



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 08:07 am BST

PDB ID : 3F87
Title : An alpha/beta-Peptide Helix Bundle with a Pure beta-Amino Acid Core and a Distinctive Quarternary Structure: GCN4pLI derivative with beta residues at a and d heptad positions - higher symmetry crystal
Authors : Giuliano, M.W.; Horne, W.S.; Gellman, S.H.
Deposited on : 2008-11-11
Resolution : 2.40 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

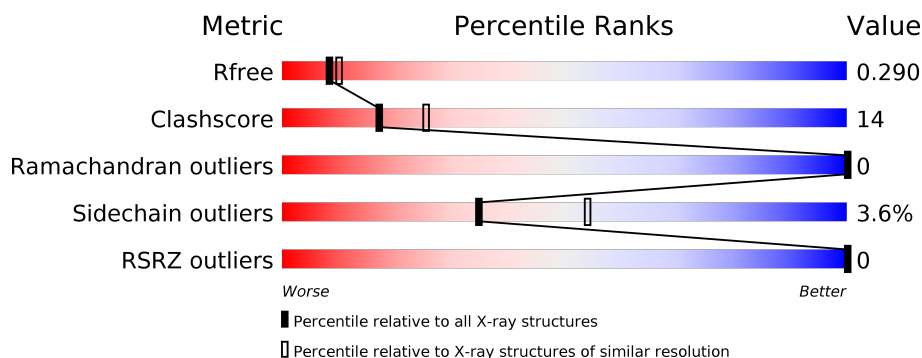
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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>44%</div> <div>47%</div> <div>9%</div> </div>
1	B	34	<div> <div>53%</div> <div>47%</div> </div>
1	C	34	<div> <div>56%</div> <div>35%</div> <div>9%</div> </div>
1	D	34	<div> <div>65%</div> <div>35%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IOD	A	34	-	-	X	-
2	IOD	A	35	-	-	X	-
2	IOD	A	36	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2643 atoms, of which 1345 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 GCN4pLI-betaAD.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	34	Total	C	H	N	O	S	97	2	0
			658	201	349	54	53	1			
1	B	34	Total	C	H	N	O	S	92	0	0
			626	191	330	51	53	1			
1	C	34	Total	C	H	N	O	S	93	2	0
			653	203	343	51	55	1			
1	D	34	Total	C	H	N	O	S	91	1	0
			618	191	323	48	55	1			

- Molecule 2 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	I	0	0
			2	2		
2	A	5	Total	I	0	0
			5	5		
2	C	2	Total	I	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total	O	0	0
			21	21		
3	B	23	Total	O	0	0
			23	23		
3	C	19	Total	O	0	0
			19	19		
3	D	16	Total	O	0	0
			16	16		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: GCN4pLI-betaAD

Chain A: 



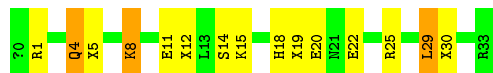
- Molecule 1: GCN4pLI-betaAD

Chain B: 



- Molecule 1: GCN4pLI-betaAD

Chain C: 



- Molecule 1: GCN4pLI-betaAD

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	71.31Å 71.31Å 97.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.40 – 2.40 44.78 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.40-2.40) 99.0 (44.78-2.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.4.0062	Depositor
R, R_{free}	0.230 , 0.296 0.230 , 0.290	Depositor DCC
R_{free} test set	490 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	21.0	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2643	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.52% 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, HMR, B3L, B3M, IOD

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	0.75	0/211	0.75	0/259
1	B	0.73	0/192	0.83	0/236
1	C	0.65	0/214	0.82	0/266
1	D	0.73	0/195	0.75	0/241
All	All	0.71	0/812	0.79	0/1002

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	9
All	All	0	37

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (37) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	ARG	Peptide
1	A	11	GLU	Peptide
1	A	15	LYS	Peptide
1	A	18[A]	HIS	Peptide
1	A	18[B]	HIS	Peptide

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Mol	Chain	Res	Type	Group
1	A	22	GLU	Peptide
1	A	25	ARG	Peptide
1	A	29	LEU	Peptide
1	A	4	GLN	Peptide
1	A	8	LYS	Peptide
1	B	1	ARG	Peptide
1	B	11	GLU	Peptide
1	B	15	LYS	Peptide
1	B	18	HIS	Peptide
1	B	22	GLU	Peptide
1	B	25	ARG	Peptide
1	B	29	LEU	Peptide
1	B	4	GLN	Peptide
1	B	8	LYS	Peptide
1	C	1	ARG	Peptide
1	C	11	GLU	Peptide
1	C	15	LYS	Peptide
1	C	18	HIS	Peptide
1	C	22	GLU	Peptide
1	C	25	ARG	Peptide
1	C	29	LEU	Peptide
1	C	4	GLN	Peptide
1	C	8	LYS	Peptide
1	D	1	ARG	Peptide
1	D	11	GLU	Peptide
1	D	15	LYS	Peptide
1	D	18	HIS	Peptide
1	D	22	GLU	Peptide
1	D	25	ARG	Peptide
1	D	29	LEU	Peptide
1	D	4	GLN	Peptide
1	D	8	LYS	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	309	349	337	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	296	330	317	10	0
1	C	310	343	332	11	0
1	D	295	323	309	3	0
2	A	5	0	0	6	0
2	B	2	0	0	1	0
2	C	2	0	0	1	0
3	A	21	0	0	0	0
3	B	23	0	0	1	0
3	C	19	0	0	0	0
3	D	16	0	0	1	0
All	All	1298	1345	1295	35	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 14.

All (35) 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:C:29:LEU:HD22	1:C:30:B3L:H2E1	1.32	1.04
1:C:29:LEU:HD22	1:C:30:B3L:CE1	1.93	0.96
1:D:10[B]:GLU:OE2	3:D:42:HOH:O	1.97	0.82
1:B:10:GLU:HG3	3:B:67:HOH:O	1.89	0.71
1:A:30:B3L:H1E2	1:B:2:B3M:CF	2.20	0.71
1:C:29:LEU:CD2	1:C:30:B3L:CE1	2.70	0.68
1:A:5:BIL:H3E1	2:A:34:IOD:I	2.64	0.67
1:C:29:LEU:CD2	1:C:30:B3L:H2E1	2.18	0.66
1:A:25:ARG:NH2	1:A:26:BIL:H3E1	2.14	0.62
2:A:35:IOD:I	2:A:36:IOD:I	3.59	0.61
1:A:19:BIL:H1D2	1:B:16:B3L:H2E2	1.84	0.60
1:B:33:HMR:HG3	2:B:35:IOD:I	2.72	0.59
1:A:27:LYS:HD2	1:B:10:GLU:HG2	1.84	0.59
1:A:30:B3L:HG	1:B:2:B3M:HF	1.85	0.58
1:C:20:GLU:OE2	1:D:20:GLU:OE1	2.22	0.58
1:A:18[A]:HIS:HD2	2:A:36:IOD:I	2.61	0.53
1:A:30:B3L:H1E2	1:B:2:B3M:HFB	1.93	0.51
1:B:21:ASN:O	1:B:24:ALA:HB3	2.15	0.47
1:A:17:TYR:CE2	1:A:21:ASN:ND2	2.83	0.46
2:C:34:IOD:I	2:C:35:IOD:I	3.73	0.46
1:A:20:GLU:OE1	1:B:20:GLU:OE2	2.34	0.45
1:A:18[A]:HIS:CD2	2:A:36:IOD:I	3.40	0.45
1:A:5:BIL:CE1	2:A:34:IOD:I	3.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:BIL:H1D2	1:C:12:BIL:HA	1.90	0.45
1:A:2:B3M:HFA	1:A:2:B3M:CB	2.48	0.44
1:A:2:B3M:O	1:A:5:BIL:HAA	2.18	0.43
1:A:15:LYS:HD3	2:A:35:IOD:I	2.88	0.43
1:D:19:BIL:HA	1:D:19:BIL:H1D2	1.82	0.42
1:A:30:B3L:H1E2	1:B:2:B3M:HFA	1.97	0.42
1:C:19:BIL:HA	1:C:19:BIL:H1D2	1.90	0.42
1:C:29:LEU:C	1:C:29:LEU:HD23	2.40	0.41
1:C:4:GLN:C	1:C:5:BIL:H2E1	2.41	0.41
1:C:4:GLN:O	1:C:5:BIL:H2E1	2.19	0.41
1:A:19:BIL:H3D2	1:A:19:BIL:H2E1	1.78	0.40
1:C:12:BIL:H2E1	1:C:12:BIL:H3D2	1.80	0.40

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	25/34 (74%)	24 (96%)	1 (4%)	0	100	100
1	B	23/34 (68%)	23 (100%)	0	0	100	100
1	C	25/34 (74%)	25 (100%)	0	0	100	100
1	D	24/34 (71%)	24 (100%)	0	0	100	100
All	All	97/136 (71%)	96 (99%)	1 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	23/21 (110%)	22 (96%)	1 (4%)	29	46
1	B	21/21 (100%)	21 (100%)	0	100	100
1	C	23/21 (110%)	21 (91%)	2 (9%)	10	15
1	D	21/21 (100%)	21 (100%)	0	100	100
All	All	88/84 (105%)	85 (97%)	3 (3%)	35	56

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	C	8	LYS
1	C	14	SER

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 ⓘ

40 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	B3L	B	16	1	8,8,9	0.58	0	7,9,11	0.89	0
1	B3L	D	30	1	8,8,9	0.61	0	7,9,11	1.14	1 (14%)
1	B3L	B	23	1	8,8,9	0.72	0	7,9,11	1.79	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	BIL	C	12	1	7,8,9	0.89	1 (14%)	5,9,11	1.97	1 (20%)
1	B3M	C	2	1	8,8,9	0.62	0	6,8,10	1.92	1 (16%)
1	B3M	A	2	1	8,8,9	0.69	0	6,8,10	0.99	0
1	B3L	A	30	1	8,8,9	0.49	0	7,9,11	1.34	2 (28%)
1	BIL	B	19	1	7,8,9	0.64	0	5,9,11	1.51	1 (20%)
1	HMR	B	33	1	9,12,12	0.30	0	9,14,14	1.60	3 (33%)
1	B3L	B	30	1	8,8,9	0.44	0	7,9,11	1.10	0
1	HMR	D	33	1	9,12,12	0.41	0	9,14,14	1.43	2 (22%)
1	B3L	C	23	1	8,8,9	0.52	0	7,9,11	0.80	0
1	B3L	A	16	1	8,8,9	0.55	0	7,9,11	0.96	0
1	BIL	D	12	1	7,8,9	0.73	0	5,9,11	1.55	1 (20%)
1	B3L	D	16	1	8,8,9	0.53	0	7,9,11	1.25	1 (14%)
1	BIL	B	26	1	7,8,9	0.56	0	5,9,11	1.41	0
1	BIL	D	19	1	7,8,9	0.59	0	5,9,11	1.72	2 (40%)
1	BIL	A	19	1	7,8,9	0.26	0	5,9,11	1.90	1 (20%)
1	BIL	A	5	1	7,8,9	0.61	0	5,9,11	1.46	2 (40%)
1	BIL	C	19	1	7,8,9	0.57	0	5,9,11	1.48	1 (20%)
1	B3M	D	2	1	7,7,9	0.70	0	5,7,10	2.10	1 (20%)
1	B3L	D	9	1	8,8,9	0.96	1 (12%)	7,9,11	1.10	1 (14%)
1	BIL	A	26	1	7,8,9	0.59	0	5,9,11	1.46	0
1	B3L	A	9	1	8,8,9	0.54	0	7,9,11	1.06	1 (14%)
1	B3L	C	9	1	8,8,9	0.37	0	7,9,11	1.01	1 (14%)
1	BIL	D	26	1	7,8,9	0.50	0	5,9,11	1.01	0
1	B3L	C	30	1	8,8,9	0.41	0	7,9,11	1.66	2 (28%)
1	BIL	D	5	1	7,8,9	0.80	0	5,9,11	1.36	1 (20%)
1	HMR	C	33	1	11,11,12	0.43	0	10,12,14	1.24	1 (10%)
1	BIL	C	5	1	7,8,9	0.75	0	5,9,11	1.29	1 (20%)
1	BIL	C	26	1	7,8,9	0.95	1 (14%)	5,9,11	1.44	1 (20%)
1	B3M	B	2	1	8,8,9	0.42	0	6,8,10	1.84	3 (50%)
1	B3L	C	16	1	8,8,9	0.78	0	7,9,11	1.07	1 (14%)
1	HMR	A	33	1	9,12,12	0.43	0	9,14,14	1.69	2 (22%)
1	B3L	A	23	1	8,8,9	0.72	0	7,9,11	1.14	1 (14%)
1	BIL	B	12	1	7,8,9	0.66	0	5,9,11	1.08	0
1	BIL	A	12	1	7,8,9	0.35	0	5,9,11	1.10	0
1	B3L	B	9	1	8,8,9	0.85	0	7,9,11	0.83	0
1	B3L	D	23	1	8,8,9	0.70	0	7,9,11	1.29	1 (14%)
1	BIL	B	5	1	7,8,9	0.72	0	5,9,11	1.49	1 (20%)

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	B3L	B	16	1	-	0/7/7/8	-
1	B3L	D	30	1	-	2/7/7/8	-
1	B3L	B	23	1	-	3/7/7/8	-
1	BIL	C	12	1	-	2/9/9/10	-
1	B3M	C	2	1	-	3/7/7/8	-
1	B3M	A	2	1	-	4/7/7/8	-
1	B3L	A	30	1	-	2/7/7/8	-
1	BIL	B	19	1	-	2/9/9/10	-
1	HMR	B	33	1	-	4/9/11/11	-
1	B3L	B	30	1	-	3/7/7/8	-
1	HMR	D	33	1	-	2/9/11/11	-
1	B3L	C	23	1	-	4/7/7/8	-
1	B3L	A	16	1	-	4/7/7/8	-
1	BIL	D	12	1	-	1/9/9/10	-
1	B3L	D	16	1	-	3/7/7/8	-
1	BIL	B	26	1	-	2/9/9/10	-
1	BIL	D	19	1	-	0/9/9/10	-
1	BIL	A	19	1	-	1/9/9/10	-
1	BIL	A	5	1	-	1/9/9/10	-
1	BIL	C	19	1	-	1/9/9/10	-
1	B3M	D	2	1	-	5/6/6/8	-
1	B3L	D	9	1	-	2/7/7/8	-
1	BIL	A	26	1	-	2/9/9/10	-
1	B3L	A	9	1	-	1/7/7/8	-
1	B3L	C	9	1	-	4/7/7/8	-
1	BIL	D	26	1	-	0/9/9/10	-
1	B3L	C	30	1	-	3/7/7/8	-
1	BIL	D	5	1	-	1/9/9/10	-
1	HMR	C	33	1	-	1/10/10/11	-
1	BIL	C	5	1	-	2/9/9/10	-
1	BIL	C	26	1	-	2/9/9/10	-
1	B3M	B	2	1	-	3/7/7/8	-
1	B3L	C	16	1	-	4/7/7/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HMR	A	33	1	-	4/9/11/11	-
1	B3L	A	23	1	-	3/7/7/8	-
1	BIL	B	12	1	-	2/9/9/10	-
1	BIL	A	12	1	-	1/9/9/10	-
1	B3L	B	9	1	-	2/7/7/8	-
1	B3L	D	23	1	-	3/7/7/8	-
1	BIL	B	5	1	-	1/9/9/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	9	B3L	CA-C	2.37	1.56	1.49
1	C	26	BIL	CA-CB	-2.33	1.50	1.53
1	C	12	BIL	CA-CB	-2.16	1.50	1.53

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	23	B3L	CB-CA-C	4.28	118.55	112.25
1	C	2	B3M	CB-CA-C	4.13	118.33	112.25
1	A	33	HMR	C-CH2-CA	-4.08	108.63	112.95
1	D	2	B3M	CG-CD-SE	-3.68	109.90	113.74
1	C	12	BIL	CA-CB-CG	-3.35	105.28	113.19
1	A	19	BIL	CA-CB-CG	-3.33	105.31	113.19
1	B	33	HMR	CG-CD-NE	-3.31	102.75	112.21
1	D	12	BIL	O-C-CA	-2.83	117.19	125.43
1	B	2	B3M	CB-CA-C	2.71	116.24	112.25
1	A	9	B3L	O-C-CA	-2.57	117.94	125.43
1	C	26	BIL	O-C-CA	-2.56	117.97	125.43
1	D	33	HMR	CB-CA-N	2.55	116.44	109.03
1	C	19	BIL	CA-CB-CG	-2.55	107.17	113.19
1	C	30	B3L	CB-CA-C	2.53	115.97	112.25
1	D	16	B3L	CB-CA-C	-2.38	108.75	112.25
1	A	23	B3L	O-C-CA	-2.36	118.56	125.43
1	B	33	HMR	NE-CZ-NH1	-2.35	116.57	120.70
1	B	5	BIL	O-C-CA	-2.31	118.71	125.43
1	C	9	B3L	O-C-CA	-2.24	118.90	125.43
1	D	33	HMR	CG-CD-NE	-2.22	105.86	112.21
1	D	5	BIL	CA-CB-CG	-2.21	107.96	113.19
1	D	19	BIL	CB-CA-C	-2.21	108.80	113.39
1	A	30	B3L	CB-CA-C	2.20	115.49	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	19	BIL	O-C-CA	-2.19	119.04	125.43
1	A	5	BIL	CA-CB-CG	-2.18	108.05	113.19
1	D	30	B3L	CB-CA-C	2.17	115.45	112.25
1	B	2	B3M	CG-CB-N	2.16	115.32	109.03
1	A	5	BIL	O-C-CA	-2.16	119.12	125.43
1	C	30	B3L	CG-CB-CA	-2.16	105.27	111.20
1	C	5	BIL	O-C-CA	-2.15	119.16	125.43
1	D	9	B3L	CB-CA-C	-2.13	109.11	112.25
1	B	2	B3M	CG-CB-CA	-2.11	103.71	111.63
1	C	16	B3L	O-C-CA	-2.06	119.43	125.43
1	B	33	HMR	NH2-CZ-NE	2.05	123.93	119.19
1	D	19	BIL	CA-CB-CG	-2.04	108.37	113.19
1	A	30	B3L	CG-CB-CA	-2.03	105.62	111.20
1	C	33	HMR	CG-CD-NE	-2.01	106.46	112.21
1	A	33	HMR	CG-CD-NE	-2.01	106.46	112.21
1	D	23	B3L	O-C-CA	-2.01	119.58	125.43

There are no chirality outliers.

All (90) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	9	B3L	N-CB-CG-CD
1	D	30	B3L	N-CB-CG-CD
1	A	30	B3L	N-CB-CG-CD
1	B	33	HMR	N-CA-CB-CG
1	B	33	HMR	CH2-CA-CB-CG
1	C	23	B3L	N-CB-CG-CD
1	A	16	B3L	N-CB-CG-CD
1	D	16	B3L	N-CB-CG-CD
1	D	9	B3L	C-CA-CB-CG
1	A	33	HMR	N-CA-CB-CG
1	A	33	HMR	CH2-CA-CB-CG
1	C	16	B3L	N-CB-CG-CD
1	A	33	HMR	NE-CD-CG-CB
1	B	30	B3L	CE1-CD-CG-CB
1	A	2	B3M	CG-CD-SE-CF
1	B	30	B3L	CE2-CD-CG-CB
1	C	30	B3L	CE1-CD-CG-CB
1	B	23	B3L	CE1-CD-CG-CB
1	C	33	HMR	NE-CD-CG-CB
1	D	33	HMR	NE-CD-CG-CB
1	C	2	B3M	CG-CD-SE-CF

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Mol	Chain	Res	Type	Atoms
1	B	33	HMR	NE-CD-CG-CB
1	D	2	B3M	SE-CD-CG-CB
1	A	2	B3M	CA-CB-CG-CD
1	D	2	B3M	CA-CB-CG-CD
1	C	30	B3L	CE2-CD-CG-CB
1	C	9	B3L	C-CA-CB-CG
1	D	16	B3L	C-CA-CB-CG
1	A	23	B3L	N-CB-CG-CD
1	A	26	BIL	C-CA-CB-N
1	C	26	BIL	C-CA-CB-N
1	C	9	B3L	O-C-CA-CB
1	D	30	B3L	O-C-CA-CB
1	B	23	B3L	O-C-CA-CB
1	C	12	BIL	O-C-CA-CB
1	C	2	B3M	O-C-CA-CB
1	A	2	B3M	O-C-CA-CB
1	A	30	B3L	O-C-CA-CB
1	B	19	BIL	O-C-CA-CB
1	B	30	B3L	O-C-CA-CB
1	C	23	B3L	O-C-CA-CB
1	A	16	B3L	O-C-CA-CB
1	D	12	BIL	O-C-CA-CB
1	C	19	BIL	O-C-CA-CB
1	D	2	B3M	O-C-CA-CB
1	D	9	B3L	O-C-CA-CB
1	A	26	BIL	O-C-CA-CB
1	C	30	B3L	O-C-CA-CB
1	C	26	BIL	O-C-CA-CB
1	C	16	B3L	O-C-CA-CB
1	A	23	B3L	O-C-CA-CB
1	B	12	BIL	O-C-CA-CB
1	B	9	B3L	O-C-CA-CB
1	B	5	BIL	O-C-CA-CB
1	D	33	HMR	N-CA-CH2-C
1	A	33	HMR	CG-CD-NE-CZ
1	C	9	B3L	C-CA-CB-N
1	C	2	B3M	C-CA-CB-N
1	C	23	B3L	C-CA-CB-N
1	A	16	B3L	C-CA-CB-N
1	D	2	B3M	C-CA-CB-N
1	A	9	B3L	C-CA-CB-N
1	B	2	B3M	C-CA-CB-N

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Mol	Chain	Res	Type	Atoms
1	C	16	B3L	C-CA-CB-N
1	A	23	B3L	C-CA-CB-N
1	B	9	B3L	C-CA-CB-N
1	D	23	B3L	C-CA-CB-N
1	C	5	BIL	CE1-CD1-CG-CB
1	B	33	HMR	CG-CD-NE-CZ
1	B	23	B3L	CE2-CD-CG-CB
1	A	2	B3M	N-CB-CG-CD
1	D	2	B3M	N-CB-CG-CD
1	D	16	B3L	O-C-CA-CB
1	B	26	BIL	O-C-CA-CB
1	A	19	BIL	O-C-CA-CB
1	A	5	BIL	O-C-CA-CB
1	D	5	BIL	O-C-CA-CB
1	C	5	BIL	O-C-CA-CB
1	B	2	B3M	O-C-CA-CB
1	A	12	BIL	O-C-CA-CB
1	D	23	B3L	O-C-CA-CB
1	C	23	B3L	C-CA-CB-CG
1	A	16	B3L	C-CA-CB-CG
1	B	2	B3M	C-CA-CB-CG
1	C	16	B3L	C-CA-CB-CG
1	D	23	B3L	N-CB-CG-CD
1	C	12	BIL	C-CA-CB-N
1	B	19	BIL	C-CA-CB-N
1	B	26	BIL	C-CA-CB-N
1	B	12	BIL	C-CA-CB-N

There are no ring outliers.

13 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	16	B3L	1	0
1	C	12	BIL	2	0
1	A	2	B3M	2	0
1	A	30	B3L	4	0
1	B	33	HMR	1	0
1	D	19	BIL	1	0
1	A	19	BIL	2	0
1	A	5	BIL	3	0
1	C	19	BIL	1	0
1	A	26	BIL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	30	B3L	4	0
1	C	5	BIL	2	0
1	B	2	B3M	4	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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, 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	23/34 (67%)	-0.20	0 100 100	14, 23, 31, 40	0
1	B	23/34 (67%)	-0.30	0 100 100	10, 19, 31, 40	0
1	C	23/34 (67%)	-0.22	0 100 100	15, 21, 34, 39	0
1	D	23/34 (67%)	-0.36	0 100 100	9, 16, 33, 36	0
All	All	92/136 (67%)	-0.27	0 100 100	9, 21, 34, 40	0

There are no RSRZ outliers to report.

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, 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	HMR	B	33	13/13	0.88	0.14	30,32,37,37	0
1	HMR	A	33	13/13	0.90	0.16	34,36,39,39	0
1	HMR	C	33	12/13	0.90	0.12	35,36,37,37	0
1	HMR	D	33	13/13	0.92	0.16	27,29,30,30	0
1	B3L	D	30	9/10	0.93	0.12	14,16,18,20	6
1	BIL	A	19	9/10	0.94	0.18	16,19,23,23	6
1	B3L	B	30	9/10	0.94	0.14	24,25,26,27	6
1	B3L	A	30	9/10	0.94	0.17	24,26,28,29	6
1	BIL	C	19	9/10	0.95	0.14	15,16,19,19	6
1	B3M	D	2	8/10	0.95	0.18	34,35,39,43	0
1	BIL	D	19	9/10	0.95	0.15	10,15,18,21	6
1	B3M	A	2	9/10	0.95	0.19	31,34,41,41	3
1	B3M	B	2	9/10	0.95	0.13	30,32,36,39	3
1	B3L	C	16	9/10	0.95	0.15	7,10,13,15	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	BIL	B	5	9/10	0.95	0.15	23,24,26,26	6
1	B3L	D	9	9/10	0.96	0.10	12,16,17,18	6
1	BIL	A	26	9/10	0.96	0.17	16,18,21,21	6
1	B3L	A	9	9/10	0.96	0.11	15,17,18,18	6
1	B3L	D	16	9/10	0.96	0.14	4,6,8,9	6
1	B3L	C	30	9/10	0.96	0.17	26,28,29,30	6
1	B3M	C	2	9/10	0.96	0.14	27,31,38,38	3
1	BIL	C	26	9/10	0.96	0.14	22,24,24,25	6
1	B3L	C	9	9/10	0.96	0.17	11,13,14,14	6
1	B3L	B	23	9/10	0.96	0.13	8,12,13,13	6
1	BIL	D	26	9/10	0.96	0.15	10,12,16,17	6
1	BIL	D	12	9/10	0.97	0.10	9,12,13,13	6
1	BIL	C	5	9/10	0.97	0.13	17,19,20,21	6
1	B3L	B	16	9/10	0.97	0.16	9,10,13,13	6
1	BIL	B	26	9/10	0.97	0.13	15,15,20,20	6
1	BIL	D	5	9/10	0.97	0.15	25,25,27,28	6
1	BIL	B	12	9/10	0.97	0.15	12,13,14,14	6
1	BIL	A	12	9/10	0.97	0.14	14,14,15,15	6
1	B3L	B	9	9/10	0.97	0.16	10,13,15,15	6
1	B3L	D	23	9/10	0.97	0.14	4,7,9,9	6
1	BIL	B	19	9/10	0.97	0.12	11,12,14,14	6
1	B3L	C	23	9/10	0.98	0.13	14,17,18,19	6
1	B3L	A	16	9/10	0.98	0.15	11,12,12,13	6
1	BIL	A	5	9/10	0.98	0.13	19,23,24,25	6
1	BIL	C	12	9/10	0.98	0.15	12,13,16,16	6
1	B3L	A	23	9/10	0.98	0.18	9,13,15,15	6

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(\AA^2)	Q<0.9
2	IOD	B	34	1/1	0.86	0.65	71,71,71,71	1
2	IOD	A	38	1/1	0.90	0.33	40,40,40,40	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	IOD	A	34	1/1	0.92	0.10	43,43,43,43	1
2	IOD	A	37	1/1	0.97	0.15	29,29,29,29	1
2	IOD	C	35	1/1	0.98	0.10	41,41,41,41	1
2	IOD	A	36	1/1	0.99	0.19	43,43,43,43	1
2	IOD	A	35	1/1	0.99	0.17	23,23,23,23	1
2	IOD	C	34	1/1	0.99	0.20	24,24,24,24	1
2	IOD	B	35	1/1	1.00	0.08	36,36,36,36	1

6.5 Other polymers [i](#)

There are no such residues in this entry.