



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 06:39 pm GMT

PDB ID : 4DWS  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28986

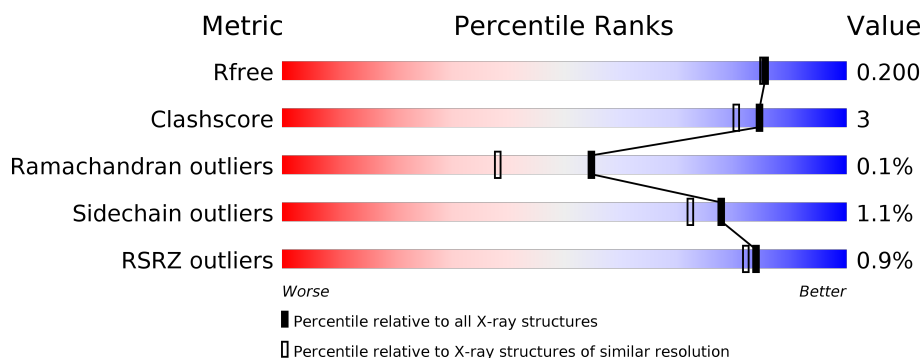
# 1 Overall quality at a glance

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))
$R_{free}$	100719	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div style="width: 92%;"></div> <div style="width: 6%;"></div> <div style="width: 2%;"></div> <div style="width: 1%;"></div> <div style="width: 1%;"></div> </div> <div>92% 6% .</div>
2	B	546	<div> <div style="width: 94%;"></div> <div style="width: 4%;"></div> <div style="width: 2%;"></div> <div style="width: 1%;"></div> <div style="width: 1%;"></div> </div> <div>94% . .</div>
3	C	546	<div> <div style="width: 89%;"></div> <div style="width: 8%;"></div> <div style="width: 2%;"></div> <div style="width: 1%;"></div> <div style="width: 1%;"></div> </div> <div>89% 8% . .</div>
4	D	546	<div> <div style="width: 90%;"></div> <div style="width: 8%;"></div> <div style="width: 2%;"></div> <div style="width: 1%;"></div> <div style="width: 1%;"></div> </div> <div>90% 8% .</div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	A	701	-	-	-	X
5	GOL	D	702	-	-	-	X

## 2 Entry composition

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
1	A	540	Total	C	N	O	S	0	4	0
			4191	2670	697	807	17			

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
2	B	538	Total	C	N	O	S	0	3	0
			4122	2628	681	795	18			

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
3	C	539	Total	C	N	O	S	0	7	0
			4201	2674	694	815	18			

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

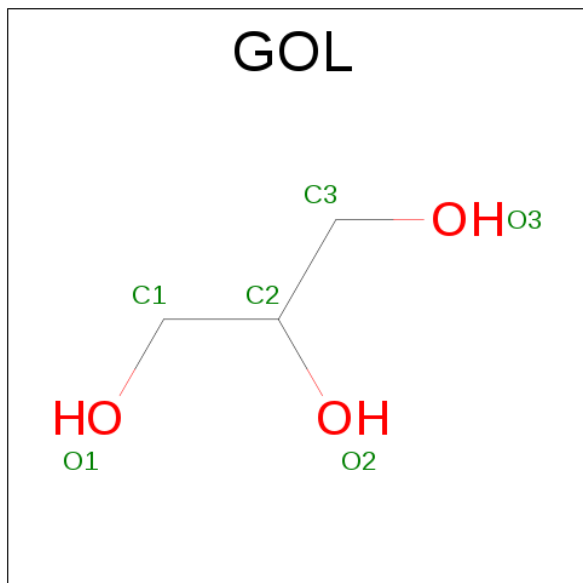
- Molecule 4 is a protein called Chi2.

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

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 (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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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		

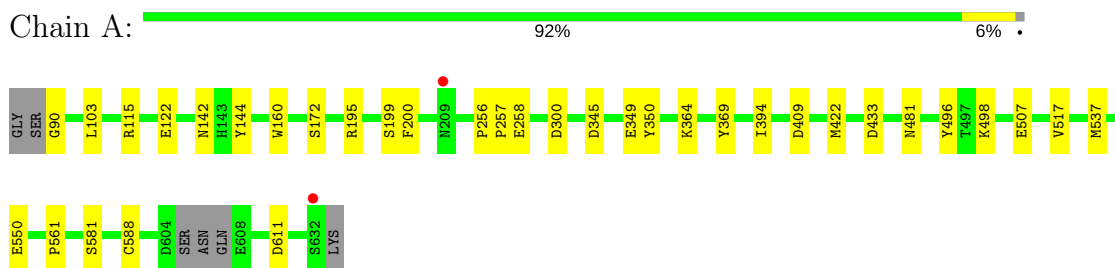
- Molecule 6 is water.

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		

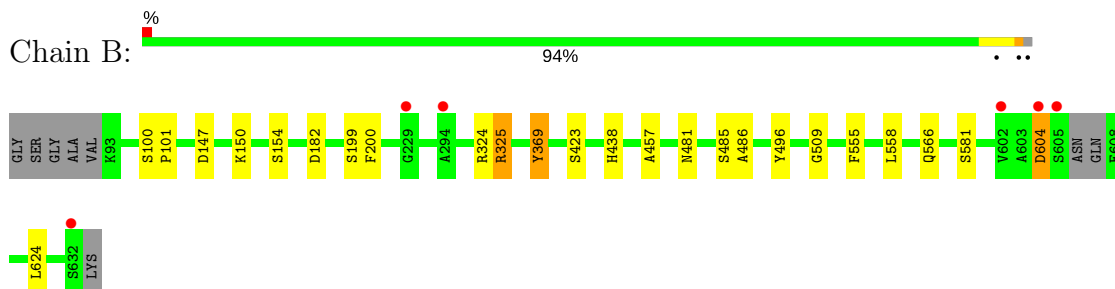
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA 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 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.

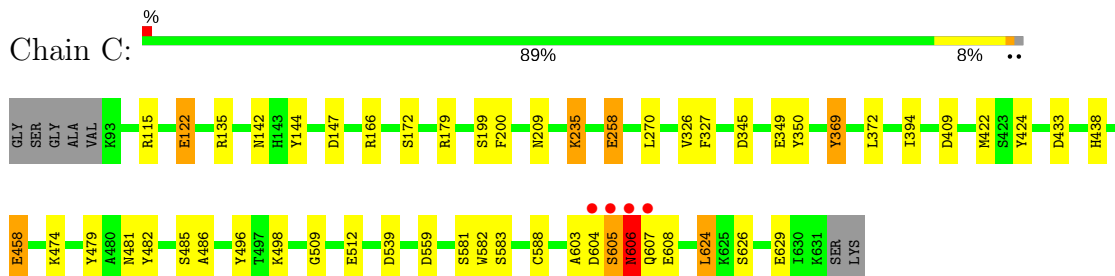
#### • Molecule 1: Chi2



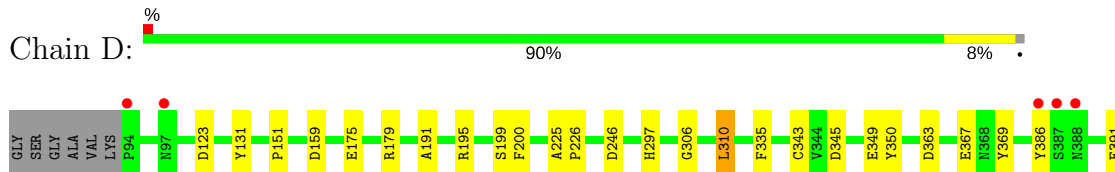
#### • Molecule 2: Chi2

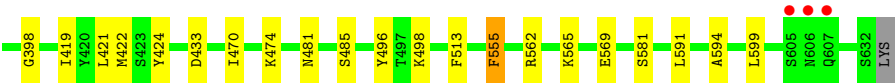


#### • Molecule 3: Chi2



#### • Molecule 4: Chi2







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.51Å 210.56Å 92.58Å 90.00° 95.27° 90.00°	Depositor
Resolution (Å)	105.28 – 1.80 19.90 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (105.28-1.80) 100.0 (19.90-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.43 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.160 , 0.199 0.160 , 0.200	Depositor DCC
$R_{free}$ test set	10651 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.5	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 47.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17938	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, MLY, M3L

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	1.14	3/4143 (0.1%)	0.99	4/5619 (0.1%)
2	B	1.05	1/4105 (0.0%)	0.95	4/5579 (0.1%)
3	C	1.22	9/4174 (0.2%)	1.04	11/5665 (0.2%)
4	D	1.15	8/4220 (0.2%)	0.99	5/5721 (0.1%)
All	All	1.14	21/16642 (0.1%)	0.99	24/22584 (0.1%)

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

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	588	CYS	CB-SG	-7.37	1.69	1.82
4	D	367	GLU	CG-CD	6.74	1.62	1.51
4	D	513	PHE	CE1-CZ	6.61	1.50	1.37
4	D	555	PHE	CE1-CZ	6.57	1.49	1.37
3	C	512	GLU	CB-CG	6.42	1.64	1.52

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	537	MET	CG-SD-CE	-8.73	86.23	100.20
2	B	324	ARG	NE-CZ-NH1	-7.68	116.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	606	ASN	CB-CA-C	7.04	124.49	110.40
3	C	166	ARG	NE-CZ-NH2	-6.82	116.89	120.30
3	C	235	LYS	CD-CE-NZ	-6.68	96.34	111.70

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	4019	20	0
2	B	4122	0	3894	14	0
3	C	4201	0	4014	30	0
4	D	4194	0	3987	21	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	15946	87	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 87 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%)	38	23
4	D	539/546 (99%)	525 (97%)	12 (2%)	2 (0%)	38	23
All	All	2122/2184 (97%)	2061 (97%)	57 (3%)	4 (0%)	55	35

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%)	410 (99%)	4 (1%)	80	75
2	B	404/435 (93%)	400 (99%)	4 (1%)	80	75
3	C	419/433 (97%)	412 (98%)	7 (2%)	66	55
4	D	422/439 (96%)	419 (99%)	3 (1%)	87	84
All	All	1659/1739 (95%)	1641 (99%)	18 (1%)	78	72

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	122	GLU
3	C	258	GLU
3	C	559	ASP
2	B	369	TYR
2	B	438	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	189	ASN
3	C	606	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	210	1	9,9,11	0.71	0	10,10,13	1.69	4 (40%)
1	MLY	A	290	1	10,10,11	1.20	1 (10%)	8,11,13	2.03	2 (25%)
1	M3L	A	364	1	11,11,12	0.93	1 (9%)	11,14,16	1.62	1 (9%)
1	M3L	A	390	1	11,11,12	0.48	0	11,14,16	4.33	6 (54%)
1	MLY	A	400	1	10,10,11	0.78	0	8,11,13	2.37	4 (50%)
1	MLY	A	402	1	10,10,11	0.71	0	8,11,13	2.00	2 (25%)
1	MLZ	A	405	1	9,9,10	0.92	1 (11%)	6,9,11	1.45	1 (16%)
1	M3L	A	498	1	11,11,12	0.78	0	11,14,16	1.03	1 (9%)
1	MLZ	A	518	1	9,9,10	0.72	0	6,9,11	1.66	2 (33%)
1	MLY	A	552	1	10,10,11	1.38	1 (10%)	8,11,13	2.31	3 (37%)
1	MLY	A	565	1	10,10,11	0.47	0	8,11,13	1.97	2 (25%)
1	M3L	A	620	1	11,11,12	0.68	0	11,14,16	0.83	0
1	MLZ	A	625	1	9,9,10	0.77	0	6,9,11	2.03	2 (33%)
1	MLY	A	93	1	10,10,11	0.54	0	8,11,13	2.33	3 (37%)
2	M3L	B	150	2	11,11,12	1.31	1 (9%)	11,14,16	1.04	0
2	MLY	B	210	2	10,10,11	1.22	1 (10%)	8,11,13	2.18	3 (37%)
2	MLY	B	235	2	10,10,11	1.01	0	8,11,13	2.17	3 (37%)
2	MLY	B	364	2	10,10,11	0.75	0	8,11,13	2.59	4 (50%)
2	MLY	B	374	2	10,10,11	0.89	1 (10%)	8,11,13	2.11	4 (50%)
2	MLY	B	390	2	10,10,11	0.83	0	8,11,13	2.30	3 (37%)
2	M3L	B	400	2	11,11,12	0.73	0	11,14,16	1.62	1 (9%)
2	MLY	B	402	2	10,10,11	0.81	0	8,11,13	2.17	3 (37%)
2	MLZ	B	405	2	9,9,10	1.19	1 (11%)	6,9,11	1.37	1 (16%)
2	M3L	B	474	2	11,11,12	1.13	1 (9%)	11,14,16	1.66	1 (9%)
2	MLY	B	498	2	10,10,11	0.71	0	8,11,13	1.94	2 (25%)
3	MLY	C	121	3	10,10,11	0.70	0	8,11,13	2.21	3 (37%)
3	MLZ	C	150	3	9,9,10	0.98	0	6,9,11	1.49	1 (16%)
3	MLY	C	210	3	10,10,11	1.33	2 (20%)	8,11,13	2.14	3 (37%)
3	MLY	C	213	3	10,10,11	1.21	2 (20%)	8,11,13	1.99	2 (25%)
3	MLY	C	364	3	10,10,11	1.16	1 (10%)	8,11,13	2.65	4 (50%)
3	MLY	C	390	3	10,10,11	1.25	1 (10%)	8,11,13	2.82	3 (37%)
3	M3L	C	400	3	11,11,12	1.57	1 (9%)	11,14,16	1.01	0
3	MLY	C	402	3	10,10,11	0.84	0	8,11,13	2.15	3 (37%)
3	M3L	C	474	3	11,11,12	0.72	0	11,14,16	1.33	2 (18%)
3	M3L	C	498	3	11,11,12	1.01	1 (9%)	11,14,16	1.05	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	MLY	C	518	3	10,10,11	0.73	0	8,11,13	2.16	4 (50%)
3	MLY	C	552	3	10,10,11	0.60	0	8,11,13	1.85	2 (25%)
3	MLZ	C	620	3	9,9,10	0.76	0	6,9,11	1.36	1 (16%)
4	MLY	D	210	4	10,10,11	1.07	1 (10%)	8,11,13	2.03	2 (25%)
4	MLZ	D	235	4	9,9,10	0.78	0	6,9,11	1.14	0
4	MLY	D	390	4	10,10,11	0.88	0	8,11,13	2.38	2 (25%)
4	M3L	D	400	4	11,11,12	0.63	0	11,14,16	1.25	2 (18%)
4	MLY	D	402	4	10,10,11	1.00	1 (10%)	8,11,13	2.06	3 (37%)
4	M3L	D	474	4	11,11,12	1.03	1 (9%)	11,14,16	1.37	3 (27%)
4	M3L	D	498	4	11,11,12	1.10	1 (9%)	11,14,16	1.54	4 (36%)

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	210	1	-	0/7/7/11	0/0/0/0
1	MLY	A	290	1	-	0/7/9/11	0/0/0/0
1	M3L	A	364	1	-	0/8/10/12	0/0/0/0
1	M3L	A	390	1	-	0/8/10/12	0/0/0/0
1	MLY	A	400	1	-	0/7/9/11	0/0/0/0
1	MLY	A	402	1	-	0/7/9/11	0/0/0/0
1	MLZ	A	405	1	-	0/6/8/10	0/0/0/0
1	M3L	A	498	1	-	0/8/10/12	0/0/0/0
1	MLZ	A	518	1	-	0/6/8/10	0/0/0/0
1	MLY	A	552	1	-	0/7/9/11	0/0/0/0
1	MLY	A	565	1	-	0/7/9/11	0/0/0/0
1	M3L	A	620	1	-	0/8/10/12	0/0/0/0
1	MLZ	A	625	1	-	0/6/8/10	0/0/0/0
1	MLY	A	93	1	-	0/7/9/11	0/0/0/0
2	M3L	B	150	2	-	0/8/10/12	0/0/0/0
2	MLY	B	210	2	-	0/7/9/11	0/0/0/0
2	MLY	B	235	2	-	0/7/9/11	0/0/0/0
2	MLY	B	364	2	-	0/7/9/11	0/0/0/0
2	MLY	B	374	2	-	0/7/9/11	0/0/0/0
2	MLY	B	390	2	-	0/7/9/11	0/0/0/0
2	M3L	B	400	2	-	0/8/10/12	0/0/0/0
2	MLY	B	402	2	-	0/7/9/11	0/0/0/0
2	MLZ	B	405	2	-	0/6/8/10	0/0/0/0
2	M3L	B	474	2	-	0/8/10/12	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLY	B	498	2	-	0/7/9/11	0/0/0/0
3	MLY	C	121	3	-	0/7/9/11	0/0/0/0
3	MLZ	C	150	3	-	0/6/8/10	0/0/0/0
3	MLY	C	210	3	-	0/7/9/11	0/0/0/0
3	MLY	C	213	3	-	0/7/9/11	0/0/0/0
3	MLY	C	364	3	-	0/7/9/11	0/0/0/0
3	MLY	C	390	3	-	0/7/9/11	0/0/0/0
3	M3L	C	400	3	-	0/8/10/12	0/0/0/0
3	MLY	C	402	3	-	0/7/9/11	0/0/0/0
3	M3L	C	474	3	-	0/8/10/12	0/0/0/0
3	M3L	C	498	3	-	0/8/10/12	0/0/0/0
3	MLY	C	518	3	-	0/7/9/11	0/0/0/0
3	MLY	C	552	3	-	0/7/9/11	0/0/0/0
3	MLZ	C	620	3	-	0/6/8/10	0/0/0/0
4	MLY	D	210	4	-	0/7/9/11	0/0/0/0
4	MLZ	D	235	4	-	0/6/8/10	0/0/0/0
4	MLY	D	390	4	-	0/7/9/11	0/0/0/0
4	M3L	D	400	4	-	0/8/10/12	0/0/0/0
4	MLY	D	402	4	-	0/7/9/11	0/0/0/0
4	M3L	D	474	4	-	0/8/10/12	0/0/0/0
4	M3L	D	498	4	-	0/8/10/12	0/0/0/0

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	374	MLY	CA-C	-2.01	1.47	1.50
4	D	498	M3L	CB-CA	2.12	1.56	1.53
3	C	213	MLY	CA-C	2.14	1.53	1.50
1	A	364	M3L	CA-C	2.22	1.53	1.50
3	C	210	MLY	CB-CA	2.24	1.56	1.53

The worst 5 of 103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	M3L	CM3-NZ-CM1	-8.08	88.53	108.98
1	A	390	M3L	CM3-NZ-CM2	-7.28	90.55	108.98
1	A	390	M3L	CM3-NZ-CE	-7.26	82.05	109.93
3	C	364	MLY	CB-CA-C	-4.97	103.46	111.65
2	B	364	MLY	CB-CA-C	-4.81	103.72	111.65

There are no chirality outliers.

There are no torsion outliers.



There are no ring outliers.

7 monomers are involved in 22 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	A	701	-	5,5,5	0.33	0	5,5,5	0.49	0
5	GOL	B	701	-	5,5,5	0.34	0	5,5,5	0.64	0
5	GOL	D	701	-	5,5,5	0.22	0	5,5,5	0.73	0
5	GOL	D	702	-	5,5,5	0.49	0	5,5,5	1.14	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
5	GOL	A	701	-	-	0/4/4/4	0/0/0/0
5	GOL	B	701	-	-	0/4/4/4	0/0/0/0
5	GOL	D	701	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	D	702	-	-	0/4/4/4	0/0/0/0

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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	701	GOL	1	0
5	D	702	GOL	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	526/546 (96%)	-0.50	2 (0%) 92 90	5, 12, 23, 39	0
2	B	527/546 (96%)	-0.24	6 (1%) 80 79	8, 18, 30, 43	0
3	C	526/546 (96%)	-0.58	4 (0%) 86 84	4, 9, 21, 46	0
4	D	532/546 (97%)	-0.45	8 (1%) 74 70	5, 13, 24, 48	0
All	All	2111/2184 (96%)	-0.44	20 (0%) 84 82	4, 13, 27, 48	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	605	SER	6.6
4	D	386[A]	TYR	5.3
3	C	605	SER	4.8
3	C	604	ASP	4.4
3	C	607	GLN	3.7

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	MLY	C	518	11/12	0.99	0.08	-	6,8,17,18	0
1	MLZ	A	625	10/11	0.95	0.11	-	12,14,34,35	0
1	MLY	A	402	11/12	0.96	0.09	-	10,14,22,28	0
1	MLY	A	290	11/12	0.96	0.11	-	12,14,24,28	0
3	MLY	C	402	11/12	0.98	0.07	-	6,8,18,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MLY	A	552	11/12	0.97	0.09	-	5,7,10,11	0
3	MLY	C	390	11/12	0.95	0.09	-	7,10,20,21	0
3	M3L	C	498	12/13	0.96	0.10	-	8,11,25,26	0
3	MLY	C	364	11/12	0.97	0.07	-	7,9,25,26	0
2	M3L	B	150	12/13	0.95	0.10	-	17,23,31,32	0
3	M3L	C	474	12/13	0.96	0.09	-	8,12,24,31	0
3	MLY	C	552	11/12	0.98	0.08	-	5,7,10,10	0
1	MLY	A	210	10/12	0.92	0.10	-	10,13,17,18	0
4	M3L	D	498	12/13	0.94	0.11	-	11,14,29,30	0
4	MLY	D	390	11/12	0.97	0.08	-	14,14,17,19	0
2	MLY	B	390	11/12	0.96	0.08	-	15,16,17,18	0
2	MLY	B	235	11/12	0.94	0.11	-	13,16,31,33	0
4	MLY	D	210	11/12	0.96	0.07	-	12,14,15,16	0
1	M3L	A	498	12/13	0.96	0.11	-	10,11,23,26	0
1	MLY	A	565	11/12	0.97	0.09	-	8,10,32,32	0
2	MLY	B	374	11/12	0.93	0.15	-	14,15,34,35	0
2	MLY	B	498	11/12	0.95	0.11	-	19,20,27,32	0
1	MLZ	A	405	10/11	0.95	0.09	-	13,14,27,29	0
3	MLY	C	121	11/12	0.95	0.11	-	7,10,28,32	0
2	MLY	B	402	11/12	0.97	0.07	-	13,14,24,26	0
4	M3L	D	400	12/13	0.94	0.09	-	9,16,26,31	0
2	M3L	B	400	12/13	0.94	0.10	-	13,16,26,32	0
3	MLY	C	213	11/12	0.96	0.11	-	7,10,32,34	0
4	MLZ	D	235	10/11	0.94	0.09	-	13,14,26,29	0
1	M3L	A	390	12/13	0.94	0.10	-	10,12,24,26	0
1	MLZ	A	518	10/11	0.97	0.08	-	7,8,23,25	0
2	MLZ	B	405	10/11	0.95	0.14	-	13,15,34,36	0
3	M3L	C	400	12/13	0.96	0.10	-	9,12,19,25	0
2	MLY	B	364	11/12	0.96	0.12	-	12,14,29,34	0
1	MLY	A	93	11/12	0.96	0.09	-	13,15,28,29	0
4	M3L	D	474	12/13	0.94	0.12	-	11,15,24,29	0
3	MLY	C	210	11/12	0.97	0.07	-	5,7,10,12	0
2	M3L	B	474	12/13	0.92	0.15	-	13,19,31,35	0
4	MLY	D	402	11/12	0.95	0.08	-	9,12,21,22	0
3	MLZ	C	150	10/11	0.93	0.10	-	12,17,28,29	0
1	M3L	A	620	12/13	0.97	0.09	-	8,13,33,34	0
1	MLY	A	400	11/12	0.96	0.09	-	12,15,20,21	0
1	M3L	A	364	12/13	0.93	0.18	-	15,24,43,45	0
3	MLZ	C	620	10/11	0.94	0.12	-	12,15,36,37	0
2	MLY	B	210	11/12	0.95	0.09	-	9,11,16,18	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	D	702	6/6	0.79	0.15	9.46	31,39,40,43	0
5	GOL	A	701	6/6	0.86	0.16	8.85	24,35,37,38	0
5	GOL	B	701	6/6	0.90	0.16	-	38,39,39,40	0
5	GOL	D	701	6/6	0.93	0.12	-	33,35,37,40	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.