Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2023 – 06:55 am GMT

PDB ID	:	4A5P
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.

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:

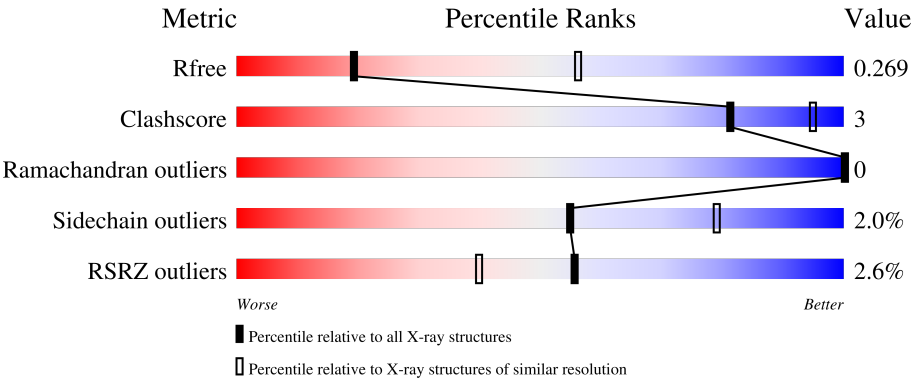
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (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 <=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	2% 71% 6% 23%
1	B	383	% 73% 7% • 20%
1	C	383	2% 71% 6% 22%

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
1	MLY	A	640	-	-	-	X
1	MLY	A	641	-	-	-	X
1	MLY	B	474	-	-	-	X
1	MLY	B	562	-	-	-	X
1	MLY	B	640	-	-	-	X
1	MLY	B	641	-	-	-	X
1	MLY	C	476	-	-	-	X
1	MLY	C	562	-	-	-	X
1	MLY	C	641	-	-	-	X

2 Entry composition (i)

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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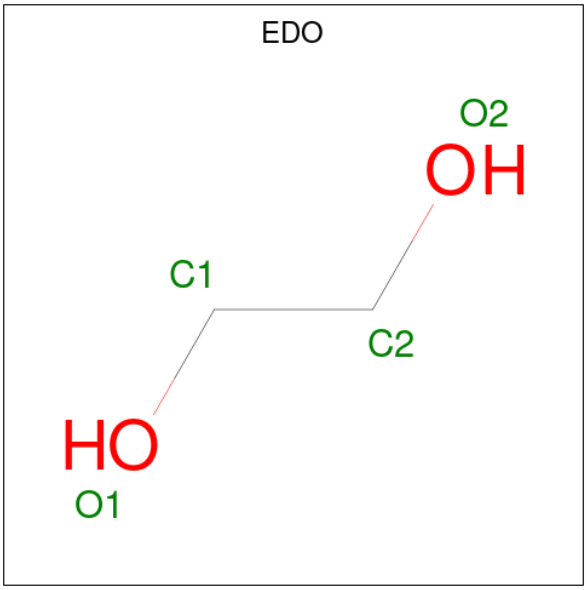
Chain	Residue	Modelled	Actual	Comment	Reference
B	313	HIS	-	expression tag	UNP P0A1I5
B	314	SER	-	expression tag	UNP P0A1I5
B	315	GLN	-	expression tag	UNP P0A1I5
B	316	ASP	-	expression tag	UNP P0A1I5
B	317	PRO	-	expression tag	UNP P0A1I5
C	304	MET	-	expression tag	UNP P0A1I5
C	305	GLY	-	expression tag	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 (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 3 is water.

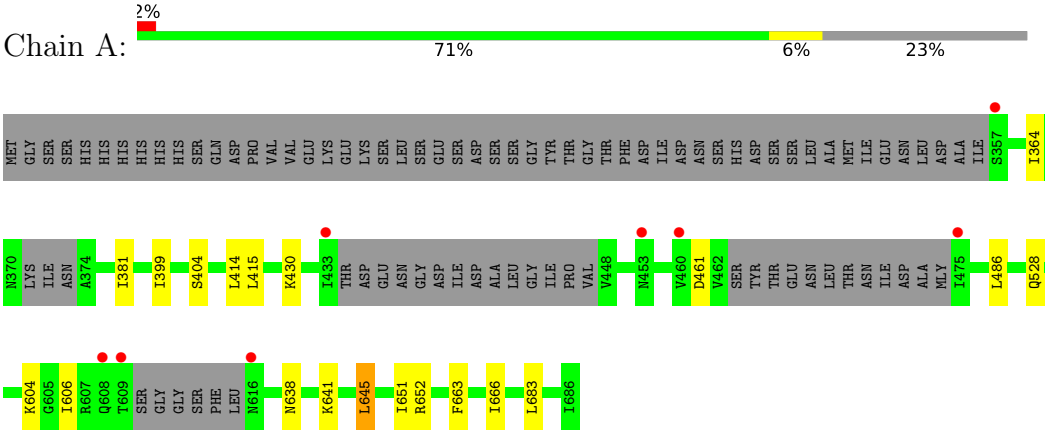
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total O 5 5	0	0
3	B	8	Total O 8 8	0	0
3	C	3	Total O 3 3	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

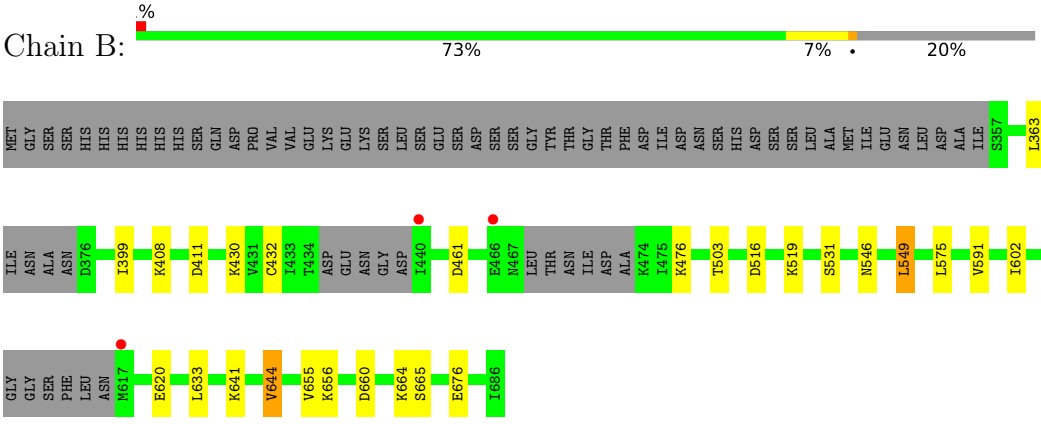
• Molecule 1: PROTEIN MXIA

Chain A:



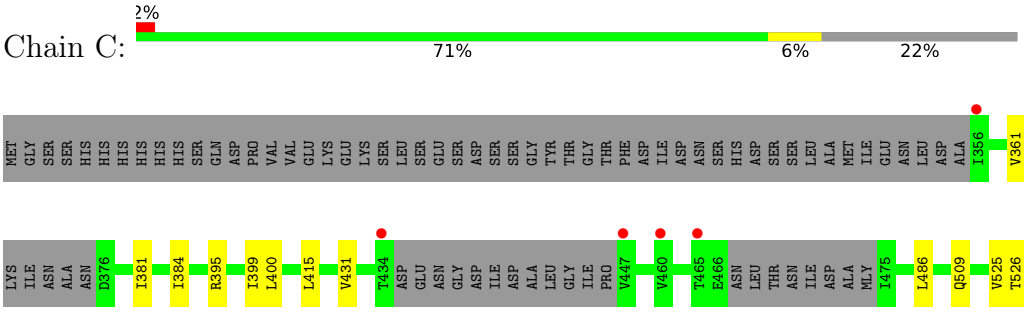
• Molecule 1: PROTEIN MXIA

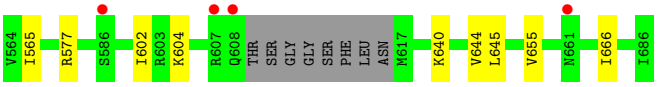
Chain B:



• Molecule 1: PROTEIN MXIA

Chain C:




V564
I565
R577
S586
I602
R603
K604
R607
Q608
THR
SER
GLY
GLY
SER
PHE
LEU
ASN
M617
K640
V644
L645
V655
N661
I666
I686

4 Data and refinement statistics (i)

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 34.07 – 3.15	Depositor EDS
% Data completeness (in resolution range)	93.4 (35.72-3.15) 93.9 (34.07-3.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 3.18Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.231 , 0.251 0.245 , 0.269	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)	0.30 , 49.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[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, EDO

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	0.42	0/2328	0.54	0/3153
1	B	0.42	0/2410	0.54	0/3268
1	C	0.42	0/2349	0.53	0/3182
All	All	0.42	0/7087	0.54	0/9603

There are no bond length outliers.

There are no bond angle outliers.

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	2429	0	2497	12	0
1	B	2517	0	2599	13	0
1	C	2451	0	2525	14	0
2	A	4	0	6	1	0
2	B	4	0	6	1	0
3	A	5	0	0	0	0
3	B	8	0	0	0	0
3	C	3	0	0	0	0
All	All	7421	0	7633	39	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 (39) 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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	255 (98%)	6 (2%)	50	76
1	B	270/337 (80%)	263 (97%)	7 (3%)	46	74
1	C	264/337 (78%)	261 (99%)	3 (1%)	73	88
All	All	795/1011 (79%)	779 (98%)	16 (2%)	55	79

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	369	GLU
1	A	528	GLN
1	A	638	ASN
1	A	645	LEU
1	A	652	ARG
1	A	663	PHE
1	B	411	ASP
1	B	549	LEU
1	B	620	GLU
1	B	633	LEU
1	B	644	VAL
1	B	665	SER
1	B	676	GLU
1	C	431	VAL
1	C	577	ARG
1	C	644	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	541	ASN
1	A	638	ASN
1	B	488	GLN
1	B	535	GLN
1	B	541	ASN
1	B	546	ASN
1	C	509	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)

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	C	519	1	9,10,11	0.54	0	6,11,13	1.27	0
1	MLY	C	656	1	9,10,11	0.48	0	6,11,13	1.11	0
1	MLY	A	476	1	7,8,11	0.51	0	3,8,13	0.66	0
1	MLY	B	430	1	9,10,11	0.52	0	6,11,13	1.13	0
1	MLY	C	476	1	9,10,11	0.63	0	6,11,13	0.52	0
1	MLY	C	640	1	9,10,11	0.49	0	6,11,13	1.21	1 (16%)
1	MLY	C	590	1	9,10,11	0.52	0	6,11,13	1.19	0
1	MLY	A	664	1	9,10,11	0.48	0	6,11,13	1.17	0
1	MLY	B	664	1	9,10,11	0.65	0	6,11,13	1.37	1 (16%)
1	MLY	B	684	1	9,10,11	0.52	0	6,11,13	1.13	0
1	MLY	A	562	1	9,10,11	0.53	0	6,11,13	1.08	0
1	MLY	B	408	1	9,10,11	0.60	0	6,11,13	0.69	0
1	MLY	A	656	1	9,10,11	0.58	0	6,11,13	0.97	0
1	MLY	A	408	1	9,10,11	0.53	0	6,11,13	1.13	0
1	MLY	C	408	1	9,10,11	0.57	0	6,11,13	0.98	0
1	MLY	B	519	1	9,10,11	0.51	0	6,11,13	1.19	0
1	MLY	A	519	1	9,10,11	0.47	0	6,11,13	1.19	0
1	MLY	A	640	1	9,10,11	0.87	0	6,11,13	0.86	0
1	MLY	B	656	1	9,10,11	0.61	0	6,11,13	1.06	0
1	MLY	C	430	1	9,10,11	0.69	0	6,11,13	0.49	0
1	MLY	C	641	1	9,10,11	0.58	0	6,11,13	1.06	0
1	MLY	B	476	1	9,10,11	0.47	0	6,11,13	1.11	0
1	MLY	A	684	1	9,10,11	0.51	0	6,11,13	1.12	0
1	MLY	B	590	1	9,10,11	0.49	0	6,11,13	1.14	0
1	MLY	B	641	1	9,10,11	0.75	0	6,11,13	0.69	0
1	MLY	B	640	1	9,10,11	0.48	0	6,11,13	1.10	0
1	MLY	C	684	1	9,10,11	0.66	0	6,11,13	0.88	0
1	MLY	C	664	1	9,10,11	0.46	0	6,11,13	1.15	0
1	MLY	A	430	1	9,10,11	0.56	0	6,11,13	1.00	0
1	MLY	A	641	1	9,10,11	0.69	0	6,11,13	0.90	0
1	MLY	A	590	1	9,10,11	0.50	0	6,11,13	1.16	0
1	MLY	B	474	1	9,10,11	0.52	0	6,11,13	1.14	0
1	MLY	C	604	1	9,10,11	0.58	0	6,11,13	1.87	2 (33%)
1	MLY	B	562	1	9,10,11	0.86	0	6,11,13	0.96	0
1	MLY	B	604	1	9,10,11	0.57	0	6,11,13	1.09	0
1	MLY	C	562	1	9,10,11	1.04	1 (11%)	6,11,13	1.30	1 (16%)
1	MLY	A	604	1	9,10,11	0.61	0	6,11,13	0.94	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	C	519	1	-	0/8/9/11	-
1	MLY	C	656	1	-	6/8/9/11	-
1	MLY	A	476	1	-	1/6/7/11	-
1	MLY	B	430	1	-	5/8/9/11	-
1	MLY	C	476	1	-	3/8/9/11	-
1	MLY	C	640	1	-	5/8/9/11	-
1	MLY	C	590	1	-	5/8/9/11	-
1	MLY	A	664	1	-	2/8/9/11	-
1	MLY	B	664	1	-	2/8/9/11	-
1	MLY	B	684	1	-	3/8/9/11	-
1	MLY	A	562	1	-	4/8/9/11	-
1	MLY	B	408	1	-	2/8/9/11	-
1	MLY	A	656	1	-	2/8/9/11	-
1	MLY	A	408	1	-	4/8/9/11	-
1	MLY	C	408	1	-	1/8/9/11	-
1	MLY	B	519	1	-	1/8/9/11	-
1	MLY	A	519	1	-	4/8/9/11	-
1	MLY	A	640	1	-	2/8/9/11	-
1	MLY	B	656	1	-	0/8/9/11	-
1	MLY	C	430	1	-	5/8/9/11	-
1	MLY	C	641	1	-	6/8/9/11	-
1	MLY	B	476	1	-	5/8/9/11	-
1	MLY	A	684	1	-	1/8/9/11	-
1	MLY	B	590	1	-	5/8/9/11	-
1	MLY	B	641	1	-	5/8/9/11	-
1	MLY	B	640	1	-	5/8/9/11	-
1	MLY	C	684	1	-	3/8/9/11	-
1	MLY	C	664	1	-	4/8/9/11	-
1	MLY	A	430	1	-	4/8/9/11	-
1	MLY	A	641	1	-	4/8/9/11	-
1	MLY	A	590	1	-	5/8/9/11	-
1	MLY	B	474	1	-	3/8/9/11	-
1	MLY	C	604	1	-	3/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	B	562	1	-	5/8/9/11	-
1	MLY	B	604	1	-	5/8/9/11	-
1	MLY	C	562	1	-	4/8/9/11	-
1	MLY	A	604	1	-	5/8/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	562	MLY	CB-CA	2.19	1.56	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	604	MLY	CH2-NZ-CH1	-2.73	102.68	109.73
1	C	604	MLY	CH1-NZ-CE	-2.67	100.17	110.74
1	B	664	MLY	CH2-NZ-CH1	-2.39	103.56	109.73
1	C	640	MLY	CD-CE-NZ	-2.16	107.94	113.79
1	C	562	MLY	CH2-NZ-CH1	-2.06	104.42	109.73

There are no chirality outliers.

All (129) 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

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Mol	Chain	Res	Type	Atoms
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	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	B	476	MLY	CD-CE-NZ-CH1
1	A	408	MLY	CD-CE-NZ-CH2
1	A	430	MLY	CD-CE-NZ-CH2
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	476	MLY	CD-CE-NZ-CH2
1	B	562	MLY	CD-CE-NZ-CH1
1	C	590	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	C	430	MLY	CG-CD-CE-NZ
1	A	562	MLY	CG-CD-CE-NZ
1	B	430	MLY	CG-CD-CE-NZ
1	B	590	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	C	641	MLY	CG-CD-CE-NZ
1	A	641	MLY	CG-CD-CE-NZ
1	A	408	MLY	CD-CE-NZ-CH1
1	A	430	MLY	CD-CE-NZ-CH1
1	B	430	MLY	CD-CE-NZ-CH2
1	B	641	MLY	CD-CE-NZ-CH2

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

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Mol	Chain	Res	Type	Atoms
1	B	640	MLY	CG-CD-CE-NZ
1	A	641	MLY	CE-CD-CG-CB
1	C	476	MLY	CA-CB-CG-CD
1	A	562	MLY	CE-CD-CG-CB
1	B	474	MLY	CA-CB-CG-CD
1	B	408	MLY	CG-CD-CE-NZ
1	A	684	MLY	CG-CD-CE-NZ
1	B	640	MLY	CA-CB-CG-CD
1	B	590	MLY	CA-CB-CG-CD
1	A	656	MLY	CE-CD-CG-CB
1	C	430	MLY	CA-CB-CG-CD
1	A	519	MLY	CG-CD-CE-NZ
1	C	408	MLY	N-CA-CB-CG
1	C	641	MLY	N-CA-CB-CG
1	C	641	MLY	C-CA-CB-CG
1	A	430	MLY	CE-CD-CG-CB
1	B	590	MLY	CD-CE-NZ-CH1
1	A	664	MLY	CE-CD-CG-CB
1	A	664	MLY	CG-CD-CE-NZ
1	B	474	MLY	CG-CD-CE-NZ
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	B	641	MLY	CG-CD-CE-NZ
1	C	640	MLY	CE-CD-CG-CB
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	430	MLY	1	0
1	B	408	MLY	1	0
1	B	519	MLY	1	0
1	B	656	MLY	1	0
1	B	476	MLY	1	0
1	B	641	MLY	1	0
1	A	430	MLY	1	0
1	A	641	MLY	1	0
1	A	590	MLY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	562	MLY	3	0
1	A	604	MLY	2	0

5.5 Carbohydrates (i)

There are no monosaccharides 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	B	1687	-	3,3,3	0.56	0	2,2,2	0.32	0
2	EDO	A	1687	-	3,3,3	0.57	0	2,2,2	0.28	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	B	1687	-	-	0/1/1/1	-
2	EDO	A	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	B	1687	EDO	1	0
2	A	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, 95^{th} 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%)	-0.07	8 (2%)	53	36	46, 70, 136, 157	0
1	B	292/383 (76%)	-0.08	5 (1%)	70	57	44, 69, 107, 119	0
1	C	285/383 (74%)	-0.04	9 (3%)	47	30	42, 71, 110, 132	0
All	All	860/1149 (74%)	-0.06	22 (2%)	56	40	42, 70, 113, 157	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	609	THR	4.9
1	A	616	ASN	4.1
1	B	440	ILE	3.5
1	C	460	VAL	3.5
1	C	586	SER	3.2
1	A	475	ILE	3.1
1	C	447	VAL	3.1
1	A	433	ILE	3.0
1	C	607	ARG	3.0
1	C	608	GLN	3.0
1	B	607	ARG	2.6
1	C	661	ASN	2.6
1	B	608	GLN	2.5
1	A	608	GLN	2.5
1	A	453	ASN	2.5
1	C	465	THR	2.5
1	B	466	GLU	2.4
1	A	460	VAL	2.3
1	C	434	THR	2.3
1	A	357	SER	2.2
1	B	617	MET	2.2
1	C	356	ILE	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	B	474	11/12	0.50	0.65	92,93,98,98	0
1	MLY	A	640	11/12	0.64	0.59	104,108,115,118	0
1	MLY	B	562	11/12	0.64	0.61	68,73,81,82	0
1	MLY	A	641	11/12	0.69	0.42	95,98,103,106	0
1	MLY	B	641	11/12	0.69	0.42	88,90,97,98	0
1	MLY	B	640	11/12	0.72	0.45	98,101,107,110	0
1	MLY	C	476	11/12	0.76	0.56	87,89,91,91	0
1	MLY	C	641	11/12	0.76	0.41	94,96,104,107	0
1	MLY	C	562	11/12	0.79	0.52	69,72,75,75	0
1	MLY	C	640	11/12	0.82	0.43	100,104,108,108	0
1	MLY	A	562	11/12	0.83	0.47	67,70,75,76	0
1	MLY	C	408	11/12	0.83	0.38	89,93,103,104	0
1	MLY	A	476	9/12	0.83	0.35	80,81,82,83	0
1	MLY	C	604	11/12	0.84	0.37	87,95,101,103	0
1	MLY	A	408	11/12	0.85	0.45	91,94,104,107	0
1	MLY	A	519	11/12	0.86	0.29	55,60,66,69	0
1	MLY	A	604	11/12	0.86	0.39	86,92,94,94	0
1	MLY	C	519	11/12	0.87	0.27	57,63,71,73	0
1	MLY	A	590	11/12	0.87	0.35	64,67,78,79	0
1	MLY	B	519	11/12	0.87	0.34	56,61,69,69	0
1	MLY	A	684	11/12	0.87	0.36	72,75,86,86	0
1	MLY	B	604	11/12	0.87	0.38	77,83,87,88	0
1	MLY	C	664	11/12	0.87	0.24	81,84,87,90	0
1	MLY	C	430	11/12	0.88	0.35	105,109,115,115	0
1	MLY	B	408	11/12	0.88	0.48	88,91,98,99	0
1	MLY	B	684	11/12	0.88	0.33	75,77,81,83	0
1	MLY	A	664	11/12	0.88	0.26	83,87,94,98	0
1	MLY	C	684	11/12	0.88	0.23	70,72,79,82	0
1	MLY	B	430	11/12	0.89	0.34	79,80,83,83	0
1	MLY	A	430	11/12	0.89	0.35	100,101,104,105	0
1	MLY	B	664	11/12	0.90	0.19	84,88,93,96	0
1	MLY	B	476	11/12	0.90	0.25	82,83,83,84	0
1	MLY	C	590	11/12	0.91	0.29	69,73,83,86	0
1	MLY	C	656	11/12	0.91	0.19	68,71,75,75	0
1	MLY	B	590	11/12	0.93	0.25	64,66,76,79	0
1	MLY	A	656	11/12	0.93	0.20	69,72,77,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	MLY	B	656	11/12	0.95	0.17	67,70,74,75	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, 95^{th} 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	EDO	B	1687	4/4	0.90	0.23	68,69,69,69	0
2	EDO	A	1687	4/4	0.91	0.28	67,67,67,67	0

6.5 Other polymers (i)

There are no such residues in this entry.