



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 9, 2026 – 09:31 PM UTC

PDB ID : 9MPK / pdb\_00009mpk  
Title : BRD3-BD1 in complex with cyclic peptide 2.1C-Y5A  
Authors : Patel, K.; Mackay, J.P.  
Deposited on : 2024-12-30  
Resolution : 2.70 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 types of validation reports are described at

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

---

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

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

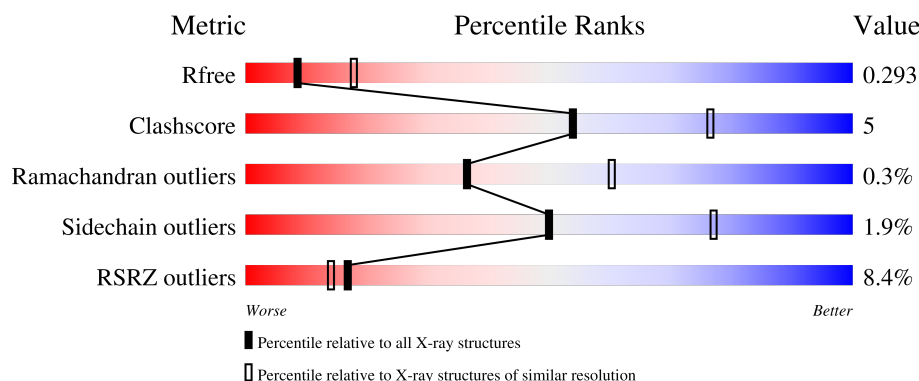
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	128	<div> <div>3%</div> <div>75%</div> <div>14%</div> <div>10%</div> </div>
1	B	128	<div> <div>8%</div> <div>87%</div> <div>11%</div> </div>
1	C	128	<div> <div>7%</div> <div>73%</div> <div>19%</div> <div>9%</div> </div>
1	D	128	<div> <div>6%</div> <div>79%</div> <div>10%</div> <div>11%</div> </div>
1	E	128	<div> <div>6%</div> <div>73%</div> <div>15%</div> <div>12%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	128	<div><div></div><div>12%</div><div>73%</div><div>15%</div><div>10%</div></div>
2	G	15	<div><div></div><div>7%</div><div>73%</div><div>27%</div></div>
2	H	15	<div><div></div><div>7%</div><div>87%</div><div>13%</div></div>
2	I	15	<div><div></div><div>7%</div><div>100%</div></div>
2	J	15	<div><div></div><div>7%</div><div>87%</div><div>13%</div></div>
2	K	15	<div><div></div><div>33%</div><div>80%</div><div>20%</div></div>
2	L	15	<div><div></div><div>100%</div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6483 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 Bromodomain-containing protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	115	Total	C	N	O	S	29	0	0
			965	625	158	173	9			
1	B	114	Total	C	N	O	S	45	0	0
			962	623	157	173	9			
1	C	117	Total	C	N	O	S	48	0	0
			979	633	161	176	9			
1	D	114	Total	C	N	O	S	46	0	0
			957	619	157	172	9			
1	E	113	Total	C	N	O	S	26	0	0
			948	614	156	169	9			
1	F	115	Total	C	N	O	S	42	0	0
			964	624	158	173	9			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLN	-	expression tag	UNP Q15059
A	21	PRO	-	expression tag	UNP Q15059
A	22	LEU	-	expression tag	UNP Q15059
A	23	GLY	-	expression tag	UNP Q15059
A	24	SER	-	expression tag	UNP Q15059
B	20	GLN	-	expression tag	UNP Q15059
B	21	PRO	-	expression tag	UNP Q15059
B	22	LEU	-	expression tag	UNP Q15059
B	23	GLY	-	expression tag	UNP Q15059
B	24	SER	-	expression tag	UNP Q15059
C	20	GLN	-	expression tag	UNP Q15059
C	21	PRO	-	expression tag	UNP Q15059
C	22	LEU	-	expression tag	UNP Q15059
C	23	GLY	-	expression tag	UNP Q15059
C	24	SER	-	expression tag	UNP Q15059
D	20	GLN	-	expression tag	UNP Q15059
D	21	PRO	-	expression tag	UNP Q15059

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	22	LEU	-	expression tag	UNP Q15059
D	23	GLY	-	expression tag	UNP Q15059
D	24	SER	-	expression tag	UNP Q15059
E	20	GLN	-	expression tag	UNP Q15059
E	21	PRO	-	expression tag	UNP Q15059
E	22	LEU	-	expression tag	UNP Q15059
E	23	GLY	-	expression tag	UNP Q15059
E	24	SER	-	expression tag	UNP Q15059
F	20	GLN	-	expression tag	UNP Q15059
F	21	PRO	-	expression tag	UNP Q15059
F	22	LEU	-	expression tag	UNP Q15059
F	23	GLY	-	expression tag	UNP Q15059
F	24	SER	-	expression tag	UNP Q15059

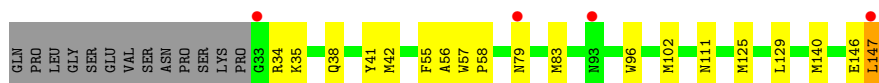
- Molecule 2 is a protein called 2.1C-Y5A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	15	Total	C	N	O	S	1	0	1
			118	80	19	18	1			
2	H	15	Total	C	N	O	S	1	0	1
			118	80	19	18	1			
2	I	15	Total	C	N	O	S	1	0	1
			118	80	19	18	1			
2	J	15	Total	C	N	O	S	1	0	1
			118	80	19	18	1			
2	K	15	Total	C	N	O	S	1	0	1
			118	80	19	18	1			
2	L	15	Total	C	N	O	S	1	0	1
			118	80	19	18	1			

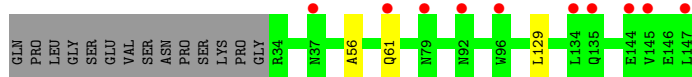
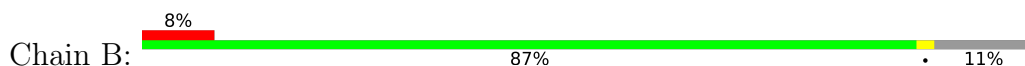
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

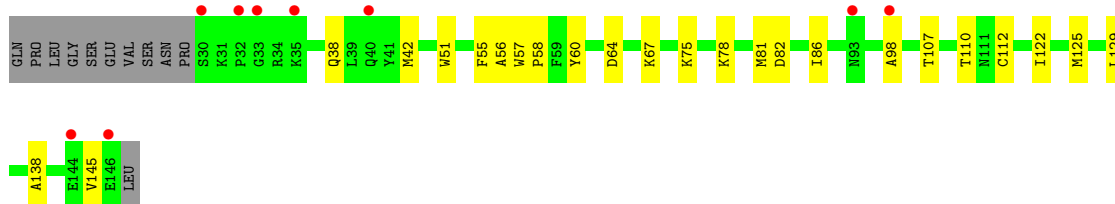
- Molecule 1: Bromodomain-containing protein 3



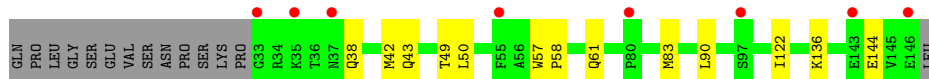
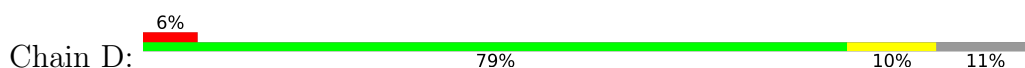
- Molecule 1: Bromodomain-containing protein 3



- Molecule 1: Bromodomain-containing protein 3

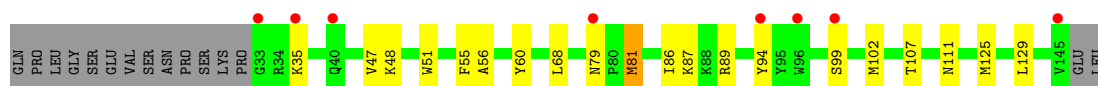


- Molecule 1: Bromodomain-containing protein 3

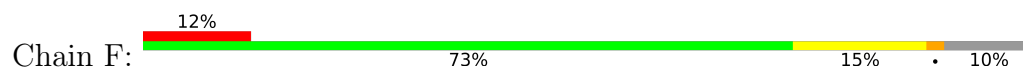


- Molecule 1: Bromodomain-containing protein 3

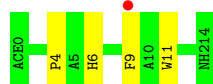
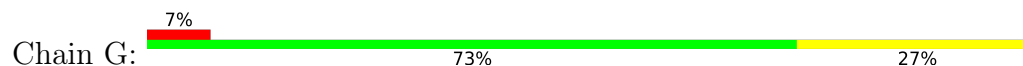




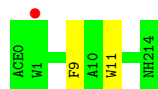
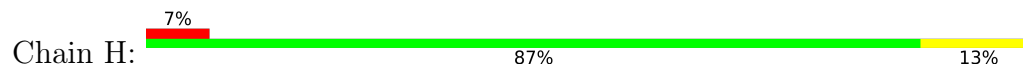
- Molecule 1: Bromodomain-containing protein 3



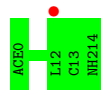
- Molecule 2: 2.1C-Y5A



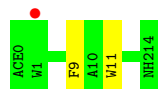
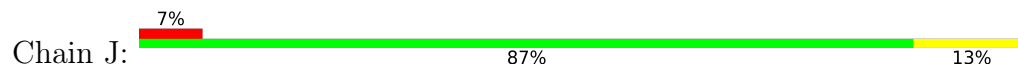
- Molecule 2: 2.1C-Y5A



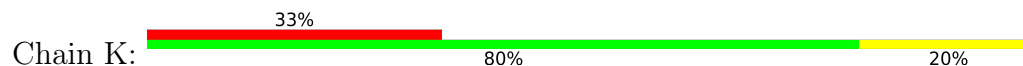
- Molecule 2: 2.1C-Y5A

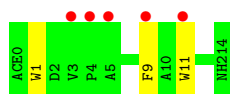


- Molecule 2: 2.1C-Y5A



- Molecule 2: 2.1C-Y5A





- Molecule 2: 2.1C-Y5A

Chain L:  100%

There are no outlier residues recorded for this chain.



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.01Å 108.69Å 178.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.42 – 2.70 46.42 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.42-2.70) 99.7 (46.42-2.70)	Depositor EDS
$R_{merge}$	0.44	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.256 , 0.295 0.255 , 0.293	Depositor DCC
$R_{free}$ test set	1363 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.3	Xtriage
Anisotropy	0.615	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 37.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6483	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	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 25.80 % 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 2.9617e-03. 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, ALY, NH2

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	0.09	0/990	0.23	0/1340
1	B	0.08	0/987	0.23	0/1335
1	C	0.09	0/1005	0.24	0/1360
1	D	0.09	0/982	0.24	0/1329
1	E	0.10	0/973	0.26	0/1317
1	F	0.10	0/990	0.30	0/1340
2	G	0.07	0/108	0.21	0/149
2	H	0.07	0/108	0.22	0/149
2	I	0.06	0/108	0.22	0/149
2	J	0.06	0/108	0.26	0/149
2	K	0.08	0/108	0.22	0/149
2	L	0.11	0/108	0.29	0/149
All	All	0.09	0/6575	0.25	0/8915

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	965	0	956	12	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	962	0	953	2	0
1	C	979	0	970	13	0
1	D	957	0	945	5	0
1	E	948	0	939	13	0
1	F	964	0	953	12	0
2	G	118	0	105	3	0
2	H	118	0	105	1	0
2	I	118	0	105	0	0
2	J	118	0	105	1	0
2	K	118	0	105	2	0
2	L	118	0	105	0	0
All	All	6483	0	6346	60	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (60) 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:50:LEU:HB2	1:D:83:MET:HE1	1.63	0.80
1:D:49:THR:HG21	1:D:136:LYS:HE3	1.65	0.79
1:F:140:MET:N	1:F:140:MET:SD	2.57	0.77
1:A:35:LYS:H	1:A:147:LEU:HD23	1.56	0.70
1:E:68:LEU:HD13	2:G:4:PRO:HA	1.77	0.66
1:E:79:ASN:O	1:E:111:ASN:ND2	2.28	0.65
1:C:81:MET:HE2	1:C:86:ILE:HG13	1.80	0.64
1:C:75:LYS:O	1:C:78:LYS:NZ	2.35	0.57
1:F:56:ALA:HA	1:F:129:LEU:HD11	1.88	0.56
1:E:56:ALA:HA	1:E:129:LEU:HD11	1.88	0.56
1:B:56:ALA:HA	1:B:129:LEU:HD11	1.90	0.54
1:F:37:ASN:ND2	1:F:140:MET:HG3	2.24	0.53
1:E:51:TRP:O	1:E:60:TYR:OH	2.25	0.52
1:F:72:ASP:OD1	1:F:72:ASP:N	2.43	0.52
1:E:47:VAL:HG11	1:E:87:LYS:HG3	1.94	0.49
1:E:89:ARG:HD2	1:E:94:TYR:CG	2.47	0.49
1:F:51:TRP:O	1:F:60:TYR:OH	2.27	0.49
1:E:55:PHE:HB3	1:E:125:MET:HB3	1.94	0.48
1:F:37:ASN:HD21	1:F:140:MET:HG3	1.78	0.48
1:D:38:GLN:O	1:D:42:MET:HG2	2.14	0.48
1:C:56:ALA:HA	1:C:129:LEU:HD11	1.96	0.47
1:C:107:THR:HA	1:C:110:THR:HG22	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:MET:HE3	1:C:82:ASP:H	1.79	0.47
1:A:79:ASN:O	1:A:111:ASN:ND2	2.47	0.47
1:C:51:TRP:O	1:C:60:TYR:OH	2.31	0.46
1:F:57:TRP:CD2	1:F:58:PRO:HD3	2.50	0.46
1:C:55:PHE:HB3	1:C:125:MET:HB3	1.98	0.46
1:C:112:CYS:SG	1:C:122:ILE:HG13	2.55	0.46
1:A:56:ALA:HA	1:A:129:LEU:HD11	1.97	0.46
2:H:9:PHE:HB3	2:H:11:TRP:NE1	2.31	0.46
1:A:55:PHE:HB3	1:A:125:MET:HB3	1.97	0.46
1:C:64:ASP:CG	1:C:67:LYS:HG3	2.40	0.46
1:E:89:ARG:HB3	1:E:94:TYR:HB3	1.97	0.46
1:A:56:ALA:HB1	1:A:83:MET:HE1	1.97	0.45
1:A:140:MET:HE2	1:A:140:MET:HB3	1.92	0.45
1:B:61:GLN:HG2	2:K:1:TRP:CZ3	2.52	0.44
1:E:68:LEU:HD11	2:G:6:HIS:ND1	2.33	0.44
1:F:68:LEU:O	1:F:70:LEU:HG	2.17	0.44
1:F:112:CYS:SG	1:F:122:ILE:HG13	2.58	0.44
1:C:38:GLN:HB3	1:C:98:ALA:HB2	1.99	0.44
1:E:107:THR:HG22	1:E:111:ASN:HD21	1.83	0.43
1:A:41:TYR:CD1	1:A:140:MET:HG3	2.54	0.43
1:C:38:GLN:O	1:C:42:MET:HG2	2.18	0.43
1:E:107:THR:HG22	1:E:111:ASN:ND2	2.34	0.43
1:A:34:ARG:NE	1:A:96:TRP:O	2.38	0.43
1:A:38:GLN:O	1:A:42:MET:HG2	2.19	0.43
1:A:140:MET:HE1	1:C:138:ALA:HB1	2.00	0.42
1:D:57:TRP:CG	1:D:58:PRO:HD3	2.54	0.42
2:G:9:PHE:HB3	2:G:11:TRP:CZ3	2.54	0.42
2:K:9:PHE:CE1	2:K:11:TRP:HB3	2.54	0.42
1:F:84:GLY:O	1:F:88:LYS:HG3	2.20	0.41
1:E:81:MET:HE3	1:E:86:ILE:HG12	2.03	0.41
1:A:57:TRP:CG	1:A:58:PRO:HD3	2.55	0.41
2:J:9:PHE:HB3	2:J:11:TRP:NE1	2.35	0.41
1:D:43:GLN:HA	1:D:90:LEU:HD13	2.02	0.41
1:F:45:VAL:HG12	1:F:136:LYS:HD3	2.01	0.41
1:A:102:MET:HE1	1:A:140:MET:HE1	2.03	0.41
1:C:57:TRP:CG	1:C:58:PRO:HD3	2.56	0.41
1:F:55:PHE:HB3	1:F:125:MET:HB3	2.02	0.41
1:E:99:SER:HA	1:E:102:MET:HE2	2.03	0.40

There are no symmetry-related clashes.

## 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	113/128 (88%)	111 (98%)	1 (1%)	1 (1%)	14	35
1	B	112/128 (88%)	110 (98%)	2 (2%)	0	100	100
1	C	115/128 (90%)	113 (98%)	2 (2%)	0	100	100
1	D	112/128 (88%)	112 (100%)	0	0	100	100
1	E	111/128 (87%)	111 (100%)	0	0	100	100
1	F	113/128 (88%)	104 (92%)	8 (7%)	1 (1%)	14	35
2	G	12/15 (80%)	11 (92%)	1 (8%)	0	100	100
2	H	12/15 (80%)	12 (100%)	0	0	100	100
2	I	12/15 (80%)	12 (100%)	0	0	100	100
2	J	12/15 (80%)	12 (100%)	0	0	100	100
2	K	12/15 (80%)	12 (100%)	0	0	100	100
2	L	12/15 (80%)	12 (100%)	0	0	100	100
All	All	748/858 (87%)	732 (98%)	14 (2%)	2 (0%)	36	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	GLU
1	F	70	LEU

### 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	107/119 (90%)	106 (99%)	1 (1%)	70	87
1	B	107/119 (90%)	107 (100%)	0	100	100
1	C	109/119 (92%)	108 (99%)	1 (1%)	70	87
1	D	106/119 (89%)	103 (97%)	3 (3%)	38	68
1	E	105/119 (88%)	102 (97%)	3 (3%)	37	67
1	F	107/119 (90%)	102 (95%)	5 (5%)	23	51
2	G	10/10 (100%)	10 (100%)	0	100	100
2	H	10/10 (100%)	10 (100%)	0	100	100
2	I	10/10 (100%)	10 (100%)	0	100	100
2	J	10/10 (100%)	10 (100%)	0	100	100
2	K	10/10 (100%)	10 (100%)	0	100	100
2	L	10/10 (100%)	10 (100%)	0	100	100
All	All	701/774 (91%)	688 (98%)	13 (2%)	50	77

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	LEU
1	C	145	VAL
1	D	61	GLN
1	D	122	ILE
1	D	144	GLU
1	E	35	LYS
1	E	48	LYS
1	E	81	MET
1	F	37	ASN
1	F	63	VAL
1	F	140	MET
1	F	144	GLU
1	F	145	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	61	GLN
1	A	142	GLN
1	B	44	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	69	ASN
1	B	127	GLN
1	C	135	GLN
1	D	43	GLN
1	D	74	HIS
1	E	43	GLN
1	E	61	GLN
1	E	139	GLN
2	I	6	HIS
1	F	37	ASN

### 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	G	7	2	10,11,12	0.88	0	7,12,14	0.58	0
2	ALY	I	7	2	10,11,12	0.88	0	7,12,14	0.66	0
2	ALY	L	7	2	10,11,12	0.86	0	7,12,14	0.65	0
2	ALY	K	7	2	10,11,12	0.89	0	7,12,14	0.71	0
2	ALY	J	7	2	10,11,12	0.87	0	7,12,14	0.63	0
2	ALY	H	7	2	10,11,12	0.87	0	7,12,14	0.71	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ALY	G	7	2	-	2/9/10/12	-
2	ALY	I	7	2	-	4/9/10/12	-
2	ALY	L	7	2	-	1/9/10/12	-
2	ALY	K	7	2	-	0/9/10/12	-
2	ALY	J	7	2	-	5/9/10/12	-
2	ALY	H	7	2	-	0/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	7	ALY	N-CA-CB-CG
2	I	7	ALY	C-CA-CB-CG
2	I	7	ALY	O-C-CA-CB
2	J	7	ALY	N-CA-CB-CG
2	J	7	ALY	C-CA-CB-CG
2	J	7	ALY	O-C-CA-CB
2	I	7	ALY	CA-CB-CG-CD
2	G	7	ALY	CE-CD-CG-CB
2	J	7	ALY	CA-CB-CG-CD
2	J	7	ALY	CE-CD-CG-CB
2	G	7	ALY	C-CA-CB-CG
2	L	7	ALY	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	115/128 (89%)	0.61	4 (3%) 47 43	17, 37, 49, 63	8 (6%)
1	B	114/128 (89%)	0.79	10 (8%) 15 13	19, 36, 57, 62	12 (10%)
1	C	117/128 (91%)	0.87	9 (7%) 19 17	17, 42, 56, 81	12 (10%)
1	D	114/128 (89%)	0.94	8 (7%) 22 19	19, 45, 64, 77	13 (11%)
1	E	113/128 (88%)	0.76	8 (7%) 22 19	21, 42, 56, 67	7 (6%)
1	F	115/128 (89%)	0.87	16 (13%) 6 5	21, 39, 52, 61	12 (10%)
2	G	12/15 (80%)	1.04	1 (8%) 17 14	44, 52, 60, 61	0
2	H	12/15 (80%)	0.83	1 (8%) 17 14	28, 34, 50, 51	0
2	I	12/15 (80%)	1.50	1 (8%) 17 14	49, 54, 64, 64	0
2	J	12/15 (80%)	0.78	1 (8%) 17 14	37, 41, 57, 60	0
2	K	12/15 (80%)	1.80	5 (41%) 0 0	49, 60, 67, 70	0
2	L	12/15 (80%)	0.33	0 100 100	31, 37, 47, 49	0
All	All	760/858 (88%)	0.83	64 (8%) 17 14	17, 41, 59, 81	64 (8%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	33	GLY	4.9
1	D	37	ASN	4.7
1	B	147	LEU	4.6
1	E	145	VAL	4.6
1	B	37	ASN	3.7
1	F	145	VAL	3.6
1	F	32	PRO	3.5
1	A	147	LEU	3.5
1	F	137	VAL	3.5
1	F	138	ALA	3.4
1	C	93	ASN	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	30	SER	3.3
1	D	33	GLY	3.3
2	K	11	TRP	3.2
1	F	79	ASN	3.1
2	J	1	TRP	3.0
1	F	92	ASN	2.8
1	F	73	TYR	2.8
1	E	99	SER	2.7
1	B	144	GLU	2.7
2	K	4	PRO	2.7
1	F	141	PRO	2.7
1	A	93	ASN	2.6
1	C	32	PRO	2.6
1	E	79	ASN	2.6
1	D	143	GLU	2.6
1	D	35	LYS	2.5
1	D	146	GLU	2.5
1	F	69	ASN	2.5
2	K	5	ALA	2.5
1	D	80	PRO	2.4
1	F	74	HIS	2.4
1	A	79	ASN	2.4
1	E	96	TRP	2.4
1	E	35	LYS	2.4
1	D	55	PHE	2.4
2	G	9	PHE	2.4
1	C	146	GLU	2.3
1	B	79	ASN	2.3
1	E	94	TYR	2.3
2	H	1	TRP	2.3
2	I	12	LEU	2.3
1	B	61	GLN	2.3
1	C	98	ALA	2.2
1	C	144	GLU	2.2
1	F	37	ASN	2.2
1	C	35	LYS	2.2
1	B	134	LEU	2.2
2	K	9	PHE	2.2
1	F	71	PRO	2.2
1	D	97	SER	2.1
1	F	63	VAL	2.1
1	F	97	SER	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	40	GLN	2.1
1	C	33	GLY	2.1
1	F	146	GLU	2.1
1	B	145	VAL	2.1
1	B	135	GLN	2.1
1	F	35	LYS	2.0
1	B	92	ASN	2.0
1	B	96	TRP	2.0
1	C	40	GLN	2.0
1	A	33	GLY	2.0
2	K	3	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. 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	G	7	12/13	0.87	0.14	32,46,51,52	0
2	ALY	I	7	12/13	0.88	0.13	29,41,51,56	0
2	ALY	J	7	12/13	0.90	0.11	22,32,41,49	0
2	ALY	H	7	12/13	0.92	0.10	17,30,34,36	0
2	ALY	K	7	12/13	0.92	0.10	23,34,50,52	0
2	ALY	L	7	12/13	0.92	0.10	25,31,37,40	0

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.