



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 08:01 PM BST

PDB ID : 6RXM  
Title : Crystal structure of CobB Ac2 (A76G, I131C, V162G) in complex with H4K16-Acetyl peptide  
Authors : Spinck, M.; Gasper, R.; Neumann, H.  
Deposited on : 2019-06-08  
Resolution : 1.92 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

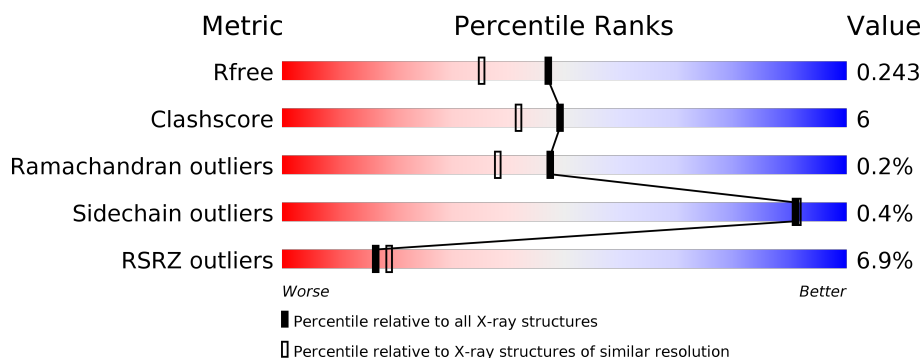
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.92 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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 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	254	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>7%</div> </div> </div>
1	B	254	<div> <div>9%</div> <div> <div></div> <div>80%</div> <div>12%</div> <div>8%</div> </div> </div>
1	C	254	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>7%</div> <div>7%</div> </div> </div>
1	D	254	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>12%</div> <div>11%</div> </div> </div>
1	E	254	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>6%</div> <div>8%</div> </div> </div>
1	F	254	<div> <div>13%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>8%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	11	<div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>27%36%36%</div>
2	H	11	<div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>27%27%9%36%</div>
2	I	11	<div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>9%36%27%36%</div>
2	J	11	<div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>55%18%27%</div>
2	K	11	<div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>9%55%18%9%18%</div>
2	L	11	<div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>64%36%</div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12179 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 NAD-dependent protein deacylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	S	0	2	0
			1838	1163	325	339	11			
1	B	234	Total	C	N	O	S	0	1	0
			1824	1152	323	338	11			
1	C	235	Total	C	N	O	S	0	2	0
			1837	1161	325	341	10			
1	D	227	Total	C	N	O	S	0	0	0
			1763	1115	310	328	10			
1	E	233	Total	C	N	O	S	0	0	0
			1813	1144	322	337	10			
1	F	233	Total	C	N	O	S	0	0	0
			1813	1144	322	337	10			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	initiating methionine	UNP P75960
A	-13	GLY	-	expression tag	UNP P75960
A	-12	SER	-	expression tag	UNP P75960
A	-11	SER	-	expression tag	UNP P75960
A	-10	HIS	-	expression tag	UNP P75960
A	-9	HIS	-	expression tag	UNP P75960
A	-8	HIS	-	expression tag	UNP P75960
A	-7	HIS	-	expression tag	UNP P75960
A	-6	HIS	-	expression tag	UNP P75960
A	-5	HIS	-	expression tag	UNP P75960
A	-4	SER	-	expression tag	UNP P75960
A	-3	GLN	-	expression tag	UNP P75960
A	-2	ASP	-	expression tag	UNP P75960
A	-1	PRO	-	expression tag	UNP P75960
A	76	GLY	ALA	engineered mutation	UNP P75960
A	131	CYS	ILE	engineered mutation	UNP P75960
A	161	ALA	VAL	engineered mutation	UNP P75960

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	MET	-	initiating methionine	UNP P75960
B	-13	GLY	-	expression tag	UNP P75960
B	-12	SER	-	expression tag	UNP P75960
B	-11	SER	-	expression tag	UNP P75960
B	-10	HIS	-	expression tag	UNP P75960
B	-9	HIS	-	expression tag	UNP P75960
B	-8	HIS	-	expression tag	UNP P75960
B	-7	HIS	-	expression tag	UNP P75960
B	-6	HIS	-	expression tag	UNP P75960
B	-5	HIS	-	expression tag	UNP P75960
B	-4	SER	-	expression tag	UNP P75960
B	-3	GLN	-	expression tag	UNP P75960
B	-2	ASP	-	expression tag	UNP P75960
B	-1	PRO	-	expression tag	UNP P75960
B	76	GLY	ALA	engineered mutation	UNP P75960
B	131	CYS	ILE	engineered mutation	UNP P75960
B	161	ALA	VAL	engineered mutation	UNP P75960
C	-14	MET	-	initiating methionine	UNP P75960
C	-13	GLY	-	expression tag	UNP P75960
C	-12	SER	-	expression tag	UNP P75960
C	-11	SER	-	expression tag	UNP P75960
C	-10	HIS	-	expression tag	UNP P75960
C	-9	HIS	-	expression tag	UNP P75960
C	-8	HIS	-	expression tag	UNP P75960
C	-7	HIS	-	expression tag	UNP P75960
C	-6	HIS	-	expression tag	UNP P75960
C	-5	HIS	-	expression tag	UNP P75960
C	-4	SER	-	expression tag	UNP P75960
C	-3	GLN	-	expression tag	UNP P75960
C	-2	ASP	-	expression tag	UNP P75960
C	-1	PRO	-	expression tag	UNP P75960
C	76	GLY	ALA	engineered mutation	UNP P75960
C	131	CYS	ILE	engineered mutation	UNP P75960
C	161	ALA	VAL	engineered mutation	UNP P75960
D	-14	MET	-	initiating methionine	UNP P75960
D	-13	GLY	-	expression tag	UNP P75960
D	-12	SER	-	expression tag	UNP P75960
D	-11	SER	-	expression tag	UNP P75960
D	-10	HIS	-	expression tag	UNP P75960
D	-9	HIS	-	expression tag	UNP P75960
D	-8	HIS	-	expression tag	UNP P75960
D	-7	HIS	-	expression tag	UNP P75960

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	HIS	-	expression tag	UNP P75960
D	-5	HIS	-	expression tag	UNP P75960
D	-4	SER	-	expression tag	UNP P75960
D	-3	GLN	-	expression tag	UNP P75960
D	-2	ASP	-	expression tag	UNP P75960
D	-1	PRO	-	expression tag	UNP P75960
D	76	GLY	ALA	engineered mutation	UNP P75960
D	131	CYS	ILE	engineered mutation	UNP P75960
D	161	ALA	VAL	engineered mutation	UNP P75960
E	-14	MET	-	initiating methionine	UNP P75960
E	-13	GLY	-	expression tag	UNP P75960
E	-12	SER	-	expression tag	UNP P75960
E	-11	SER	-	expression tag	UNP P75960
E	-10	HIS	-	expression tag	UNP P75960
E	-9	HIS	-	expression tag	UNP P75960
E	-8	HIS	-	expression tag	UNP P75960
E	-7	HIS	-	expression tag	UNP P75960
E	-6	HIS	-	expression tag	UNP P75960
E	-5	HIS	-	expression tag	UNP P75960
E	-4	SER	-	expression tag	UNP P75960
E	-3	GLN	-	expression tag	UNP P75960
E	-2	ASP	-	expression tag	UNP P75960
E	-1	PRO	-	expression tag	UNP P75960
E	76	GLY	ALA	engineered mutation	UNP P75960
E	131	CYS	ILE	engineered mutation	UNP P75960
E	161	ALA	VAL	engineered mutation	UNP P75960
F	-14	MET	-	initiating methionine	UNP P75960
F	-13	GLY	-	expression tag	UNP P75960
F	-12	SER	-	expression tag	UNP P75960
F	-11	SER	-	expression tag	UNP P75960
F	-10	HIS	-	expression tag	UNP P75960
F	-9	HIS	-	expression tag	UNP P75960
F	-8	HIS	-	expression tag	UNP P75960
F	-7	HIS	-	expression tag	UNP P75960
F	-6	HIS	-	expression tag	UNP P75960
F	-5	HIS	-	expression tag	UNP P75960
F	-4	SER	-	expression tag	UNP P75960
F	-3	GLN	-	expression tag	UNP P75960
F	-2	ASP	-	expression tag	UNP P75960
F	-1	PRO	-	expression tag	UNP P75960
F	76	GLY	ALA	engineered mutation	UNP P75960
F	131	CYS	ILE	engineered mutation	UNP P75960

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
F	161	ALA	VAL	engineered mutation	UNP P75960

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	7	Total	C	N	O	0	0	0
			57	33	16	8			
2	H	7	Total	C	N	O	0	1	0
			65	38	19	8			
2	I	7	Total	C	N	O	0	0	0
			57	33	16	8			
2	J	8	Total	C	N	O	0	0	0
			66	39	18	9			
2	K	9	Total	C	N	O	0	0	0
			74	45	19	10			
2	L	11	Total	C	N	O	0	0	0
			87	54	21	12			

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	161	Total	O	0	0
			161	161		
4	B	89	Total	O	0	0
			89	89		

*Continued on next page...*

*Continued from previous page...*

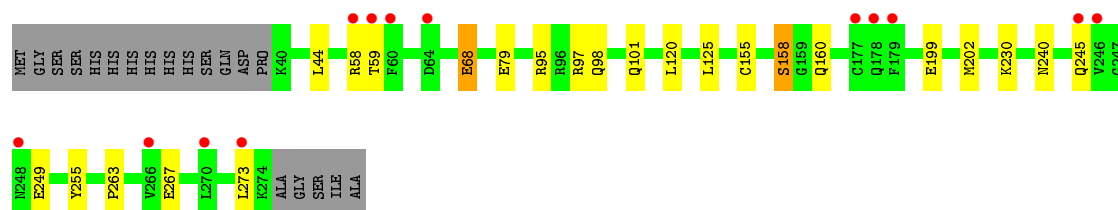
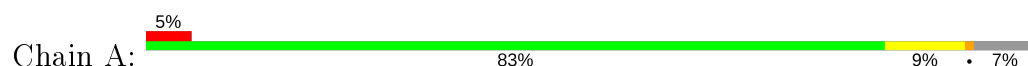
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	185	Total 185	O 185	0	0
4	D	85	Total 85	O 85	0	0
4	E	211	Total 211	O 211	0	0
4	F	95	Total 95	O 95	0	0
4	G	7	Total 7	O 7	0	0
4	H	7	Total 7	O 7	0	0
4	I	10	Total 10	O 10	0	0
4	J	7	Total 7	O 7	0	0
4	K	10	Total 10	O 10	0	0
4	L	12	Total 12	O 12	0	0



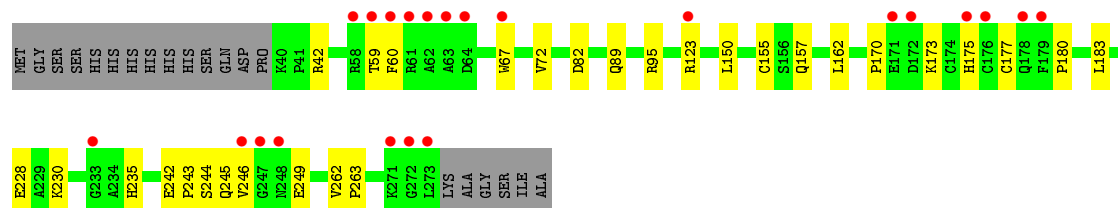
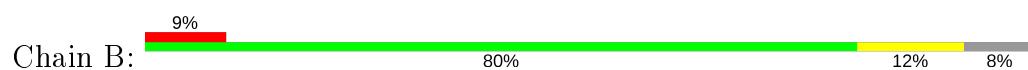
### 3 Residue-property plots

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.

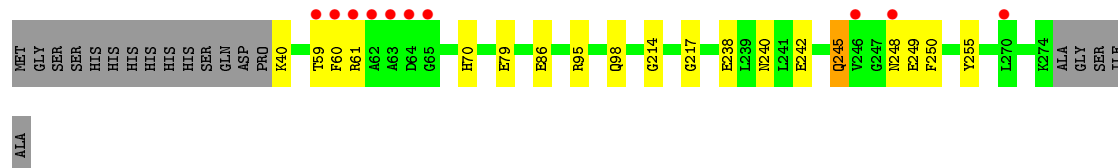
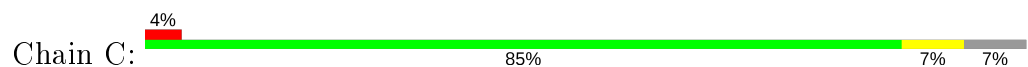
- Molecule 1: NAD-dependent protein deacylase



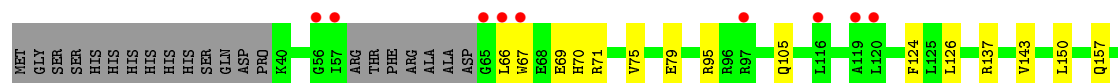
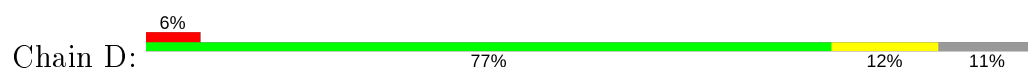
- Molecule 1: NAD-dependent protein deacylase



- Molecule 1: NAD-dependent protein deacylase

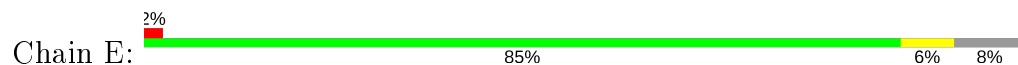


- Molecule 1: NAD-dependent protein deacylase

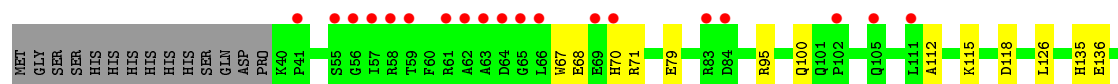
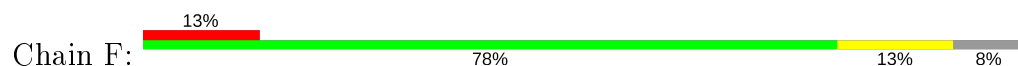




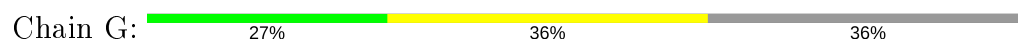
- Molecule 1: NAD-dependent protein deacylase



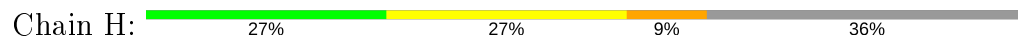
- Molecule 1: NAD-dependent protein deacylase



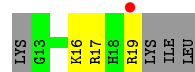
- Molecule 2: Histone H4



- Molecule 2: Histone H4



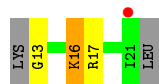
- Molecule 2: Histone H4



- Molecule 2: Histone H4



## ● Molecule 2: Histone H4



## ● Molecule 2: Histone H4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.30Å 95.38Å 168.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.47 – 1.92 48.47 – 1.92	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.47-1.92) 100.0 (48.47-1.92)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 1.92Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.204 , 0.242 0.205 , 0.243	Depositor DCC
$R_{free}$ test set	1998 reflections (1.75%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.3	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 48.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.055 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12179	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.5796e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.333 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: ZN, ALY

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	0.48	0/1889	0.64	0/2564
1	B	0.47	0/1872	0.61	0/2542
1	C	0.51	0/1888	0.62	0/2563
1	D	0.42	0/1806	0.58	0/2452
1	E	0.53	0/1858	0.64	0/2523
1	F	0.46	0/1858	0.60	0/2523
2	G	0.44	0/44	0.61	0/54
2	H	0.40	0/54	0.51	0/65
2	I	0.49	0/44	0.64	0/54
2	J	0.39	0/53	0.69	0/65
2	K	0.47	0/61	0.49	0/76
2	L	0.46	0/74	0.55	0/94
All	All	0.48	0/11501	0.62	0/15575

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
2	H	0	1
2	K	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	16	ALY	Mainchain
2	K	16	ALY	Mainchain

## 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	1838	0	1792	17	0
1	B	1824	0	1769	29	0
1	C	1837	0	1788	16	0
1	D	1763	0	1706	30	0
1	E	1813	0	1752	16	0
1	F	1813	0	1752	27	0
2	G	57	0	57	2	0
2	H	65	0	70	3	0
2	I	57	0	57	2	0
2	J	66	0	70	2	0
2	K	74	0	81	3	0
2	L	87	0	94	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	161	0	0	3	2
4	B	89	0	0	4	1
4	C	185	0	0	3	1
4	D	85	0	0	2	0
4	E	211	0	0	3	0
4	F	95	0	0	1	0
4	G	7	0	0	1	0
4	H	7	0	0	1	0
4	I	10	0	0	0	0
4	J	7	0	0	0	0
4	K	10	0	0	1	0
4	L	12	0	0	0	0
All	All	12179	0	10988	132	2

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 (132) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:79:GLU:OE2	2:K:17:ARG:NH2	1.98	0.96
1:C:248:ASN:HD21	1:E:61:ARG:HH12	1.11	0.93
1:B:170:PRO:O	1:B:173:LYS:NZ	2.03	0.89
1:D:69:GLU:OE2	1:F:95:ARG:NH2	2.11	0.83
1:B:157:GLN:NE2	1:B:177:CYS:SG	2.55	0.80
1:D:79:GLU:OE2	2:I:17:ARG:NH1	2.14	0.79
1:E:201:TYR:HH	2:K:13:GLY:N	1.82	0.78
1:D:67:TRP:HE1	1:D:69:GLU:HB2	1.50	0.77
1:A:230:LYS:HE3	1:A:249:GLU:HA	1.66	0.76
1:B:246:VAL:HG21	1:D:245:GLN:HG3	1.68	0.75
1:D:67:TRP:NE1	1:D:69:GLU:HB2	2.01	0.74
1:F:230:LYS:NZ	4:F:401:HOH:O	2.08	0.73
1:A:101:GLN:NE2	4:A:402:HOH:O	2.22	0.73
2:G:13:GLY:N	4:G:101:HOH:O	2.23	0.72
1:A:79:GLU:OE1	2:H:17:ARG:NH2	2.16	0.72
1:B:230:LYS:NZ	1:B:249:GLU:HA	2.03	0.72
1:D:69:GLU:HG2	1:F:95:ARG:HH22	1.54	0.70
1:B:155:CYS:SG	1:B:157:GLN:HG3	2.32	0.69
1:B:60:PHE:CD2	1:B:72:VAL:HG12	2.28	0.69
1:C:248:ASN:ND2	1:E:61:ARG:HH12	1.87	0.69
1:A:245:GLN:HG3	1:A:249:GLU:HG2	1.75	0.68
1:A:97:ARG:NH1	4:A:404:HOH:O	2.27	0.67
1:B:60:PHE:HD2	1:B:72:VAL:HG12	1.60	0.66
1:A:249:GLU:OE1	1:A:249:GLU:N	2.28	0.66
1:C:79:GLU:OE1	2:J:17:ARG:NH2	2.24	0.65
1:B:82:ASP:OD1	4:B:401:HOH:O	2.13	0.65
1:B:230:LYS:HZ3	1:B:249:GLU:HA	1.61	0.64
2:K:13:GLY:N	4:K:101:HOH:O	2.31	0.62
1:B:60:PHE:CZ	1:B:67:TRP:CE3	2.91	0.59
1:B:95:ARG:HB3	1:B:150:LEU:HD21	1.86	0.58
1:D:227:HIS:HD2	1:D:249:GLU:OE1	1.86	0.58
1:B:60:PHE:CD2	1:B:67:TRP:HB2	2.38	0.57
1:C:249:GLU:N	1:C:249:GLU:OE1	2.32	0.57
1:F:190:PHE:HD1	2:L:17:ARG:HA	1.71	0.56
1:F:126:LEU:HD23	1:F:143:VAL:HG22	1.88	0.55
1:C:217:GLY:O	2:I:19:ARG:NH2	2.40	0.55
1:A:58:ARG:HD2	1:A:95:ARG:HE	1.72	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:GLU:O	1:D:271:LYS:HD2	2.06	0.54
1:D:267:GLU:OE1	1:D:271:LYS:NZ	2.36	0.54
1:A:58:ARG:HE	1:A:98:GLN:HG3	1.71	0.54
1:F:67:TRP:HZ2	1:F:190:PHE:CE2	2.27	0.53
1:A:245:GLN:HG3	1:A:249:GLU:CG	2.38	0.53
1:E:268:LYS:HE2	4:E:423:HOH:O	2.08	0.53
1:E:193:MET:HG2	1:F:193:MET:HE3	1.91	0.53
1:E:40:LYS:N	4:E:411:HOH:O	2.41	0.53
1:C:70:HIS:HD2	4:C:556:HOH:O	1.91	0.53
1:C:86:GLU:HG2	4:C:428:HOH:O	2.09	0.53
1:D:258:ALA:O	1:D:262:VAL:HG13	2.09	0.52
1:F:172:ASP:O	1:F:173:LYS:HD3	2.09	0.52
1:D:67:TRP:HD1	1:D:70:HIS:HD1	1.51	0.52
1:C:248:ASN:HD21	1:E:61:ARG:NH1	1.93	0.52
1:A:199:GLU:HA	1:A:202:MET:HE2	1.91	0.51
1:D:246:VAL:C	1:D:248:ASN:H	2.13	0.51
1:D:95:ARG:HB3	1:D:150:LEU:HD21	1.93	0.50
1:B:230:LYS:HZ1	1:B:249:GLU:HA	1.76	0.50
1:D:240:ASN:O	1:D:255:TYR:HA	2.12	0.50
1:D:71:ARG:HG3	1:F:71:ARG:HG2	1.94	0.50
1:B:157:GLN:HE22	1:B:177:CYS:HB2	1.78	0.49
1:C:95:ARG:HH21	1:C:98:GLN:NE2	2.11	0.48
1:F:67:TRP:HZ2	1:F:190:PHE:CD2	2.30	0.48
1:D:246:VAL:O	1:D:248:ASN:N	2.46	0.48
1:A:120:LEU:HD21	1:A:273:LEU:HD11	1.95	0.48
1:B:245:GLN:NE2	1:B:249:GLU:HG3	2.29	0.48
1:F:160:GLN:OE1	1:F:176:CYS:SG	2.73	0.47
2:H:18:HIS:ND1	2:H:19[A]:ARG:HG3	2.29	0.47
1:C:255:TYR:CG	1:E:243:PRO:HD3	2.49	0.47
1:E:65:GLY:HA2	2:L:22:LEU:CD1	2.45	0.47
1:E:60:PHE:CD1	1:E:60:PHE:N	2.77	0.47
2:J:19:ARG:O	2:J:19:ARG:HG2	2.15	0.47
1:D:105:GLN:OE1	1:D:137:ARG:NH2	2.49	0.46
1:D:66:LEU:CD1	1:D:75:VAL:HG23	2.45	0.46
1:B:95:ARG:HA	1:B:95:ARG:HD3	1.83	0.46
1:A:263:PRO:O	1:A:267:GLU:HG3	2.17	0.45
1:B:245:GLN:HE22	1:B:249:GLU:HG3	1.81	0.45
1:E:214:GLY:N	1:E:240:ASN:OD1	2.47	0.45
1:B:235:HIS:ND1	4:B:408:HOH:O	2.36	0.45
1:F:100:GLN:HE22	1:F:165:THR:HB	1.81	0.45
1:E:218:HIS:NE2	1:E:245:GLN:HG3	2.32	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:GLN:OE1	4:A:401:HOH:O	2.20	0.45
1:D:67:TRP:CD1	1:D:70:HIS:ND1	2.77	0.45
1:B:228:GLU:OE2	4:B:402:HOH:O	2.21	0.45
1:B:59:THR:OG1	1:B:60:PHE:N	2.50	0.44
1:F:240:ASN:O	1:F:255:TYR:HA	2.17	0.44
1:E:126:LEU:HD21	1:E:135:HIS:CG	2.53	0.44
1:F:115:LYS:O	1:F:118:ASP:HB2	2.17	0.44
1:F:126:LEU:HD21	1:F:135:HIS:CG	2.53	0.44
1:F:266:VAL:O	1:F:270:LEU:HG	2.18	0.43
1:D:126:LEU:HD23	1:D:143:VAL:HG22	2.01	0.43
1:F:157:GLN:NE2	1:F:181:ALA:HB2	2.34	0.43
2:G:18:HIS:O	2:G:19:ARG:HB2	2.18	0.43
2:L:21:ILE:HG22	2:L:22:LEU:HD23	2.00	0.43
1:F:267:GLU:O	1:F:271:LYS:HG3	2.19	0.43
1:B:89:GLN:NE2	1:B:183:LEU:O	2.49	0.43
1:B:173:LYS:HB3	1:B:180:PRO:HB3	2.01	0.42
1:D:227:HIS:CD2	1:D:249:GLU:OE1	2.71	0.42
1:F:162:LEU:HA	1:F:162:LEU:HD23	1.85	0.42
1:E:199:GLU:OE1	4:E:401:HOH:O	2.22	0.42
1:E:65:GLY:HA2	2:L:22:LEU:HD12	2.01	0.42
1:A:44[A]:LEU:HD13	1:A:125:LEU:HB3	2.02	0.42
1:B:42:ARG:HG2	1:B:123:ARG:HD3	2.01	0.42
1:A:155:CYS:SG	1:A:158:SER:HB3	2.60	0.42
1:C:242:GLU:HG2	1:E:248:ASN:HD21	1.84	0.42
1:D:175:HIS:HA	4:D:440:HOH:O	2.18	0.42
1:F:112:ALA:O	1:F:115:LYS:HB3	2.20	0.42
2:H:19[A]:ARG:NH2	4:H:101:HOH:O	2.40	0.42
1:D:249:GLU:O	1:D:249:GLU:HG2	2.20	0.42
1:D:67:TRP:HB2	1:D:95:ARG:HH21	1.85	0.41
1:C:98:GLN:HG3	4:C:454:HOH:O	2.19	0.41
1:F:136:GLU:OE2	1:F:145:HIS:NE2	2.43	0.41
1:F:178:GLN:O	1:F:180:PRO:HD3	2.20	0.41
1:C:238:GLU:HB2	1:C:250:PHE:CG	2.56	0.41
1:A:59:THR:HG22	1:A:68:GLU:HG3	2.02	0.41
1:D:243:PRO:HA	1:D:255:TYR:CE1	2.56	0.41
1:F:68:GLU:OE2	1:F:70:HIS:HD2	2.03	0.41
1:A:240:ASN:O	1:A:255:TYR:HA	2.21	0.41
1:D:124:PHE:CZ	1:D:126:LEU:HB2	2.55	0.41
1:D:157:GLN:HE21	1:D:157:GLN:HB2	1.63	0.41
1:D:162:LEU:HD22	1:D:175:HIS:CE1	2.56	0.41
1:D:69:GLU:CG	1:F:95:ARG:HH22	2.30	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:21:ILE:HD13	2:L:21:ILE:HA	1.87	0.41
1:B:244:SER:O	4:B:403:HOH:O	2.22	0.41
1:C:214:GLY:N	1:C:240:ASN:OD1	2.53	0.41
1:B:157:GLN:HE22	1:B:177:CYS:CB	2.34	0.40
1:D:273:LEU:O	4:D:401:HOH:O	2.22	0.40
1:B:242:GLU:HG3	1:B:243:PRO:HD2	2.02	0.40
1:B:262:VAL:HB	1:B:263:PRO:HD3	2.02	0.40
1:C:245:GLN:CD	1:C:245:GLN:H	2.19	0.40
1:C:59:THR:HG23	1:C:60:PHE:O	2.20	0.40
1:B:95:ARG:CB	1:B:150:LEU:HD21	2.49	0.40
1:F:67:TRP:CZ2	1:F:190:PHE:CE2	3.07	0.40
1:F:243:PRO:HA	1:F:255:TYR:CE1	2.57	0.40
1:B:162:LEU:HD21	1:B:175:HIS:CE1	2.57	0.40

All (2) 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)
4:A:405:HOH:O	4:B:413:HOH:O 3_544	2.10	0.10
4:A:431:HOH:O	4:C:424:HOH:O 3_644	2.12	0.08

## 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	235/254 (92%)	231 (98%)	3 (1%)	1 (0%)	34	24
1	B	233/254 (92%)	231 (99%)	2 (1%)	0	100	100
1	C	235/254 (92%)	231 (98%)	3 (1%)	1 (0%)	34	24
1	D	223/254 (88%)	221 (99%)	1 (0%)	1 (0%)	34	24
1	E	231/254 (91%)	229 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	231/254 (91%)	228 (99%)	3 (1%)	0	100	100
2	G	4/11 (36%)	4 (100%)	0	0	100	100
2	H	4/11 (36%)	4 (100%)	0	0	100	100
2	I	4/11 (36%)	4 (100%)	0	0	100	100
2	J	5/11 (46%)	5 (100%)	0	0	100	100
2	K	6/11 (54%)	6 (100%)	0	0	100	100
2	L	8/11 (73%)	8 (100%)	0	0	100	100
All	All	1419/1590 (89%)	1402 (99%)	14 (1%)	3 (0%)	47	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	245	GLN
1	A	68	GLU
1	D	247	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	194/207 (94%)	193 (100%)	1 (0%)	88	89
1	B	192/207 (93%)	192 (100%)	0	100	100
1	C	194/207 (94%)	192 (99%)	2 (1%)	76	75
1	D	186/207 (90%)	186 (100%)	0	100	100
1	E	190/207 (92%)	189 (100%)	1 (0%)	88	89
1	F	190/207 (92%)	189 (100%)	1 (0%)	88	89
2	G	3/7 (43%)	3 (100%)	0	100	100
2	H	4/7 (57%)	4 (100%)	0	100	100
2	I	3/7 (43%)	3 (100%)	0	100	100
2	J	4/7 (57%)	4 (100%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	5/7 (71%)	5 (100%)	0	100	100
2	L	6/7 (86%)	6 (100%)	0	100	100
All	All	1171/1284 (91%)	1166 (100%)	5 (0%)	91	91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	SER
1	C	40	LYS
1	C	61	ARG
1	E	60	PHE
1	F	230	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	248	ASN
1	B	157	GLN
1	B	175	HIS
1	B	245	GLN
1	C	175	HIS
1	C	248	ASN
1	D	157	GLN
1	D	175	HIS
1	D	227	HIS
1	E	227	HIS
1	E	248	ASN
1	F	70	HIS
1	F	100	GLN
1	F	157	GLN
1	F	218	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	ALY	H	16	2	10,11,12	1.46	1 (10%)	7,12,14	1.17	1 (14%)
2	ALY	J	16	2	10,11,12	0.79	0	7,12,14	0.86	0
2	ALY	I	16	2	10,11,12	0.80	0	7,12,14	0.98	1 (14%)
2	ALY	K	16	2	10,11,12	1.43	1 (10%)	7,12,14	1.39	1 (14%)
2	ALY	G	16	2	10,11,12	1.51	1 (10%)	7,12,14	1.92	2 (28%)
2	ALY	L	16	2	10,11,12	1.51	1 (10%)	7,12,14	1.04	1 (14%)

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	ALY	H	16	2	-	0/9/10/12	-
2	ALY	J	16	2	-	0/9/10/12	-
2	ALY	I	16	2	-	0/9/10/12	-
2	ALY	K	16	2	-	0/9/10/12	-
2	ALY	G	16	2	-	0/9/10/12	-
2	ALY	L	16	2	-	0/9/10/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	16	ALY	O-C	4.23	1.36	1.19
2	L	16	ALY	O-C	4.11	1.36	1.19
2	H	16	ALY	O-C	3.90	1.35	1.19
2	K	16	ALY	O-C	3.89	1.35	1.19

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	16	ALY	CE-NZ-CH	-3.70	116.86	122.56
2	G	16	ALY	CD-CG-CB	-2.67	104.18	113.62

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	16	ALY	CD-CG-CB	-2.65	104.25	113.62
2	K	16	ALY	CD-CG-CB	-2.54	104.64	113.62
2	I	16	ALY	CD-CG-CB	-2.51	104.74	113.62
2	L	16	ALY	CD-CG-CB	-2.46	104.94	113.62

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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	235/254 (92%)	0.35	13 (5%) 25 28	22, 34, 72, 84	0
1	B	234/254 (92%)	0.53	22 (9%) 8 10	24, 40, 80, 97	0
1	C	235/254 (92%)	0.25	10 (4%) 35 38	20, 32, 65, 92	0
1	D	227/254 (89%)	0.47	15 (6%) 18 20	24, 43, 71, 93	0
1	E	233/254 (91%)	0.16	5 (2%) 63 66	20, 29, 51, 88	0
1	F	233/254 (91%)	0.82	32 (13%) 3 3	23, 44, 73, 99	0
2	G	6/11 (54%)	0.33	0 100 100	27, 33, 39, 58	0
2	H	6/11 (54%)	0.28	0 100 100	26, 39, 47, 47	0
2	I	6/11 (54%)	0.36	1 (16%) 1 1	23, 29, 42, 59	0
2	J	7/11 (63%)	0.27	0 100 100	26, 34, 55, 59	0
2	K	8/11 (72%)	0.57	1 (12%) 3 4	26, 34, 54, 62	0
2	L	10/11 (90%)	0.40	0 100 100	26, 37, 54, 55	0
All	All	1440/1590 (90%)	0.43	99 (6%) 16 19	20, 37, 71, 99	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	273	LEU	7.4
1	B	59	THR	7.3
1	D	65	GLY	7.2
1	C	63	ALA	6.5
1	E	60	PHE	6.3
1	A	246	VAL	6.2
1	E	59	THR	5.8
1	F	61	ARG	5.8
1	D	269	LEU	5.7
1	D	57	ILE	5.7
1	F	171	GLU	5.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	246	VAL	5.4
1	A	58	ARG	5.4
1	B	246	VAL	5.3
1	F	269	LEU	5.3
1	C	65	GLY	5.1
1	F	175	HIS	4.9
1	B	176	CYS	4.8
1	A	64	ASP	4.6
1	F	62	ALA	4.6
1	B	61	ARG	4.5
1	E	61	ARG	4.4
1	E	64	ASP	4.4
1	F	111	LEU	4.3
1	B	58	ARG	4.0
1	B	62	ALA	4.0
1	C	64	ASP	3.9
1	A	179	PHE	3.9
1	F	246	VAL	3.7
1	D	56	GLY	3.7
1	D	67	TRP	3.6
1	F	58	ARG	3.5
1	B	60	PHE	3.4
1	F	63	ALA	3.4
1	F	162	LEU	3.4
1	F	270	LEU	3.3
1	A	59	THR	3.3
1	D	245	GLN	3.3
1	F	41	PRO	3.2
1	A	177	CYS	3.2
1	B	248	ASN	3.2
1	B	272	GLY	3.1
1	A	270	LEU	3.1
1	F	64	ASP	3.1
1	B	67	TRP	3.1
1	A	245	GLN	3.0
1	D	116	LEU	3.0
1	F	66	LEU	3.0
1	C	270	LEU	2.9
1	B	123	ARG	2.9
1	F	105	GLN	2.9
1	B	63	ALA	2.9
1	E	58	ARG	2.8

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	102	PRO	2.8
2	K	21	ILE	2.8
1	F	55	SER	2.8
1	A	248	ASN	2.8
1	B	178	GLN	2.7
1	D	273	LEU	2.7
1	C	61	ARG	2.7
1	D	66	LEU	2.7
1	C	59	THR	2.7
1	F	170	PRO	2.6
1	F	56	GLY	2.6
1	F	272	GLY	2.6
1	D	120	LEU	2.5
1	F	266	VAL	2.5
1	B	179	PHE	2.5
1	C	246	VAL	2.4
1	F	59	THR	2.4
1	F	267	GLU	2.4
1	A	178	GLN	2.4
1	D	247	GLY	2.4
1	B	175	HIS	2.3
1	C	62	ALA	2.3
1	F	65	GLY	2.3
1	A	60	PHE	2.3
1	C	248	ASN	2.3
1	A	266	VAL	2.3
1	C	60	PHE	2.2
1	D	271	LYS	2.2
2	I	19	ARG	2.2
1	B	172	ASP	2.2
1	B	233	GLY	2.2
1	F	57	ILE	2.2
1	F	83	ARG	2.2
1	B	247	GLY	2.2
1	B	171	GLU	2.2
1	F	70	HIS	2.1
1	F	245	GLN	2.1
1	B	64	ASP	2.1
1	F	84	ASP	2.1
1	F	165	THR	2.1
1	D	97	ARG	2.1
1	B	271	LYS	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	254	TYR	2.0
1	D	119	ALA	2.0
1	B	273	LEU	2.0
1	F	69	GLU	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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	ALY	L	16	12/13	0.94	0.10	22,27,36,45	0
2	ALY	G	16	12/13	0.95	0.11	16,23,31,33	0
2	ALY	J	16	12/13	0.95	0.11	22,27,38,39	0
2	ALY	K	16	12/13	0.96	0.11	23,25,35,39	0
2	ALY	H	16	12/13	0.96	0.10	21,24,33,39	0
2	ALY	I	16	12/13	0.96	0.10	18,23,35,40	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	ZN	A	300	1/1	0.95	0.05	51,51,51,51	0
3	ZN	B	301	1/1	0.96	0.06	59,59,59,59	0
3	ZN	F	301	1/1	0.98	0.06	54,54,54,54	0
3	ZN	D	301	1/1	0.98	0.05	40,40,40,40	0
3	ZN	C	300	1/1	0.98	0.07	41,41,41,41	0
3	ZN	E	301	1/1	0.99	0.08	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.