



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 14, 2020 – 01:19 pm BST

PDB ID : 2MYS
Title : MYOSIN SUBFRAGMENT-1, ALPHA CARBON COORDINATES ONLY
FOR THE TWO LIGHT CHAINS
Authors : Rayment, I.; Holden, H.M.
Deposited on : 1996-06-27
Resolution : 2.80 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 ⓘ 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)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

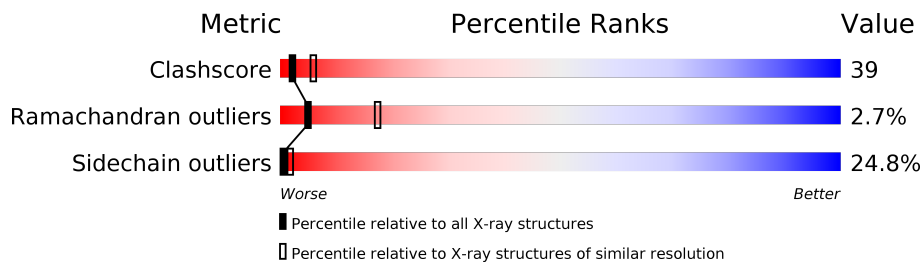
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	843	
2	B	166	
3	C	149	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	5000	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6788 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 MYOSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	800	6510	4206	1081	1187	36	0	0	0

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	30	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	35	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	45	GLN	GLU	CONFLICT	UNP P13538
A	49	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	55	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	59	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	63	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	84	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	87	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	107	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	130	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	138	MLY	GLU	CONFLICT	UNP P13538
A	190	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	236	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	248	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	272	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	295	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	296	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	317	GLU	GLN	CONFLICT	UNP P13538
A	348	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	353	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	367	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	369	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	385	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	407	GLY	LYS	CONFLICT	UNP P13538
A	412	ALA	PHE	CONFLICT	UNP P13538

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Chain	Residue	Modelled	Actual	Comment	Reference
A	415	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	417	GLU	GLN	CONFLICT	UNP P13538
A	421	GLU	GLN	CONFLICT	UNP P13538
A	431	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	436	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	486	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	504	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	505	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	528	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	551	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	553	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	557	GLU	GLN	CONFLICT	UNP P13538
A	598	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	600	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	613	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	617	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	659	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	681	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	750	GLY	SER	CONFLICT	UNP P13538
A	751	GLY	ILE	CONFLICT	UNP P13538
A	759	ALA	ARG	CONFLICT	UNP P13538
A	764	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	768	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	782	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	789	ALA	ARG	CONFLICT	UNP P13538
A	805	ALA	ARG	CONFLICT	UNP P13538
A	827	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	833	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	837	MLY	LYS	MODIFIED RESIDUE	UNP P13538
A	839	MLY	LYS	MODIFIED RESIDUE	UNP P13538

- Molecule 2 is a protein called MYOSIN.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	B	138	Total C 138 138	0	0	138

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	21	GLU	GLN	CONFLICT	UNP P02609
B	23	GLU	GLN	CONFLICT	UNP P02609

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Chain	Residue	Modelled	Actual	Comment	Reference
B	25	GLU	GLN	CONFLICT	UNP P02609
B	26	ASP	GLU	CONFLICT	UNP P02609
B	38	ALA	ARG	CONFLICT	UNP P02609
B	124	GLY	GLN	CONFLICT	UNP P02609
B	125	GLY	CYS	CONFLICT	UNP P02609
B	126	GLY	ASP	CONFLICT	UNP P02609
B	163	ALA	LYS	CONFLICT	UNP P02609

- Molecule 3 is a protein called MYOSIN.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	C	134	Total C 134 134	0	0	134

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	4	LYS	PRO	CONFLICT	UNP P02605
C	5	ALA	ASP	CONFLICT	UNP P02605
C	6	ALA	GLN	CONFLICT	UNP P02605
C	7	ALA	ILE	CONFLICT	UNP P02605
C	27	ALA	LEU	CONFLICT	UNP P02605
C	34	ALA	VAL	CONFLICT	UNP P02605
C	61	ALA	LYS	CONFLICT	UNP P02605
C	62	ALA	LYS	CONFLICT	UNP P02605

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

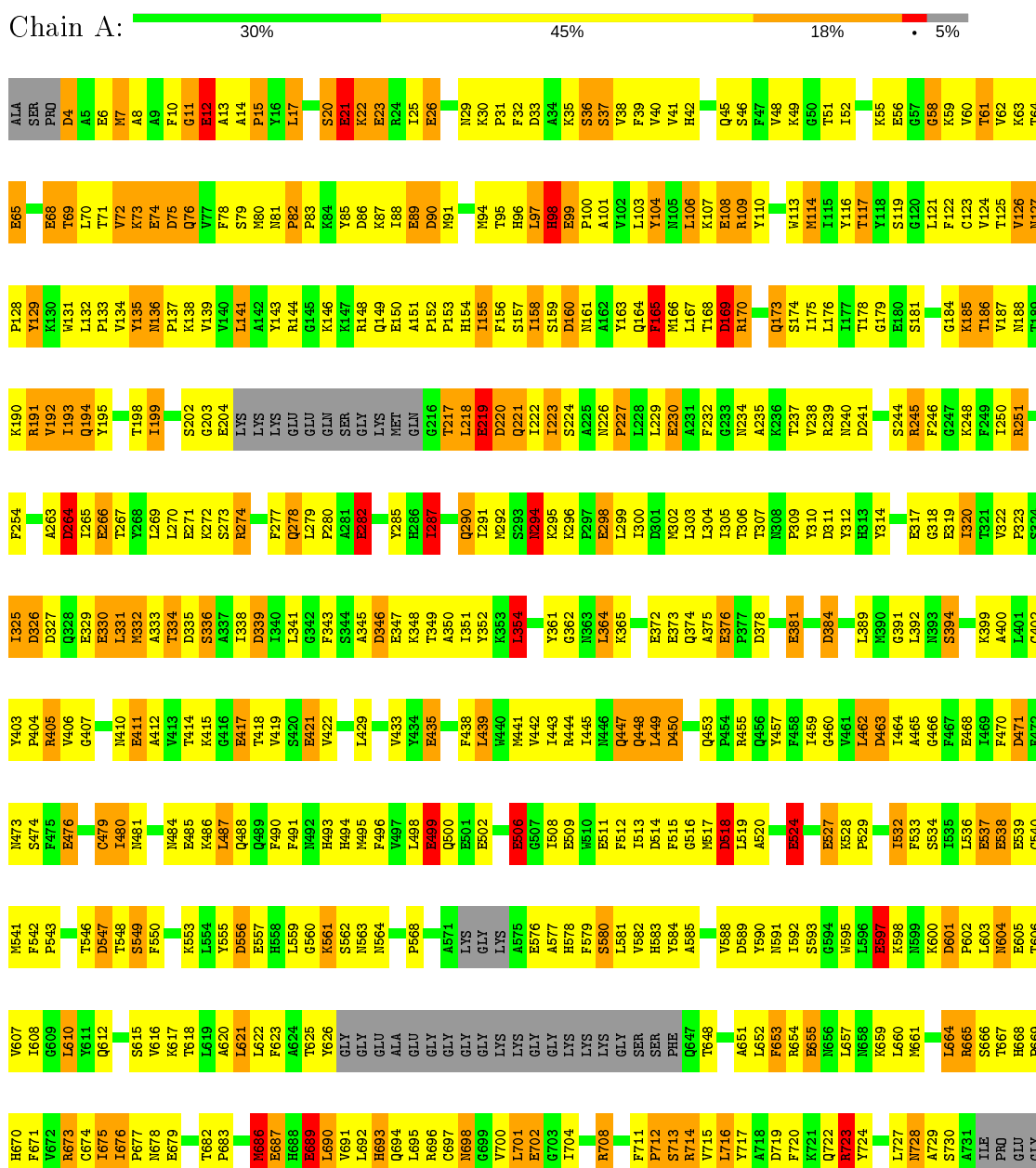
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		

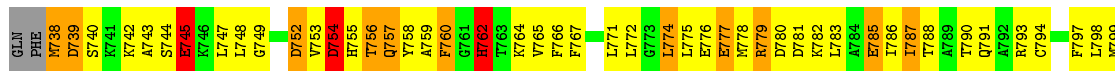
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

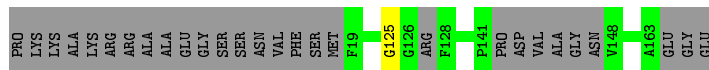
- Molecule 1: MYOSIN





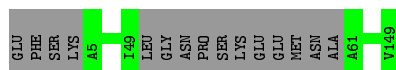
- Molecule 2: MYOSIN

Chain B: 83% 17%



- Molecule 3: MYOSIN

Chain C: 90% 10%



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	98.40 Å 124.20 Å 274.90 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.80)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.223 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6788	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

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: MG, MLY, SO4

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	1.25	58/6156 (0.9%)	1.51	91/8350 (1.1%)

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	1

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	476	GLU	CD-OE1	8.78	1.35	1.25
1	A	576	GLU	CD-OE1	8.71	1.35	1.25
1	A	204	GLU	CD-OE2	8.33	1.34	1.25
1	A	745	GLU	CD-OE2	8.26	1.34	1.25
1	A	411	GLU	CD-OE1	8.20	1.34	1.25

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	800	ARG	NE-CZ-NH2	-16.34	112.13	120.30
1	A	98	HIS	CB-CA-C	-11.56	87.28	110.40
1	A	327	ASP	CB-CG-OD1	-9.97	109.33	118.30
1	A	241	ASP	CB-CG-OD1	-9.78	109.50	118.30
1	A	264	ASP	CB-CG-OD2	-9.48	109.77	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	98	HIS	Mainchain

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	6510	0	6500	524	1
2	B	138	0	0	1	0
3	C	134	0	0	0	0
4	A	5	0	0	2	0
5	B	1	0	0	0	0
All	All	6788	0	6500	524	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 39.

The worst 5 of 524 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:72:VAL:HG13	1:A:76:GLN:HB3	1.36	1.03
1:A:98:HIS:HB3	1:A:100:PRO:HD2	1.42	0.99
1:A:56:GLU:HB2	1:A:59:MLY:HB3	1.40	0.99
1:A:174:SER:HB3	1:A:667:THR:HG21	1.44	0.97
1:A:546:THR:HG22	1:A:548:THR:H	1.32	0.94

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)
1:A:561:LYS:NZ	1:A:561:LYS:NZ[4_566]	2.17	0.03

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	745/843 (88%)	619 (83%)	106 (14%)	20 (3%)	5 17

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	LYS
1	A	712	PRO
1	A	729	ALA
1	A	757	GLN
1	A	762	HIS

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	645/674 (96%)	485 (75%)	160 (25%)	0 2

5 of 160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	365	LYS
1	A	462	LEU
1	A	787	ILE
1	A	376	GLU
1	A	410	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	424	ASN
1	A	481	ASN
1	A	757	GLN
1	A	447	GLN
1	A	453	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

45 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	0.87	0	6,11,13	0.49	0
1	MLY	A	436	1	9,10,11	1.07	1 (11%)	6,11,13	0.49	0
1	MLY	A	19	1	9,10,11	1.19	1 (11%)	6,11,13	0.57	0
1	MLY	A	190	1	9,10,11	1.24	1 (11%)	6,11,13	0.52	0
1	MLY	A	369	1	9,10,11	0.69	0	6,11,13	0.45	0
1	MLY	A	505	1	9,10,11	0.89	1 (11%)	6,11,13	0.35	0
1	MLY	A	768	1	9,10,11	0.77	0	6,11,13	0.41	0
1	MLY	A	431	1	9,10,11	0.52	0	6,11,13	0.45	0
1	MLY	A	296	1	9,10,11	0.65	0	6,11,13	0.37	0
1	MLY	A	248	1	9,10,11	0.82	0	6,11,13	0.61	0
1	MLY	A	107	1	9,10,11	0.47	0	6,11,13	0.33	0
1	MLY	A	681	1	9,10,11	0.61	0	6,11,13	0.45	0
1	MLY	A	348	1	9,10,11	0.83	0	6,11,13	0.47	0
1	MLY	A	486	1	9,10,11	0.64	0	6,11,13	0.39	0
1	MLY	A	600	1	9,10,11	0.52	0	6,11,13	0.37	0
1	MLY	A	55	1	9,10,11	0.72	0	6,11,13	0.79	0
1	MLY	A	827	1	9,10,11	0.70	0	6,11,13	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	A	63	1	9,10,11	0.93	1 (11%)	6,11,13	0.43	0
1	MLY	A	385	1	9,10,11	0.99	1 (11%)	6,11,13	0.44	0
1	MLY	A	613	1	9,10,11	0.57	0	6,11,13	0.64	0
1	MLY	A	49	1	9,10,11	1.10	1 (11%)	6,11,13	0.74	0
1	MLY	A	415	1	9,10,11	0.77	0	6,11,13	0.18	0
1	MLY	A	30	1	9,10,11	0.88	0	6,11,13	0.31	0
1	MLY	A	837	1	9,10,11	0.60	0	6,11,13	0.55	0
1	MLY	A	130	1	9,10,11	0.78	0	6,11,13	0.74	0
1	MLY	A	236	1	9,10,11	0.79	1 (11%)	6,11,13	0.48	0
1	MLY	A	617	1	9,10,11	0.95	1 (11%)	6,11,13	0.34	0
1	MLY	A	84	1	9,10,11	0.50	0	6,11,13	0.80	0
1	MLY	A	295	1	9,10,11	0.80	0	6,11,13	0.34	0
1	MLY	A	353	1	9,10,11	0.86	0	6,11,13	0.79	0
1	MLY	A	659	1	9,10,11	0.83	0	6,11,13	0.59	0
1	MLY	A	87	1	9,10,11	1.22	1 (11%)	6,11,13	0.43	0
1	MLY	A	528	1	9,10,11	0.89	0	6,11,13	0.65	0
1	MLY	A	35	1	9,10,11	0.74	0	6,11,13	0.38	0
1	MLY	A	272	1	9,10,11	1.00	1 (11%)	6,11,13	0.55	0
1	MLY	A	367	1	9,10,11	0.63	0	6,11,13	0.37	0
1	MLY	A	504	1	9,10,11	0.87	0	6,11,13	0.23	0
1	MLY	A	553	1	9,10,11	0.65	0	6,11,13	0.54	0
1	MLY	A	551	1	9,10,11	0.52	0	6,11,13	0.19	0
1	MLY	A	833	1	9,10,11	1.16	1 (11%)	6,11,13	0.31	0
1	MLY	A	138	1	9,10,11	1.34	1 (11%)	6,11,13	0.84	0
1	MLY	A	782	1	9,10,11	0.78	0	6,11,13	0.35	0
1	MLY	A	598	1	9,10,11	0.88	1 (11%)	6,11,13	0.44	0
1	MLY	A	764	1	9,10,11	0.86	0	6,11,13	0.36	0
1	MLY	A	839	1	9,10,11	0.72	0	6,11,13	0.78	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	-	3/8/9/11	-
1	MLY	A	436	1	-	4/8/9/11	-
1	MLY	A	19	1	-	4/8/9/11	-
1	MLY	A	190	1	-	5/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	369	1	-	2/8/9/11	-
1	MLY	A	505	1	-	5/8/9/11	-
1	MLY	A	768	1	-	4/8/9/11	-
1	MLY	A	431	1	-	4/8/9/11	-
1	MLY	A	296	1	-	4/8/9/11	-
1	MLY	A	248	1	-	6/8/9/11	-
1	MLY	A	107	1	-	2/8/9/11	-
1	MLY	A	681	1	-	4/8/9/11	-
1	MLY	A	348	1	-	5/8/9/11	-
1	MLY	A	486	1	-	2/8/9/11	-
1	MLY	A	600	1	-	3/8/9/11	-
1	MLY	A	55	1	-	6/8/9/11	-
1	MLY	A	827	1	-	0/8/9/11	-
1	MLY	A	63	1	-	4/8/9/11	-
1	MLY	A	385	1	-	2/8/9/11	-
1	MLY	A	613	1	-	4/8/9/11	-
1	MLY	A	49	1	-	3/8/9/11	-
1	MLY	A	415	1	-	3/8/9/11	-
1	MLY	A	30	1	-	2/8/9/11	-
1	MLY	A	837	1	-	5/8/9/11	-
1	MLY	A	130	1	-	5/8/9/11	-
1	MLY	A	236	1	-	3/8/9/11	-
1	MLY	A	617	1	-	1/8/9/11	-
1	MLY	A	84	1	-	4/8/9/11	-
1	MLY	A	295	1	-	2/8/9/11	-
1	MLY	A	353	1	-	4/8/9/11	-
1	MLY	A	659	1	-	3/8/9/11	-
1	MLY	A	87	1	-	2/8/9/11	-
1	MLY	A	528	1	-	4/8/9/11	-
1	MLY	A	35	1	-	3/8/9/11	-
1	MLY	A	272	1	-	3/8/9/11	-
1	MLY	A	367	1	-	2/8/9/11	-
1	MLY	A	504	1	-	4/8/9/11	-
1	MLY	A	553	1	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	551	1	-	3/8/9/11	-
1	MLY	A	833	1	-	6/8/9/11	-
1	MLY	A	138	1	-	4/8/9/11	-
1	MLY	A	782	1	-	6/8/9/11	-
1	MLY	A	598	1	-	5/8/9/11	-
1	MLY	A	764	1	-	2/8/9/11	-
1	MLY	A	839	1	-	3/8/9/11	-

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	138	MLY	CB-CA	-3.64	1.48	1.53
1	A	19	MLY	CB-CA	-3.21	1.49	1.53
1	A	87	MLY	CB-CA	-3.13	1.49	1.53
1	A	436	MLY	CB-CA	-2.96	1.49	1.53
1	A	49	MLY	CB-CA	-2.86	1.49	1.53

There are no bond angle outliers.

There are no chirality outliers.

5 of 159 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	436	MLY	C-CA-CB-CG
1	A	19	MLY	C-CA-CB-CG
1	A	505	MLY	N-CA-CB-CG
1	A	505	MLY	C-CA-CB-CG
1	A	248	MLY	N-CA-CB-CG

There are no ring outliers.

27 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	59	MLY	3	0
1	A	190	MLY	2	0
1	A	296	MLY	3	0
1	A	248	MLY	2	0
1	A	107	MLY	3	0
1	A	348	MLY	5	0
1	A	486	MLY	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	600	MLY	1	0
1	A	55	MLY	1	0
1	A	63	MLY	3	0
1	A	49	MLY	4	0
1	A	415	MLY	1	0
1	A	30	MLY	1	0
1	A	837	MLY	1	0
1	A	617	MLY	1	0
1	A	295	MLY	6	0
1	A	659	MLY	2	0
1	A	87	MLY	2	0
1	A	528	MLY	3	0
1	A	35	MLY	1	0
1	A	272	MLY	1	0
1	A	553	MLY	2	0
1	A	138	MLY	1	0
1	A	782	MLY	1	0
1	A	598	MLY	1	0
1	A	764	MLY	1	0
1	A	839	MLY	4	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z > 2$
4	SO4	A	5000	-	4,4,4	0.37	0	6,6,6	0.25	0

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	5000	SO4	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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.