W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Jun 19, 2024 – 12:29 AM EDT

PDB ID	:	4BHU
Title	:	Crystal structure of BslA - A bacterial hydrophobin
Authors	:	Rao, F.V.; Hobley, L.; Ostrowski, A.; Bromley, K.M.; Porter, M.; Prescott, A.R.; Swedlow, J.R.; MacPhee, C.E.; van Aalten, D.M.F.; Stanley-Wall, N.R.
Deposited on	:	2013-04-08
Resolution	:	1.91 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1
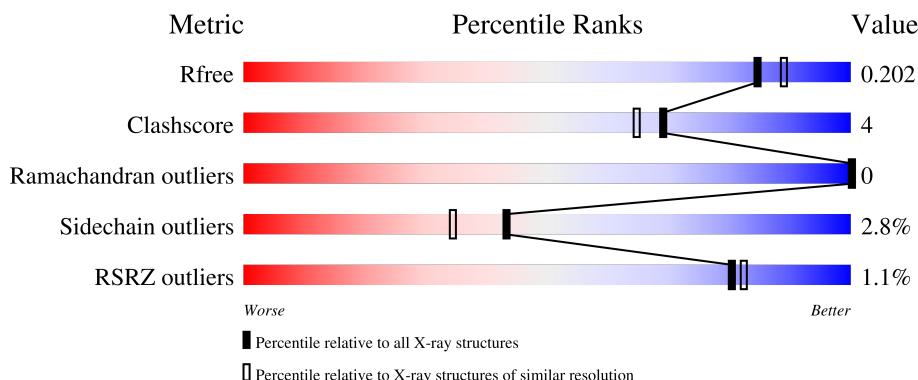
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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	Percentile Ranks	Value
Rfree		0.202
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		2.8%
RSRZ outliers		1.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
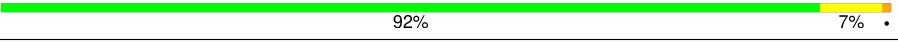
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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	130	91% 8% ·
1	B	130	97% · ·
1	C	130	86% 11% · ·
1	D	130	88% 8% · ·
1	E	130	97% ·

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Mol	Chain	Length	Quality of chain
1	F	130	92% 7%
1	G	130	% 92% 6%
1	H	130	84% 12%
1	J	130	2% 82% 8% 9%
2	I	130	8% 82% 9% 8%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 21151 atoms, of which 9970 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 UNCHARACTERIZED PROTEIN YUAB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	128	Total	C	H	N	O	Se	0	5	0
			2008	632	1016	165	193	2			
1	B	129	Total	C	H	N	O	Se	0	3	0
			1998	629	1009	166	192	2			
1	C	130	Total	C	H	N	O	Se	0	3	0
			2021	636	1023	167	193	2			
1	D	129	Total	C	H	N	O	Se	0	2	0
			1992	627	1006	166	191	2			
1	E	130	Total	C	H	N	O	Se	0	0	0
			1991	627	1005	166	191	2			
1	F	130	Total	C	H	N	O	Se	0	0	0
			1990	627	1004	166	191	2			
1	G	128	Total	C	H	N	O	Se	0	2	0
			1982	624	1002	165	189	2			
1	H	128	Total	C	H	N	O	Se	0	2	0
			1982	624	1002	165	189	2			
1	J	118	Total	C	H	N	O	Se	0	2	0
			1837	580	925	153	177	2			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	GLY	-	expression tag	UNP P71014
A	44	PRO	-	expression tag	UNP P71014
A	45	LEU	-	expression tag	UNP P71014
A	46	GLY	-	expression tag	UNP P71014
A	47	SER	-	expression tag	UNP P71014
A	98	MSE	LEU	engineered mutation	UNP P71014
B	43	GLY	-	expression tag	UNP P71014
B	44	PRO	-	expression tag	UNP P71014
B	45	LEU	-	expression tag	UNP P71014
B	46	GLY	-	expression tag	UNP P71014
B	47	SER	-	expression tag	UNP P71014

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Chain	Residue	Modelled	Actual	Comment	Reference
B	98	MSE	LEU	engineered mutation	UNP P71014
C	43	GLY	-	expression tag	UNP P71014
C	44	PRO	-	expression tag	UNP P71014
C	45	LEU	-	expression tag	UNP P71014
C	46	GLY	-	expression tag	UNP P71014
C	47	SER	-	expression tag	UNP P71014
C	98	MSE	LEU	engineered mutation	UNP P71014
D	43	GLY	-	expression tag	UNP P71014
D	44	PRO	-	expression tag	UNP P71014
D	45	LEU	-	expression tag	UNP P71014
D	46	GLY	-	expression tag	UNP P71014
D	47	SER	-	expression tag	UNP P71014
D	98	MSE	LEU	engineered mutation	UNP P71014
E	43	GLY	-	expression tag	UNP P71014
E	44	PRO	-	expression tag	UNP P71014
E	45	LEU	-	expression tag	UNP P71014
E	46	GLY	-	expression tag	UNP P71014
E	47	SER	-	expression tag	UNP P71014
E	98	MSE	LEU	engineered mutation	UNP P71014
F	43	GLY	-	expression tag	UNP P71014
F	44	PRO	-	expression tag	UNP P71014
F	45	LEU	-	expression tag	UNP P71014
F	46	GLY	-	expression tag	UNP P71014
F	47	SER	-	expression tag	UNP P71014
F	98	MSE	LEU	engineered mutation	UNP P71014
G	43	GLY	-	expression tag	UNP P71014
G	44	PRO	-	expression tag	UNP P71014
G	45	LEU	-	expression tag	UNP P71014
G	46	GLY	-	expression tag	UNP P71014
G	47	SER	-	expression tag	UNP P71014
G	98	MSE	LEU	engineered mutation	UNP P71014
H	43	GLY	-	expression tag	UNP P71014
H	44	PRO	-	expression tag	UNP P71014
H	45	LEU	-	expression tag	UNP P71014
H	46	GLY	-	expression tag	UNP P71014
H	47	SER	-	expression tag	UNP P71014
H	98	MSE	LEU	engineered mutation	UNP P71014
J	43	GLY	-	expression tag	UNP P71014
J	44	PRO	-	expression tag	UNP P71014
J	45	LEU	-	expression tag	UNP P71014
J	46	GLY	-	expression tag	UNP P71014
J	47	SER	-	expression tag	UNP P71014

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Chain	Residue	Modelled	Actual	Comment	Reference
J	98	MSE	LEU	engineered mutation	UNP P71014
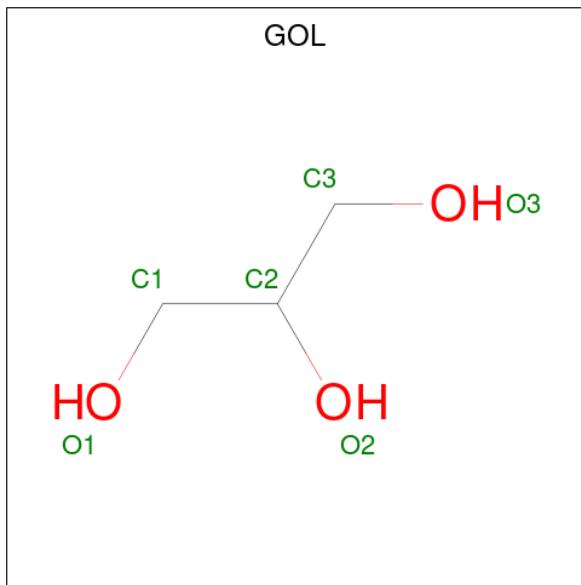
- Molecule 2 is a protein called UNCHARACTERIZED PROTEIN YUAB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	I	119	Total 1845	C 580	H 930	N 153	O 180	Se 2	0	2	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	43	GLY	-	expression tag	UNP P71014
I	44	PRO	-	expression tag	UNP P71014
I	45	LEU	-	expression tag	UNP P71014
I	46	GLY	-	expression tag	UNP P71014
I	47	SER	-	expression tag	UNP P71014
I	74	ASP	ASN	conflict	UNP P71014
I	98	MSE	LEU	engineered mutation	UNP P71014

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 14	C 3	H 8	O 3	0	0
3	B	1	Total 14	C 3	H 8	O 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total 14	C 3	H 8	O 3	0	0
3	F	1	Total 14	C 3	H 8	O 3	0	0
3	F	1	Total 14	C 3	H 8	O 3	0	0
3	J	1	Total 14	C 3	H 8	O 3	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Cl 1	0	0
4	B	1	Total 1	Cl 1	0	0
4	C	2	Total 2	Cl 2	0	0
4	E	2	Total 2	Cl 2	0	0
4	F	1	Total 1	Cl 1	0	0
4	H	1	Total 1	Cl 1	0	0
4	I	2	Total 2	Cl 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	162	Total 162	O 162	0	0
5	B	161	Total 161	O 161	0	0
5	C	191	Total 191	O 191	0	0
5	D	145	Total 145	O 145	0	0
5	E	180	Total 180	O 180	0	0
5	F	166	Total 166	O 166	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	117	Total 117	O 117	0	0
5	H	145	Total 145	O 145	0	0
5	I	59	Total 59	O 59	0	0
5	J	85	Total 85	O 85	0	0

3 Residue-property plots ⓘ
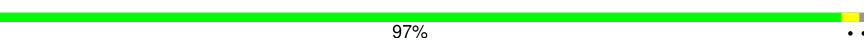
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: UNCHARACTERIZED PROTEIN YUAB

Chain A:

91%   8%
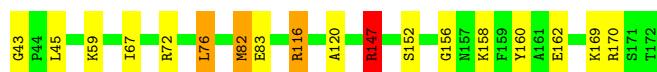
G43 E68 T75 L124 K130 L131 K132 E149 N150 K151 I155 K169 R170 SER THR

- Molecule 1: UNCHARACTERIZED PROTEIN YUAB

Chain B:

97%

G43 K113 K130 E149 S171 THR

- Molecule 1: UNCHARACTERIZED PROTEIN YUAB

Chain C:

86%   11%

G43 P44 L45 K59 I67 R72 L76 M82 E83 R116 A120 R147 S152 G156 N157 K158 F159 Y160 A161 E162 K169 R170 S171 T172

- Molecule 1: UNCHARACTERIZED PROTEIN YUAB

Chain D:

88%   8%

G43 P44 L45 M82 E83 R104 T105 R116 A120 L123 L124 E149 G156 N157 K158 R170 S171 THR

- Molecule 1: UNCHARACTERIZED PROTEIN YUAB

Chain E:

97%

G43 M82 N111 K130 R170 S171 T172

- Molecule 1: UNCHARACTERIZED PROTEIN YUAB

Chain F:

92%   7%

G43 E61 L86 P87 S88 K113 R147 A148 E149 L153 K158 R170 S171 T172

• Molecule 1: UNCHARACTERIZED PROTEIN YUAB

Chain G:

%

92%   6% ••

G43 P44 L45 T53 G56 K59 I67 K130 K151 G156 N157 R170 SER THR

• Molecule 1: UNCHARACTERIZED PROTEIN YUAB

Chain H:

84%   12%   •••

G43 T53 K59 T60 E61 I67 R72 L76 L79 M82 R116 A120 F129 K130 L131 K132 R147 Y160 A161 E162 D166 R170 SER THR

• Molecule 1: UNCHARACTERIZED PROTEIN YUAB

Chain J:

2%

82%   8%   •   9%

GLY PRO LEU GLY S47 G56 A57 S58 K59 I67 P73 N74 T75 L79 M82 R104 L109 S152 LEU SER ILE GLY ASN MLY F159 I165 R170 SER THR
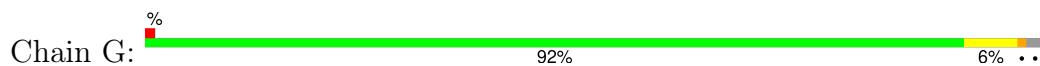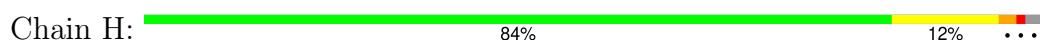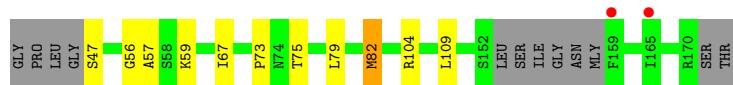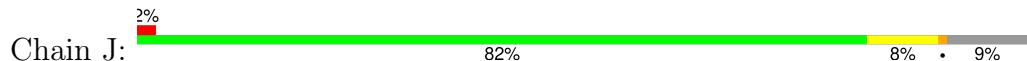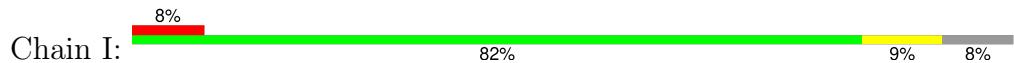
• Molecule 2: UNCHARACTERIZED PROTEIN YUAB

Chain I:

8%

82%   9%   8%

GLY PRO LEU GLY S47 F51 A52 T53 A57 S58 K59 T60 S63 F64 I67 P73 D74 L109 R116 L119 N135 T143 Y144 R147 S154 ILE GLY ASN MLY PHE Y160 D166 R170 SER THR

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.70Å 95.98Å 259.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.19 – 1.91 77.20 – 1.91	Depositor EDS
% Data completeness (in resolution range)	100.0 (77.19-1.91) 97.6 (77.20-1.91)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.73 (at 1.91Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.165 , 0.199 0.169 , 0.202	Depositor DCC
R_{free} test set	6835 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	23.9	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 52.2	EDS
L-test for twinning[2]	$<|L|> = 0.47$, $<L^2> = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	21151	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MLY, GOL, CL

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	0.55	0/990	0.69	0/1341
1	B	0.52	0/981	0.69	0/1329
1	C	0.58	0/990	0.77	2/1342 (0.1%)
1	D	0.55	0/975	0.69	0/1321
1	E	0.62	0/967	0.69	0/1310
1	F	0.61	0/967	0.71	0/1310
1	G	0.56	0/969	0.72	0/1313
1	H	0.53	0/969	0.79	4/1313 (0.3%)
1	J	0.48	0/910	0.62	0/1231
2	I	0.45	0/912	0.63	0/1234
All	All	0.55	0/9630	0.70	6/13044 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	147	ARG	NE-CZ-NH2	-8.09	116.25	120.30
1	H	72	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	H	72	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	C	147	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	C	72	ARG	NE-CZ-NH2	-5.64	117.48	120.30

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	992	1016	1003	4	0
1	B	989	1009	997	2	0
1	C	998	1023	1011	11	0
1	D	986	1006	993	11	0
1	E	986	1005	1003	2	0
1	F	986	1004	1003	9	0
1	G	980	1002	987	7	0
1	H	980	1002	988	14	0
1	J	912	925	911	7	0
2	I	915	930	916	6	0
3	A	6	8	8	0	0
3	B	6	8	8	0	0
3	E	6	8	8	0	0
3	F	12	16	16	1	0
3	J	6	8	8	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	1	0
4	E	2	0	0	0	0
4	F	1	0	0	1	0
4	H	1	0	0	0	0
4	I	2	0	0	0	0
5	A	162	0	0	1	0
5	B	161	0	0	2	0
5	C	191	0	0	3	0
5	D	145	0	0	4	0
5	E	180	0	0	2	1
5	F	166	0	0	4	1
5	G	117	0	0	4	0
5	H	145	0	0	3	0
5	I	59	0	0	2	0
5	J	85	0	0	0	0
All	All	11181	9970	9860	73	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 4.

The worst 5 of 73 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:43:GLY:N	5:C:2001:HOH:O	1.97	0.96
1:D:158:MLY:O	5:D:2122:HOH:O	1.92	0.85
1:F:61:GLU:OE2	1:F:170:ARG:CD	2.25	0.85
1:F:61:GLU:OE2	1:F:170:ARG:HD2	1.78	0.83
1:G:157:ASN:ND2	5:G:2009:HOH:O	2.13	0.81

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)
5:E:2037:HOH:O	5:F:2155:HOH:O[1_655]	2.06	0.14

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	128/130 (98%)	127 (99%)	1 (1%)	0	100	100
1	B	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
1	C	128/130 (98%)	126 (98%)	2 (2%)	0	100	100
1	D	126/130 (97%)	124 (98%)	2 (2%)	0	100	100
1	E	125/130 (96%)	124 (99%)	1 (1%)	0	100	100
1	F	125/130 (96%)	124 (99%)	1 (1%)	0	100	100
1	G	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
1	H	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
1	J	114/130 (88%)	109 (96%)	5 (4%)	0	100	100
2	I	115/130 (88%)	112 (97%)	3 (3%)	0	100	100
All	All	1238/1300 (95%)	1218 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

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	106/101 (105%)	103 (97%)	3 (3%)	43	34
1	B	105/101 (104%)	105 (100%)	0	100	100
1	C	106/101 (105%)	100 (94%)	6 (6%)	20	10
1	D	104/101 (103%)	101 (97%)	3 (3%)	42	33
1	E	103/101 (102%)	102 (99%)	1 (1%)	76	75
1	F	103/101 (102%)	101 (98%)	2 (2%)	57	51
1	G	103/101 (102%)	101 (98%)	2 (2%)	57	51
1	H	103/101 (102%)	97 (94%)	6 (6%)	20	10
1	J	97/101 (96%)	93 (96%)	4 (4%)	30	20
2	I	98/101 (97%)	93 (95%)	5 (5%)	24	13
All	All	1028/1010 (102%)	996 (97%)	32 (3%)	43	30

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	47	SER
1	J	79	LEU
1	E	111	ASN
1	D	124	LEU
1	J	82	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	110	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

28 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	MLY	A	59	1	9,10,11	0.84	0	6,11,13	0.64	0
1	MLY	C	158	1	9,10,11	0.62	0	6,11,13	0.76	0
1	MLY	E	158	1	9,10,11	0.70	0	6,11,13	0.64	0
1	MLY	D	130	1	9,10,11	0.81	0	6,11,13	1.12	0
1	MLY	H	59	1	9,10,11	0.73	0	6,11,13	0.77	0
2	MLY	I	59	2	9,10,11	0.75	0	6,11,13	0.84	0
1	MLY	F	59	1	9,10,11	0.79	0	6,11,13	0.63	0
1	MLY	B	130	1	9,10,11	1.00	0	6,11,13	1.51	1 (16%)
1	MLY	D	59	1	9,10,11	0.57	0	6,11,13	0.94	0
1	MLY	D	158	1	9,10,11	0.66	0	6,11,13	0.76	0
1	MLY	J	59	1	9,10,11	0.88	0	6,11,13	0.91	0
1	MLY	J	130	1	9,10,11	0.64	0	6,11,13	0.85	0
1	MLY	B	158	1	9,10,11	0.78	0	6,11,13	0.95	0
1	MLY	G	130	1	9,10,11	0.74	0	6,11,13	1.34	1 (16%)
2	MLY	I	130	2	9,10,11	0.78	0	6,11,13	0.78	0
1	MLY	A	130	1	9,10,11	0.88	0	6,11,13	1.19	1 (16%)
1	MLY	C	59	1	9,10,11	0.67	0	6,11,13	0.66	0
1	MLY	G	158	1	9,10,11	0.61	0	6,11,13	0.68	0
1	MLY	H	130	1	9,10,11	0.94	0	6,11,13	1.05	1 (16%)
1	MLY	F	130	1	9,10,11	0.67	0	6,11,13	1.17	0
1	MLY	A	158	1	9,10,11	0.78	0	6,11,13	0.96	0
1	MLY	E	130	1	9,10,11	0.76	0	6,11,13	1.27	2 (33%)
1	MLY	H	158	1	9,10,11	0.74	0	6,11,13	0.49	0
1	MLY	B	59	1	9,10,11	0.76	0	6,11,13	0.69	0
1	MLY	C	130	1	9,10,11	0.66	0	6,11,13	0.84	0
1	MLY	G	59	1	9,10,11	0.44	0	6,11,13	1.02	0
1	MLY	F	158	1	9,10,11	0.87	1 (11%)	6,11,13	0.81	0
1	MLY	E	59	1	9,10,11	0.93	0	6,11,13	0.97	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	MLY	A	59	1	-	1/8/9/11	-
1	MLY	C	158	1	-	0/8/9/11	-
1	MLY	E	158	1	-	0/8/9/11	-
1	MLY	D	130	1	-	0/8/9/11	-
1	MLY	H	59	1	-	5/8/9/11	-
2	MLY	I	59	2	-	6/8/9/11	-
1	MLY	F	59	1	-	0/8/9/11	-
1	MLY	B	130	1	-	0/8/9/11	-
1	MLY	D	59	1	-	3/8/9/11	-
1	MLY	D	158	1	-	1/8/9/11	-
1	MLY	J	59	1	-	3/8/9/11	-
1	MLY	J	130	1	-	1/8/9/11	-
1	MLY	B	158	1	-	0/8/9/11	-
1	MLY	G	130	1	-	0/8/9/11	-
2	MLY	I	130	2	-	0/8/9/11	-
1	MLY	A	130	1	-	0/8/9/11	-
1	MLY	C	59	1	-	4/8/9/11	-
1	MLY	G	158	1	-	0/8/9/11	-
1	MLY	H	130	1	-	1/8/9/11	-
1	MLY	F	130	1	-	0/8/9/11	-
1	MLY	A	158	1	-	0/8/9/11	-
1	MLY	E	130	1	-	3/8/9/11	-
1	MLY	H	158	1	-	1/8/9/11	-
1	MLY	B	59	1	-	2/8/9/11	-
1	MLY	C	130	1	-	1/8/9/11	-
1	MLY	G	59	1	-	4/8/9/11	-
1	MLY	F	158	1	-	1/8/9/11	-
1	MLY	E	59	1	-	1/8/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	158	MLY	CE-NZ	2.05	1.53	1.46

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	130	MLY	CH2-NZ-CE	-2.90	99.24	110.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	130	MLY	CD-CE-NZ	-2.60	106.99	113.71
1	G	130	MLY	CH1-NZ-CE	-2.58	100.52	110.75
1	E	130	MLY	CH2-NZ-CH1	-2.15	104.20	109.72
1	E	130	MLY	CH2-NZ-CE	-2.08	102.52	110.75

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	59	MLY	O-C-CA-CB
1	C	59	MLY	O-C-CA-CB
1	D	59	MLY	O-C-CA-CB
1	E	59	MLY	O-C-CA-CB
1	G	59	MLY	O-C-CA-CB

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	158	MLY	1	0
1	H	59	MLY	1	0
1	D	158	MLY	1	0
1	J	59	MLY	2	0
1	C	59	MLY	1	0
1	G	59	MLY	1	0

5.5   Carbohydrates   ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry   ⓘ

Of 16 ligands modelled in this entry, 10 are monoatomic - leaving 6 for Mogul analysis.

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	GOL	F	1174	-	5,5,5	0.67	0	5,5,5	0.88	0
3	GOL	J	1171	-	5,5,5	0.38	0	5,5,5	0.41	0
3	GOL	E	1173	-	5,5,5	0.62	0	5,5,5	1.42	1 (20%)
3	GOL	A	1171	-	5,5,5	0.36	0	5,5,5	0.66	0
3	GOL	B	1172	-	5,5,5	0.27	0	5,5,5	0.79	0
3	GOL	F	1173	-	5,5,5	0.45	0	5,5,5	0.52	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	GOL	F	1174	-	-	1/4/4/4	-
3	GOL	J	1171	-	-	2/4/4/4	-
3	GOL	E	1173	-	-	3/4/4/4	-
3	GOL	A	1171	-	-	0/4/4/4	-
3	GOL	B	1172	-	-	0/4/4/4	-
3	GOL	F	1173	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	1173	GOL	O3-C3-C2	-2.55	98.91	110.38

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1173	GOL	C1-C2-C3-O3
3	E	1173	GOL	O2-C2-C3-O3
3	J	1171	GOL	C1-C2-C3-O3
3	E	1173	GOL	O1-C1-C2-O2
3	J	1171	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1174	GOL	1	0

5.7 Other polymers ⓘ

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 ⓘ

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	123/130 (94%)	-0.09	0	100	100	16, 24, 34, 61	0
1	B	124/130 (95%)	0.00	0	100	100	15, 26, 37, 54	0
1	C	125/130 (96%)	-0.10	0	100	100	15, 22, 34, 44	0
1	D	124/130 (95%)	0.03	0	100	100	16, 25, 38, 57	0
1	E	125/130 (96%)	-0.12	0	100	100	15, 21, 32, 43	0
1	F	125/130 (96%)	-0.08	0	100	100	15, 21, 32, 43	0
1	G	123/130 (94%)	-0.08	1 (0%)	86	87	15, 23, 37, 47	0
1	H	123/130 (94%)	0.02	0	100	100	15, 24, 36, 46	0
1	J	114/130 (87%)	0.24	2 (1%)	68	71	23, 36, 50, 59	0
2	I	115/130 (88%)	0.63	10 (8%)	10	12	23, 39, 57, 66	0
All	All	1221/1300 (93%)	0.04	13 (1%)	80	82	15, 25, 44, 66	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	159	PHE	5.6
2	I	160	TYR	3.5
2	I	51	PHE	3.0
2	I	57	ALA	2.9
2	I	64	PHE	2.8

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
2	MLY	I	59	11/12	0.87	0.27	44,64,73,73	0
1	MLY	J	59	11/12	0.92	0.21	37,51,72,72	0
1	MLY	C	59	11/12	0.93	0.18	25,41,58,58	0
1	MLY	H	59	11/12	0.93	0.14	27,41,57,57	0
1	MLY	A	59	11/12	0.94	0.14	26,35,52,52	0
2	MLY	I	130	11/12	0.94	0.18	29,47,67,67	0
1	MLY	B	59	11/12	0.94	0.18	27,42,53,53	0
1	MLY	G	59	11/12	0.95	0.14	26,36,56,56	0
1	MLY	D	59	11/12	0.96	0.13	29,38,47,47	0
1	MLY	D	158	11/12	0.96	0.12	22,35,54,54	0
1	MLY	F	158	11/12	0.96	0.13	14,28,52,52	0
1	MLY	A	130	11/12	0.96	0.13	15,26,41,41	0
1	MLY	J	130	11/12	0.96	0.11	27,45,55,58	0
1	MLY	F	59	11/12	0.97	0.11	16,20,23,24	0
1	MLY	F	130	11/12	0.97	0.14	16,28,49,49	0
1	MLY	A	158	11/12	0.97	0.13	15,28,44,44	0
1	MLY	C	130	11/12	0.97	0.12	14,27,46,46	0
1	MLY	C	158	11/12	0.97	0.10	17,27,45,45	0
1	MLY	B	130	11/12	0.97	0.12	16,31,44,44	0
1	MLY	B	158	11/12	0.97	0.11	15,29,47,47	0
1	MLY	E	130	11/12	0.97	0.13	17,30,50,50	0
1	MLY	E	158	11/12	0.97	0.12	14,26,43,43	0
1	MLY	H	158	11/12	0.98	0.11	17,27,40,40	0
1	MLY	G	130	11/12	0.98	0.11	17,29,47,47	0
1	MLY	G	158	11/12	0.98	0.10	20,28,35,40	0
1	MLY	D	130	11/12	0.98	0.11	18,32,54,54	0
1	MLY	H	130	11/12	0.98	0.12	14,29,48,48	0
1	MLY	E	59	11/12	0.99	0.11	16,20,24,24	0

6.3 Carbohydrates (i)

There are no monosaccharides 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(Å^2)	Q<0.9
3	GOL	F	1174	6/6	0.84	0.15	30,37,45,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
4	CL	C	1174	1/1	0.88	0.07	40,40,40,40	0
4	CL	H	1171	1/1	0.88	0.20	59,59,59,59	0
3	GOL	J	1171	6/6	0.90	0.10	49,58,67,69	0
4	CL	I	1172	1/1	0.90	0.18	39,39,39,39	0
4	CL	I	1171	1/1	0.92	0.25	61,61,61,61	0
3	GOL	E	1173	6/6	0.92	0.15	22,30,34,36	0
3	GOL	F	1173	6/6	0.93	0.14	24,30,35,39	0
4	CL	C	1173	1/1	0.95	0.27	52,52,52,52	0
3	GOL	B	1172	6/6	0.96	0.10	21,27,30,32	0
3	GOL	A	1171	6/6	0.96	0.12	19,25,30,32	0
4	CL	E	1175	1/1	0.97	0.05	42,42,42,42	0
4	CL	B	1173	1/1	0.99	0.11	16,16,16,16	0
4	CL	E	1174	1/1	0.99	0.12	17,17,17,17	0
4	CL	F	1175	1/1	1.00	0.15	16,16,16,16	0
4	CL	A	1172	1/1	1.00	0.13	17,17,17,17	0

6.5 Other polymers ⓘ

There are no such residues in this entry.