Full wwPDB X-ray Structure Validation Report (i)

Nov 5, 2023 – 08:11 PM EST

PDB ID	:	3F86
Title	:	An alpha/beta-Peptide Helix Bundle with a Pure beta-Amino Acid Core and a Distinctive Quaternary Structure: GCN4pLI derivative with beta residues at a and d heptad positions
Authors	:	Giuliano, M.W.; Horne, W.S.; Gellman, S.H.
Deposited on	:	2008-11-11
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 (i) 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 (i)) were used in the production of this report:

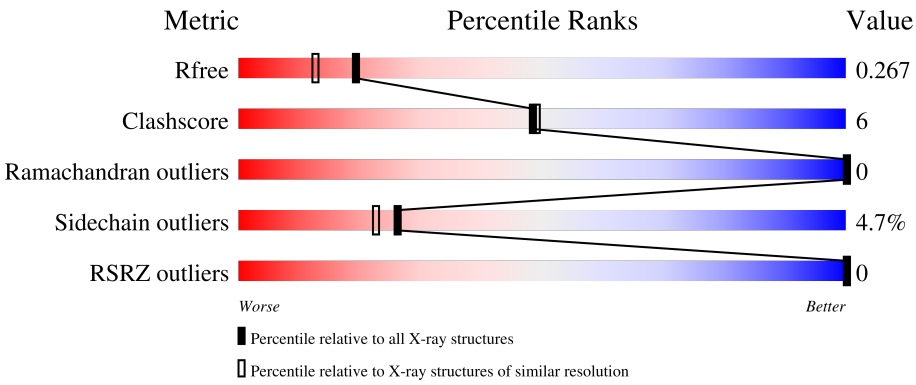
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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 of 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 <=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	50% 44% • •
1	B	34	56% 29% 15%
1	C	34	47% 38% 12% •
1	D	34	59% 26% 12% •
1	E	34	53% 38% 6% •

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Mol	Chain	Length	Quality of chain
1	F	34	62% 21% 12%
1	G	34	53% 32% 12%
1	H	34	56% 35% 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4931 atoms, of which 2517 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
			Total	C	H	N	O	S			
1	A	34	612	190	322	47	52	1	93	0	0
1	B	34	599	187	313	46	52	1	92	0	0
1	C	34	611	191	322	45	53		97	1	0
1	D	34	609	188	319	48	53	1	91	0	0
1	E	34	611	188	321	48	53	1	94	0	0
1	F	33	575	181	300	42	51	1	92	0	0
1	G	33	593	185	311	45	51	1	90	0	0
1	H	34	593	186	309	44	53	1	92	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	21	21	21	0	0
2	B	15	15	15	0	0
2	C	8	8	8	0	0
2	D	26	26	26	0	0
2	E	25	25	25	0	0
2	F	12	12	12	0	0

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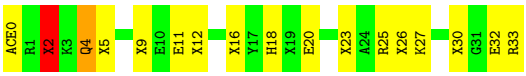
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	G	12	12	12	0	0
			Total	O		
2	H	9	9	9	0	0

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.

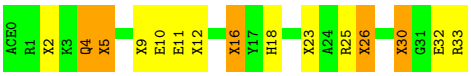
- Molecule 1: GCN4pLI-betaAD

Chain A:



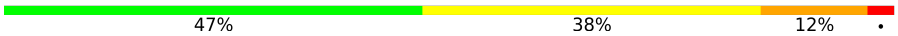
- Molecule 1: GCN4pLI-betaAD

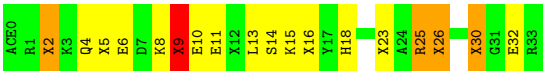
Chain B:



- Molecule 1: GCN4pLI-betaAD

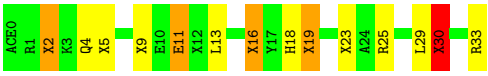
Chain C:





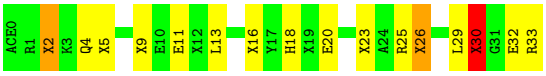
- Molecule 1: GCN4pLI-betaAD

Chain D:



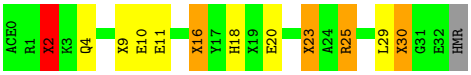
- Molecule 1: GCN4pLI-betaAD

Chain E:



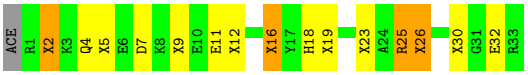
- Molecule 1: GCN4pLI-betaAD

Chain F:



• Molecule 1: GCN4pLI-betaAD

Chain G:



• Molecule 1: GCN4pLI-betaAD

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	38.38Å 68.72Å 48.30Å 90.00° 100.93° 90.00°	Depositor
Resolution (Å)	47.40 – 2.00 39.03 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (47.40-2.00) 99.1 (39.03-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.4.0062	Depositor
R, R_{free}	0.200 , 0.266 0.206 , 0.267	Depositor DCC
R_{free} test set	842 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	23.3	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 55.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4931	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.35% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, BIL, B3L, B3M, HMR

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	0.64	0/187	0.78	0/230
1	B	0.58	0/183	0.73	0/226
1	C	0.73	0/193	0.91	0/236
1	D	0.69	0/186	0.94	1/229 (0.4%)
1	E	0.66	0/186	0.89	0/229
1	F	0.55	0/184	0.81	0/227
1	G	0.54	0/184	0.63	0/226
1	H	0.65	0/180	0.81	1/222 (0.5%)
All	All	0.63	0/1483	0.82	2/1825 (0.1%)

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	15
1	B	0	15
1	C	0	14
1	D	0	14
1	E	0	15
1	F	0	14
1	G	0	15
1	H	0	15
All	All	0	117

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	13	LEU	CA-CB-CG	6.64	130.57	115.30
1	H	13	LEU	CA-CB-CG	6.49	130.23	115.30

There are no chirality outliers.

All (117) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	GLU	Peptide
1	A	16	B3L	Mainchain,Peptide
1	A	18	HIS	Peptide
1	A	2	B3M	Mainchain,Peptide
1	A	23	B3L	Mainchain,Peptide
1	A	25	ARG	Peptide
1	A	30	B3L	Mainchain,Peptide
1	A	32	GLU	Peptide
1	A	4	GLN	Peptide
1	A	9	B3L	Mainchain,Peptide
1	B	11	GLU	Peptide
1	B	16	B3L	Mainchain,Peptide
1	B	18	HIS	Peptide
1	B	2	B3M	Mainchain,Peptide
1	B	23	B3L	Mainchain,Peptide
1	B	25	ARG	Peptide
1	B	30	B3L	Mainchain,Peptide
1	B	32	GLU	Peptide
1	B	4	GLN	Peptide
1	B	9	B3L	Mainchain,Peptide
1	C	11	GLU	Peptide
1	C	16	B3L	Mainchain,Peptide
1	C	18	HIS	Peptide
1	C	2	B3M	Mainchain
1	C	23	B3L	Mainchain,Peptide
1	C	25	ARG	Peptide
1	C	30	B3L	Mainchain,Peptide
1	C	32	GLU	Peptide
1	C	4	GLN	Peptide
1	C	9	B3L	Mainchain,Peptide
1	D	11	GLU	Peptide
1	D	16	B3L	Mainchain,Peptide
1	D	18	HIS	Peptide
1	D	2	B3M	Mainchain,Peptide
1	D	23	B3L	Mainchain,Peptide
1	D	25	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	D	30	B3L	Mainchain,Peptide
1	D	4	GLN	Peptide
1	D	9	B3L	Mainchain,Peptide
1	E	11	GLU	Peptide
1	E	16	B3L	Mainchain,Peptide
1	E	18	HIS	Peptide
1	E	2	B3M	Mainchain,Peptide
1	E	23	B3L	Mainchain,Peptide
1	E	25	ARG	Peptide
1	E	30	B3L	Mainchain,Peptide
1	E	32	GLU	Peptide
1	E	4	GLN	Peptide
1	E	9	B3L	Mainchain,Peptide
1	F	11	GLU	Peptide
1	F	16	B3L	Mainchain,Peptide
1	F	18	HIS	Peptide
1	F	2	B3M	Mainchain,Peptide
1	F	23	B3L	Mainchain,Peptide
1	F	25	ARG	Peptide
1	F	30	B3L	Mainchain,Peptide
1	F	4	GLN	Peptide
1	F	9	B3L	Mainchain,Peptide
1	G	11	GLU	Peptide
1	G	16	B3L	Mainchain,Peptide
1	G	18	HIS	Peptide
1	G	2	B3M	Mainchain,Peptide
1	G	23	B3L	Mainchain,Peptide
1	G	25	ARG	Peptide
1	G	30	B3L	Mainchain,Peptide
1	G	32	GLU	Peptide
1	G	4	GLN	Peptide
1	G	9	B3L	Mainchain,Peptide
1	H	11	GLU	Peptide
1	H	16	B3L	Mainchain,Peptide
1	H	18	HIS	Peptide
1	H	2	B3M	Mainchain,Peptide
1	H	23	B3L	Mainchain,Peptide
1	H	25	ARG	Peptide
1	H	30	B3L	Mainchain,Peptide
1	H	32	GLU	Peptide
1	H	4	GLN	Peptide
1	H	9	B3L	Mainchain,Peptide

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	290	322	285	3	0
1	B	286	313	272	4	0
1	C	289	322	282	8	0
1	D	290	319	284	4	0
1	E	290	321	284	4	0
1	F	275	300	269	4	0
1	G	282	311	276	3	0
1	H	284	309	268	6	0
2	A	21	0	0	2	0
2	B	15	0	0	0	0
2	C	8	0	0	0	0
2	D	26	0	0	1	0
2	E	25	0	0	0	0
2	F	12	0	0	0	0
2	G	12	0	0	1	0
2	H	9	0	0	1	0
All	All	2414	2517	2220	27	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 6.

All (27) 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:A:0:ACE:H3	2:A:126:HOH:O	1.57	1.04
1:G:7:ASP:OD1	2:G:111:HOH:O	2.04	0.74
1:D:11:GLU:OE1	2:D:103:HOH:O	2.11	0.69
2:A:126:HOH:O	1:D:29:LEU:HD12	1.99	0.63
1:H:1:ARG:HA	1:H:4:GLN:CG	2.28	0.63
1:F:2:B3M:HFB	1:H:2:B3M:SE	2.52	0.60
1:E:26:BIL:H2E1	1:E:29:LEU:HD22	1.84	0.59
1:C:15[A]:LYS:NZ	1:E:20:GLU:OE1	2.41	0.54
1:H:21:ASN:ND2	2:H:35:HOH:O	2.41	0.53
1:B:26:BIL:H3E1	1:C:8:LYS:HG2	1.91	0.53
1:A:2:B3M:HF	1:D:30:B3L:H3E1	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2:B3M:CF	1:H:2:B3M:SE	3.09	0.51
1:B:26:BIL:CE1	1:C:8:LYS:HG2	2.43	0.49
1:E:20:GLU:OE1	1:F:20:GLU:OE2	2.32	0.48
1:G:25:ARG:CZ	1:G:26:BIL:H3E1	2.45	0.46
1:C:25:ARG:CZ	1:C:26:BIL:H3E1	2.45	0.46
1:H:1:ARG:HA	1:H:4:GLN:HG2	1.98	0.46
1:B:4:GLN:C	1:B:5:BIL:H2E1	2.37	0.45
1:E:30:B3L:H3E2	1:H:2:B3M:HFB	1.99	0.45
1:F:25:ARG:O	1:F:29:LEU:HD13	2.17	0.44
1:C:10:GLU:HA	1:C:13:LEU:HD23	2.01	0.43
1:A:27:LYS:HE2	1:B:10:GLU:CG	2.50	0.42
1:C:9:B3L:O	1:C:13:LEU:HD22	2.20	0.42
1:C:15[A]:LYS:HA	1:C:15[A]:LYS:HD3	1.88	0.42
1:G:5:BIL:H1D2	1:G:5:BIL:HA	1.94	0.41
1:C:15[B]:LYS:HA	1:C:15[B]:LYS:HD3	1.98	0.41
1:D:19:BIL:H2E1	1:D:19:BIL:H3D2	1.90	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	23/34 (68%)	23 (100%)	0	0	100	100
1	B	23/34 (68%)	23 (100%)	0	0	100	100
1	C	24/34 (71%)	24 (100%)	0	0	100	100
1	D	23/34 (68%)	22 (96%)	1 (4%)	0	100	100
1	E	23/34 (68%)	23 (100%)	0	0	100	100
1	F	22/34 (65%)	22 (100%)	0	0	100	100
1	G	22/34 (65%)	22 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	23/34 (68%)	22 (96%)	1 (4%)	0	100	100
All	All	183/272 (67%)	181 (99%)	2 (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	19/21 (90%)	17 (90%)	2 (10%)	7	4
1	B	18/21 (86%)	18 (100%)	0	100	100
1	C	20/21 (95%)	18 (90%)	2 (10%)	7	4
1	D	19/21 (90%)	19 (100%)	0	100	100
1	E	20/21 (95%)	19 (95%)	1 (5%)	24	20
1	F	18/21 (86%)	17 (94%)	1 (6%)	21	17
1	G	19/21 (90%)	19 (100%)	0	100	100
1	H	17/21 (81%)	16 (94%)	1 (6%)	19	15
All	All	150/168 (89%)	143 (95%)	7 (5%)	26	22

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	20	GLU
1	C	6	GLU
1	C	14	SER
1	E	13	LEU
1	F	10	GLU
1	H	3	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	B	18	HIS
1	H	21	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

79 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	BIL	H	12	1	7,8,9	0.50	0	5,9,11	1.02	0
1	BIL	E	12	1	7,8,9	0.57	0	5,9,11	0.65	0
1	BIL	B	12	1	7,8,9	0.30	0	5,9,11	1.12	1 (20%)
1	B3M	G	2	1	8,8,9	0.75	0	6,8,10	1.13	1 (16%)
1	B3L	B	30	1	8,8,9	0.56	0	7,9,11	1.25	1 (14%)
1	B3L	F	16	1	8,8,9	0.72	0	7,9,11	1.47	1 (14%)
1	BIL	F	12	1	7,8,9	0.56	0	5,9,11	0.77	0
1	BIL	B	26	1	7,8,9	1.46	1 (14%)	5,9,11	1.36	1 (20%)
1	B3L	D	16	1	8,8,9	0.84	0	7,9,11	1.09	1 (14%)
1	BIL	A	5	1	7,8,9	0.32	0	5,9,11	1.50	1 (20%)
1	B3L	A	16	1	8,8,9	0.66	0	7,9,11	0.88	0
1	B3L	F	23	1	8,8,9	0.82	0	7,9,11	1.50	2 (28%)
1	B3M	D	2	1	8,8,9	0.46	0	6,8,10	1.25	1 (16%)
1	B3L	C	16	1	8,8,9	0.65	0	7,9,11	0.73	0
1	B3L	G	30	1	8,8,9	0.61	0	7,9,11	0.80	0
1	BIL	F	5	1	7,8,9	0.53	0	5,9,11	1.29	0
1	B3L	E	16	1	8,8,9	0.36	0	7,9,11	1.06	0
1	BIL	D	19	1	7,8,9	0.44	0	5,9,11	1.41	1 (20%)
1	B3L	H	9	1	8,8,9	0.47	0	7,9,11	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	BIL	D	12	1	7,8,9	0.57	0	5,9,11	1.43	0
1	HMR	A	33	1	11,11,12	0.38	0	10,12,14	1.53	2 (20%)
1	BIL	B	5	1	7,8,9	0.54	0	5,9,11	1.23	1 (20%)
1	B3L	B	23	1	8,8,9	0.34	0	7,9,11	0.99	0
1	B3M	B	2	1	8,8,9	0.49	0	6,8,10	1.09	0
1	BIL	H	19	1	7,8,9	0.67	0	5,9,11	0.80	0
1	B3L	G	23	1	8,8,9	0.60	0	7,9,11	0.94	0
1	B3L	H	16	1	8,8,9	0.64	0	7,9,11	0.80	0
1	BIL	G	5	1	7,8,9	0.32	0	5,9,11	1.16	0
1	B3L	H	30	1	8,8,9	0.40	0	7,9,11	1.30	1 (14%)
1	BIL	C	26	1	7,8,9	0.63	0	5,9,11	1.21	1 (20%)
1	B3L	A	30	1	8,8,9	0.49	0	7,9,11	0.90	0
1	BIL	A	19	1	7,8,9	0.74	0	5,9,11	0.90	0
1	BIL	B	19	1	7,8,9	0.39	0	5,9,11	1.10	0
1	BIL	H	26	1	7,8,9	0.36	0	5,9,11	1.37	2 (40%)
1	B3M	H	2	1	8,8,9	0.55	0	6,8,10	1.22	0
1	BIL	C	5	1	7,8,9	0.48	0	5,9,11	1.24	1 (20%)
1	B3L	C	30	1	8,8,9	0.58	0	7,9,11	1.19	1 (14%)
1	B3L	C	23	1	8,8,9	0.70	0	7,9,11	0.91	0
1	BIL	F	26	1	7,8,9	0.43	0	5,9,11	1.28	0
1	B3L	D	23	1	8,8,9	0.49	0	7,9,11	1.05	0
1	BIL	F	19	1	7,8,9	0.55	0	5,9,11	0.73	0
1	HMR	E	33	1	12,12,12	0.51	0	11,14,14	1.44	2 (18%)
1	B3L	E	23	1	8,8,9	0.44	0	7,9,11	0.92	0
1	B3M	A	2	1	8,8,9	1.25	1 (12%)	6,8,10	2.17	1 (16%)
1	B3L	F	30	1	8,8,9	0.60	0	7,9,11	1.26	1 (14%)
1	B3L	E	9	1	8,8,9	0.45	0	7,9,11	0.75	0
1	HMR	D	33	1	12,12,12	0.49	0	11,14,14	1.30	1 (9%)
1	BIL	D	5	1	7,8,9	0.47	0	5,9,11	1.35	1 (20%)
1	B3L	B	9	1	8,8,9	0.47	0	7,9,11	0.76	0
1	BIL	G	26	1	7,8,9	0.47	0	5,9,11	1.64	2 (40%)
1	B3L	E	30	1	8,8,9	0.50	0	7,9,11	1.12	1 (14%)
1	B3L	G	16	1	8,8,9	0.59	0	7,9,11	1.39	1 (14%)
1	B3L	F	9	1	8,8,9	0.64	0	7,9,11	0.98	0
1	B3L	A	23	1	8,8,9	0.64	0	7,9,11	0.79	0
1	BIL	A	26	1	7,8,9	1.58	1 (14%)	5,9,11	1.06	0
1	BIL	A	12	1	7,8,9	0.75	0	5,9,11	1.47	1 (20%)
1	BIL	G	12	1	7,8,9	0.33	0	5,9,11	1.26	1 (20%)
1	HMR	G	33	1	8,8,12	0.42	0	7,8,14	1.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	B3M	C	2	1	6,6,9	1.76	1 (16%)	4,6,10	2.95	1 (25%)
1	BIL	E	26	1	7,8,9	0.55	0	5,9,11	1.37	1 (20%)
1	B3L	D	30	1	8,8,9	0.59	0	7,9,11	1.39	1 (14%)
1	HMR	C	33	1	8,8,12	0.64	0	7,9,14	1.15	0
1	B3L	H	23	1	8,8,9	0.54	0	7,9,11	1.15	0
1	BIL	C	19	1	7,8,9	0.42	0	5,9,11	1.36	0
1	B3L	G	9	1	8,8,9	0.44	0	7,9,11	0.82	0
1	B3L	A	9	1	8,8,9	0.51	0	7,9,11	1.00	0
1	B3M	F	2	1	8,8,9	0.60	0	6,8,10	1.46	1 (16%)
1	BIL	C	12	1	7,8,9	0.37	0	5,9,11	1.09	0
1	BIL	G	19	1	7,8,9	0.39	0	5,9,11	1.72	2 (40%)
1	B3L	D	9	1	8,8,9	0.64	0	7,9,11	0.74	0
1	HMR	B	33	1	11,11,12	0.41	0	10,12,14	1.34	2 (20%)
1	B3L	C	9	1	8,8,9	1.08	1 (12%)	7,9,11	1.38	1 (14%)
1	B3M	E	2	1	8,8,9	0.60	0	6,8,10	1.19	1 (16%)
1	BIL	H	5	1	7,8,9	0.55	0	5,9,11	0.93	0
1	BIL	E	5	1	7,8,9	0.46	0	5,9,11	1.23	1 (20%)
1	B3L	B	16	1	8,8,9	0.83	0	7,9,11	0.94	1 (14%)
1	BIL	E	19	1	7,8,9	0.49	0	5,9,11	1.55	0
1	BIL	D	26	1	7,8,9	0.58	0	5,9,11	1.11	0
1	HMR	H	33	1	12,12,12	0.50	0	11,14,14	1.10	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	BIL	H	12	1	-	2/9/9/10	-
1	BIL	E	12	1	-	1/9/9/10	-
1	BIL	B	12	1	-	2/9/9/10	-
1	B3M	G	2	1	-	3/7/7/8	-
1	B3L	B	30	1	-	3/7/7/8	-
1	B3L	F	16	1	-	1/7/7/8	-
1	BIL	F	12	1	-	2/9/9/10	-
1	BIL	B	26	1	-	2/9/9/10	-
1	B3L	D	16	1	-	3/7/7/8	-
1	BIL	A	5	1	-	1/9/9/10	-
1	B3L	A	16	1	-	2/7/7/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	B3L	F	23	1	-	4/7/7/8	-
1	B3M	D	2	1	-	4/7/7/8	-
1	B3L	C	16	1	-	2/7/7/8	-
1	B3L	G	30	1	-	2/7/7/8	-
1	BIL	F	5	1	-	1/9/9/10	-
1	B3L	E	16	1	-	2/7/7/8	-
1	BIL	D	19	1	-	2/9/9/10	-
1	B3L	H	9	1	-	2/7/7/8	-
1	BIL	D	12	1	-	2/9/9/10	-
1	HMR	A	33	1	-	2/10/10/11	-
1	BIL	B	5	1	-	3/9/9/10	-
1	B3L	B	23	1	-	4/7/7/8	-
1	B3M	B	2	1	-	4/7/7/8	-
1	BIL	H	19	1	-	2/9/9/10	-
1	B3L	G	23	1	-	2/7/7/8	-
1	B3L	H	16	1	-	2/7/7/8	-
1	BIL	G	5	1	-	1/9/9/10	-
1	B3L	H	30	1	-	3/7/7/8	-
1	BIL	C	26	1	-	1/9/9/10	-
1	B3L	A	30	1	-	3/7/7/8	-
1	BIL	A	19	1	-	0/9/9/10	-
1	BIL	B	19	1	-	1/9/9/10	-
1	BIL	H	26	1	-	3/9/9/10	-
1	B3M	H	2	1	-	4/7/7/8	-
1	BIL	C	5	1	-	1/9/9/10	-
1	B3L	C	30	1	-	1/7/7/8	-
1	B3L	C	23	1	-	3/7/7/8	-
1	BIL	F	26	1	-	3/9/9/10	-
1	B3L	D	23	1	-	1/7/7/8	-
1	BIL	F	19	1	-	2/9/9/10	-
1	HMR	E	33	1	-	1/11/11/11	-
1	B3L	E	23	1	-	1/7/7/8	-
1	B3M	A	2	1	-	3/7/7/8	-
1	B3L	F	30	1	-	2/7/7/8	-
1	B3L	E	9	1	-	2/7/7/8	-
1	HMR	D	33	1	-	2/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	BIL	D	5	1	-	2/9/9/10	-
1	B3L	B	9	1	-	1/7/7/8	-
1	BIL	G	26	1	-	1/9/9/10	-
1	B3L	E	30	1	-	1/7/7/8	-
1	B3L	G	16	1	-	2/7/7/8	-
1	B3L	F	9	1	-	2/7/7/8	-
1	B3L	A	23	1	-	1/7/7/8	-
1	BIL	A	26	1	-	1/9/9/10	-
1	BIL	A	12	1	-	1/9/9/10	-
1	BIL	G	12	1	-	2/9/9/10	-
1	HMR	G	33	1	-	2/7/7/11	-
1	B3M	C	2	1	-	3/5/5/8	-
1	BIL	E	26	1	-	1/9/9/10	-
1	B3L	D	30	1	-	4/7/7/8	-
1	HMR	C	33	1	-	2/7/7/11	-
1	B3L	H	23	1	-	3/7/7/8	-
1	BIL	C	19	1	-	1/9/9/10	-
1	B3L	G	9	1	-	2/7/7/8	-
1	B3L	A	9	1	-	2/7/7/8	-
1	B3M	F	2	1	-	3/7/7/8	-
1	BIL	C	12	1	-	1/9/9/10	-
1	BIL	G	19	1	-	1/9/9/10	-
1	B3L	D	9	1	-	2/7/7/8	-
1	HMR	B	33	1	-	3/10/10/11	-
1	B3L	C	9	1	-	2/7/7/8	-
1	B3M	E	2	1	-	5/7/7/8	-
1	BIL	H	5	1	-	1/9/9/10	-
1	BIL	E	5	1	-	1/9/9/10	-
1	B3L	B	16	1	-	3/7/7/8	-
1	BIL	E	19	1	-	3/9/9/10	-
1	BIL	D	26	1	-	1/9/9/10	-
1	HMR	H	33	1	-	3/11/11/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2	B3M	CB-CA	-4.14	1.47	1.53
1	A	26	BIL	CA-CB	-4.04	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	26	BIL	CA-CB	-3.78	1.48	1.53
1	A	2	B3M	CB-CA	-3.18	1.49	1.53
1	C	9	B3L	CB-CA	-2.81	1.49	1.53

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	2	B3M	CA-CB-C	5.71	120.66	112.25
1	A	2	B3M	CA-CB-C	4.97	119.57	112.25
1	F	16	B3L	CA-CB-C	3.25	117.03	112.25
1	C	9	B3L	CA-CB-C	3.15	116.89	112.25
1	F	2	B3M	CA-CB-C	2.94	116.58	112.25
1	E	33	HMR	CG-CD-NE	-2.86	104.03	112.21
1	G	16	B3L	CA-CB-C	2.80	116.37	112.25
1	B	26	BIL	CA-CB-CG	-2.76	106.68	113.19
1	G	26	BIL	CA-CB-CG	-2.72	106.77	113.19
1	F	23	B3L	CA-CB-C	2.61	116.10	112.25
1	D	30	B3L	CA-CB-C	2.56	116.01	112.25
1	B	33	HMR	CG-CD-NE	-2.55	104.91	112.21
1	B	33	HMR	O-C-CA	-2.48	118.19	125.43
1	D	19	BIL	O-C-CA	-2.48	118.20	125.43
1	F	30	B3L	CA-CB-C	2.47	115.89	112.25
1	E	33	HMR	CC-CB-N	-2.45	101.91	109.03
1	G	19	BIL	O-C-CA	-2.44	118.30	125.43
1	B	30	B3L	CA-CB-C	2.34	115.70	112.25
1	A	33	HMR	CG-CD-NE	-2.33	105.56	112.21
1	D	5	BIL	O-C-CA	-2.32	118.68	125.43
1	H	30	B3L	CG-CA-CB	-2.30	104.90	111.20
1	D	2	B3M	CA-CB-C	2.27	115.59	112.25
1	D	33	HMR	CG-CD-NE	-2.26	105.76	112.21
1	G	12	BIL	O-C-CA	-2.25	118.86	125.43
1	G	19	BIL	CA-CB-CG	-2.25	107.88	113.19
1	E	30	B3L	CG-CA-CB	-2.24	105.05	111.20
1	G	2	B3M	CG-CA-CB	-2.19	103.40	111.63
1	B	5	BIL	O-C-CA	-2.14	119.20	125.43
1	A	5	BIL	CA-CB-CG	-2.14	108.14	113.19
1	C	30	B3L	CA-CB-C	2.14	115.40	112.25
1	C	26	BIL	CA-CB-CG	-2.14	108.15	113.19
1	E	26	BIL	CA-CB-CG	-2.13	108.16	113.19
1	D	16	B3L	O-C-CB	-2.10	119.30	125.43
1	E	5	BIL	O-C-CA	-2.09	119.32	125.43
1	C	5	BIL	CA-CB-CG	-2.09	108.25	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	2	B3M	CF-SE-CD	2.09	107.57	100.40
1	F	23	B3L	CE1-CD-CG	2.08	118.76	111.11
1	H	26	BIL	O-C-CA	-2.08	119.36	125.43
1	G	26	BIL	CB-CA-C	2.07	117.69	113.39
1	H	26	BIL	CA-CB-CG	-2.06	108.34	113.19
1	A	12	BIL	O-C-CA	-2.03	119.51	125.43
1	B	16	B3L	CA-CB-C	-2.02	109.29	112.25
1	B	12	BIL	O-C-CA	-2.01	119.57	125.43
1	A	33	HMR	CC-CB-N	2.00	114.85	109.03

There are no chirality outliers.

All (163) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	33	HMR	N-CB-CC-CG
1	B	33	HMR	CA-CB-CC-CG
1	C	33	HMR	N-CB-CC-CG
1	C	33	HMR	CA-CB-CC-CG
1	D	33	HMR	CA-CB-CC-CG
1	G	33	HMR	N-CB-CC-CG
1	G	33	HMR	CA-CB-CC-CG
1	B	2	B3M	N-CA-CG-CD
1	B	2	B3M	CB-CA-CG-CD
1	C	2	B3M	N-CA-CG-CD
1	C	2	B3M	CB-CA-CG-CD
1	D	2	B3M	CG-CA-CB-C
1	E	2	B3M	N-CA-CG-CD
1	E	2	B3M	CB-CA-CG-CD
1	H	2	B3M	CG-CA-CB-C
1	D	16	B3L	N-CA-CG-CD
1	B	23	B3L	N-CA-CG-CD
1	A	30	B3L	N-CA-CG-CD
1	G	30	B3L	N-CA-CG-CD
1	H	33	HMR	NE-CD-CG-CC
1	E	2	B3M	CG-CD-SE-CF
1	A	33	HMR	NE-CD-CG-CC
1	D	33	HMR	NE-CD-CG-CC
1	B	5	BIL	CE1-CD1-CG-CB
1	F	19	BIL	CE1-CD1-CG-CD2
1	H	30	B3L	CE2-CD-CG-CA
1	H	30	B3L	CE1-CD-CG-CA
1	H	23	B3L	CE1-CD-CG-CA

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Mol	Chain	Res	Type	Atoms
1	F	23	B3L	CE1-CD-CG-CA
1	D	30	B3L	CE1-CD-CG-CA
1	B	30	B3L	CE1-CD-CG-CA
1	F	23	B3L	CE2-CD-CG-CA
1	A	2	B3M	CG-CD-SE-CF
1	B	2	B3M	CG-CD-SE-CF
1	D	2	B3M	CG-CD-SE-CF
1	H	33	HMR	CB-CC-CG-CD
1	H	2	B3M	CG-CD-SE-CF
1	F	2	B3M	CG-CD-SE-CF
1	G	2	B3M	CG-CD-SE-CF
1	D	30	B3L	CE2-CD-CG-CA
1	C	2	B3M	O-C-CB-CA
1	F	26	BIL	CE1-CD1-CG-CB
1	H	23	B3L	CE2-CD-CG-CA
1	B	5	BIL	CE1-CD1-CG-CD2
1	F	26	BIL	CE1-CD1-CG-CD2
1	E	19	BIL	CA-CB-CG-CD2
1	F	30	B3L	CE1-CD-CG-CA
1	C	23	B3L	N-CA-CG-CD
1	D	12	BIL	C-CA-CB-N
1	H	12	BIL	C-CA-CB-N
1	B	33	HMR	O-C-CA-CB
1	B	2	B3M	O-C-CB-CA
1	D	2	B3M	O-C-CB-CA
1	F	2	B3M	O-C-CB-CA
1	G	2	B3M	O-C-CB-CA
1	H	2	B3M	O-C-CB-CA
1	C	5	BIL	O-C-CA-CB
1	E	5	BIL	O-C-CA-CB
1	F	5	BIL	O-C-CA-CB
1	A	9	B3L	O-C-CB-CA
1	B	9	B3L	O-C-CB-CA
1	C	9	B3L	O-C-CB-CA
1	D	9	B3L	O-C-CB-CA
1	F	9	B3L	O-C-CB-CA
1	A	12	BIL	O-C-CA-CB
1	B	12	BIL	O-C-CA-CB
1	D	12	BIL	O-C-CA-CB
1	G	12	BIL	O-C-CA-CB
1	H	12	BIL	O-C-CA-CB
1	A	16	B3L	O-C-CB-CA

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Mol	Chain	Res	Type	Atoms
1	D	16	B3L	O-C-CB-CA
1	G	16	B3L	O-C-CB-CA
1	H	16	B3L	O-C-CB-CA
1	F	19	BIL	O-C-CA-CB
1	H	19	BIL	O-C-CA-CB
1	B	23	B3L	O-C-CB-CA
1	D	23	B3L	O-C-CB-CA
1	F	23	B3L	O-C-CB-CA
1	A	26	BIL	O-C-CA-CB
1	B	26	BIL	O-C-CA-CB
1	C	26	BIL	O-C-CA-CB
1	F	26	BIL	O-C-CA-CB
1	G	26	BIL	O-C-CA-CB
1	H	26	BIL	O-C-CA-CB
1	A	30	B3L	O-C-CB-CA
1	B	30	B3L	O-C-CB-CA
1	C	30	B3L	O-C-CB-CA
1	D	30	B3L	O-C-CB-CA
1	E	30	B3L	O-C-CB-CA
1	F	30	B3L	O-C-CB-CA
1	G	30	B3L	O-C-CB-CA
1	D	2	B3M	N-CA-CB-C
1	E	2	B3M	N-CA-CB-C
1	F	2	B3M	N-CA-CB-C
1	G	2	B3M	N-CA-CB-C
1	H	2	B3M	N-CA-CB-C
1	A	9	B3L	N-CA-CB-C
1	C	9	B3L	N-CA-CB-C
1	D	9	B3L	N-CA-CB-C
1	E	9	B3L	N-CA-CB-C
1	G	9	B3L	N-CA-CB-C
1	H	9	B3L	N-CA-CB-C
1	A	16	B3L	N-CA-CB-C
1	B	16	B3L	N-CA-CB-C
1	D	16	B3L	N-CA-CB-C
1	E	16	B3L	N-CA-CB-C
1	B	23	B3L	N-CA-CB-C
1	C	23	B3L	N-CA-CB-C
1	F	23	B3L	N-CA-CB-C
1	G	23	B3L	N-CA-CB-C
1	A	30	B3L	N-CA-CB-C
1	D	30	B3L	N-CA-CB-C

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Mol	Chain	Res	Type	Atoms
1	A	33	HMR	CG-CD-NE-CZ
1	B	30	B3L	CE2-CD-CG-CA
1	E	33	HMR	CB-CC-CG-CD
1	D	5	BIL	CE1-CD1-CG-CB
1	H	33	HMR	OXT-C-CA-CB
1	E	19	BIL	CA-CB-CG-CD1
1	H	26	BIL	CA-CB-CG-CD1
1	A	2	B3M	O-C-CB-CA
1	E	2	B3M	O-C-CB-CA
1	A	5	BIL	O-C-CA-CB
1	B	5	BIL	O-C-CA-CB
1	D	5	BIL	O-C-CA-CB
1	G	5	BIL	O-C-CA-CB
1	H	5	BIL	O-C-CA-CB
1	E	9	B3L	O-C-CB-CA
1	G	9	B3L	O-C-CB-CA
1	H	9	B3L	O-C-CB-CA
1	F	12	BIL	O-C-CA-CB
1	B	16	B3L	O-C-CB-CA
1	C	16	B3L	O-C-CB-CA
1	E	16	B3L	O-C-CB-CA
1	F	16	B3L	O-C-CB-CA
1	B	19	BIL	O-C-CA-CB
1	C	19	BIL	O-C-CA-CB
1	D	19	BIL	O-C-CA-CB
1	E	19	BIL	O-C-CA-CB
1	G	19	BIL	O-C-CA-CB
1	A	23	B3L	O-C-CB-CA
1	C	23	B3L	O-C-CB-CA
1	E	23	B3L	O-C-CB-CA
1	G	23	B3L	O-C-CB-CA
1	H	23	B3L	O-C-CB-CA
1	D	26	BIL	O-C-CA-CB
1	E	26	BIL	O-C-CA-CB
1	H	30	B3L	O-C-CB-CA
1	A	2	B3M	CG-CA-CB-C
1	F	9	B3L	N-CA-CG-CD
1	B	16	B3L	N-CA-CG-CD
1	C	16	B3L	N-CA-CG-CD
1	G	16	B3L	CG-CA-CB-C
1	H	16	B3L	N-CA-CG-CD
1	B	23	B3L	CG-CA-CB-C

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Mol	Chain	Res	Type	Atoms
1	B	12	BIL	C-CA-CB-N
1	C	12	BIL	C-CA-CB-N
1	E	12	BIL	C-CA-CB-N
1	F	12	BIL	C-CA-CB-N
1	G	12	BIL	C-CA-CB-N
1	D	19	BIL	C-CA-CB-N
1	H	19	BIL	C-CA-CB-N
1	B	26	BIL	C-CA-CB-N
1	H	26	BIL	C-CA-CB-N

There are no ring outliers.

13 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	26	BIL	2	0
1	D	19	BIL	1	0
1	B	5	BIL	1	0
1	G	5	BIL	1	0
1	C	26	BIL	1	0
1	H	2	B3M	3	0
1	A	2	B3M	1	0
1	G	26	BIL	1	0
1	E	30	B3L	1	0
1	E	26	BIL	1	0
1	D	30	B3L	1	0
1	F	2	B3M	2	0
1	C	9	B3L	1	0

5.5 Carbohydrates (i)

There are no monosaccharides 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 (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	23/34 (67%)	-0.34	0	100	100	16, 21, 30, 39	0
1	B	23/34 (67%)	-0.50	0	100	100	17, 22, 30, 33	0
1	C	23/34 (67%)	-0.25	0	100	100	14, 22, 37, 40	0
1	D	23/34 (67%)	-0.35	0	100	100	17, 21, 31, 45	0
1	E	23/34 (67%)	-0.31	0	100	100	17, 23, 34, 39	0
1	F	23/34 (67%)	-0.24	0	100	100	20, 24, 36, 43	0
1	G	23/34 (67%)	-0.36	0	100	100	18, 23, 31, 37	0
1	H	23/34 (67%)	-0.37	0	100	100	18, 24, 34, 38	0
All	All	184/272 (67%)	-0.34	0	100	100	14, 23, 37, 45	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	HMR	C	33	9/13	0.78	0.16	36,38,39,39	2
1	HMR	G	33	9/13	0.78	0.17	36,36,38,38	0
1	HMR	D	33	13/13	0.81	0.20	44,47,51,51	0
1	HMR	H	33	13/13	0.81	0.17	37,41,43,44	0
1	B3M	C	2	7/10	0.81	0.15	38,39,41,41	2
1	HMR	A	33	12/13	0.83	0.16	39,42,46,46	0
1	HMR	E	33	13/13	0.86	0.20	33,34,36,36	0
1	B3L	F	30	9/10	0.86	0.17	37,38,38,40	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	B3M	G	2	9/10	0.87	0.17	29,31,35,35	3
1	B3M	H	2	9/10	0.89	0.14	36,37,39,41	3
1	B3M	B	2	9/10	0.90	0.14	31,33,39,40	3
1	B3L	A	30	9/10	0.91	0.12	29,29,30,31	6
1	B3M	E	2	9/10	0.91	0.12	35,39,42,43	3
1	BIL	C	5	9/10	0.92	0.15	29,32,34,34	6
1	BIL	E	5	9/10	0.92	0.10	28,31,32,32	6
1	B3L	A	9	9/10	0.92	0.14	15,18,18,18	6
1	B3L	F	23	9/10	0.92	0.13	19,20,21,21	6
1	B3M	A	2	9/10	0.92	0.11	22,27,33,35	3
1	B3L	B	30	9/10	0.92	0.12	22,23,24,24	6
1	HMR	B	33	12/13	0.92	0.12	31,35,42,42	0
1	B3L	H	30	9/10	0.92	0.14	29,31,33,33	6
1	BIL	F	19	9/10	0.93	0.16	17,21,27,27	6
1	BIL	H	5	9/10	0.93	0.11	25,26,28,28	6
1	B3L	D	30	9/10	0.93	0.12	32,33,34,36	6
1	B3L	H	23	9/10	0.93	0.13	14,18,19,19	6
1	BIL	H	26	9/10	0.93	0.12	22,23,24,24	6
1	B3M	D	2	9/10	0.94	0.11	24,27,34,36	3
1	BIL	A	26	9/10	0.94	0.13	20,22,24,24	6
1	BIL	D	26	9/10	0.94	0.14	21,22,24,24	6
1	BIL	F	26	9/10	0.94	0.12	25,27,27,28	6
1	BIL	F	12	9/10	0.94	0.11	19,20,20,21	6
1	B3M	F	2	9/10	0.95	0.12	23,27,36,36	3
1	BIL	G	12	9/10	0.95	0.10	17,19,20,20	6
1	B3L	E	16	9/10	0.95	0.14	15,16,17,18	6
1	BIL	G	5	9/10	0.95	0.14	24,26,29,29	6
1	B3L	G	30	9/10	0.95	0.13	21,22,24,26	6
1	B3L	C	9	9/10	0.95	0.11	18,19,19,20	6
1	B3L	F	16	9/10	0.96	0.10	17,18,19,19	6
1	BIL	A	19	9/10	0.96	0.11	13,14,17,17	6
1	BIL	E	19	9/10	0.96	0.12	13,16,24,24	6
1	B3L	F	9	9/10	0.96	0.13	20,21,21,21	6
1	BIL	H	19	9/10	0.96	0.10	16,18,20,20	6
1	B3L	B	23	9/10	0.96	0.09	12,15,17,18	6
1	B3L	H	9	9/10	0.96	0.10	15,18,19,20	6
1	BIL	A	12	9/10	0.96	0.10	17,19,25,25	6
1	BIL	B	12	9/10	0.96	0.10	17,18,19,19	6
1	BIL	B	26	9/10	0.96	0.10	18,20,23,23	6
1	BIL	C	26	9/10	0.96	0.11	18,20,23,23	6
1	BIL	C	12	9/10	0.96	0.09	15,16,18,18	6
1	BIL	E	26	9/10	0.96	0.11	19,21,25,25	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	BIL	D	12	9/10	0.96	0.10	14,15,18,18	6
1	BIL	G	26	9/10	0.96	0.13	18,19,22,22	6
1	BIL	B	5	9/10	0.96	0.08	21,24,24,24	6
1	BIL	F	5	9/10	0.96	0.12	17,18,20,20	6
1	BIL	H	12	9/10	0.96	0.09	19,20,26,26	6
1	B3L	A	16	9/10	0.96	0.09	13,14,14,14	6
1	B3L	E	30	9/10	0.96	0.10	23,24,25,26	6
1	B3L	B	16	9/10	0.96	0.10	13,14,15,15	6
1	B3L	D	16	9/10	0.96	0.10	9,12,13,14	6
1	BIL	D	5	9/10	0.96	0.11	19,21,23,23	6
1	B3L	H	16	9/10	0.97	0.08	13,15,15,16	6
1	BIL	A	5	9/10	0.97	0.11	17,21,24,24	6
1	BIL	B	19	9/10	0.97	0.11	15,17,18,18	6
1	BIL	D	19	9/10	0.97	0.11	16,18,22,22	6
1	BIL	E	12	9/10	0.97	0.10	18,20,20,20	6
1	B3L	C	16	9/10	0.97	0.10	12,13,15,15	6
1	BIL	G	19	9/10	0.97	0.10	16,18,24,24	6
1	B3L	D	9	9/10	0.97	0.10	10,14,14,14	6
1	B3L	E	9	9/10	0.97	0.12	19,20,22,22	6
1	B3L	C	23	9/10	0.97	0.09	13,14,15,15	6
1	B3L	C	30	9/10	0.97	0.09	18,23,25,26	6
1	B3L	D	23	9/10	0.97	0.11	15,16,17,17	6
1	B3L	E	23	9/10	0.97	0.11	14,15,16,16	6
1	B3L	B	9	9/10	0.97	0.10	15,17,17,17	6
1	B3L	G	23	9/10	0.97	0.09	16,18,18,18	6
1	B3L	G	16	9/10	0.97	0.10	16,17,18,18	6
1	B3L	A	23	9/10	0.98	0.11	10,14,16,17	6
1	BIL	C	19	9/10	0.98	0.09	13,15,23,23	6
1	B3L	G	9	9/10	0.98	0.09	15,18,19,19	6

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.