	S	55	0	0
			1731	1070	313	329	19			
1	B	211	Total	C	N	O	S	88	0	0
			1714	1060	308	327	19			
1	C	154	Total	C	N	O	S	30	0	0
			1265	787	229	242	7			
1	D	152	Total	C	N	O	S	42	0	0
			1250	778	226	240	6			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	133	SER	-	EXPRESSION TAG	UNP Q96T88
A	?	-	SER	DELETION	UNP Q96T88
A	?	-	ARG	DELETION	UNP Q96T88
A	?	-	ASP	DELETION	UNP Q96T88
A	?	-	GLU	DELETION	UNP Q96T88
A	?	-	PRO	DELETION	UNP Q96T88
A	?	-	CYS	DELETION	UNP Q96T88
A	?	-	SER	DELETION	UNP Q96T88
A	?	-	SER	DELETION	UNP Q96T88
A	?	-	THR	DELETION	UNP Q96T88
B	133	SER	-	EXPRESSION TAG	UNP Q96T88
B	?	-	SER	DELETION	UNP Q96T88
B	?	-	ARG	DELETION	UNP Q96T88
B	?	-	ASP	DELETION	UNP Q96T88
B	?	-	GLU	DELETION	UNP Q96T88
B	?	-	PRO	DELETION	UNP Q96T88
B	?	-	CYS	DELETION	UNP Q96T88
B	?	-	SER	DELETION	UNP Q96T88
B	?	-	SER	DELETION	UNP Q96T88
B	?	-	THR	DELETION	UNP Q96T88
C	133	SER	-	EXPRESSION TAG	UNP Q96T88

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	SER	DELETION	UNP Q96T88
C	?	-	ARG	DELETION	UNP Q96T88
C	?	-	ASP	DELETION	UNP Q96T88
C	?	-	GLU	DELETION	UNP Q96T88
C	?	-	PRO	DELETION	UNP Q96T88
C	?	-	CYS	DELETION	UNP Q96T88
C	?	-	SER	DELETION	UNP Q96T88
C	?	-	SER	DELETION	UNP Q96T88
C	?	-	THR	DELETION	UNP Q96T88
D	133	SER	-	EXPRESSION TAG	UNP Q96T88
D	?	-	SER	DELETION	UNP Q96T88
D	?	-	ARG	DELETION	UNP Q96T88
D	?	-	ASP	DELETION	UNP Q96T88
D	?	-	GLU	DELETION	UNP Q96T88
D	?	-	PRO	DELETION	UNP Q96T88
D	?	-	CYS	DELETION	UNP Q96T88
D	?	-	SER	DELETION	UNP Q96T88
D	?	-	SER	DELETION	UNP Q96T88
D	?	-	THR	DELETION	UNP Q96T88

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	10	Total	C	N	O	6	0	0
			82	49	19	14			
2	Q	9	Total	C	N	O	4	0	0
			76	46	18	12			
2	R	1	Total	C	N	O	4	0	0
			12	9	2	1			

- 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		

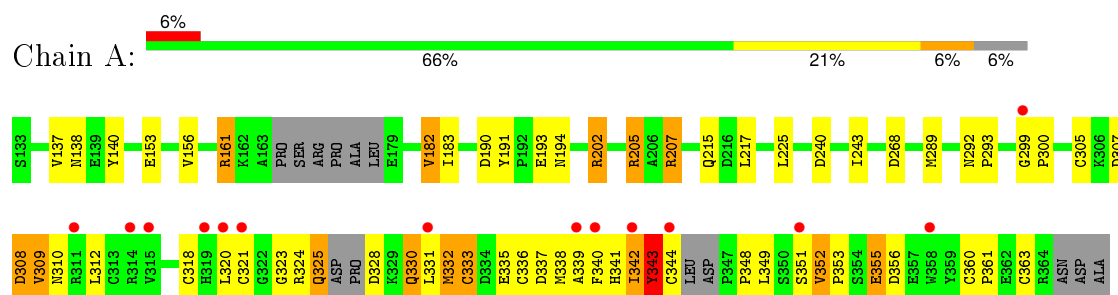
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total 3	O 3	0	0
4	C	1	Total 1	O 1	0	0

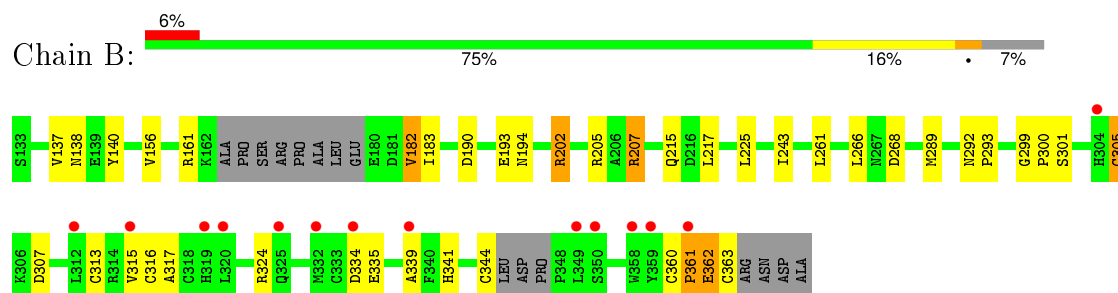
### 3 Residue-property plots

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.

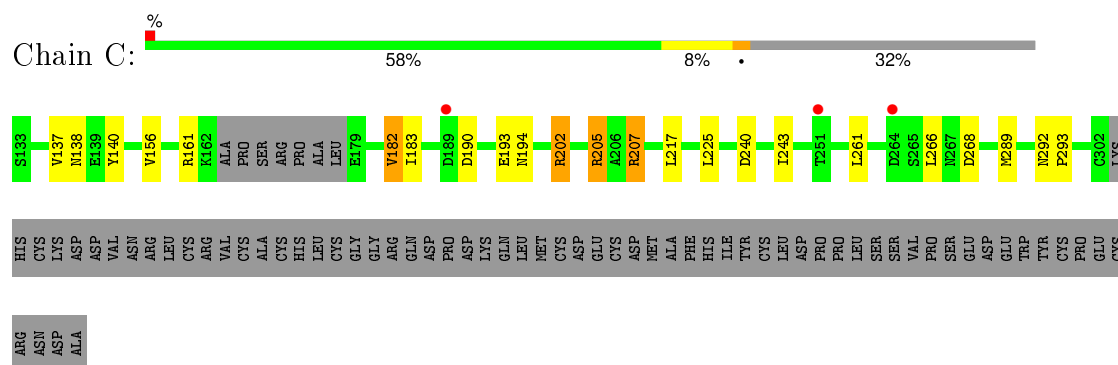
- Molecule 1: E3 ubiquitin-protein ligase UHRF1



- Molecule 1: E3 ubiquitin-protein ligase UHRF1

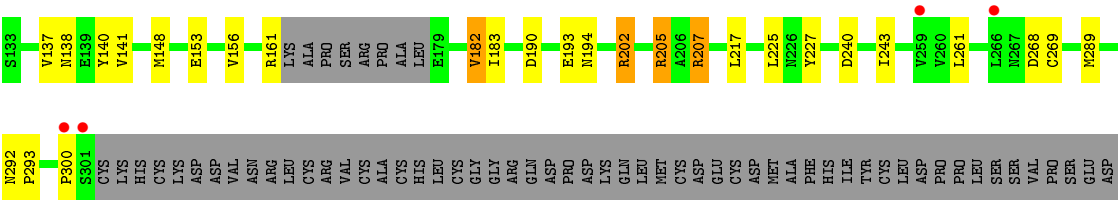


- Molecule 1: E3 ubiquitin-protein ligase UHRF1



- Molecule 1: E3 ubiquitin-protein ligase UHRF1





GLU  
TRP  
TYR  
CYS  
PRO  
GLU  
CYS  
ARG  
ASN  
ASP  
ALA

● Molecule 2: Histone H3.3



A1  
R2  
T3  
K4  
Q5  
T6  
A7  
R8  
S10  
THR  
GLY  
GLY

● Molecule 2: Histone H3.3



A1  
R2  
T3  
A7  
R8  
T9  
SER  
THR  
GLY  
GLY

● Molecule 2: Histone H3.3



ALA  
ARG  
THR  
LYS  
GLN  
THR  
ALA  
ARG  
K9  
SER  
THR  
GLY  
GLY



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 <sub>2</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.18 Å   145.18 Å   125.41 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	40.27 – 2.90 40.27 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.6 (40.27-2.90) 97.6 (40.27-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.65 (at 2.90 Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.243   ,   0.286 0.238   ,   0.234	Depositor DCC
$R_{free}$ test set	2965 reflections (10.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	70.5	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 40.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 29459 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6141	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.49	0/1765	1.01	8/2380 (0.3%)
1	B	0.42	0/1749	0.85	7/2361 (0.3%)
1	C	0.42	0/1289	0.68	6/1741 (0.3%)
1	D	0.41	0/1274	0.69	6/1722 (0.3%)
2	P	0.40	0/69	0.63	0/90
2	Q	0.30	0/63	0.54	0/82
All	All	0.44	0/6209	0.83	27/8376 (0.3%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	202	ARG	NE-CZ-NH1	-19.89	110.36	120.30
1	A	207	ARG	NE-CZ-NH2	-19.81	110.39	120.30
1	B	202	ARG	NE-CZ-NH2	18.64	129.62	120.30
1	A	161	ARG	NE-CZ-NH1	-17.79	111.40	120.30
1	A	161	ARG	NE-CZ-NH2	17.11	128.85	120.30
1	A	207	ARG	NE-CZ-NH1	16.87	128.73	120.30
1	B	202	ARG	CD-NE-CZ	9.34	136.67	123.60
1	A	207	ARG	CD-NE-CZ	8.77	135.88	123.60
1	A	161	ARG	CD-NE-CZ	8.46	135.44	123.60
1	D	207	ARG	NE-CZ-NH1	-7.90	116.35	120.30
1	C	207	ARG	NE-CZ-NH1	-7.79	116.41	120.30
1	B	207	ARG	NE-CZ-NH1	-7.42	116.59	120.30
1	A	202	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	C	202	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	D	202	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	202	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	B	161	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	C	161	ARG	NE-CZ-NH2	-6.12	117.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	161	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	D	202	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	C	202	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	C	161	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	D	161	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	161	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	D	207	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	C	207	ARG	NE-CZ-NH2	5.57	123.08	120.30
1	B	207	ARG	NE-CZ-NH2	5.22	122.91	120.30

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	1731	0	1645	48	1
1	B	1714	0	1626	23	0
1	C	1265	0	1224	11	0
1	D	1250	0	1206	14	0
2	P	82	0	96	6	0
2	Q	76	0	91	0	0
2	R	12	0	20	2	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	1	0	0	0	0
4	A	3	0	0	0	0
4	C	1	0	0	0	0
All	All	6141	0	5908	99	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 9.

All (99) 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:A:336:CYS:HB3	1:A:363:CYS:SG	2.10	0.90
1:B:360:CYS:HB2	1:B:361:PRO:HD2	1.62	0.81
1:A:333:CYS:HB2	1:A:360:CYS:SG	2.28	0.73
1:A:340:PHE:CE2	1:A:360:CYS:SG	2.82	0.73
1:B:317:ALA:O	1:B:339:ALA:HB3	1.89	0.72
1:C:193:GLU:HG2	1:C:194:ASN:HD22	1.55	0.71
1:D:193:GLU:HG2	1:D:194:ASN:HD22	1.57	0.70
1:B:193:GLU:HG2	1:B:194:ASN:HD22	1.57	0.70
1:B:140:TYR:HB2	1:B:289:MET:HG2	1.75	0.67
1:A:193:GLU:HG2	1:A:194:ASN:HD22	1.59	0.67
1:C:140:TYR:HB2	1:C:289:MET:HG2	1.76	0.67
1:B:305:CYS:HB3	1:B:313:CYS:SG	2.34	0.66
1:A:193:GLU:HG2	1:A:194:ASN:ND2	2.11	0.66
1:D:193:GLU:HG2	1:D:194:ASN:ND2	2.10	0.66
1:A:341:HIS:CD2	1:A:343:TYR:CE1	2.84	0.66
1:C:193:GLU:HG2	1:C:194:ASN:ND2	2.12	0.65
1:A:321:CYS:SG	1:A:341:HIS:HE1	2.19	0.65
1:D:140:TYR:HB2	1:D:289:MET:HG2	1.77	0.65
1:A:328:ASP:N	1:A:330:GLN:HE22	1.95	0.64
1:B:193:GLU:HG2	1:B:194:ASN:ND2	2.12	0.64
1:A:335:GLU:HB3	1:A:363:CYS:HB3	1.79	0.63
1:A:137:VAL:O	1:A:138:ASN:HB2	1.99	0.63
1:A:191:TYR:CE1	2:P:9:M3L:HE2	2.33	0.62
1:A:341:HIS:CD2	1:A:343:TYR:OH	2.52	0.62
1:A:341:HIS:CG	1:A:343:TYR:CE1	2.87	0.62
1:A:341:HIS:CD2	1:A:343:TYR:CZ	2.88	0.62
1:B:299:GLY:HA2	1:B:300:PRO:O	2.00	0.61
1:D:182:VAL:HG23	1:D:183:ILE:N	2.16	0.61
1:D:137:VAL:O	1:D:138:ASN:HB2	2.00	0.61
1:B:301:SER:HB2	1:B:307:ASP:OD2	2.00	0.60
1:A:182:VAL:HG23	1:A:183:ILE:N	2.16	0.60
1:A:140:TYR:HB2	1:A:289:MET:HG2	1.82	0.60
1:C:207:ARG:HG2	1:C:289:MET:HE3	1.82	0.60
1:A:330:GLN:O	2:P:3:THR:HA	2.02	0.60
1:B:313:CYS:O	1:B:317:ALA:HB3	2.01	0.60
1:B:137:VAL:O	1:B:138:ASN:HB2	2.01	0.60
1:B:335:GLU:HB3	1:B:363:CYS:SG	2.42	0.59
1:A:330:GLN:HE21	1:A:330:GLN:N	2.00	0.59
1:B:360:CYS:HB2	1:B:361:PRO:CD	2.31	0.59
1:A:309:VAL:O	1:A:309:VAL:HG22	2.04	0.57
1:A:336:CYS:SG	1:A:338:MET:HB2	2.45	0.57
1:D:137:VAL:HA	1:D:156:VAL:HG12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:TYR:HD1	1:A:344:CYS:H	1.54	0.56
1:B:182:VAL:HG23	1:B:183:ILE:N	2.19	0.56
1:A:308:ASP:C	1:A:310:ASN:H	2.09	0.56
1:C:137:VAL:HA	1:C:156:VAL:HG12	1.88	0.56
1:D:207:ARG:HG2	1:D:289:MET:HE3	1.89	0.55
1:B:313:CYS:HB3	1:B:316:CYS:SG	2.46	0.54
1:C:182:VAL:HG23	1:C:183:ILE:N	2.21	0.54
1:A:318:CYS:HB2	1:A:341:HIS:CE1	2.42	0.54
1:A:307:ASP:O	1:A:309:VAL:N	2.40	0.53
1:C:137:VAL:O	1:C:138:ASN:HB2	2.08	0.52
1:A:323:GLY:C	1:A:325:GLN:H	2.12	0.52
1:B:341:HIS:HB2	1:B:344:CYS:SG	2.49	0.52
1:A:330:GLN:C	1:A:331:LEU:HD12	2.30	0.52
1:A:137:VAL:HA	1:A:156:VAL:HG12	1.92	0.51
1:A:193:GLU:HG3	2:P:5:GLN:OE1	2.10	0.51
1:A:335:GLU:HB3	1:A:363:CYS:CB	2.41	0.51
1:B:217:LEU:HD22	1:B:243:ILE:CD1	2.41	0.50
1:A:340:PHE:CZ	1:A:360:CYS:SG	3.05	0.49
1:B:361:PRO:O	1:B:362:GLU:C	2.52	0.48
1:D:205:ARG:NH2	1:D:240:ASP:OD2	2.46	0.48
1:A:339:ALA:C	1:A:340:PHE:CD2	2.87	0.48
1:A:323:GLY:HA3	1:A:325:GLN:HG2	1.95	0.48
1:B:289:MET:SD	1:B:293:PRO:HG3	2.54	0.48
1:A:205:ARG:NH2	1:A:240:ASP:OD2	2.47	0.47
1:A:308:ASP:O	1:A:310:ASN:N	2.46	0.47
1:C:217:LEU:HD22	1:C:243:ILE:CD1	2.45	0.47
1:C:205:ARG:NH2	1:C:240:ASP:OD2	2.48	0.47
1:B:137:VAL:HA	1:B:156:VAL:HG12	1.96	0.46
1:D:292:ASN:HA	1:D:293:PRO:HD3	1.77	0.46
2:P:7:ALA:C	2:P:9:M3L:N	2.69	0.46
1:D:148:MET:SD	2:R:9:M3L:HB2	2.56	0.46
1:B:207:ARG:HB3	1:B:289:MET:HE2	1.97	0.46
2:P:6:THR:HG22	2:P:7:ALA:N	2.31	0.46
1:A:217:LEU:HD22	1:A:243:ILE:CD1	2.47	0.45
1:D:217:LEU:HD22	1:D:243:ILE:CD1	2.47	0.45
1:C:261:LEU:HD11	1:C:266:LEU:HD22	1.99	0.45
1:A:340:PHE:CZ	1:A:360:CYS:HB2	2.53	0.44
1:A:318:CYS:CB	1:A:341:HIS:CE1	3.00	0.44
1:A:339:ALA:O	1:A:340:PHE:CD2	2.72	0.43
1:B:292:ASN:HA	1:B:293:PRO:HD3	1.75	0.43
1:A:325:GLN:NE2	1:A:343:TYR:OH	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:HIS:HD2	1:A:343:TYR:OH	1.98	0.43
1:A:292:ASN:HA	1:A:293:PRO:HD3	1.76	0.42
2:R:9:M3L:HD3	2:R:9:M3L:HM22	1.89	0.42
1:B:261:LEU:HD11	1:B:266:LEU:HD22	2.02	0.42
1:A:299:GLY:HA3	1:A:300:PRO:HA	1.67	0.42
1:D:227:TYR:CE2	1:D:269:CYS:SG	3.05	0.42
2:P:7:ALA:O	2:P:9:M3L:N	2.53	0.41
1:C:292:ASN:HA	1:C:293:PRO:HD3	1.76	0.41
1:A:215:GLN:HB3	1:B:215:GLN:O	2.20	0.41
1:A:336:CYS:CB	1:A:363:CYS:SG	2.88	0.41
1:D:141:VAL:HB	1:D:205:ARG:O	2.21	0.41
1:D:227:TYR:HE2	1:D:269:CYS:HG	1.57	0.41
1:A:352:VAL:HG23	1:A:352:VAL:O	2.22	0.40
1:A:323:GLY:C	1:A:325:GLN:N	2.75	0.40
1:A:318:CYS:SG	1:A:320:LEU:HB2	2.62	0.40
1:A:332:MET:HB3	1:A:332:MET:HE3	1.84	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:194:ASN:OD1	1:A:356:ASP:OD1[8_556]	2.17	0.03

## 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	205/226 (91%)	171 (83%)	23 (11%)	11 (5%)	2	7
1	B	205/226 (91%)	182 (89%)	20 (10%)	3 (2%)	13	42
1	C	150/226 (66%)	142 (95%)	8 (5%)	0	100	100
1	D	148/226 (66%)	139 (94%)	8 (5%)	1 (1%)	26	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	7/13 (54%)	6 (86%)	1 (14%)	0	100	100
2	Q	7/13 (54%)	6 (86%)	1 (14%)	0	100	100
All	All	722/930 (78%)	646 (90%)	61 (8%)	15 (2%)	9	32

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	308	ASP
1	A	355	GLU
1	A	309	VAL
1	A	342	ILE
1	A	361	PRO
1	A	343	TYR
1	A	351	SER
1	B	362	GLU
1	A	352	VAL
1	B	324	ARG
1	B	361	PRO
1	A	333	CYS
1	A	348	PRO
1	A	353	PRO
1	D	300	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	192/203 (95%)	172 (90%)	20 (10%)	9	26
1	B	191/203 (94%)	182 (95%)	9 (5%)	32	68
1	C	138/203 (68%)	132 (96%)	6 (4%)	35	71
1	D	136/203 (67%)	128 (94%)	8 (6%)	24	58
2	P	7/8 (88%)	6 (86%)	1 (14%)	4	12
2	Q	6/8 (75%)	5 (83%)	1 (17%)	3	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	670/828 (81%)	625 (93%)	45 (7%)	20	50

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	GLU
1	A	161	ARG
1	A	182	VAL
1	A	190	ASP
1	A	202	ARG
1	A	205	ARG
1	A	207	ARG
1	A	225	LEU
1	A	268	ASP
1	A	305	CYS
1	A	312	LEU
1	A	324	ARG
1	A	325	GLN
1	A	330	GLN
1	A	332	MET
1	A	337	ASP
1	A	342	ILE
1	A	343	TYR
1	A	349	LEU
1	A	355	GLU
1	B	182	VAL
1	B	190	ASP
1	B	202	ARG
1	B	205	ARG
1	B	225	LEU
1	B	268	ASP
1	B	305	CYS
1	B	315	VAL
1	B	334	ASP
1	C	182	VAL
1	C	190	ASP
1	C	202	ARG
1	C	205	ARG
1	C	225	LEU
1	C	268	ASP
1	D	153	GLU
1	D	182	VAL

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Mol	Chain	Res	Type
1	D	190	ASP
1	D	202	ARG
1	D	205	ARG
1	D	225	LEU
1	D	261	LEU
1	D	268	ASP
2	P	2	ARG
2	Q	3	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	ASN
1	A	194	ASN
1	A	231	ASN
1	A	267	ASN
1	A	325	GLN
1	A	330	GLN
1	A	341	HIS
1	B	147	ASN
1	B	194	ASN
1	B	231	ASN
1	B	267	ASN
1	C	147	ASN
1	C	194	ASN
1	C	231	ASN
1	C	267	ASN
1	D	147	ASN
1	D	194	ASN
1	D	231	ASN
1	D	267	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	P	9	2	10,11,12	1.27	1 (10%)	12,14,16	1.90	3 (25%)
2	M3L	Q	9	2	10,11,12	1.03	0	12,14,16	2.08	3 (25%)
2	M3L	R	9	-	10,11,12	0.96	0	12,14,16	1.87	4 (33%)

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	P	9	2	-	0/8/10/12	0/0/0/0
2	M3L	Q	9	2	-	0/8/10/12	0/0/0/0
2	M3L	R	9	-	-	0/8/10/12	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	9	M3L	CB-CA	2.46	1.56	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	9	M3L	CM3-NZ-CM2	-2.99	101.29	108.98
2	Q	9	M3L	CM3-NZ-CM2	-2.95	101.40	108.98
2	P	9	M3L	CM3-NZ-CM2	-2.53	102.48	108.98
2	Q	9	M3L	CM2-NZ-CE	-2.12	101.47	109.90
2	R	9	M3L	O-C-CA	-2.06	120.13	125.49
2	R	9	M3L	CE-CD-CG	2.17	119.32	110.64
2	P	9	M3L	CD-CG-CB	2.19	121.44	113.66
2	P	9	M3L	CM3-NZ-CE	3.87	125.31	109.90
2	R	9	M3L	CM3-NZ-CE	4.11	126.23	109.90
2	Q	9	M3L	CM3-NZ-CE	4.83	129.09	109.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	9	M3L	3	0
2	R	9	M3L	2	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	213/226 (94%)	0.25	14 (6%) 22 16	38, 66, 112, 129	14 (6%)
1	B	211/226 (93%)	0.35	14 (6%) 22 16	38, 67, 134, 151	22 (10%)
1	C	154/226 (68%)	-0.03	3 (1%) 70 66	42, 64, 97, 133	7 (4%)
1	D	152/226 (67%)	0.02	4 (2%) 59 54	43, 65, 94, 131	10 (6%)
2	P	9/13 (69%)	0.25	1 (11%) 7 4	66, 73, 90, 105	2 (22%)
2	Q	8/13 (61%)	1.81	4 (50%) 0 0	79, 93, 113, 119	1 (12%)
2	R	0/13	-	-	-	-
All	All	747/943 (79%)	0.19	40 (5%) 29 23	38, 66, 121, 151	56 (7%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	351	SER	5.7
1	A	320	LEU	4.5
1	A	315	VAL	4.2
1	B	319	HIS	4.1
2	Q	2	ARG	3.9
1	A	314	ARG	3.6
1	B	320	LEU	3.4
2	Q	7	ALA	3.4
1	D	300	PRO	3.3
1	A	319	HIS	3.2
1	A	340	PHE	3.2
1	B	358	TRP	3.1
2	Q	1	ALA	3.0
1	B	350	SER	3.0
1	A	321	CYS	3.0
1	A	344	CYS	2.9
1	B	325	GLN	2.9
1	B	334	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	259	VAL	2.8
1	A	331	LEU	2.7
1	D	301	SER	2.7
1	B	361	PRO	2.7
1	B	359	TYR	2.5
1	C	264	ASP	2.4
1	A	339	ALA	2.4
1	B	315	VAL	2.4
1	B	349	LEU	2.3
1	A	342	ILE	2.3
1	A	311	ARG	2.3
1	C	189	ASP	2.2
1	B	304	HIS	2.2
1	B	332	MET	2.2
1	B	312	LEU	2.2
2	P	1	ALA	2.2
1	A	358	TRP	2.2
2	Q	3	THR	2.1
1	C	251	THR	2.1
1	D	266	LEU	2.1
1	B	339	ALA	2.0
1	A	299	GLY	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	M3L	Q	9	12/13	0.94	0.20	-	48,72,85,88	0
2	M3L	P	9	12/13	0.96	0.19	-	37,51,102,109	0
2	M3L	R	9	12/13	0.92	0.28	-	57,98,102,116	4

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	ZN	A	503	1/1	0.92	0.06	-1.26	109,109,109,109	0
3	ZN	A	502	1/1	0.89	0.05	-1.67	122,122,122,122	0
3	ZN	A	501	1/1	0.86	0.09	-1.93	130,130,130,130	0
3	ZN	B	504	1/1	0.93	0.05	-2.00	125,125,125,125	0
3	ZN	B	505	1/1	0.98	0.07	-2.19	135,135,135,135	0
3	ZN	B	506	1/1	0.99	0.07	-2.25	150,150,150,150	0
3	ZN	C	501	1/1	0.89	0.11	-	106,106,106,106	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.