



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2025 – 02:06 PM EDT

PDB ID : 4KVV  
Title : Crystal structure of an alkylated Cys mutant of CC-Hex  
Authors : Burton, A.J.; Agnew, C.; Brady, R.L.; Woolfson, D.N.  
Deposited on : 2013-05-23  
Resolution : 1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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>.

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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 : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.21  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.004 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41.4

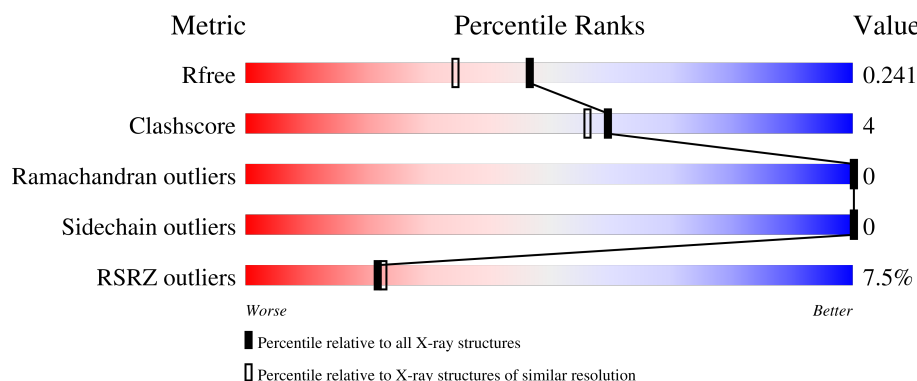
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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 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	33	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	33	<div> <div>79%</div> <div>9%</div> <div>12%</div> </div>
1	C	33	<div> <div>6%</div> <div>76%</div> <div>•</div> <div>6%</div> <div>15%</div> </div>
1	D	33	<div> <div>9%</div> <div>79%</div> <div>12%</div> <div>9%</div> </div>
1	E	33	<div> <div>6%</div> <div>82%</div> <div>•</div> <div>•</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	33	<div><div></div><div>6%</div><div>82%</div><div>6%</div><div>9%</div></div>
1	G	33	<div><div></div><div>6%</div><div>79%</div><div>6%</div><div>12%</div></div>
1	H	33	<div><div></div><div>9%</div><div>88%</div><div>6%</div><div>6%</div></div>
1	I	33	<div><div></div><div>6%</div><div>82%</div><div>9%</div><div>9%</div></div>
1	J	33	<div><div></div><div>9%</div><div>82%</div><div>6%</div><div>12%</div></div>
1	K	33	<div><div></div><div>3%</div><div>88%</div><div></div><div>9%</div></div>
1	L	33	<div><div></div><div>9%</div><div>76%</div><div>15%</div><div>6%</div></div>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 5393 atoms, of which 2619 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 6-HELIX COILED COIL CC-HEX-L24C PEPTIDE with an alkylated Cys mutation.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	30	Total	Br	C	H	N	O	S	39	0	0
			440	1	144	216	37	41	1			
1	B	29	Total	Br	C	H	N	O	S	38	0	0
			432	1	139	217	35	39	1			
1	C	28	Total	Br	C	H	N	O	S	7	0	0
			422	1	136	212	34	38	1			
1	D	30	Total	Br	C	H	N	O	S	18	0	0
			448	1	144	224	37	41	1			
1	E	29	Total	Br	C	H	N	O	S	23	0	0
			431	1	139	216	35	39	1			
1	F	30	Total	Br	C	H	N	O	S	13	0	0
			440	1	144	216	37	41	1			
1	G	29	Total	Br	C	H	N	O	S	17	0	0
			421	1	139	206	35	39	1			
1	H	31	Total	Br	C	H	N	O	S	11	0	0
			456	1	146	228	38	42	1			
1	I	30	Total	Br	C	H	N	O	S	29	0	0
			449	1	144	225	37	41	1			
1	J	29	Total	Br	C	H	N	O	S	25	0	0
			432	1	139	217	35	39	1			
1	K	30	Total	Br	C	H	N	O	S	38	0	0
			449	1	144	225	37	41	1			
1	L	31	Total	Br	C	H	N	O	S	32	0	0
			445	1	146	217	38	42	1			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	9	Total	O	0	0
			9	9		
2	B	12	Total	O	0	0
			12	12		

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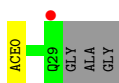
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	16	Total 16	O 16	0	0
2	D	13	Total 13	O 13	0	0
2	E	8	Total 8	O 8	0	0
2	F	11	Total 11	O 11	0	0
2	G	14	Total 14	O 14	0	0
2	H	12	Total 12	O 12	0	0
2	I	7	Total 7	O 7	0	0
2	J	7	Total 7	O 7	0	0
2	K	13	Total 13	O 13	0	0
2	L	6	Total 6	O 6	0	0

### 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.

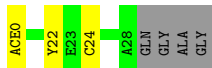
- Molecule 1: 6-HELIX COILED COIL CC-HEX-L24C PEPTIDE with an alkylated Cys mutation

Chain A: 




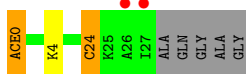
- Molecule 1: 6-HELIX COILED COIL CC-HEX-L24C PEPTIDE with an alkylated Cys mutation

Chain B: 




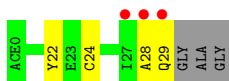
- Molecule 1: 6-HELIX COILED COIL CC-HEX-L24C PEPTIDE with an alkylated Cys mutation

Chain C: 




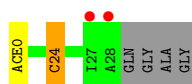
- Molecule 1: 6-HELIX COILED COIL CC-HEX-L24C PEPTIDE with an alkylated Cys mutation

Chain D: 

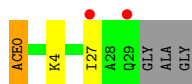
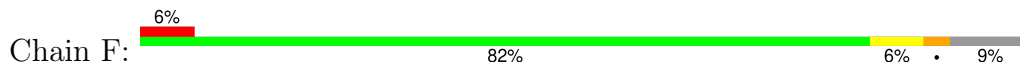


- Molecule 1: 6-HELIX COILED COIL CC-HEX-L24C PEPTIDE with an alkylated Cys mutation

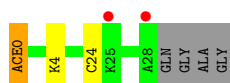
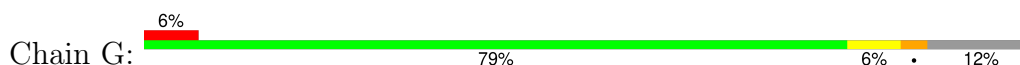
Chain E: 



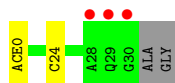
- Molecule 1: 6-HELIX COILED COIL CC-HEX-L24C PEPTIDE with an alkylated Cys mutation



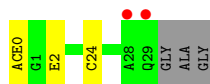
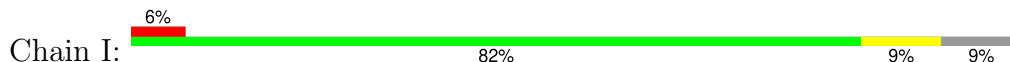
- Molecule 1: 6-HELIX COILED COIL CC-HEX-L24C PEPTIDE with an alkylated Cys mutation



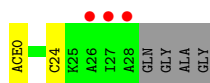
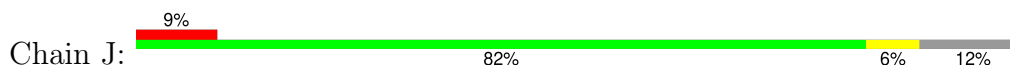
- Molecule 1: 6-HELIX COILED COIL CC-HEX-L24C PEPTIDE with an alkylated Cys mutation



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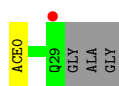


- Molecule 1: 6-HELIX COILED COIL CC-HEX-L24C PEPTIDE with an alkylated Cys mutation

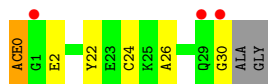
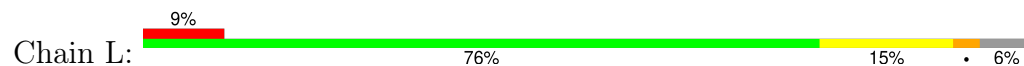


- Molecule 1: 6-HELIX COILED COIL CC-HEX-L24C PEPTIDE with an alkylated Cys mutation





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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.02Å 56.02Å 286.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.34 – 1.90 36.34 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (36.34-1.90) 99.9 (36.34-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 1.89Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.203 , 0.232 0.213 , 0.241	Depositor DCC
$R_{free}$ test set	1872 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.4	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 52.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5393	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.65% 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, 0.333 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: YCM, ACE, 4BF

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	0.51	0/197	2.04	2/258 (0.8%)
1	B	0.61	0/188	1.67	2/246 (0.8%)
1	C	0.61	0/183	1.27	2/239 (0.8%)
1	D	0.67	0/197	0.68	0/258
1	E	0.57	0/188	1.21	2/246 (0.8%)
1	F	0.54	0/197	1.89	2/258 (0.8%)
1	G	0.61	0/188	2.27	2/246 (0.8%)
1	H	0.58	0/201	2.06	2/263 (0.8%)
1	I	0.58	0/197	1.74	2/258 (0.8%)
1	J	0.62	0/188	1.63	2/246 (0.8%)
1	K	0.53	0/197	1.49	2/258 (0.8%)
1	L	0.56	0/201	1.10	2/263 (0.8%)
All	All	0.58	0/2322	1.65	22/3039 (0.7%)

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	0	ACE	O-C-N	-31.44	69.75	123.20
1	H	0	ACE	O-C-N	27.90	170.63	123.20
1	A	0	ACE	O-C-N	26.85	168.84	123.20
1	F	0	ACE	O-C-N	-25.49	79.87	123.20
1	I	0	ACE	O-C-N	22.13	160.82	123.20

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	224	216	243	0	0
1	B	215	217	236	3	0
1	C	210	212	231	3	0
1	D	224	224	244	2	0
1	E	215	216	236	4	0
1	F	224	216	244	2	0
1	G	215	206	236	3	0
1	H	228	228	246	1	0
1	I	224	225	243	2	0
1	J	215	217	236	4	0
1	K	224	225	244	0	0
1	L	228	217	247	5	0
2	A	9	0	0	0	0
2	B	12	0	0	1	0
2	C	16	0	0	0	0
2	D	13	0	0	0	0
2	E	8	0	0	0	0
2	F	11	0	0	0	0
2	G	14	0	0	0	0
2	H	12	0	0	0	0
2	I	7	0	0	0	0
2	J	7	0	0	0	0
2	K	13	0	0	0	0
2	L	6	0	0	0	0
All	All	2774	2619	2886	22	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 4.

The worst 5 of 22 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:J:24:YCM:HD2	1:L:24:YCM:HZ21	1.34	0.92
1:G:0:ACE:H1	1:G:4:LYS:H	1.50	0.77
1:J:24:YCM:HD2	1:L:24:YCM:NZ2	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:YCM:HZ21	1:B:24:YCM:HB2	1.57	0.70
1:C:0:ACE:H1	1:C:4:LYS:H	1.57	0.69

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	26/33 (79%)	26 (100%)	0	0	100	100
1	B	25/33 (76%)	25 (100%)	0	0	100	100
1	C	24/33 (73%)	24 (100%)	0	0	100	100
1	D	26/33 (79%)	26 (100%)	0	0	100	100
1	E	25/33 (76%)	25 (100%)	0	0	100	100
1	F	26/33 (79%)	26 (100%)	0	0	100	100
1	G	25/33 (76%)	25 (100%)	0	0	100	100
1	H	27/33 (82%)	27 (100%)	0	0	100	100
1	I	26/33 (79%)	26 (100%)	0	0	100	100
1	J	25/33 (76%)	25 (100%)	0	0	100	100
1	K	26/33 (79%)	26 (100%)	0	0	100	100
1	L	27/33 (82%)	27 (100%)	0	0	100	100
All	All	308/396 (78%)	308 (100%)	0	0	100	100

There are no Ramachandran outliers to report.

### 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	18/18 (100%)	18 (100%)	0	100	100
1	B	17/18 (94%)	17 (100%)	0	100	100
1	C	17/18 (94%)	17 (100%)	0	100	100
1	D	18/18 (100%)	18 (100%)	0	100	100
1	E	17/18 (94%)	17 (100%)	0	100	100
1	F	18/18 (100%)	18 (100%)	0	100	100
1	G	17/18 (94%)	17 (100%)	0	100	100
1	H	18/18 (100%)	18 (100%)	0	100	100
1	I	18/18 (100%)	18 (100%)	0	100	100
1	J	17/18 (94%)	17 (100%)	0	100	100
1	K	18/18 (100%)	18 (100%)	0	100	100
1	L	18/18 (100%)	18 (100%)	0	100	100
All	All	211/216 (98%)	211 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

24 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
1	YCM	G	24	1	7,9,10	1.04	0	5,10,12	0.67	0
1	4BF	A	22	1	11,12,13	0.91	0	10,15,17	0.83	0
1	4BF	D	22	1	11,12,13	1.14	1 (9%)	10,15,17	0.55	0
1	YCM	D	24	1	7,9,10	1.19	0	5,10,12	0.99	0
1	YCM	C	24	1	7,9,10	1.49	1 (14%)	5,10,12	1.49	2 (40%)
1	YCM	L	24	1	7,9,10	1.09	0	5,10,12	0.62	0
1	4BF	H	22	1	11,12,13	0.87	0	10,15,17	0.54	0
1	YCM	H	24	1	7,9,10	1.23	0	5,10,12	0.39	0
1	4BF	J	22	1	11,12,13	1.04	0	10,15,17	0.63	0
1	4BF	C	22	1	11,12,13	0.82	0	10,15,17	0.93	0
1	4BF	E	22	1	11,12,13	0.92	0	10,15,17	0.76	0
1	4BF	B	22	1	11,12,13	1.38	1 (9%)	10,15,17	0.91	0
1	4BF	F	22	1	11,12,13	0.97	0	10,15,17	0.68	0
1	4BF	I	22	1	11,12,13	1.01	0	10,15,17	0.84	0
1	YCM	J	24	1	7,9,10	1.00	0	5,10,12	0.68	0
1	YCM	I	24	1	7,9,10	1.16	0	5,10,12	0.59	0
1	4BF	K	22	1	11,12,13	1.21	0	10,15,17	0.82	0
1	YCM	A	24	1	7,9,10	0.97	0	5,10,12	0.70	0
1	YCM	K	24	1	7,9,10	1.11	0	5,10,12	0.53	0
1	YCM	E	24	1	7,9,10	1.18	1 (14%)	5,10,12	1.49	1 (20%)
1	YCM	F	24	1	7,9,10	1.10	0	5,10,12	0.42	0
1	4BF	L	22	1	11,12,13	1.06	0	10,15,17	1.26	1 (10%)
1	YCM	B	24	1	7,9,10	1.21	0	5,10,12	1.11	0
1	4BF	G	22	1	11,12,13	1.06	0	10,15,17	0.68	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
1	YCM	G	24	1	-	2/6/8/10	-
1	4BF	A	22	1	-	1/5/6/8	0/1/1/1
1	4BF	D	22	1	-	1/5/6/8	0/1/1/1
1	YCM	D	24	1	-	0/6/8/10	-
1	YCM	C	24	1	-	0/6/8/10	-
1	YCM	L	24	1	-	2/6/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4BF	H	22	1	-	0/5/6/8	0/1/1/1
1	YCM	H	24	1	-	2/6/8/10	-
1	4BF	J	22	1	-	0/5/6/8	0/1/1/1
1	4BF	C	22	1	-	0/5/6/8	0/1/1/1
1	4BF	E	22	1	-	1/5/6/8	0/1/1/1
1	4BF	B	22	1	-	1/5/6/8	0/1/1/1
1	4BF	F	22	1	-	0/5/6/8	0/1/1/1
1	4BF	I	22	1	-	1/5/6/8	0/1/1/1
1	YCM	J	24	1	-	1/6/8/10	-
1	YCM	I	24	1	-	2/6/8/10	-
1	4BF	K	22	1	-	0/5/6/8	0/1/1/1
1	YCM	A	24	1	-	1/6/8/10	-
1	YCM	K	24	1	-	2/6/8/10	-
1	YCM	E	24	1	-	3/6/8/10	-
1	YCM	F	24	1	-	3/6/8/10	-
1	4BF	L	22	1	-	1/5/6/8	0/1/1/1
1	YCM	B	24	1	-	2/6/8/10	-
1	4BF	G	22	1	-	0/5/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	24	YCM	CD-SG	-2.36	1.75	1.81
1	C	24	YCM	CD-SG	-2.31	1.75	1.81
1	D	22	4BF	CD2-CE2	2.13	1.42	1.38
1	B	22	4BF	CD2-CE2	2.00	1.42	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	24	YCM	CB-CA-C	-2.33	104.48	110.80
1	E	24	YCM	CB-CA-C	-2.29	104.57	110.80
1	C	24	YCM	CE-CD-SG	-2.19	106.90	113.81
1	L	22	4BF	CE1-CD1-CG	-2.16	118.17	121.00

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	24	YCM	SG-CD-CE-NZ2

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Mol	Chain	Res	Type	Atoms
1	E	24	YCM	CA-CB-SG-CD
1	F	24	YCM	SG-CD-CE-NZ2
1	G	24	YCM	SG-CD-CE-NZ2
1	I	24	YCM	SG-CD-CE-OZ1

There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	24	YCM	1	0
1	D	24	YCM	1	0
1	C	24	YCM	2	0
1	L	24	YCM	2	0
1	H	24	YCM	1	0
1	J	24	YCM	4	0
1	I	24	YCM	1	0
1	E	24	YCM	4	0
1	B	24	YCM	3	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	27/33 (81%)	-0.07	1 (3%) 45 47	17, 27, 43, 45	6 (22%)
1	B	26/33 (78%)	-0.19	0 100 100	11, 27, 45, 47	5 (19%)
1	C	25/33 (75%)	0.03	2 (8%) 20 21	21, 26, 48, 65	1 (4%)
1	D	27/33 (81%)	0.06	3 (11%) 12 12	15, 26, 47, 80	3 (11%)
1	E	26/33 (78%)	0.10	2 (7%) 21 22	19, 24, 52, 65	4 (15%)
1	F	27/33 (81%)	-0.10	2 (7%) 22 23	10, 27, 46, 64	1 (3%)
1	G	26/33 (78%)	-0.10	2 (7%) 21 22	20, 26, 47, 51	4 (15%)
1	H	28/33 (84%)	0.24	3 (10%) 12 13	21, 30, 48, 75	2 (7%)
1	I	27/33 (81%)	0.11	2 (7%) 22 23	21, 28, 41, 47	4 (14%)
1	J	26/33 (78%)	0.21	3 (11%) 11 11	18, 27, 52, 62	4 (15%)
1	K	27/33 (81%)	-0.20	1 (3%) 45 47	13, 27, 45, 46	5 (18%)
1	L	28/33 (84%)	0.13	3 (10%) 12 13	16, 27, 47, 67	5 (17%)
All	All	320/396 (80%)	0.02	24 (7%) 22 23	10, 27, 50, 80	44 (13%)

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	29	GLN	5.6
1	H	30	GLY	5.2
1	E	28	ALA	5.0
1	L	30	GLY	4.8
1	D	29	GLN	4.5

### 6.2 Non-standard residues in protein, DNA, RNA chains

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
1	YCM	C	24	10/11	0.79	0.23	27,41,83,85	0
1	YCM	B	24	10/11	0.86	0.16	27,33,43,45	0
1	YCM	G	24	10/11	0.87	0.18	26,39,72,86	0
1	YCM	J	24	10/11	0.90	0.19	32,36,82,88	0
1	YCM	E	24	10/11	0.91	0.16	32,43,60,77	0
1	YCM	I	24	10/11	0.93	0.15	23,29,64,67	0
1	4BF	C	22	12/13	0.94	0.12	26,39,48,69	0
1	4BF	B	22	12/13	0.94	0.12	23,29,43,57	1
1	YCM	H	24	10/11	0.95	0.14	26,31,60,80	0
1	4BF	I	22	12/13	0.95	0.11	21,28,45,45	1
1	4BF	G	22	12/13	0.95	0.09	21,27,33,34	1
1	4BF	D	22	12/13	0.95	0.11	19,27,49,50	1
1	4BF	K	22	12/13	0.95	0.09	24,30,37,40	1
1	YCM	K	24	10/11	0.95	0.14	24,29,69,82	0
1	4BF	L	22	12/13	0.95	0.08	18,24,30,43	1
1	YCM	F	24	10/11	0.96	0.11	23,27,55,72	0
1	YCM	D	24	10/11	0.96	0.10	24,30,55,55	0
1	YCM	A	24	10/11	0.96	0.12	25,30,50,64	0
1	4BF	J	22	12/13	0.96	0.09	28,33,38,42	1
1	YCM	L	24	10/11	0.96	0.10	20,25,47,63	0
1	4BF	A	22	12/13	0.97	0.10	28,45,51,66	0
1	4BF	F	22	12/13	0.97	0.08	18,23,32,34	1
1	4BF	H	22	12/13	0.97	0.11	25,29,37,37	1
1	4BF	E	22	12/13	0.97	0.12	24,33,43,53	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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.