



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 09:01 am BST

PDB ID : 3C3F
Title : alpha/beta-Peptide helix bundles: The GCN4-pLI side chain sequence on an (alpha-alpha-alpha-beta) backbone
Authors : Horne, W.S.; Price, J.L.; Gellman, S.H.
Deposited on : 2008-01-28
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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 : 2.11
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) : 2.11

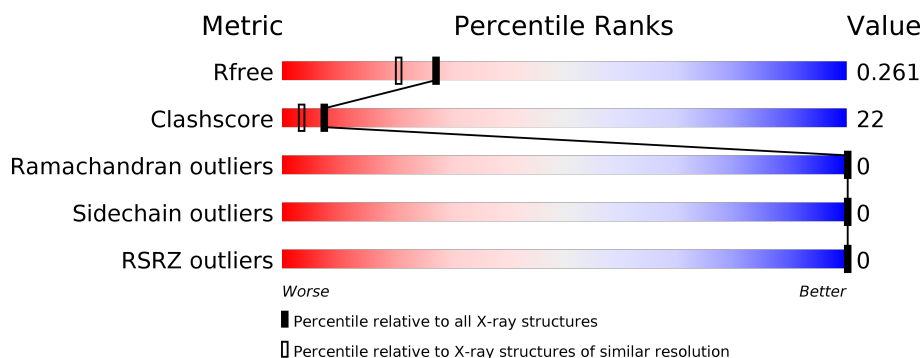
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	34	<div> <div style="width: 65%; background-color: green;"></div> <div style="width: 29%; background-color: yellow;"></div> <div style="width: 6%; background-color: orange;"></div> <div style="width: 0%; background-color: red;"></div> <div style="width: 0%; background-color: grey;"></div> </div> <div>65% 29% . .</div>
1	B	34	<div> <div style="width: 74%; background-color: green;"></div> <div style="width: 21%; background-color: yellow;"></div> <div style="width: 5%; background-color: orange;"></div> <div style="width: 0%; background-color: red;"></div> <div style="width: 0%; background-color: grey;"></div> </div> <div>74% 21% . .</div>
1	C	34	<div> <div style="width: 68%; background-color: green;"></div> <div style="width: 26%; background-color: yellow;"></div> <div style="width: 6%; background-color: orange;"></div> <div style="width: 0%; background-color: red;"></div> <div style="width: 0%; background-color: grey;"></div> </div> <div>68% 26% . .</div>
1	D	34	<div> <div style="width: 62%; background-color: green;"></div> <div style="width: 29%; background-color: yellow;"></div> <div style="width: 6%; background-color: orange;"></div> <div style="width: 0%; background-color: red;"></div> <div style="width: 0%; background-color: grey;"></div> </div> <div>62% 29% 6% .</div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2545 atoms, of which 1274 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 alpha/beta peptide with the GCN4-pLI side chain sequence on an (alpha-alpha-alpha-beta) backbone.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	33	Total	C	H	N	O	S	97	2	1
			595	183	316	45	49	2			
1	B	33	Total	C	H	N	O	S	99	2	1
			586	182	309	44	49	2			
1	C	33	Total	C	H	N	O	S	95	1	1
			580	179	307	45	47	2			
1	D	33	Total	C	H	N	O	S	103	4	1
			633	193	342	48	48	2			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	42	Total	O	0	0
			42	42		
2	B	34	Total	O	0	0
			34	34		
2	C	36	Total	O	0	0
			36	36		
2	D	39	Total	O	0	0
			39	39		

i

- Molecule 1: alpha/beta peptide with the GCN4-pLI side chain sequence on an (alpha-alpha-alpha-beta) backbone



Token	Count (approx.)
?0	10
R1	8
M2	2
E6	7
E10	7
S14	7
H18	7
E22	7
I26	7
L30	7
?31	10
E32	7
ARG	1

70	R1	M2		I5	E6		E10		S14		H18		E22	X23		I26		L30	731	E32	ARG
----	----	----	--	----	----	--	-----	--	-----	--	-----	--	-----	-----	--	-----	--	-----	-----	-----	-----

[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	35.24Å 35.23Å 47.31Å 90.00° 90.87° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00 24.91 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.2 (25.00-2.00) 95.0 (24.91-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.185 , 0.265 0.191 , 0.261	Depositor DCC
R_{free} test set	362 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	17.0	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.389 for k,h,-l 0.398 for -k,-h,-l 0.367 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2545	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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: BIL, ACE, B3L, B3K, B3D, B3E, BAL

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	0/202	0.64	0/253
1	B	0.55	0/204	0.70	0/258
1	C	0.60	0/197	0.76	0/248
1	D	0.51	0/211	0.69	0/264
All	All	0.54	0/814	0.70	0/1023

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	10
1	B	0	9
1	C	0	9
1	D	0	10
All	All	0	38

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (38) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	GLU	Peptide
1	A	14[A]	SER	Peptide
1	A	14[B]	SER	Peptide
1	A	18	HIS	Peptide
1	A	2[A]	MET	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	2[B]	MET	Peptide
1	A	22	GLU	Peptide
1	A	26	ILE	Peptide
1	A	30	LEU	Peptide
1	A	6	GLU	Peptide
1	B	10	GLU	Peptide
1	B	14	SER	Peptide
1	B	18	HIS	Peptide
1	B	2[A]	MET	Peptide
1	B	2[B]	MET	Peptide
1	B	22	GLU	Peptide
1	B	26	ILE	Peptide
1	B	30	LEU	Peptide
1	B	6	GLU	Peptide
1	C	10	GLU	Peptide
1	C	14	SER	Peptide
1	C	18	HIS	Peptide
1	C	2[A]	MET	Peptide
1	C	2[B]	MET	Peptide
1	C	22	GLU	Peptide
1	C	26	ILE	Peptide
1	C	30	LEU	Peptide
1	C	6	GLU	Peptide
1	D	10	GLU	Peptide
1	D	14[A]	SER	Peptide
1	D	14[B]	SER	Peptide
1	D	18	HIS	Peptide
1	D	2[A]	MET	Peptide
1	D	2[B]	MET	Peptide
1	D	22	GLU	Peptide
1	D	26	ILE	Peptide
1	D	30	LEU	Peptide
1	D	6	GLU	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	279	316	304	21	0
1	B	277	309	295	30	0
1	C	273	307	292	28	0
1	D	291	342	332	20	0
2	A	42	0	0	0	1
2	B	34	0	0	0	0
2	C	36	0	0	0	0
2	D	39	0	0	0	0
All	All	1271	1274	1223	52	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 22.

All (52) 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:B:2[B]:MET:CE	1:C:2[B]:MET:HE3	1.31	1.53
1:C:2[A]:MET:CE	1:D:2[A]:MET:HE3	1.51	1.41
1:A:2[B]:MET:HE3	1:D:2[B]:MET:SD	1.76	1.26
1:B:2[B]:MET:CE	1:C:2[B]:MET:CE	2.15	1.23
1:A:2[B]:MET:HE1	1:B:2[B]:MET:HE3	1.21	1.16
1:A:2[A]:MET:HE2	1:D:2[A]:MET:CE	1.75	1.16
1:C:2[A]:MET:HE1	1:D:2[A]:MET:CE	1.77	1.12
1:B:2[B]:MET:SD	1:C:2[B]:MET:CE	2.38	1.11
1:A:2[A]:MET:CE	1:D:2[A]:MET:HE2	1.81	1.10
1:B:2[B]:MET:SD	1:C:2[B]:MET:HE3	1.95	1.04
1:A:2[B]:MET:CE	1:B:2[B]:MET:HE3	1.89	1.02
1:B:2[A]:MET:HE2	1:C:2[A]:MET:HE2	1.39	1.02
1:A:2[A]:MET:HE1	1:B:2[A]:MET:CE	1.90	1.01
1:A:2[A]:MET:HE1	1:B:2[A]:MET:HE3	1.43	0.98
1:B:2[B]:MET:HE3	1:C:2[B]:MET:HE3	0.98	0.98
1:C:2[A]:MET:CE	1:D:2[A]:MET:CE	2.34	0.97
1:A:2[B]:MET:CE	1:D:2[B]:MET:SD	2.55	0.94
1:A:2[B]:MET:HE1	1:B:2[B]:MET:CE	1.98	0.92
1:B:2[B]:MET:SD	1:C:2[B]:MET:HE2	2.08	0.91
1:A:2[B]:MET:SD	1:B:2[B]:MET:CE	2.65	0.84
1:A:15:B3K:NZ	1:D:20:GLU:OE1	2.11	0.83
1:B:2[B]:MET:HE3	1:C:2[B]:MET:CE	1.91	0.81
1:A:2[A]:MET:HE2	1:D:2[A]:MET:HE2	0.88	0.80
1:B:2[B]:MET:HE1	1:C:2[B]:MET:CE	2.11	0.79
1:C:2[A]:MET:HE1	1:D:2[A]:MET:HE3	0.83	0.79
1:A:2[A]:MET:CE	1:B:2[A]:MET:HE3	2.12	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2[A]:MET:CE	1:C:2[A]:MET:HE2	2.14	0.77
1:A:2[B]:MET:SD	1:B:2[B]:MET:HE2	2.25	0.77
1:B:2[A]:MET:HE2	1:C:2[A]:MET:CE	2.15	0.76
1:B:2[A]:MET:CE	1:C:2[A]:MET:CE	2.65	0.75
1:A:2[A]:MET:CE	1:D:2[A]:MET:CE	2.54	0.73
1:A:2[A]:MET:CE	1:B:2[A]:MET:CE	2.64	0.73
1:A:2[B]:MET:SD	1:B:2[B]:MET:HE3	2.29	0.69
1:B:2[B]:MET:HE1	1:C:5:ILE:HD13	1.77	0.66
1:C:2[A]:MET:HE2	1:D:2[A]:MET:CE	2.25	0.65
1:A:2[A]:MET:HE1	1:B:2[A]:MET:HE2	1.79	0.64
1:A:2[B]:MET:CE	1:B:2[B]:MET:CE	2.63	0.62
1:B:2[B]:MET:HE1	1:C:5:ILE:CD1	2.34	0.57
1:B:2[A]:MET:HE1	1:C:2[A]:MET:HE3	1.89	0.55
1:B:2[A]:MET:CE	1:C:2[A]:MET:HE3	2.37	0.54
1:D:2[B]:MET:CE	1:D:5:ILE:HD12	2.38	0.53
1:A:2[A]:MET:CE	1:B:2[A]:MET:HE2	2.35	0.53
1:C:2[B]:MET:HE1	1:D:5:ILE:HD13	1.93	0.51
1:B:2[A]:MET:HE1	1:C:2[A]:MET:CE	2.39	0.50
1:A:16:LEU:HA	1:A:19:BIL:H2E1	1.96	0.47
1:C:2[B]:MET:HE2	1:C:2[B]:MET:HA	1.96	0.47
1:C:23:B3L:H1E1	1:D:26:ILE:CD1	2.46	0.46
1:C:2[A]:MET:HE2	1:D:2[A]:MET:HE2	1.98	0.44
1:C:23:B3L:H1E2	1:D:19:BIL:H2D2	2.00	0.42
1:D:28[B]:LYS:CB	1:D:28[B]:LYS:NZ	2.82	0.42
1:C:2[B]:MET:HE1	1:D:5:ILE:CD1	2.48	0.42
1:D:19:BIL:HA	1:D:19:BIL:H1D2	1.91	0.42

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)
2:A:57:HOH:O	2:A:73:HOH:O[1_554]	1.93	0.27

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	25/34 (74%)	25 (100%)	0	0	100	100
1	B	25/34 (74%)	25 (100%)	0	0	100	100
1	C	24/34 (71%)	24 (100%)	0	0	100	100
1	D	26/34 (76%)	26 (100%)	0	0	100	100
All	All	100/136 (74%)	100 (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	23/24 (96%)	23 (100%)	0	100	100
1	B	23/24 (96%)	23 (100%)	0	100	100
1	C	22/24 (92%)	22 (100%)	0	100	100
1	D	24/24 (100%)	24 (100%)	0	100	100
All	All	92/96 (96%)	92 (100%)	0	100	100

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

Some 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 ⓘ

33 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	B3K	B	27	1	9,9,10	0.47	0	8,9,11	1.18	1 (12%)
1	B3K	D	3	1	9,9,10	0.51	0	8,9,11	0.97	0
1	B3K	D	15[A]	-	9,9,10	0.38	0	8,9,11	0.69	0
1	BAL	D	31	1	4,4,5	0.43	0	3,3,5	0.83	0
1	B3K	C	27	1	9,9,10	0.31	0	8,9,11	1.71	2 (25%)
1	B3K	D	15[B]	-	9,9,10	0.46	0	8,9,11	0.60	0
1	B3K	A	3	1	9,9,10	0.72	0	8,9,11	0.90	0
1	B3D	C	7	1	5,8,9	0.45	0	4,9,11	1.52	1 (25%)
1	B3D	B	7	1	5,8,9	0.51	0	4,9,11	1.54	1 (25%)
1	B3D	A	7	1	5,8,9	0.72	0	4,9,11	1.51	1 (25%)
1	B3K	A	27	1	9,9,10	0.37	0	8,9,11	1.59	1 (12%)
1	B3E	D	11	1	6,9,10	1.09	1 (16%)	6,10,12	1.05	0
1	B3D	D	7	1	5,8,9	0.57	0	4,9,11	1.44	1 (25%)
1	BAL	B	31	1	4,4,5	0.62	0	3,3,5	0.97	0
1	B3E	C	11	1	6,9,10	0.79	0	6,10,12	1.35	1 (16%)
1	BIL	A	19	1	7,8,9	0.36	0	5,9,11	1.15	0
1	BIL	D	19	1	7,8,9	0.59	0	5,9,11	1.31	1 (20%)
1	B3K	C	15	1	6,6,10	0.52	0	4,6,11	0.99	0
1	B3K	A	15	1	9,9,10	0.54	0	8,9,11	1.04	0
1	B3K	C	3	1	9,9,10	0.72	0	8,9,11	0.88	0
1	B3E	A	11	1	6,9,10	1.05	1 (16%)	6,10,12	1.02	0
1	B3K	B	3	1	9,9,10	0.60	0	8,9,11	0.79	0
1	B3K	B	15	1	6,6,10	0.68	0	4,6,11	1.35	0
1	BIL	C	19	1	7,8,9	0.55	0	5,9,11	1.06	0
1	BIL	B	19	1	7,8,9	0.45	0	5,9,11	0.93	0
1	BAL	A	31	1	4,4,5	0.51	0	3,3,5	0.77	0
1	BAL	C	31	1	4,4,5	0.40	0	3,3,5	1.23	0
1	B3E	B	11	1	6,9,10	0.90	0	6,10,12	1.71	1 (16%)
1	B3K	D	27	1	9,9,10	0.35	0	8,9,11	1.90	2 (25%)
1	B3L	D	23	1	8,8,9	0.34	0	7,9,11	0.99	0
1	B3L	B	23	1	8,8,9	0.51	0	7,9,11	0.93	0
1	B3L	C	23	1	8,8,9	0.42	0	7,9,11	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	B3L	A	23	1	8,8,9	0.31	0	7,9,11	0.88	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	B3K	B	27	1	-	3/8/8/9	-
1	B3K	D	3	1	-	1/8/8/9	-
1	B3K	D	15[A]	-	-	6/8/8/9	-
1	BAL	D	31	1	-	0/1/2/3	-
1	B3K	C	27	1	-	2/8/8/9	-
1	B3K	D	15[B]	-	-	4/8/8/9	-
1	B3K	A	3	1	-	2/8/8/9	-
1	B3D	C	7	1	-	1/5/7/8	-
1	B3D	B	7	1	-	2/5/7/8	-
1	B3D	A	7	1	-	1/5/7/8	-
1	B3K	A	27	1	-	4/8/8/9	-
1	B3E	D	11	1	-	3/6/8/9	-
1	B3D	D	7	1	-	2/5/7/8	-
1	BAL	B	31	1	-	0/1/2/3	-
1	B3E	C	11	1	-	3/6/8/9	-
1	BIL	A	19	1	-	4/9/9/10	-
1	BIL	D	19	1	-	1/9/9/10	-
1	B3K	C	15	1	-	2/5/5/9	-
1	B3K	A	15	1	-	5/8/8/9	-
1	B3K	C	3	1	-	2/8/8/9	-
1	B3E	A	11	1	-	2/6/8/9	-
1	B3K	B	3	1	-	2/8/8/9	-
1	B3K	B	15	1	-	1/5/5/9	-
1	BIL	C	19	1	-	1/9/9/10	-
1	BIL	B	19	1	-	3/9/9/10	-
1	BAL	A	31	1	-	0/1/2/3	-
1	BAL	C	31	1	-	0/1/2/3	-
1	B3E	B	11	1	-	2/6/8/9	-
1	B3K	D	27	1	-	4/8/8/9	-
1	B3L	D	23	1	-	1/7/7/8	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	B3L	B	23	1	-	1/7/7/8	-
1	B3L	C	23	1	-	1/7/7/8	-
1	B3L	A	23	1	-	1/7/7/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	11	B3E	CA-CB	-2.51	1.50	1.53
1	A	11	B3E	CA-CB	-2.47	1.50	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	B3K	CB-CA-C	4.08	118.26	112.25
1	D	27	B3K	CB-CA-C	4.06	118.23	112.25
1	C	27	B3K	CB-CA-C	3.78	117.81	112.25
1	B	11	B3E	CD-CG-CB	-3.41	105.58	112.74
1	C	11	B3E	CD-CG-CB	-2.69	107.08	112.74
1	C	7	B3D	CA-CB-CG	-2.55	107.12	110.81
1	B	7	B3D	CA-CB-CG	-2.49	107.21	110.81
1	D	27	B3K	CG-CB-CA	-2.31	102.96	111.63
1	B	27	B3K	CG-CB-CA	-2.25	103.16	111.63
1	A	7	B3D	CB-CA-C	2.21	115.50	112.25
1	C	27	B3K	CG-CB-CA	-2.16	103.52	111.63
1	D	7	B3D	CD-CG-CB	-2.10	110.74	112.95
1	D	19	BIL	O-C-CA	-2.05	119.46	125.43

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	15[A]	B3K	N-CB-CG-CD
1	D	15[A]	B3K	CA-CB-CG-CD
1	A	27	B3K	N-CB-CG-CD
1	A	27	B3K	CA-CB-CG-CD
1	A	19	BIL	CA-CB-CG-CD1
1	A	15	B3K	N-CB-CG-CD
1	A	15	B3K	CA-CB-CG-CD
1	D	23	B3L	C-CA-CB-CG
1	A	15	B3K	CD-CE-CF-NZ
1	A	27	B3K	CG-CD-CE-CF

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	C	11	B3E	CE-CD-CG-CB
1	D	15[A]	B3K	CG-CD-CE-CF
1	B	27	B3K	CE-CD-CG-CB
1	A	19	BIL	N-CB-CG-CD1
1	B	19	BIL	CE1-CD1-CG-CB
1	D	11	B3E	CE-CD-CG-CB
1	A	15	B3K	CG-CD-CE-CF
1	C	27	B3K	CG-CD-CE-CF
1	D	15[B]	B3K	CD-CE-CF-NZ
1	A	19	BIL	N-CB-CG-CD2
1	D	15[A]	B3K	O-C-CA-CB
1	D	15[B]	B3K	O-C-CA-CB
1	C	7	B3D	O-C-CA-CB
1	B	7	B3D	O-C-CA-CB
1	A	27	B3K	O-C-CA-CB
1	C	11	B3E	O-C-CA-CB
1	A	19	BIL	O-C-CA-CB
1	D	19	BIL	O-C-CA-CB
1	C	15	B3K	O-C-CA-CB
1	C	3	B3K	O-C-CA-CB
1	C	19	BIL	O-C-CA-CB
1	B	19	BIL	O-C-CA-CB
1	D	27	B3K	O-C-CA-CB
1	B	23	B3L	O-C-CA-CB
1	C	23	B3L	O-C-CA-CB
1	A	23	B3L	O-C-CA-CB
1	D	3	B3K	C-CA-CB-N
1	D	15[A]	B3K	C-CA-CB-N
1	D	15[B]	B3K	C-CA-CB-N
1	A	3	B3K	C-CA-CB-N
1	B	7	B3D	C-CA-CB-N
1	A	7	B3D	C-CA-CB-N
1	D	11	B3E	C-CA-CB-N
1	D	7	B3D	C-CA-CB-N
1	C	11	B3E	C-CA-CB-N
1	C	15	B3K	C-CA-CB-N
1	C	3	B3K	C-CA-CB-N
1	A	11	B3E	C-CA-CB-N
1	B	3	B3K	C-CA-CB-N
1	B	15	B3K	C-CA-CB-N
1	B	11	B3E	C-CA-CB-N
1	D	27	B3K	C-CA-CB-N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	B	27	B3K	CD-CE-CF-NZ
1	D	27	B3K	CG-CD-CE-CF
1	D	15[B]	B3K	CG-CD-CE-CF
1	B	27	B3K	O-C-CA-CB
1	C	27	B3K	O-C-CA-CB
1	A	3	B3K	O-C-CA-CB
1	D	11	B3E	O-C-CA-CB
1	D	7	B3D	O-C-CA-CB
1	A	15	B3K	O-C-CA-CB
1	A	11	B3E	O-C-CA-CB
1	B	3	B3K	O-C-CA-CB
1	B	11	B3E	O-C-CA-CB
1	D	27	B3K	C-CA-CB-CG
1	B	19	BIL	CE1-CD1-CG-CD2
1	D	15[A]	B3K	CD-CE-CF-NZ

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	19	BIL	1	0
1	D	19	BIL	2	0
1	A	15	B3K	1	0
1	C	23	B3L	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates 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

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	24/34 (70%)	-0.30	0 100 100	8, 16, 22, 25	0
1	B	24/34 (70%)	-0.31	0 100 100	11, 17, 22, 23	0
1	C	24/34 (70%)	-0.19	0 100 100	8, 17, 23, 24	0
1	D	24/34 (70%)	-0.19	0 100 100	8, 16, 22, 23	0
All	All	96/136 (70%)	-0.25	0 100 100	8, 17, 23, 25	0

There are no RSRZ outliers to report.

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	B3K	A	27	10/11	0.84	0.20	18,20,24,24	3
1	BAL	D	31	5/6	0.86	0.13	17,19,21,23	0
1	B3L	D	23	9/10	0.88	0.14	19,21,24,24	6
1	B3E	C	11	10/11	0.89	0.13	10,11,25,25	0
1	B3K	A	15	10/11	0.89	0.17	11,15,25,25	3
1	BAL	C	31	5/6	0.89	0.11	19,20,22,22	0
1	B3K	D	27	10/11	0.89	0.15	18,20,24,25	3
1	B3K	C	27	10/11	0.89	0.16	20,21,30,30	3
1	B3E	A	11	10/11	0.90	0.12	10,11,26,27	0
1	B3E	B	11	10/11	0.90	0.12	12,13,26,27	0
1	B3L	C	23	9/10	0.90	0.14	19,21,22,22	6
1	B3E	D	11	10/11	0.91	0.13	9,11,27,27	0
1	BIL	C	19	9/10	0.92	0.12	16,17,19,19	6
1	BIL	D	19	9/10	0.92	0.14	17,20,22,22	6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	BAL	B	31	5/6	0.93	0.17	19,20,22,22	0
1	B3K	B	27	10/11	0.93	0.13	19,22,31,31	3
1	B3K	B	15	7/11	0.93	0.13	13,13,18,18	2
1	B3D	C	7	9/10	0.93	0.12	11,11,18,18	0
1	BAL	A	31	5/6	0.93	0.15	18,19,20,21	0
1	B3K	D	15[A]	10/11	0.94	0.15	12,13,14,14	18
1	B3D	A	7	9/10	0.94	0.10	8,9,19,19	0
1	BIL	A	19	9/10	0.94	0.15	16,18,21,21	6
1	B3K	D	15[B]	10/11	0.94	0.15	12,13,15,15	18
1	B3K	A	3	10/11	0.94	0.10	10,12,14,15	3
1	B3K	C	3	10/11	0.94	0.10	13,16,17,17	3
1	B3D	D	7	9/10	0.94	0.11	9,9,17,18	0
1	B3L	B	23	9/10	0.94	0.14	17,18,21,21	6
1	B3K	B	3	10/11	0.94	0.11	14,15,18,19	3
1	BIL	B	19	9/10	0.95	0.11	16,17,18,18	6
1	B3K	D	3	10/11	0.95	0.11	10,14,17,17	3
1	B3D	B	7	9/10	0.95	0.11	11,11,17,19	0
1	B3K	C	15	7/11	0.95	0.12	13,13,18,18	2
1	B3L	A	23	9/10	0.95	0.12	16,18,20,21	6

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.