



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:07 PM UTC

PDB ID : 1W6Q / pdb_00001w6q
Title : X-RAY CRYSTAL STRUCTURE OF R111H HUMAN GALECTIN-1
Authors : Lopez-Lucendo, M.I.F.; Gabius, H.J.; Romero, A.
Deposited on : 2004-08-21
Resolution : 2.10 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 types of validation reports are described at

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

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

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

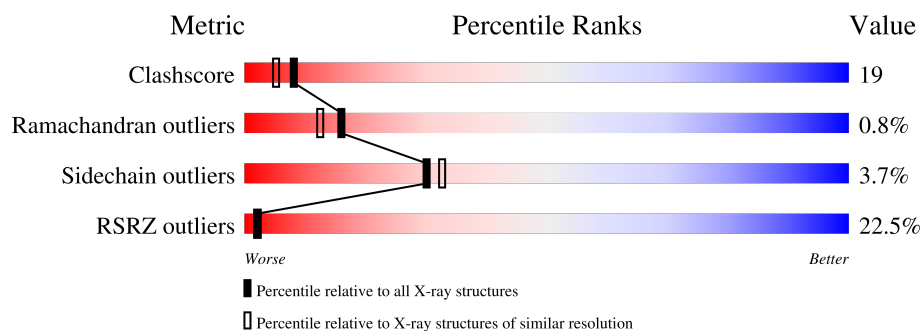
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 $\leq 5\%$. 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	134	21% 65% 31% ..
2	B	134	24% 63% 31% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2211 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called GALECTIN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	134	Total	C	N	O	S	0	0	0
			1025	646	177	195	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1111	HIS	ARG	engineered mutation	UNP P09382

- Molecule 2 is a protein called GALECTIN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	134	Total	C	N	O	S	0	0	0
			1024	646	177	194	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2111	HIS	ARG	engineered mutation	UNP P09382

- Molecule 3 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		

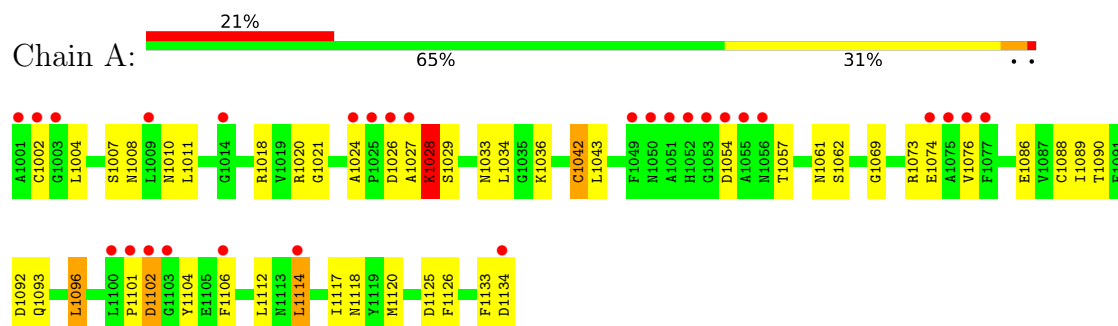
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	70	Total	O	0	0
			70	70		
4	B	68	Total	O	0	0
			68	68		

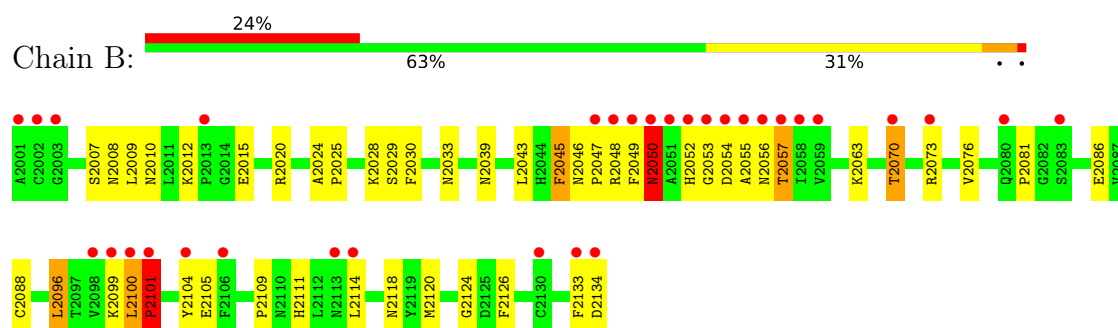
3 Residue-property plots

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: GALECTIN-1



• Molecule 2: GALECTIN-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	43.13Å 58.18Å 111.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.65 – 2.10 34.65 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.7 (34.65-2.10) 96.8 (34.65-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.34 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.242 , 0.283 0.239 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.679	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2211	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.84% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CSO, BME

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	0.38	0/1040	0.91	3/1407 (0.2%)
2	B	0.56	1/1047 (0.1%)	1.07	7/1418 (0.5%)
All	All	0.48	1/2087 (0.0%)	0.99	10/2825 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2045	PHE	C-N	7.37	1.43	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2045	PHE	CA-C-N	-8.86	113.11	122.85
2	B	2045	PHE	C-N-CA	-8.86	113.11	122.85
1	A	1096	LEU	N-CA-C	-6.46	99.19	109.59
2	B	2096	LEU	N-CA-C	-6.38	99.29	109.76
1	A	1042	CYS	N-CA-C	-5.77	105.73	112.89
1	A	1028	LYS	N-CA-C	-5.70	106.45	113.41
2	B	2053	GLY	N-CA-C	-5.39	108.57	115.42
2	B	2048	ARG	NE-CZ-NH2	5.32	123.98	119.20
2	B	2100	LEU	CA-C-N	5.27	126.42	119.84
2	B	2100	LEU	C-N-CA	5.27	126.42	119.84

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	1025	0	981	41	0
2	B	1024	0	981	40	0
3	A	12	0	15	5	0
3	B	12	0	15	3	0
4	A	70	0	0	6	0
4	B	68	0	0	1	0
All	All	2211	0	1992	79	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 19.

All (79) 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:1020:ARG:HG3	1:A:1086:GLU:HG2	1.58	0.84
1:A:1034:LEU:HD11	1:A:1089:ILE:HD13	1.64	0.79
2:B:2050:ASN:CG	2:B:2050:ASN:O	2.30	0.74
2:B:2030:PHE:CZ	2:B:2047:PRO:HG2	2.23	0.73
1:A:1061:ASN:HD22	1:A:1062:SER:H	1.38	0.69
2:B:2100:LEU:HB3	2:B:2101:PRO:HD2	1.75	0.66
1:A:1076:VAL:HG23	1:A:1106:PHE:HE1	1.60	0.66
1:A:1061:ASN:ND2	1:A:1062:SER:H	1.93	0.66
1:A:1018:ARG:HD3	4:A:2015:HOH:O	1.97	0.64
2:B:2043:LEU:HB2	2:B:2096:LEU:CD2	2.27	0.64
1:A:1054:ASP:HB3	1:A:1057:THR:CG2	2.28	0.63
1:A:1088:CYS:HB2	3:A:2136:BME:H11	1.79	0.63
1:A:1112:LEU:HB3	1:A:1114:LEU:HD13	1.79	0.63
1:A:1043:LEU:HB2	1:A:1096:LEU:HD22	1.82	0.62
2:B:2070:THR:HG23	4:B:4045:HOH:O	2.01	0.61
1:A:1027:ALA:HA	1:A:1125:ASP:OD1	2.02	0.59
1:A:1076:VAL:CG2	1:A:1106:PHE:HE1	2.16	0.59
2:B:2015:GLU:HG2	2:B:2134:ASP:CG	2.27	0.59
2:B:2099:LYS:HD3	2:B:2105:GLU:OE1	2.02	0.58
1:A:1061:ASN:HD21	1:A:1069:GLY:C	2.10	0.58
2:B:2052:HIS:C	2:B:2054:ASP:H	2.10	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2076:VAL:HG21	2:B:2104:TYR:CD2	2.39	0.58
1:A:1073:ARG:HG3	1:A:1073:ARG:HH11	1.69	0.57
1:A:1024:ALA:HB3	1:A:1125:ASP:HB3	1.87	0.57
2:B:2009:LEU:HD22	2:B:2133:PHE:CE1	2.40	0.56
2:B:2015:GLU:HG2	2:B:2134:ASP:OD1	2.05	0.56
2:B:2050:ASN:HA	2:B:2054:ASP:O	2.07	0.55
2:B:2010:ASN:H	2:B:2118:ASN:ND2	2.05	0.55
1:A:1074:GLU:HG2	3:A:2135:BME:O1	2.07	0.55
2:B:2088:CYS:HB3	3:B:3135:BME:S2	2.47	0.54
2:B:2039:ASN:HA	2:B:2063:LYS:HE3	1.89	0.54
1:A:1088:CYS:CB	3:A:2136:BME:H11	2.37	0.53
1:A:1036:LYS:HB2	1:A:1114:LEU:HD21	1.92	0.52
1:A:1042:CYS:SG	1:A:1096:LEU:HD21	2.50	0.52
2:B:2030:PHE:HA	2:B:2124:GLY:HA3	1.92	0.52
1:A:1010:ASN:H	1:A:1118:ASN:ND2	2.08	0.51
2:B:2050:ASN:O	2:B:2050:ASN:ND2	2.44	0.51
2:B:2100:LEU:HB3	2:B:2101:PRO:CD	2.41	0.51
2:B:2054:ASP:HB3	2:B:2057:THR:CG2	2.41	0.51
1:A:1061:ASN:HD22	1:A:1062:SER:N	2.07	0.50
2:B:2012:LYS:O	2:B:2015:GLU:HB2	2.11	0.50
2:B:2030:PHE:CG	2:B:2126:PHE:HB2	2.46	0.50
2:B:2010:ASN:H	2:B:2118:ASN:HD22	1.63	0.47
1:A:1102:ASP:OD2	1:A:1104:TYR:HD1	1.97	0.46
2:B:2046:ASN:ND2	2:B:2046:ASN:C	2.72	0.46
1:A:1011:LEU:HD23	1:A:1117:ILE:HD12	1.97	0.46
2:B:2076:VAL:HG21	2:B:2104:TYR:CG	2.51	0.46
2:B:2086:GLU:HB3	3:B:3136:BME:H11	1.98	0.46
2:B:2033:ASN:O	2:B:2120:MET:HA	2.17	0.45
2:B:2007:SER:O	2:B:2008:ASN:HB2	2.16	0.45
2:B:2020:ARG:HB2	3:B:3137:BME:H12	1.98	0.45
1:A:1026:ASP:HB3	4:A:2001:HOH:O	2.15	0.45
1:A:1093:GLN:HG2	4:A:2057:HOH:O	2.17	0.44
2:B:2028:LYS:O	2:B:2029:SER:HB3	2.17	0.44
1:A:1133:PHE:O	1:A:1134:ASP:C	2.58	0.44
1:A:1010:ASN:H	1:A:1118:ASN:HD22	1.67	0.43
2:B:2046:ASN:O	2:B:2046:ASN:CG	2.61	0.43
2:B:2055:ALA:O	2:B:2056:ASN:C	2.61	0.43
1:A:1021:GLY:HA3	1:A:1126:PHE:CZ	2.53	0.43
2:B:2030:PHE:CE1	2:B:2047:PRO:HG2	2.54	0.43
1:A:1101:PRO:N	3:A:2136:BME:H21	2.34	0.43
1:A:1004:LEU:HD13	2:B:2009:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1033:ASN:O	1:A:1120:MET:HA	2.20	0.42
1:A:1054:ASP:HB3	1:A:1057:THR:HG21	2.00	0.42
1:A:1002:CYS:HA	4:A:2069:HOH:O	2.19	0.42
1:A:1020:ARG:HD3	4:A:2052:HOH:O	2.18	0.42
2:B:2045:PHE:CE2	2:B:2047:PRO:HG3	2.54	0.42
2:B:2052:HIS:C	2:B:2054:ASP:N	2.78	0.42
1:A:1074:GLU:HG2	3:A:2135:BME:C1	2.50	0.41
2:B:2049:PHE:CD2	2:B:2081:PRO:HG3	2.55	0.41
2:B:2024:ALA:HA	2:B:2025:PRO:HD3	1.93	0.41
2:B:2073:ARG:HG3	2:B:2073:ARG:HH11	1.85	0.41
1:A:1011:LEU:HB3	1:A:1117:ILE:HB	2.01	0.41
2:B:2109:PRO:HG2	2:B:2111:HIS:NE2	2.35	0.41
1:A:1007:SER:O	1:A:1008:ASN:HB2	2.21	0.40
1:A:1090:THR:HG22	4:A:2055:HOH:O	2.21	0.40
1:A:1092:ASP:C	1:A:1092:ASP:OD2	2.64	0.40
1:A:1028:LYS:O	1:A:1029:SER:HB3	2.22	0.40
1:A:1004:LEU:CD1	2:B:2009:LEU:HD23	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	131/134 (98%)	125 (95%)	6 (5%)	0	100	100
2	B	132/134 (98%)	123 (93%)	7 (5%)	2 (2%)	8	4
All	All	263/268 (98%)	248 (94%)	13 (5%)	2 (1%)	16	12

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	2050	ASN

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Mol	Chain	Res	Type
2	B	2101	PRO

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	108/108 (100%)	105 (97%)	3 (3%)	38	43
2	B	109/109 (100%)	104 (95%)	5 (5%)	24	25
All	All	217/217 (100%)	209 (96%)	8 (4%)	30	33

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1028	LYS
1	A	1102	ASP
1	A	1114	LEU
2	B	2050	ASN
2	B	2057	THR
2	B	2070	THR
2	B	2101	PRO
2	B	2114	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1008	ASN
1	A	1056	ASN
1	A	1061	ASN
1	A	1080	GLN
1	A	1118	ASN
2	B	2008	ASN
2	B	2050	ASN
2	B	2056	ASN
2	B	2118	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	CSO	A	1016	1	3,6,7	0.79	0	1,6,8	0.75	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	CSO	A	1016	1	-	0/1/5/7	-

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.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

6 ligands 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	$\# Z > 2$
3	BME	A	2136	1	3,3,3	0.33	0	2,2,2	0.24	0
3	BME	B	3136	2	3,3,3	0.35	0	2,2,2	0.25	0
3	BME	B	3135	-	3,3,3	0.34	0	2,2,2	0.24	0
3	BME	B	3137	2	3,3,3	0.27	0	2,2,2	0.20	0
3	BME	A	2137	1	3,3,3	0.31	0	2,2,2	0.17	0
3	BME	A	2135	1	3,3,3	0.21	0	2,2,2	0.12	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
3	BME	A	2136	1	-	0/1/1/1	-
3	BME	B	3136	2	-	1/1/1/1	-
3	BME	B	3135	-	-	0/1/1/1	-
3	BME	B	3137	2	-	1/1/1/1	-
3	BME	A	2137	1	-	1/1/1/1	-
3	BME	A	2135	1	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2135	BME	O1-C1-C2-S2
3	A	2137	BME	O1-C1-C2-S2
3	B	3136	BME	O1-C1-C2-S2
3	B	3137	BME	O1-C1-C2-S2

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2136	BME	3	0
3	B	3136	BME	1	0
3	B	3135	BME	1	0
3	B	3137	BME	1	0
3	A	2135	BME	2	0

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	133/134 (99%)	1.21	28 (21%) 2 2	21, 36, 58, 65	0
2	B	134/134 (100%)	1.43	32 (23%) 2 2	25, 38, 58, 68	0
All	All	267/268 (99%)	1.32	60 (22%) 2 2	21, 38, 58, 68	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1075	ALA	7.5
2	B	2054	ASP	4.6
1	A	1001	ALA	4.4
1	A	1056	ASN	4.3
2	B	2001	ALA	4.3
1	A	1102	ASP	4.2
2	B	2051	ALA	4.2
1	A	1002	CYS	4.2
2	B	2133	PHE	4.1
2	B	2052	HIS	4.1
2	B	2104	TYR	4.0
2	B	2057	THR	3.9
2	B	2056	ASN	3.9
2	B	2002	CYS	3.8
1	A	1026	ASP	3.6
2	B	2114	LEU	3.6
1	A	1052	HIS	3.4
2	B	2050	ASN	3.4
1	A	1076	VAL	3.4
1	A	1051	ALA	3.4
2	B	2101	PRO	3.4
1	A	1055	ALA	3.4
1	A	1106	PHE	3.3
2	B	2055	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	2049	PHE	3.3
1	A	1027	ALA	3.2
1	A	1050	ASN	3.1
2	B	2083	SER	3.1
1	A	1054	ASP	3.0
1	A	1077	PHE	2.9
1	A	1134	ASP	2.8
2	B	2130	CYS	2.7
2	B	2073	ARG	2.7
2	B	2003	GLY	2.6
1	A	1101	PRO	2.6
2	B	2053	GLY	2.6
1	A	1049	PHE	2.5
1	A	1103	GLY	2.5
1	A	1024	ALA	2.4
1	A	1100	LEU	2.4
1	A	1003	GLY	2.4
2	B	2047	PRO	2.4
1	A	1074	GLU	2.3
1	A	1053	GLY	2.3
2	B	2106	PHE	2.3
2	B	2099	LYS	2.3
2	B	2058	ILE	2.3
2	B	2080	GLN	2.2
1	A	1114	LEU	2.2
1	A	1025	PRO	2.1
2	B	2100	LEU	2.1
1	A	1014	GLY	2.1
2	B	2098	VAL	2.1
1	A	1009	LEU	2.1
2	B	2134	ASP	2.1
2	B	2048	ARG	2.1
2	B	2059	VAL	2.1
2	B	2113	ASN	2.0
2	B	2013	PRO	2.0
2	B	2070	THR	2.0

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($\text{\AA}^2$)	Q<0.9
1	CSO	A	1016	7/8	0.92	0.11	33,36,44,47	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	BME	A	2136	4/4	0.47	0.39	51,51,53,58	0
3	BME	B	3135	4/4	0.71	0.27	51,51,53,58	0
3	BME	B	3136	4/4	0.77	0.21	51,51,53,58	0
3	BME	B	3137	4/4	0.81	0.19	51,53,54,54	0
3	BME	A	2135	4/4	0.95	0.09	48,51,53,53	0
3	BME	A	2137	4/4	0.96	0.11	45,47,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.