



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:56 AM UTC

PDB ID : 4A5P / pdb_00004a5p
Title : Structure of the Shigella flexneri MxiA protein
Authors : Abrusci, P.; Vegara-Irigaray, M.; Johnson, S.; Roversi, P.; Friede, M.E.; Deane, J.E.; Tang, C.M.; Lea, S.M.
Deposited on : 2011-10-26
Resolution : 3.15 Å(reported)

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

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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

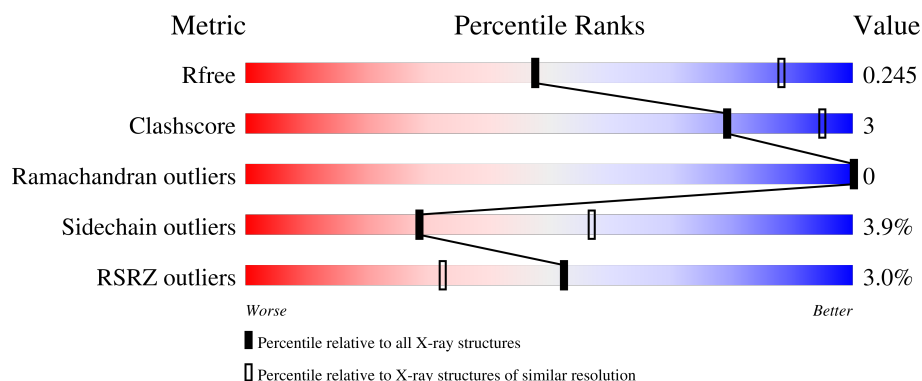
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	383	
1	B	383	
1	C	383	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7421 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 PROTEIN MXIA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	0	0
			2429	1559	413	449	8			
1	B	305	Total	C	N	O	S	0	1	0
			2517	1621	424	464	8			
1	C	297	Total	C	N	O	S	0	0	0
			2451	1578	412	453	8			

There are 42 discrepancies between the modelled and reference sequences:

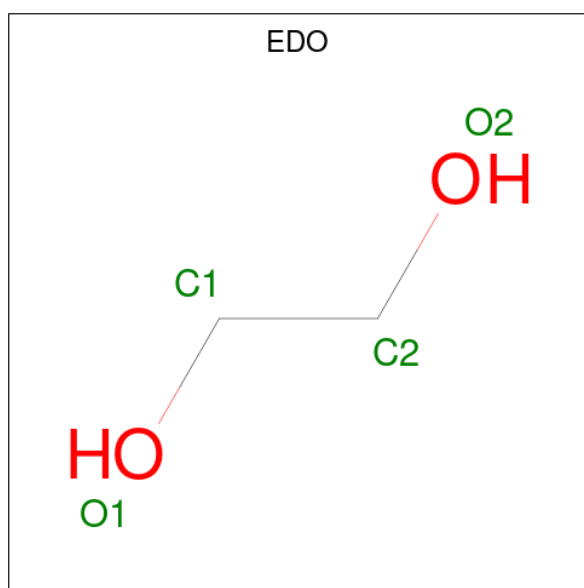
Chain	Residue	Modelled	Actual	Comment	Reference
A	304	MET	-	expression tag	UNP P0A1I5
A	305	GLY	-	expression tag	UNP P0A1I5
A	306	SER	-	expression tag	UNP P0A1I5
A	307	SER	-	expression tag	UNP P0A1I5
A	308	HIS	-	expression tag	UNP P0A1I5
A	309	HIS	-	expression tag	UNP P0A1I5
A	310	HIS	-	expression tag	UNP P0A1I5
A	311	HIS	-	expression tag	UNP P0A1I5
A	312	HIS	-	expression tag	UNP P0A1I5
A	313	HIS	-	expression tag	UNP P0A1I5
A	314	SER	-	expression tag	UNP P0A1I5
A	315	GLN	-	expression tag	UNP P0A1I5
A	316	ASP	-	expression tag	UNP P0A1I5
A	317	PRO	-	expression tag	UNP P0A1I5
B	304	MET	-	expression tag	UNP P0A1I5
B	305	GLY	-	expression tag	UNP P0A1I5
B	306	SER	-	expression tag	UNP P0A1I5
B	307	SER	-	expression tag	UNP P0A1I5
B	308	HIS	-	expression tag	UNP P0A1I5
B	309	HIS	-	expression tag	UNP P0A1I5
B	310	HIS	-	expression tag	UNP P0A1I5
B	311	HIS	-	expression tag	UNP P0A1I5
B	312	HIS	-	expression tag	UNP P0A1I5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	313	HIS	-	expression tag	UNP P0A1I5
B	314	SER	-	expression tag	UNP P0A1I5
B	315	GLN	-	expression tag	UNP P0A1I5
B	316	ASP	-	expression tag	UNP P0A1I5
B	317	PRO	-	expression tag	UNP P0A1I5
C	304	MET	-	expression tag	UNP P0A1I5
C	305	GLY	-	expression tag	UNP P0A1I5
C	306	SER	-	expression tag	UNP P0A1I5
C	307	SER	-	expression tag	UNP P0A1I5
C	308	HIS	-	expression tag	UNP P0A1I5
C	309	HIS	-	expression tag	UNP P0A1I5
C	310	HIS	-	expression tag	UNP P0A1I5
C	311	HIS	-	expression tag	UNP P0A1I5
C	312	HIS	-	expression tag	UNP P0A1I5
C	313	HIS	-	expression tag	UNP P0A1I5
C	314	SER	-	expression tag	UNP P0A1I5
C	315	GLN	-	expression tag	UNP P0A1I5
C	316	ASP	-	expression tag	UNP P0A1I5
C	317	PRO	-	expression tag	UNP P0A1I5

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

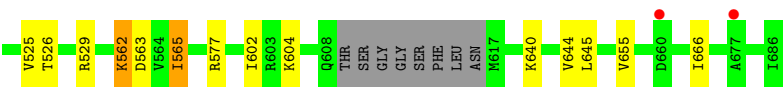
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total 5	O 5	0	0
3	B	8	Total 8	O 8	0	0
3	C	3	Total 3	O 3	0	0

i

- Molecule 1: PROTEIN MXIA





4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	160.61Å 160.61Å 100.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.72 – 3.15 35.72 – 3.15	Depositor EDS
% Data completeness (in resolution range)	93.4 (35.72-3.15) 93.8 (35.72-3.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.18Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.231 , 0.251 (Not available) , 0.245	Depositor DCC
R_{free} test set	1226 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	70.8	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.046 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7421	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.78	0/2328	1.23	2/3153 (0.1%)
1	B	0.77	0/2410	1.21	0/3268
1	C	0.77	0/2349	1.23	0/3182
All	All	0.77	0/7087	1.22	2/9603 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	638	ASN	CA-C-N	5.84	132.21	121.70
1	A	638	ASN	C-N-CA	5.84	132.21	121.70

There are no chirality outliers.

There are no planarity outliers.

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	2429	0	2497	13	0
1	B	2517	0	2599	13	0
1	C	2451	0	2527	14	0
2	A	4	0	6	1	0
2	B	4	0	6	1	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	8	0	0	0	0
3	C	3	0	0	0	0
All	All	7421	0	7635	40	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 3.

All (40) 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:B:516:ASP:HA	1:B:519:MLY:HD3	1.77	0.66
1:B:641:MLY:HH13	1:B:641:MLY:HG3	1.83	0.61
1:A:604:MLY:HA	1:A:604:MLY:HH22	1.83	0.59
1:C:562:MLY:HH22	1:C:563:ASP:HA	1.87	0.55
1:C:562:MLY:HE2	1:C:563:ASP:HA	1.89	0.55
1:A:430:MLY:HD2	1:A:461:ASP:HA	1.88	0.55
1:B:503:THR:HG21	1:B:531:SER:HA	1.88	0.55
1:A:641:MLY:HA	1:A:641:MLY:HE2	1.88	0.54
1:C:395:ARG:HH22	1:C:509:GLN:HE22	1.55	0.54
1:B:575:LEU:HD23	2:B:1687:EDO:H22	1.93	0.50
1:B:656:MLY:HE2	1:B:660:ASP:HB3	1.92	0.50
1:A:543:SER:HB3	2:A:1687:EDO:H12	1.94	0.49
1:A:366:LEU:HD22	1:A:404:SER:HB2	1.96	0.47
1:B:430:MLY:HG3	1:B:461:ASP:HA	1.97	0.46
1:C:526:THR:H	1:C:529:ARG:HD2	1.79	0.46
1:C:361:VAL:HG23	1:C:364:ILE:HD11	1.98	0.46
1:C:529:ARG:NH2	1:C:562:MLY:HH12	2.32	0.46
1:C:602:ILE:HD13	1:C:655:VAL:HG22	1.98	0.46
1:B:591:VAL:HG12	1:B:644:VAL:HG12	1.98	0.45
1:A:593:MET:HE2	1:A:646:LEU:HD23	1.99	0.45
1:B:363:LEU:HB3	1:B:399:ILE:HG23	1.99	0.45
1:C:645:LEU:HB2	1:C:666:ILE:HD11	1.98	0.45
1:A:381:ILE:HG23	1:A:399:ILE:HD12	1.99	0.44
1:A:645:LEU:HB2	1:A:666:ILE:HD11	2.00	0.43
1:C:381:ILE:HG23	1:C:399:ILE:HD12	1.99	0.43
1:A:364:ILE:HB	1:A:415:LEU:HB2	1.99	0.43
1:B:432:CYS:HB2	1:B:476:MLY:HB2	2.00	0.43
1:A:590:MLY:HB2	1:A:683:LEU:HD11	2.01	0.43
1:B:363:LEU:HD22	1:B:399:ILE:HG12	2.00	0.43
1:A:606:ILE:HD11	1:A:651:ILE:HG22	2.01	0.42
1:C:525:VAL:HG12	1:C:529:ARG:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:ASN:HD21	1:B:549:LEU:HD13	1.83	0.41
1:C:384:ILE:HG21	1:C:486:LEU:HD23	2.01	0.41
1:B:602:ILE:HD13	1:B:655:VAL:HG22	2.01	0.41
1:B:408:MLY:HH22	1:B:408:MLY:HD3	1.93	0.41
1:C:565:ILE:H	1:C:565:ILE:HG13	1.76	0.41
1:C:364:ILE:HG12	1:C:400:LEU:HD23	2.02	0.40
1:A:414:LEU:HD13	1:A:486:LEU:HD11	2.02	0.40
1:A:604:MLY:HE3	1:A:604:MLY:HB3	1.78	0.40
1:C:364:ILE:HB	1:C:415:LEU:HB2	2.03	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	273/383 (71%)	268 (98%)	5 (2%)	0	100	100
1	B	284/383 (74%)	278 (98%)	6 (2%)	0	100	100
1	C	275/383 (72%)	269 (98%)	6 (2%)	0	100	100
All	All	832/1149 (72%)	815 (98%)	17 (2%)	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	261/337 (77%)	252 (97%)	9 (3%)	32	60
1	B	270/337 (80%)	257 (95%)	13 (5%)	23	52
1	C	264/337 (78%)	255 (97%)	9 (3%)	32	60
All	All	795/1011 (79%)	764 (96%)	31 (4%)	28	57

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	369	GLU
1	A	475	ILE
1	A	525	VAL
1	A	527	ILE
1	A	638	ASN
1	A	645	LEU
1	A	663	PHE
1	A	666	ILE
1	A	674	ILE
1	B	364	ILE
1	B	411	ASP
1	B	426	ILE
1	B	443	LEU
1	B	527	ILE
1	B	549	LEU
1	B	620	GLU
1	B	633	LEU
1	B	644	VAL
1	B	662	ARG
1	B	665	SER
1	B	674	ILE
1	B	676	GLU
1	C	364	ILE
1	C	366	LEU
1	C	426	ILE
1	C	431	VAL
1	C	433	ILE
1	C	475	ILE
1	C	565	ILE
1	C	577	ARG
1	C	644	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	387	GLN
1	A	405	ASN
1	A	425	ASN
1	A	535	GLN
1	A	541	ASN
1	A	638	ASN
1	B	405	ASN
1	B	425	ASN
1	B	535	GLN
1	B	546	ASN
1	B	631	HIS
1	B	638	ASN
1	B	661	ASN
1	C	405	ASN
1	C	505	ASN
1	C	509	GLN
1	C	541	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

37 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	B	476	1	9,10,11	0.48	0	6,11,13	1.12	0
1	MLY	B	430	1	9,10,11	0.52	0	6,11,13	1.13	0
1	MLY	A	640	1	9,10,11	0.84	0	6,11,13	0.86	0
1	MLY	C	562	1	9,10,11	0.99	0	6,11,13	1.32	1 (16%)
1	MLY	C	590	1	9,10,11	0.52	0	6,11,13	1.18	0
1	MLY	B	656	1	9,10,11	0.59	0	6,11,13	1.06	0
1	MLY	A	604	1	9,10,11	0.62	0	6,11,13	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	C	604	1	9,10,11	0.55	0	6,11,13	1.86	2 (33%)
1	MLY	C	664	1	9,10,11	0.47	0	6,11,13	1.15	0
1	MLY	A	656	1	9,10,11	0.57	0	6,11,13	0.96	0
1	MLY	B	684	1	9,10,11	0.52	0	6,11,13	1.12	0
1	MLY	B	664	1	9,10,11	0.63	0	6,11,13	1.37	1 (16%)
1	MLY	C	476	1	9,10,11	0.64	0	6,11,13	0.52	0
1	MLY	B	474	1	9,10,11	0.52	0	6,11,13	1.14	0
1	MLY	A	430	1	9,10,11	0.55	0	6,11,13	1.00	0
1	MLY	C	656	1	9,10,11	0.49	0	6,11,13	1.10	0
1	MLY	A	590	1	9,10,11	0.51	0	6,11,13	1.16	0
1	MLY	A	562	1	9,10,11	0.53	0	6,11,13	1.08	0
1	MLY	B	519	1	9,10,11	0.51	0	6,11,13	1.17	0
1	MLY	C	519	1	9,10,11	0.53	0	6,11,13	1.25	0
1	MLY	A	476	1	7,8,11	0.52	0	3,8,13	0.62	0
1	MLY	A	641	1	9,10,11	0.68	0	6,11,13	0.90	0
1	MLY	A	408	1	9,10,11	0.53	0	6,11,13	1.14	0
1	MLY	B	562	1	9,10,11	0.82	0	6,11,13	0.95	0
1	MLY	C	641	1	9,10,11	0.57	0	6,11,13	1.06	0
1	MLY	A	684	1	9,10,11	0.52	0	6,11,13	1.11	0
1	MLY	C	640	1	9,10,11	0.50	0	6,11,13	1.23	1 (16%)
1	MLY	B	408	1	9,10,11	0.60	0	6,11,13	0.68	0
1	MLY	C	408	1	9,10,11	0.56	0	6,11,13	0.97	0
1	MLY	B	590	1	9,10,11	0.50	0	6,11,13	1.14	0
1	MLY	C	430	1	9,10,11	0.67	0	6,11,13	0.48	0
1	MLY	C	684	1	9,10,11	0.65	0	6,11,13	0.87	0
1	MLY	B	604	1	9,10,11	0.56	0	6,11,13	1.07	0
1	MLY	A	664	1	9,10,11	0.48	0	6,11,13	1.17	0
1	MLY	B	641	1	9,10,11	0.73	0	6,11,13	0.70	0
1	MLY	B	640	1	9,10,11	0.49	0	6,11,13	1.10	0
1	MLY	A	519	1	9,10,11	0.47	0	6,11,13	1.19	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	B	476	1	-	5/8/9/11	-
1	MLY	B	430	1	-	5/8/9/11	-
1	MLY	A	640	1	-	2/8/9/11	-
1	MLY	C	562	1	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	C	590	1	-	5/8/9/11	-
1	MLY	B	656	1	-	0/8/9/11	-
1	MLY	A	604	1	-	5/8/9/11	-
1	MLY	C	604	1	-	3/8/9/11	-
1	MLY	C	664	1	-	4/8/9/11	-
1	MLY	A	656	1	-	2/8/9/11	-
1	MLY	B	684	1	-	3/8/9/11	-
1	MLY	B	664	1	-	2/8/9/11	-
1	MLY	C	476	1	-	3/8/9/11	-
1	MLY	B	474	1	-	3/8/9/11	-
1	MLY	A	430	1	-	4/8/9/11	-
1	MLY	C	656	1	-	6/8/9/11	-
1	MLY	A	590	1	-	5/8/9/11	-
1	MLY	A	562	1	-	4/8/9/11	-
1	MLY	B	519	1	-	1/8/9/11	-
1	MLY	C	519	1	-	1/8/9/11	-
1	MLY	A	476	1	-	2/6/7/11	-
1	MLY	A	641	1	-	4/8/9/11	-
1	MLY	A	408	1	-	4/8/9/11	-
1	MLY	B	562	1	-	5/8/9/11	-
1	MLY	C	641	1	-	6/8/9/11	-
1	MLY	A	684	1	-	1/8/9/11	-
1	MLY	C	640	1	-	5/8/9/11	-
1	MLY	B	408	1	-	2/8/9/11	-
1	MLY	C	408	1	-	1/8/9/11	-
1	MLY	B	590	1	-	5/8/9/11	-
1	MLY	C	430	1	-	5/8/9/11	-
1	MLY	C	684	1	-	3/8/9/11	-
1	MLY	B	604	1	-	5/8/9/11	-
1	MLY	A	664	1	-	2/8/9/11	-
1	MLY	B	641	1	-	5/8/9/11	-
1	MLY	B	640	1	-	5/8/9/11	-
1	MLY	A	519	1	-	5/8/9/11	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	604	MLY	CH2-NZ-CH1	-2.74	102.68	109.72
1	C	604	MLY	CH1-NZ-CE	-2.67	100.17	110.75
1	B	664	MLY	CH2-NZ-CH1	-2.40	103.56	109.72
1	C	640	MLY	CD-CE-NZ	-2.23	107.94	113.71
1	C	562	MLY	CH2-NZ-CH1	-2.07	104.42	109.72

There are no chirality outliers.

All (132) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	562	MLY	N-CA-CB-CG
1	A	562	MLY	C-CA-CB-CG
1	A	590	MLY	C-CA-CB-CG
1	A	604	MLY	N-CA-CB-CG
1	A	604	MLY	C-CA-CB-CG
1	A	641	MLY	C-CA-CB-CG
1	B	430	MLY	C-CA-CB-CG
1	B	474	MLY	C-CA-CB-CG
1	B	476	MLY	N-CA-CB-CG
1	B	476	MLY	C-CA-CB-CG
1	B	590	MLY	C-CA-CB-CG
1	B	590	MLY	O-C-CA-CB
1	B	604	MLY	N-CA-CB-CG
1	B	604	MLY	C-CA-CB-CG
1	B	640	MLY	N-CA-CB-CG
1	B	640	MLY	C-CA-CB-CG
1	B	640	MLY	O-C-CA-CB
1	B	641	MLY	C-CA-CB-CG
1	B	641	MLY	O-C-CA-CB
1	B	684	MLY	N-CA-CB-CG
1	B	684	MLY	C-CA-CB-CG
1	C	430	MLY	N-CA-CB-CG
1	C	430	MLY	C-CA-CB-CG
1	C	562	MLY	N-CA-CB-CG
1	C	562	MLY	C-CA-CB-CG
1	C	590	MLY	N-CA-CB-CG
1	C	590	MLY	C-CA-CB-CG
1	C	604	MLY	C-CA-CB-CG
1	C	640	MLY	C-CA-CB-CG
1	C	656	MLY	N-CA-CB-CG
1	C	656	MLY	C-CA-CB-CG
1	C	664	MLY	C-CA-CB-CG
1	A	408	MLY	CD-CE-NZ-CH2

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Mol	Chain	Res	Type	Atoms
1	A	430	MLY	CD-CE-NZ-CH2
1	B	476	MLY	CD-CE-NZ-CH1
1	C	640	MLY	CD-CE-NZ-CH1
1	C	640	MLY	CD-CE-NZ-CH2
1	C	656	MLY	CD-CE-NZ-CH1
1	C	656	MLY	CD-CE-NZ-CH2
1	C	664	MLY	CD-CE-NZ-CH2
1	A	656	MLY	CG-CD-CE-NZ
1	B	430	MLY	CG-CD-CE-NZ
1	B	590	MLY	CG-CD-CE-NZ
1	C	430	MLY	CG-CD-CE-NZ
1	A	562	MLY	CG-CD-CE-NZ
1	A	590	MLY	CG-CD-CE-NZ
1	A	604	MLY	CE-CD-CG-CB
1	C	476	MLY	CG-CD-CE-NZ
1	A	408	MLY	CD-CE-NZ-CH1
1	A	430	MLY	CD-CE-NZ-CH1
1	A	519	MLY	CD-CE-NZ-CH1
1	A	590	MLY	CD-CE-NZ-CH2
1	B	430	MLY	CD-CE-NZ-CH1
1	B	430	MLY	CD-CE-NZ-CH2
1	B	476	MLY	CD-CE-NZ-CH2
1	B	562	MLY	CD-CE-NZ-CH1
1	B	641	MLY	CD-CE-NZ-CH2
1	C	590	MLY	CD-CE-NZ-CH1
1	C	641	MLY	CD-CE-NZ-CH1
1	C	641	MLY	CD-CE-NZ-CH2
1	C	664	MLY	CD-CE-NZ-CH1
1	A	641	MLY	CG-CD-CE-NZ
1	C	641	MLY	CG-CD-CE-NZ
1	A	604	MLY	CG-CD-CE-NZ
1	B	664	MLY	CE-CD-CG-CB
1	C	664	MLY	CG-CD-CE-NZ
1	B	604	MLY	CA-CB-CG-CD
1	C	590	MLY	CG-CD-CE-NZ
1	B	519	MLY	CG-CD-CE-NZ
1	A	408	MLY	CA-CB-CG-CD
1	B	562	MLY	CG-CD-CE-NZ
1	A	604	MLY	CA-CB-CG-CD
1	B	476	MLY	CG-CD-CE-NZ
1	B	562	MLY	CA-CB-CG-CD
1	C	656	MLY	CA-CB-CG-CD

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Mol	Chain	Res	Type	Atoms
1	B	604	MLY	CE-CD-CG-CB
1	B	684	MLY	CE-CD-CG-CB
1	C	562	MLY	CE-CD-CG-CB
1	C	476	MLY	CE-CD-CG-CB
1	B	604	MLY	CG-CD-CE-NZ
1	B	430	MLY	CE-CD-CG-CB
1	C	656	MLY	CE-CD-CG-CB
1	A	408	MLY	CE-CD-CG-CB
1	C	604	MLY	CE-CD-CG-CB
1	C	684	MLY	CG-CD-CE-NZ
1	C	640	MLY	CA-CB-CG-CD
1	A	640	MLY	CE-CD-CG-CB
1	C	684	MLY	CE-CD-CG-CB
1	A	476	MLY	CA-CB-CG-CD
1	A	430	MLY	CA-CB-CG-CD
1	B	408	MLY	CE-CD-CG-CB
1	A	640	MLY	CD-CE-NZ-CH1
1	B	664	MLY	CA-CB-CG-CD
1	C	604	MLY	CA-CB-CG-CD
1	B	562	MLY	CE-CD-CG-CB
1	B	640	MLY	CG-CD-CE-NZ
1	C	430	MLY	CE-CD-CG-CB
1	A	519	MLY	CE-CD-CG-CB
1	A	641	MLY	CE-CD-CG-CB
1	A	590	MLY	CD-CE-NZ-CH1
1	A	684	MLY	CG-CD-CE-NZ
1	B	408	MLY	CG-CD-CE-NZ
1	A	562	MLY	CE-CD-CG-CB
1	B	562	MLY	CD-CE-NZ-CH2
1	C	641	MLY	C-CA-CB-CG
1	A	519	MLY	CD-CE-NZ-CH2
1	C	590	MLY	CD-CE-NZ-CH2
1	A	656	MLY	CE-CD-CG-CB
1	C	476	MLY	CA-CB-CG-CD
1	C	408	MLY	N-CA-CB-CG
1	C	641	MLY	N-CA-CB-CG
1	B	474	MLY	CA-CB-CG-CD
1	A	519	MLY	CG-CD-CE-NZ
1	A	430	MLY	CE-CD-CG-CB
1	B	640	MLY	CA-CB-CG-CD
1	B	590	MLY	CA-CB-CG-CD
1	A	664	MLY	CE-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
1	C	430	MLY	CA-CB-CG-CD
1	A	664	MLY	CG-CD-CE-NZ
1	B	474	MLY	CG-CD-CE-NZ
1	B	590	MLY	CD-CE-NZ-CH1
1	A	590	MLY	CE-CD-CG-CB
1	C	641	MLY	CE-CD-CG-CB
1	C	684	MLY	CA-CB-CG-CD
1	A	519	MLY	C-CA-CB-CG
1	C	519	MLY	C-CA-CB-CG
1	B	641	MLY	CG-CD-CE-NZ
1	C	640	MLY	CE-CD-CG-CB
1	A	476	MLY	CG-CD-CE-NZ
1	C	562	MLY	CD-CE-NZ-CH1
1	A	641	MLY	N-CA-CB-CG
1	B	641	MLY	N-CA-CB-CG

There are no ring outliers.

11 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	476	MLY	1	0
1	B	430	MLY	1	0
1	C	562	MLY	3	0
1	B	656	MLY	1	0
1	A	604	MLY	2	0
1	A	430	MLY	1	0
1	A	590	MLY	1	0
1	B	519	MLY	1	0
1	A	641	MLY	1	0
1	B	408	MLY	1	0
1	B	641	MLY	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
2	EDO	A	1687	-	3,3,3	0.50	0	2,2,2	0.33	0
2	EDO	B	1687	-	3,3,3	0.50	0	2,2,2	0.36	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
2	EDO	A	1687	-	-	0/1/1/1	-
2	EDO	B	1687	-	-	0/1/1/1	-

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1687	EDO	1	0
2	B	1687	EDO	1	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	283/383 (73%)	0.37	11 (3%) 43 25	46, 70, 136, 157	0
1	B	292/383 (76%)	0.38	8 (2%) 56 35	38, 69, 107, 119	1 (0%)
1	C	285/383 (74%)	0.36	7 (2%) 58 37	42, 71, 110, 132	0
All	All	860/1149 (74%)	0.37	26 (3%) 52 32	38, 70, 113, 157	1 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	660	ASP	4.1
1	B	440	ILE	3.9
1	A	457	ILE	3.4
1	B	661	ASN	3.3
1	B	448	VAL	3.2
1	C	460	VAL	3.2
1	C	660	ASP	3.1
1	C	356	ILE	2.8
1	A	433	ILE	2.7
1	C	447	VAL	2.5
1	A	357	SER	2.4
1	C	488	GLN	2.4
1	B	637	ARG	2.3
1	A	462	VAL	2.3
1	A	450	THR	2.3
1	A	621	VAL	2.3
1	B	462	VAL	2.2
1	A	663	PHE	2.2
1	A	666	ILE	2.2
1	B	458	SER	2.2
1	A	454	GLU	2.2
1	A	637	ARG	2.1
1	B	445	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	677	ALA	2.1
1	A	358	SER	2.0
1	C	456	VAL	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(Å ²)	Q<0.9
1	MLY	A	640	11/12	0.38	0.23	104,108,115,118	0
1	MLY	B	640	11/12	0.56	0.28	98,101,107,110	0
1	MLY	C	476	11/12	0.56	0.18	87,89,91,91	0
1	MLY	B	474	11/12	0.60	0.22	92,93,98,98	0
1	MLY	B	562	11/12	0.62	0.26	68,73,81,82	0
1	MLY	C	562	11/12	0.65	0.24	69,72,75,75	0
1	MLY	B	604	11/12	0.66	0.20	77,83,87,88	0
1	MLY	C	640	11/12	0.68	0.22	100,104,108,108	0
1	MLY	A	684	11/12	0.69	0.18	72,75,86,86	0
1	MLY	A	408	11/12	0.70	0.18	91,94,104,107	0
1	MLY	A	641	11/12	0.71	0.20	95,98,103,106	0
1	MLY	C	604	11/12	0.74	0.18	87,95,101,103	0
1	MLY	B	641	11/12	0.74	0.19	88,90,97,98	0
1	MLY	A	476	9/12	0.76	0.14	80,81,82,83	0
1	MLY	C	430	11/12	0.76	0.21	105,109,115,115	0
1	MLY	C	641	11/12	0.77	0.18	94,96,104,107	0
1	MLY	A	604	11/12	0.78	0.24	86,92,94,94	0
1	MLY	A	562	11/12	0.79	0.17	67,70,75,76	0
1	MLY	A	664	11/12	0.79	0.19	83,87,94,98	0
1	MLY	B	664	11/12	0.82	0.17	84,88,93,96	0
1	MLY	C	408	11/12	0.82	0.19	89,93,103,104	0
1	MLY	B	684	11/12	0.83	0.15	75,77,81,83	0
1	MLY	B	590	11/12	0.83	0.14	64,66,76,79	0
1	MLY	C	684	11/12	0.83	0.14	70,72,79,82	0
1	MLY	C	519	11/12	0.84	0.14	57,63,71,73	0
1	MLY	C	664	11/12	0.84	0.18	81,84,87,90	0
1	MLY	B	408	11/12	0.84	0.15	88,91,98,99	0
1	MLY	A	590	11/12	0.85	0.13	64,67,78,79	0
1	MLY	B	430	11/12	0.85	0.15	79,80,83,83	0
1	MLY	C	656	11/12	0.86	0.18	68,71,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	MLY	C	590	11/12	0.86	0.17	69,73,83,86	0
1	MLY	A	519	11/12	0.86	0.15	55,60,66,69	0
1	MLY	B	476	11/12	0.87	0.16	82,83,83,84	0
1	MLY	B	656	11/12	0.87	0.14	67,70,74,75	0
1	MLY	B	519	11/12	0.87	0.16	56,61,69,69	0
1	MLY	A	656	11/12	0.87	0.17	69,72,77,78	0
1	MLY	A	430	11/12	0.88	0.12	100,101,104,105	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
2	EDO	B	1687	4/4	0.88	0.14	68,69,69,69	0
2	EDO	A	1687	4/4	0.91	0.12	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.