



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 04:37 PM UTC

PDB ID : 4DWS / pdb_00004dws
Title : Crystal Structure of a chitinase from the Yersinia entomophaga toxin complex
Authors : Busby, J.N.; Hurst, M.R.H.; Lott, J.S.
Deposited on : 2012-02-26
Resolution : 1.80 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 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

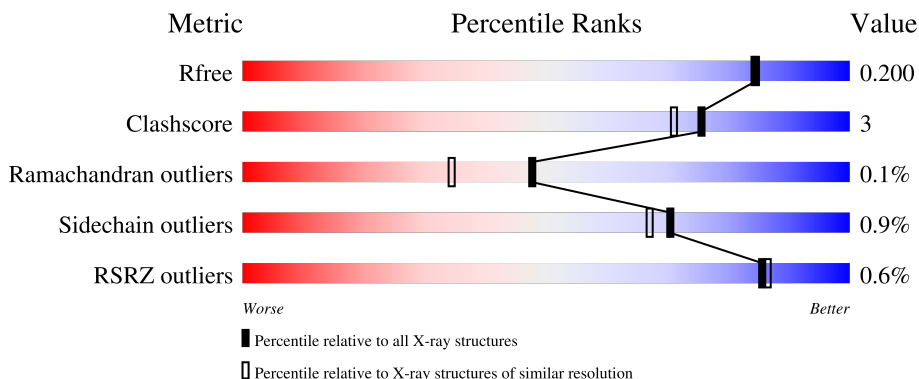
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


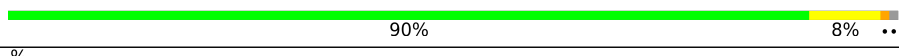
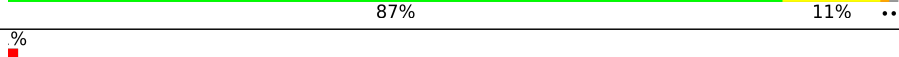
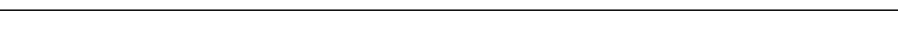
The reported resolution of this entry is 1.80 Å.

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))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 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	546	 89% 10% .
2	B	546	 90% 8% ..
3	C	546	 87% 11% ..
4	D	546	 88% 10% .

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 17938 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 Chi2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	540	4191	2670	697	807	17	0	4	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	88	GLY	-	expression tag	UNP B6A879
A	89	SER	-	expression tag	UNP B6A879
A	90	GLY	-	expression tag	UNP B6A879
A	91	ALA	-	expression tag	UNP B6A879

- Molecule 2 is a protein called Chi2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	538	4122	2628	681	795	18	0	3	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	88	GLY	-	expression tag	UNP B6A879
B	89	SER	-	expression tag	UNP B6A879
B	90	GLY	-	expression tag	UNP B6A879
B	91	ALA	-	expression tag	UNP B6A879

- Molecule 3 is a protein called Chi2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	539	4201	2674	694	815	18	0	7	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	88	GLY	-	expression tag	UNP B6A879
C	89	SER	-	expression tag	UNP B6A879
C	90	GLY	-	expression tag	UNP B6A879
C	91	ALA	-	expression tag	UNP B6A879

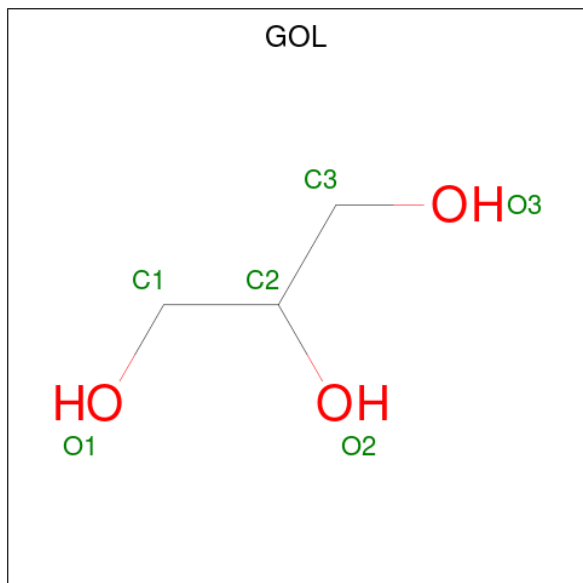
- Molecule 4 is a protein called Chi2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	539	4194	2662	702	812	18	0	9	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	88	GLY	-	expression tag	UNP B6A879
D	89	SER	-	expression tag	UNP B6A879
D	90	GLY	-	expression tag	UNP B6A879
D	91	ALA	-	expression tag	UNP B6A879

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	6	3	3	0	0
5	B	1	6	3	3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

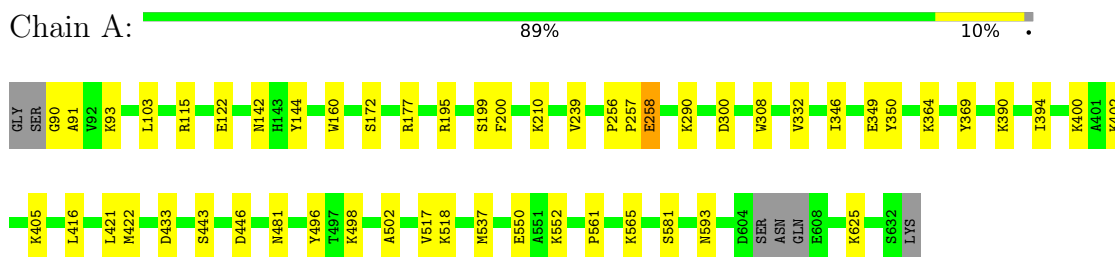
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	305	Total	O	0	0
			305	305		
6	B	203	Total	O	0	0
			203	203		
6	C	394	Total	O	0	0
			394	394		
6	D	304	Total	O	0	0
			304	304		

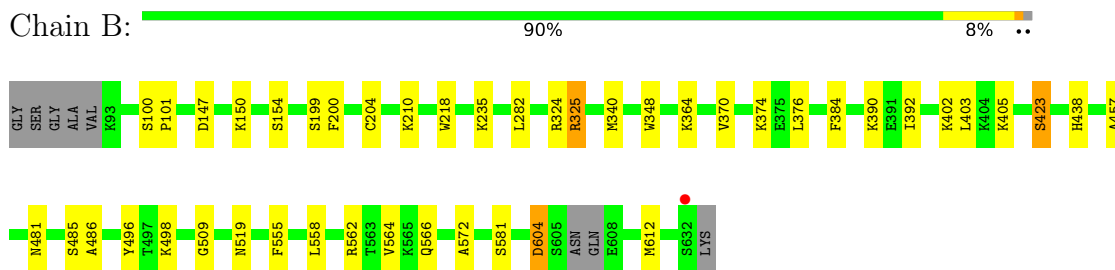
3 Residue-property plots [i](#)

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.

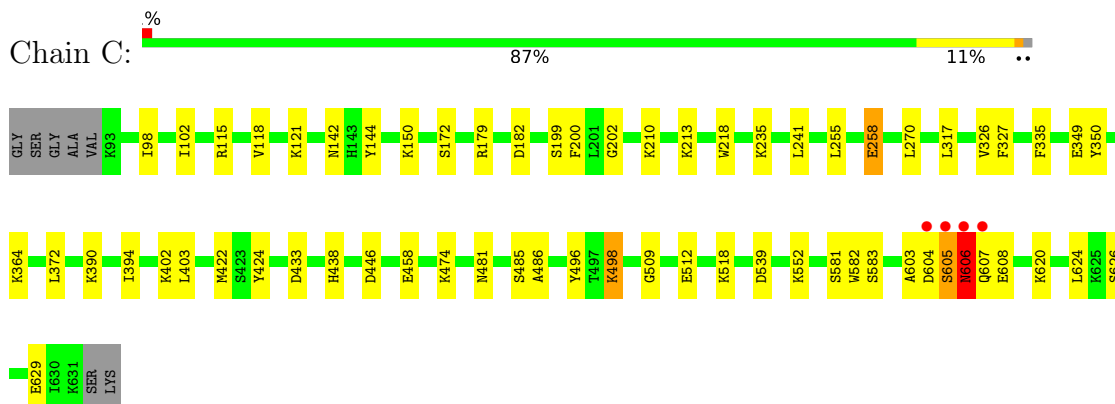
- Molecule 1: Chi2



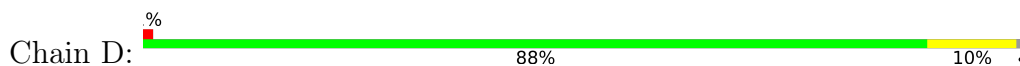
- Molecule 2: Chi2



- Molecule 3: Chi2



- Molecule 4: Chi2





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.51Å 210.56Å 92.58Å 90.00° 95.27° 90.00°	Depositor
Resolution (Å)	105.28 – 1.80 105.28 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (105.28-1.80) 99.9 (105.28-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 1.80Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.160 , 0.199 0.160 , 0.200	Depositor DCC
R_{free} test set	10654 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	13.5	Xtrriage
Anisotropy	0.026	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17938	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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: MLZ, GOL, M3L, 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	1.30	8/4143 (0.2%)	1.16	8/5619 (0.1%)
2	B	1.21	3/4105 (0.1%)	1.16	8/5579 (0.1%)
3	C	1.38	9/4174 (0.2%)	1.19	10/5665 (0.2%)
4	D	1.33	9/4220 (0.2%)	1.18	12/5721 (0.2%)
All	All	1.31	29/16642 (0.2%)	1.17	38/22584 (0.2%)

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
2	B	0	1
3	C	0	2
All	All	0	3

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	98	ILE	N-CA	7.05	1.52	1.46
4	D	594	ALA	CA-CB	6.88	1.64	1.53
1	A	446	ASP	C-O	6.79	1.27	1.23
3	C	446	ASP	CA-CB	6.70	1.57	1.52
4	D	446	ASP	C-O	6.59	1.27	1.23

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	613	GLY	CA-C-N	-8.48	111.03	120.45
4	D	613	GLY	C-N-CA	-8.48	111.03	120.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	100	SER	CA-C-N	-7.50	112.28	119.85
4	D	100	SER	C-N-CA	-7.50	112.28	119.85
1	A	308	TRP	N-CA-C	7.36	119.30	111.28

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	604	ASP	Peptide
3	C	603	ALA	Peptide
3	C	605	SER	Peptide

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	4191	0	4020	23	0
2	B	4122	0	3897	19	0
3	C	4201	0	4015	32	0
4	D	4194	0	3989	23	0
5	A	6	0	8	1	0
5	B	6	0	8	0	0
5	D	12	0	16	2	0
6	A	305	0	0	1	0
6	B	203	0	0	3	0
6	C	394	0	0	4	0
6	D	304	0	0	3	0
All	All	17938	0	15953	99	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.

The worst 5 of 99 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:433:ASP:OD1	1:A:498:M3L:CM1	2.06	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:ASP:OD1	1:A:498:M3L:HM11	1.58	1.02
4:D:433:ASP:OD1	4:D:498:M3L:HM33	1.64	0.97
3:C:433:ASP:OD1	3:C:498:M3L:CM2	2.17	0.93
3:C:433:ASP:OD1	3:C:498:M3L:HM23	1.72	0.86

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	526/546 (96%)	513 (98%)	13 (2%)	0	100	100
2	B	526/546 (96%)	510 (97%)	16 (3%)	0	100	100
3	C	531/546 (97%)	513 (97%)	16 (3%)	2 (0%)	30	19
4	D	539/546 (99%)	525 (97%)	12 (2%)	2 (0%)	30	19
All	All	2122/2184 (97%)	2061 (97%)	57 (3%)	4 (0%)	48	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	606	ASN
3	C	607	GLN
4	D	386[A]	TYR
4	D	386[B]	TYR

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	414/432 (96%)	409 (99%)	5 (1%)	63	57
2	B	404/435 (93%)	401 (99%)	3 (1%)	76	73
3	C	419/433 (97%)	416 (99%)	3 (1%)	76	73
4	D	422/439 (96%)	418 (99%)	4 (1%)	70	67
All	All	1659/1739 (95%)	1644 (99%)	15 (1%)	70	67

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	438	HIS
4	D	561	PRO
3	C	258	GLU
4	D	624	LEU
4	D	363	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	274	GLN
3	C	606	ASN
4	D	574	ASN
4	D	162	GLN
4	D	525	HIS

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	M3L	A	390	1	10,11,12	0.44	0	9,14,16	4.59	7 (77%)
4	M3L	D	400	4	10,11,12	0.67	0	9,14,16	0.87	0
4	M3L	D	498	4	10,11,12	1.13	0	9,14,16	1.35	3 (33%)
2	MLZ	B	405	2	8,9,10	1.21	1 (12%)	4,9,11	0.80	0
1	M3L	A	620	1	10,11,12	0.74	0	9,14,16	0.73	0
2	M3L	B	400	2	10,11,12	0.76	0	9,14,16	0.68	0
2	MLY	B	235	2	9,10,11	0.96	1 (11%)	6,11,13	2.54	4 (66%)
4	M3L	D	474	4	10,11,12	0.82	0	9,14,16	1.04	1 (11%)
3	M3L	C	498	3	10,11,12	0.82	0	9,14,16	1.11	1 (11%)
4	MLY	D	402	4	9,10,11	0.60	0	6,11,13	2.20	2 (33%)
3	MLY	C	390	3	9,10,11	0.85	0	6,11,13	2.88	2 (33%)
1	MLY	A	400	1	9,10,11	0.78	0	6,11,13	2.27	2 (33%)
1	MLY	A	290	1	9,10,11	0.96	0	6,11,13	2.33	2 (33%)
3	MLY	C	518	3	9,10,11	0.80	0	6,11,13	2.17	2 (33%)
1	M3L	A	498	1	10,11,12	0.84	0	9,14,16	0.72	0
2	M3L	B	474	2	10,11,12	0.82	0	9,14,16	1.12	0
1	M3L	A	364	1	10,11,12	0.73	0	9,14,16	0.71	0
1	MLY	A	402	1	9,10,11	0.73	0	6,11,13	2.17	2 (33%)
3	MLY	C	402	3	9,10,11	0.89	0	6,11,13	1.99	2 (33%)
4	MLY	D	210	4	9,10,11	0.88	0	6,11,13	2.24	2 (33%)
3	M3L	C	474	3	10,11,12	0.48	0	9,14,16	0.97	0
2	MLY	B	402	2	9,10,11	0.88	0	6,11,13	2.34	3 (50%)
1	MLZ	A	405	1	8,9,10	0.51	0	4,9,11	1.61	1 (25%)
2	MLY	B	498	2	9,10,11	0.77	0	6,11,13	2.20	2 (33%)
1	MLZ	A	518	1	8,9,10	0.72	0	4,9,11	1.66	1 (25%)
2	M3L	B	150	2	10,11,12	0.68	0	9,14,16	0.73	0
1	MLY	A	552	1	9,10,11	1.26	1 (11%)	6,11,13	2.38	2 (33%)
4	MLZ	D	235	4	8,9,10	0.80	0	4,9,11	1.24	0
3	MLZ	C	150	3	8,9,10	0.83	0	4,9,11	1.50	1 (25%)
3	MLY	C	552	3	9,10,11	0.63	0	6,11,13	2.08	2 (33%)
1	MLY	A	210	1	9,9,11	0.74	0	10,10,13	1.67	3 (30%)
3	MLY	C	210	3	9,10,11	0.98	0	6,11,13	2.21	2 (33%)
3	MLY	C	364	3	9,10,11	0.76	0	6,11,13	2.17	2 (33%)
2	MLY	B	374	2	9,10,11	0.67	0	6,11,13	2.00	3 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MLY	B	364	2	9,10,11	0.66	0	6,11,13	2.11	2 (33%)
3	MLZ	C	620	3	8,9,10	0.76	0	4,9,11	1.62	1 (25%)
1	MLZ	A	625	1	8,9,10	0.81	0	4,9,11	1.88	1 (25%)
3	M3L	C	400	3	10,11,12	0.98	0	9,14,16	0.81	0
2	MLY	B	390	2	9,10,11	0.85	1 (11%)	6,11,13	2.24	2 (33%)
3	MLY	C	213	3	9,10,11	1.01	1 (11%)	6,11,13	2.21	2 (33%)
1	MLY	A	565	1	9,10,11	0.52	0	6,11,13	2.24	2 (33%)
1	MLY	A	93	1	9,10,11	0.55	0	6,11,13	2.37	2 (33%)
3	MLY	C	121	3	9,10,11	0.75	0	6,11,13	2.56	3 (50%)
2	MLY	B	210	2	9,10,11	1.25	1 (11%)	6,11,13	2.07	2 (33%)
4	MLY	D	390	4	9,10,11	0.92	0	6,11,13	2.71	2 (33%)

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	M3L	A	390	1	-	3/9/10/12	-
4	M3L	D	400	4	-	0/9/10/12	-
4	M3L	D	498	4	-	4/9/10/12	-
2	MLZ	B	405	2	-	0/7/8/10	-
1	M3L	A	620	1	-	0/9/10/12	-
2	M3L	B	400	2	-	0/9/10/12	-
2	MLY	B	235	2	-	2/8/9/11	-
4	M3L	D	474	4	-	1/9/10/12	-
3	M3L	C	498	3	-	2/9/10/12	-
4	MLY	D	402	4	-	1/8/9/11	-
3	MLY	C	390	3	-	3/8/9/11	-
1	MLY	A	400	1	-	1/8/9/11	-
1	MLY	A	290	1	-	2/8/9/11	-
3	MLY	C	518	3	-	2/8/9/11	-
1	M3L	A	498	1	-	2/9/10/12	-
2	M3L	B	474	2	-	0/9/10/12	-
1	M3L	A	364	1	-	4/9/10/12	-
1	MLY	A	402	1	-	1/8/9/11	-
3	MLY	C	402	3	-	1/8/9/11	-
4	MLY	D	210	4	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	M3L	C	474	3	-	1/9/10/12	-
2	MLY	B	402	2	-	1/8/9/11	-
1	MLZ	A	405	1	-	0/7/8/10	-
2	MLY	B	498	2	-	2/8/9/11	-
1	MLZ	A	518	1	-	2/7/8/10	-
2	M3L	B	150	2	-	2/9/10/12	-
1	MLY	A	552	1	-	3/8/9/11	-
4	MLZ	D	235	4	-	2/7/8/10	-
3	MLZ	C	150	3	-	0/7/8/10	-
3	MLY	C	552	3	-	2/8/9/11	-
1	MLY	A	210	1	-	2/7/7/11	-
3	MLY	C	210	3	-	2/8/9/11	-
3	MLY	C	364	3	-	1/8/9/11	-
2	MLY	B	374	2	-	2/8/9/11	-
2	MLY	B	364	2	-	1/8/9/11	-
3	MLZ	C	620	3	-	0/7/8/10	-
1	MLZ	A	625	1	-	1/7/8/10	-
3	M3L	C	400	3	-	0/9/10/12	-
2	MLY	B	390	2	-	1/8/9/11	-
3	MLY	C	213	3	-	2/8/9/11	-
1	MLY	A	565	1	-	3/8/9/11	-
1	MLY	A	93	1	-	2/8/9/11	-
3	MLY	C	121	3	-	2/8/9/11	-
2	MLY	B	210	2	-	2/8/9/11	-
4	MLY	D	390	4	-	3/8/9/11	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	552	MLY	CB-CA	3.25	1.58	1.53
2	B	405	MLZ	CB-CA	2.61	1.57	1.53
2	B	210	MLY	CB-CA	2.45	1.57	1.53
3	C	213	MLY	CB-CA	2.33	1.57	1.53
2	B	235	MLY	O-C	2.14	1.28	1.20

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	M3L	CM3-NZ-CM1	-7.78	88.53	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	M3L	CM3-NZ-CM2	-7.01	90.55	108.98
1	A	390	M3L	CM3-NZ-CE	-7.01	82.05	109.91
3	C	390	MLY	CH2-NZ-CH1	5.58	124.03	109.72
4	D	390	MLY	CH2-NZ-CH1	5.15	122.91	109.72

There are no chirality outliers.

5 of 70 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	518	MLZ	CD-CE-NZ-CM
1	A	625	MLZ	CD-CE-NZ-CM
2	B	210	MLY	O-C-CA-CB
3	C	210	MLY	O-C-CA-CB
4	D	210	MLY	O-C-CA-CB

There are no ring outliers.

7 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	498	M3L	3	0
4	D	474	M3L	3	0
3	C	498	M3L	5	0
1	A	498	M3L	6	0
1	A	364	M3L	1	0
3	C	474	M3L	2	0
2	B	150	M3L	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
5	GOL	D	701	-	5,5,5	0.22	0	5,5,5	0.82	0
5	GOL	D	702	-	5,5,5	0.51	0	5,5,5	1.28	0
5	GOL	B	701	-	5,5,5	0.36	0	5,5,5	0.68	0
5	GOL	A	701	-	5,5,5	0.37	0	5,5,5	0.53	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	D	701	-	-	1/4/4/4	-
5	GOL	D	702	-	-	3/4/4/4	-
5	GOL	B	701	-	-	2/4/4/4	-
5	GOL	A	701	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	702	GOL	O2-C2-C3-O3
5	D	702	GOL	O1-C1-C2-C3
5	D	702	GOL	C1-C2-C3-O3
5	B	701	GOL	O1-C1-C2-O2
5	D	701	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	702	GOL	2	0
5	A	701	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	526/546 (96%)	-0.74	0 100 100	5, 12, 23, 39	4 (0%)
2	B	527/546 (96%)	-0.32	1 (0%) 91 91	8, 18, 30, 43	3 (0%)
3	C	526/546 (96%)	-0.86	4 (0%) 82 83	4, 9, 21, 46	7 (1%)
4	D	532/546 (97%)	-0.65	8 (1%) 72 72	5, 12, 23, 48	9 (1%)
All	All	2111/2184 (96%)	-0.64	13 (0%) 85 86	4, 13, 27, 48	23 (1%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	607	GLN	4.1
3	C	604	ASP	3.9
4	D	386[A]	TYR	3.4
3	C	605	SER	3.3
3	C	606	ASN	3.0

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, 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	210	10/12	0.87	0.07	10,13,17,18	0
2	M3L	B	150	12/13	0.91	0.10	17,23,31,32	0
2	M3L	B	474	12/13	0.92	0.10	13,19,31,35	0
3	MLZ	C	150	10/11	0.93	0.09	12,17,28,29	0
2	MLY	B	210	11/12	0.94	0.07	9,11,16,18	0
2	MLY	B	235	11/12	0.94	0.09	13,16,31,33	0
2	M3L	B	400	12/13	0.94	0.09	13,16,26,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	MLZ	A	405	10/11	0.94	0.08	13,14,27,29	0
1	M3L	A	390	12/13	0.94	0.08	10,12,24,26	0
4	M3L	D	400	12/13	0.94	0.08	9,16,26,31	0
1	MLY	A	290	11/12	0.95	0.07	12,14,24,28	0
2	MLY	B	498	11/12	0.95	0.07	19,20,27,32	0
2	MLY	B	374	11/12	0.95	0.08	14,15,34,35	0
3	MLY	C	390	11/12	0.95	0.06	7,10,20,21	0
3	MLZ	C	620	10/11	0.95	0.09	12,15,36,37	0
4	MLY	D	210	11/12	0.95	0.06	12,14,15,16	0
4	MLY	D	390	11/12	0.95	0.06	14,14,17,19	0
1	M3L	A	364	12/13	0.95	0.11	15,24,43,45	0
3	MLY	C	121	11/12	0.96	0.09	7,10,28,32	0
2	MLY	B	390	11/12	0.96	0.06	15,16,17,18	0
3	MLY	C	213	11/12	0.96	0.08	7,10,32,34	0
1	MLY	A	93	11/12	0.96	0.07	13,15,28,29	0
3	M3L	C	400	12/13	0.96	0.07	9,12,19,25	0
3	M3L	C	474	12/13	0.96	0.07	8,12,24,31	0
2	MLY	B	402	11/12	0.96	0.07	13,14,24,26	0
2	MLZ	B	405	10/11	0.96	0.08	13,15,34,36	0
4	MLZ	D	235	10/11	0.96	0.07	13,14,26,29	0
1	M3L	A	498	12/13	0.96	0.07	10,11,23,26	0
1	MLY	A	400	11/12	0.96	0.06	12,15,20,21	0
4	MLY	D	402	11/12	0.96	0.06	9,12,21,22	0
4	M3L	D	474	12/13	0.96	0.08	11,15,24,29	0
4	M3L	D	498	12/13	0.96	0.08	11,14,29,30	0
3	MLY	C	402	11/12	0.97	0.06	6,8,18,19	0
1	MLY	A	552	11/12	0.97	0.05	5,7,10,11	0
3	M3L	C	498	12/13	0.97	0.06	8,11,25,26	0
2	MLY	B	364	11/12	0.97	0.08	12,14,29,34	0
1	MLY	A	565	11/12	0.97	0.07	8,10,32,32	0
1	M3L	A	620	12/13	0.97	0.07	8,13,33,34	0
3	MLY	C	210	11/12	0.97	0.05	5,7,10,12	0
1	MLZ	A	625	10/11	0.97	0.07	12,14,34,35	0
3	MLY	C	364	11/12	0.97	0.07	7,9,25,26	0
1	MLY	A	402	11/12	0.97	0.06	10,14,22,28	0
1	MLZ	A	518	10/11	0.97	0.06	7,8,23,25	0
3	MLY	C	518	11/12	0.98	0.05	6,8,17,18	0
3	MLY	C	552	11/12	0.98	0.04	5,7,10,10	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(Å ²)	Q<0.9
5	GOL	D	702	6/6	0.74	0.16	31,39,40,43	0
5	GOL	B	701	6/6	0.90	0.09	38,39,39,40	0
5	GOL	D	701	6/6	0.91	0.08	33,35,37,40	0
5	GOL	A	701	6/6	0.91	0.10	24,35,37,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.