



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:57 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 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

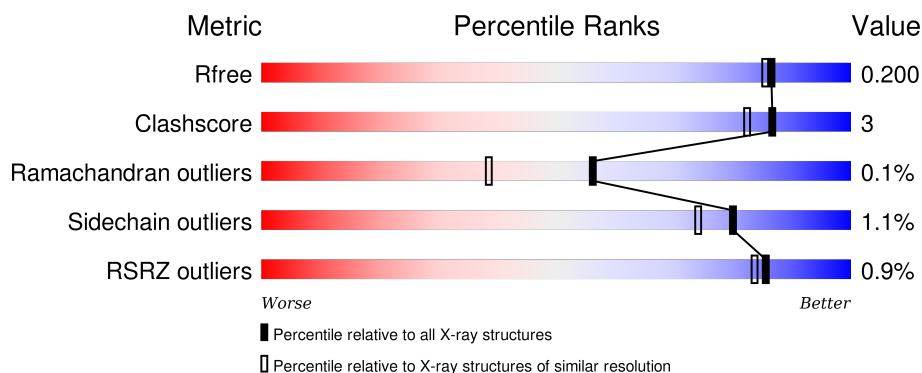
1 Overall quality at a glance

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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (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 ≥ 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>92%</div> <div>6% .</div> </div>
2	B	546	<div> <div>%</div> <div>94%</div> <div>. . .</div> </div>
3	C	546	<div> <div>%</div> <div>89%</div> <div>8% ..</div> </div>
4	D	546	<div> <div>%</div> <div>90%</div> <div>8% .</div> </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 criteria:

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
			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

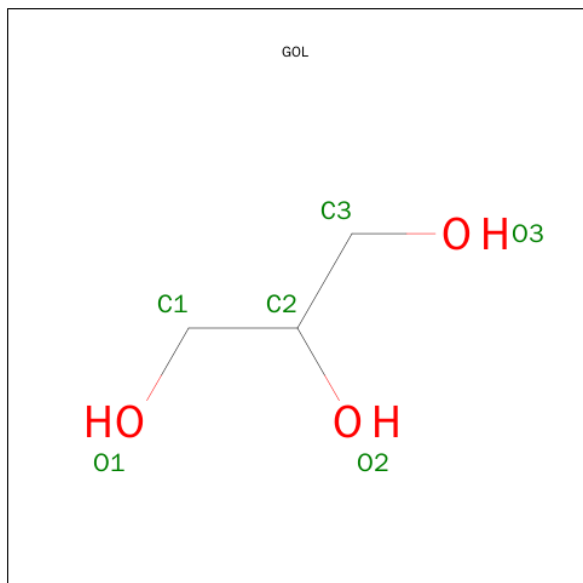
- Molecule 4 is a protein called Chi2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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: C₃H₈O₃).



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		

Continued on next page...

Continued from previous page...

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		

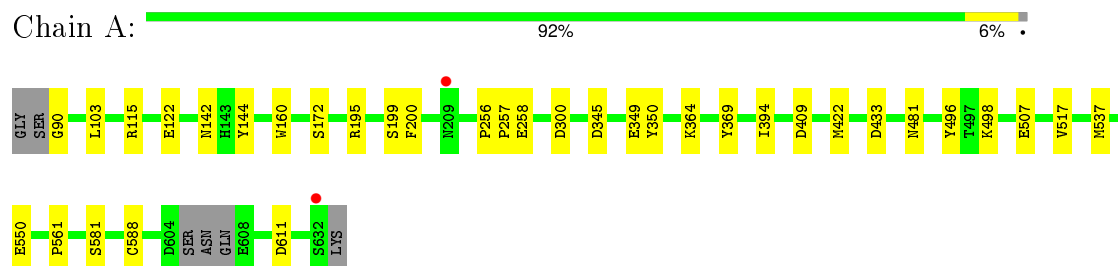
- Molecule 6 is water.

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		

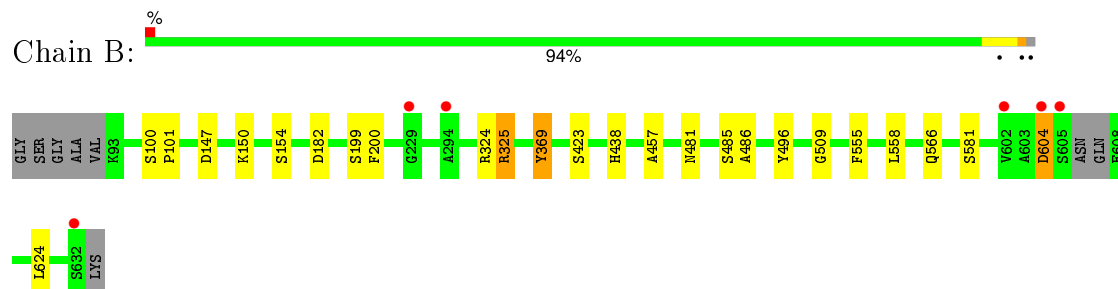
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

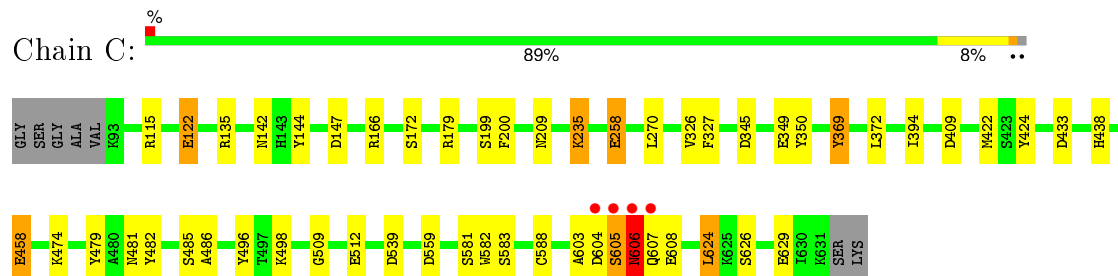
• Molecule 1: Chi2



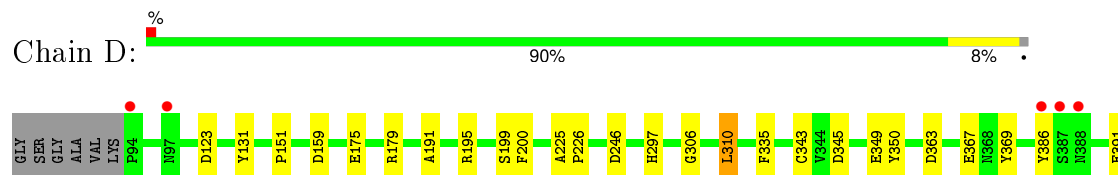
• Molecule 2: Chi2

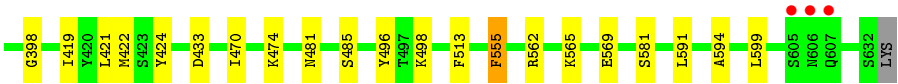


• Molecule 3: Chi2



• 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 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
$\langle I/\sigma(I) \rangle$ ¹	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	10654 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	13.5	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 212074 reflections	Xtriage
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

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.*

¹Intensities estimated from amplitudes.

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

All (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
1	A	507	GLU	CG-CD	5.96	1.60	1.51
3	C	479	TYR	CD1-CE1	5.73	1.48	1.39
3	C	588	CYS	CB-SG	-5.71	1.72	1.81
3	C	458[A]	GLU	CB-CG	5.66	1.62	1.52
3	C	458[B]	GLU	CB-CG	5.66	1.62	1.52
4	D	424	TYR	CD1-CE1	5.63	1.47	1.39
3	C	458[A]	GLU	CG-CD	5.62	1.60	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	458[B]	GLU	CG-CD	5.62	1.60	1.51
3	C	122	GLU	CD-OE2	5.61	1.31	1.25
1	A	90	GLY	N-CA	5.57	1.54	1.46
4	D	594	ALA	CA-CB	5.51	1.64	1.52
4	D	335	PHE	CE1-CZ	5.49	1.47	1.37
4	D	175	GLU	CG-CD	5.36	1.59	1.51
4	D	131	TYR	CG-CD2	5.28	1.46	1.39
2	B	369	TYR	CG-CD1	5.23	1.46	1.39
3	C	486	ALA	CA-CB	5.02	1.62	1.52

All (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
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
1	A	422	MET	CA-CB-CG	-6.59	102.10	113.30
2	B	324	ARG	NE-CZ-NH2	6.44	123.52	120.30
1	A	611	ASP	CB-CG-OD1	6.22	123.90	118.30
3	C	369	TYR	CB-CG-CD2	-6.08	117.35	121.00
3	C	135	ARG	NE-CZ-NH1	5.91	123.25	120.30
2	B	624	LEU	CA-CB-CG	5.70	128.40	115.30
4	D	422	MET	CG-SD-CE	-5.68	91.12	100.20
1	A	409	ASP	CB-CG-OD1	5.66	123.39	118.30
3	C	147	ASP	CB-CG-OD1	5.63	123.37	118.30
3	C	409	ASP	CB-CG-OD1	5.54	123.28	118.30
3	C	326	VAL	CG1-CB-CG2	-5.52	102.06	110.90
4	D	123	ASP	CB-CG-OD1	5.49	123.24	118.30
4	D	562	ARG	NE-CZ-NH2	5.43	123.02	120.30
3	C	624	LEU	CB-CG-CD2	-5.17	102.21	111.00
3	C	482	TYR	CG-CD1-CE1	-5.15	117.18	121.30
4	D	310	LEU	CB-CG-CD2	5.14	119.74	111.00
2	B	182	ASP	CB-CG-OD1	5.09	122.89	118.30
3	C	270	LEU	CB-CG-CD1	5.04	119.57	111.00
4	D	591	LEU	CB-CG-CD1	-5.04	102.44	111.00

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

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.

All (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
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
1:A:550[B]:GLU:CD	1:A:550[B]:GLU:H	1.82	0.81
4:D:433:ASP:OD1	4:D:498:M3L:CM3	2.29	0.80
1:A:433:ASP:OD1	1:A:498:M3L:HM13	1.83	0.78
3:C:604:ASP:O	3:C:606:ASN:ND2	2.18	0.76
4:D:474:M3L:HM33	4:D:474:M3L:HG3	1.69	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:474:M3L:HM33	3:C:474:M3L:HG3	1.68	0.74
4:D:343[B]:CYS:HB3	4:D:391:GLU:HB2	1.68	0.74
3:C:433:ASP:OD1	3:C:498:M3L:HM21	1.87	0.72
4:D:474:M3L:CG	4:D:474:M3L:HM33	2.23	0.69
3:C:422[B]:MET:HE1	6:C:1002:HOH:O	1.93	0.68
2:B:325:ARG:HD2	6:B:963:HOH:O	1.94	0.66
2:B:150:M3L:HM13	2:B:150:M3L:HG3	1.78	0.65
3:C:606:ASN:C	3:C:608:GLU:H	2.01	0.62
4:D:481:ASN:ND2	4:D:581:SER:OG	2.33	0.61
1:A:433:ASP:HA	1:A:498:M3L:HM13	1.82	0.61
3:C:433:ASP:HA	3:C:498:M3L:HM23	1.82	0.60
2:B:566:GLN:CG	6:B:891:HOH:O	2.49	0.59
3:C:606:ASN:C	3:C:608:GLU:N	2.54	0.59
2:B:147:ASP:OD2	2:B:150:M3L:HE3	2.03	0.59
5:D:702:GOL:C3	6:D:1048:HOH:O	2.49	0.58
1:A:122:GLU:CD	1:A:122:GLU:H	2.11	0.54
1:A:160:TRP:NE1	5:A:701:GOL:H11	2.23	0.54
5:D:702:GOL:H31	6:D:1048:HOH:O	2.06	0.53
3:C:539:ASP:HB2	3:C:624:LEU:HD12	1.91	0.53
4:D:195:ARG:NH1	4:D:343[B]:CYS:SG	2.84	0.51
1:A:481:ASN:ND2	1:A:581:SER:OG	2.39	0.50
2:B:481:ASN:ND2	2:B:581:SER:OG	2.44	0.49
3:C:481:ASN:ND2	3:C:581:SER:OG	2.45	0.48
3:C:474:M3L:HM33	3:C:474:M3L:CG	2.41	0.48
3:C:115[B]:ARG:CZ	3:C:172:SER:HA	2.44	0.48
3:C:209[B]:ASN:OD1	6:C:1067:HOH:O	2.20	0.47
3:C:349:GLU:HA	3:C:350:TYR:CD1	2.50	0.47
3:C:496:TYR:CE2	3:C:498:M3L:HA	2.50	0.47
4:D:398:GLY:HA2	4:D:421:LEU:HD11	1.97	0.47
4:D:496:TYR:CE2	4:D:498:M3L:HA	2.49	0.46
2:B:485:SER:HA	2:B:555:PHE:O	2.16	0.46
4:D:151:PRO:HB2	4:D:599:LEU:HD22	1.98	0.46
1:A:142:ASN:HB2	1:A:144:TYR:CE1	2.51	0.46
3:C:422[B]:MET:CE	6:C:1002:HOH:O	2.58	0.45
2:B:325:ARG:CD	6:B:963:HOH:O	2.56	0.45
1:A:115:ARG:CZ	1:A:172:SER:HA	2.46	0.45
2:B:486:ALA:HB1	2:B:496:TYR:CD2	2.51	0.45
1:A:199:SER:HA	1:A:200:PHE:HA	1.83	0.45
2:B:485:SER:OG	2:B:509:GLY:HA2	2.16	0.45
4:D:485:SER:HA	4:D:555:PHE:O	2.18	0.44
1:A:349:GLU:HA	1:A:350:TYR:CD1	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:191:ALA:HA	4:D:297:HIS:CD2	2.53	0.44
3:C:258:GLU:H	3:C:258:GLU:CD	2.20	0.44
4:D:159:ASP:OD2	4:D:246:ASP:OD1	2.36	0.44
1:A:496:TYR:CE2	1:A:498:M3L:HA	2.53	0.43
4:D:349:GLU:HA	4:D:350:TYR:CD1	2.53	0.43
3:C:605:SER:O	3:C:606:ASN:C	2.56	0.43
6:A:1094:HOH:O	3:C:235:LYS:HE2	2.17	0.43
4:D:225:ALA:N	4:D:226:PRO:CD	2.82	0.43
3:C:349:GLU:HA	3:C:350:TYR:CG	2.54	0.43
4:D:474:M3L:CG	4:D:474:M3L:CM3	2.96	0.42
3:C:179:ARG:HD3	6:C:793:HOH:O	2.19	0.42
3:C:626:SER:OG	3:C:629:GLU:HG3	2.18	0.42
1:A:257:PRO:HD2	1:A:258:GLU:OE2	2.19	0.42
1:A:195:ARG:HA	1:A:300:ASP:O	2.19	0.42
3:C:199[A]:SER:HA	3:C:200:PHE:HA	1.83	0.42
3:C:142:ASN:HB2	3:C:144:TYR:CE1	2.55	0.42
1:A:256:PRO:HA	1:A:257:PRO:HD3	1.89	0.41
2:B:100:SER:HA	2:B:101:PRO:HD2	1.91	0.41
3:C:327:PHE:CD2	3:C:372:LEU:HD11	2.55	0.41
4:D:419:ILE:HD12	4:D:470:ILE:HG21	2.01	0.41
2:B:604:ASP:OD1	2:B:604:ASP:C	2.58	0.41
2:B:199:SER:HA	2:B:200:PHE:HA	1.85	0.41
1:A:364:M3L:HM33	1:A:364:M3L:HD3	1.79	0.41
4:D:199:SER:HA	4:D:200:PHE:HA	1.77	0.41
3:C:582:TRP:HA	3:C:583[B]:SER:HA	1.87	0.41
3:C:485:SER:OG	3:C:509:GLY:HA2	2.21	0.41
1:A:349:GLU:HA	1:A:350:TYR:CG	2.56	0.41
2:B:423:SER:HB2	2:B:457:ALA:HB2	2.02	0.41
3:C:422[B]:MET:HE2	3:C:424:TYR:CE1	2.56	0.41
4:D:565:LYS:HE3	4:D:569:GLU:OE2	2.20	0.41
1:A:498:M3L:HD3	1:A:498:M3L:HM12	1.73	0.41
4:D:179:ARG:HD3	6:D:890:HOH:O	2.19	0.41
4:D:306:GLY:O	4:D:310:LEU:HB2	2.21	0.41
2:B:558:LEU:HD23	2:B:558:LEU:H	1.85	0.41
1:A:103:LEU:HD21	1:A:517:VAL:HG12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	39	23
4	D	539/546 (99%)	525 (97%)	12 (2%)	2 (0%)	39	23
All	All	2122/2184 (97%)	2061 (97%)	57 (3%)	4 (0%)	56	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

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%)	82	77
2	B	404/435 (93%)	400 (99%)	4 (1%)	82	77
3	C	419/433 (97%)	412 (98%)	7 (2%)	68	57
4	D	422/439 (96%)	419 (99%)	3 (1%)	88	86
All	All	1659/1739 (95%)	1641 (99%)	18 (1%)	80	74

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	345	ASP
1	A	369	TYR
1	A	394	ILE
1	A	561	PRO
2	B	154	SER
2	B	325	ARG
2	B	369	TYR
2	B	438	HIS
3	C	122	GLU
3	C	258	GLU
3	C	345	ASP
3	C	369	TYR
3	C	394	ILE
3	C	438	HIS
3	C	559	ASP
4	D	345	ASP
4	D	363	ASP
4	D	369	TYR

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	0.78	0	10,10,13	1.74	4 (40%)
1	MLY	A	290	1	9,10,11	0.95	0	9,11,13	1.96	2 (22%)
1	M3L	A	364	1	10,11,12	0.67	0	12,14,16	0.90	1 (8%)
1	M3L	A	390	1	10,11,12	0.43	0	12,14,16	4.07	7 (58%)
1	MLY	A	400	1	9,10,11	0.84	0	9,11,13	2.03	3 (33%)
1	MLY	A	402	1	9,10,11	0.67	0	9,11,13	1.87	2 (22%)
1	MLZ	A	405	1	8,9,10	0.50	0	7,9,11	1.53	2 (28%)
1	M3L	A	498	1	10,11,12	0.82	0	12,14,16	1.01	1 (8%)
1	MLZ	A	518	1	8,9,10	0.72	0	7,9,11	1.56	2 (28%)
1	MLY	A	552	1	9,10,11	1.75	1 (11%)	9,11,13	2.20	3 (33%)
1	MLY	A	565	1	9,10,11	0.49	0	9,11,13	1.91	2 (22%)
1	M3L	A	620	1	10,11,12	0.71	0	12,14,16	0.99	0
1	MLZ	A	625	1	8,9,10	0.84	0	7,9,11	1.60	1 (14%)
1	MLY	A	93	1	9,10,11	0.55	0	9,11,13	2.07	2 (22%)
2	M3L	B	150	2	10,11,12	0.66	0	12,14,16	1.06	1 (8%)
2	MLY	B	210	2	9,10,11	1.50	1 (11%)	9,11,13	1.92	3 (33%)
2	MLY	B	235	2	9,10,11	0.87	0	9,11,13	2.13	4 (44%)
2	MLY	B	364	2	9,10,11	0.71	0	9,11,13	1.87	3 (33%)
2	MLY	B	374	2	9,10,11	0.72	0	9,11,13	1.70	3 (33%)
2	MLY	B	390	2	9,10,11	0.75	0	9,11,13	1.88	2 (22%)
2	M3L	B	400	2	10,11,12	0.88	1 (10%)	12,14,16	1.21	1 (8%)
2	MLY	B	402	2	9,10,11	0.79	0	9,11,13	2.03	3 (33%)
2	MLZ	B	405	2	8,9,10	1.55	1 (12%)	7,9,11	1.07	0
2	M3L	B	474	2	10,11,12	0.90	0	12,14,16	1.14	1 (8%)
2	MLY	B	498	2	9,10,11	0.84	0	9,11,13	1.92	2 (22%)
3	MLY	C	121	3	9,10,11	0.74	0	9,11,13	2.25	3 (33%)
3	MLZ	C	150	3	8,9,10	0.78	0	7,9,11	1.39	2 (28%)
3	MLY	C	210	3	9,10,11	1.19	1 (11%)	9,11,13	1.88	2 (22%)
3	MLY	C	213	3	9,10,11	1.30	1 (11%)	9,11,13	1.95	3 (33%)
3	MLY	C	364	3	9,10,11	0.77	0	9,11,13	1.91	3 (33%)
3	MLY	C	390	3	9,10,11	0.80	0	9,11,13	2.37	2 (22%)
3	M3L	C	400	3	10,11,12	0.98	0	12,14,16	0.97	0
3	MLY	C	402	3	9,10,11	1.01	1 (11%)	9,11,13	1.87	3 (33%)
3	M3L	C	474	3	10,11,12	0.44	0	12,14,16	1.23	1 (8%)
3	M3L	C	498	3	10,11,12	0.77	0	12,14,16	1.13	1 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MLY	C	518	3	9,10,11	0.74	0	9,11,13	1.92	3 (33%)
3	MLY	C	552	3	9,10,11	0.64	0	9,11,13	1.77	2 (22%)
3	MLZ	C	620	3	8,9,10	0.83	0	7,9,11	1.35	1 (14%)
4	MLY	D	210	4	9,10,11	0.79	0	9,11,13	1.96	2 (22%)
4	MLZ	D	235	4	8,9,10	0.85	0	7,9,11	1.15	0
4	MLY	D	390	4	9,10,11	0.90	0	9,11,13	2.24	2 (22%)
4	M3L	D	400	4	10,11,12	0.64	0	12,14,16	1.04	1 (8%)
4	MLY	D	402	4	9,10,11	0.64	0	9,11,13	1.95	3 (33%)
4	M3L	D	474	4	10,11,12	0.78	0	12,14,16	1.29	2 (16%)
4	M3L	D	498	4	10,11,12	1.26	1 (10%)	12,14,16	1.52	4 (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	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

Continued on next page...

Continued from previous page...

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	MLY	CB-CA	-2.19	1.51	1.53
2	B	400	M3L	CB-CA	2.22	1.55	1.53
4	D	498	M3L	CB-CA	2.79	1.56	1.53
3	C	210	MLY	CB-CA	2.96	1.56	1.53
3	C	213	MLY	CB-CA	3.50	1.57	1.53
2	B	210	MLY	CB-CA	3.69	1.57	1.53
2	B	405	MLZ	CB-CA	3.95	1.57	1.53
1	A	552	MLY	CB-CA	4.95	1.58	1.53

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	M3L	CM3-NZ-CM1	-7.95	88.53	108.98
1	A	390	M3L	CM3-NZ-CM2	-7.16	90.55	108.98
1	A	390	M3L	CM3-NZ-CE	-7.00	82.05	109.90
3	C	121	MLY	CD-CE-NZ	-3.07	106.00	113.92
4	D	498	M3L	O-C-CA	-2.92	117.88	125.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	498	M3L	CM3-NZ-CM1	-2.84	101.66	108.98
1	A	552	MLY	O-C-CA	-2.79	118.21	125.49
1	A	552	MLY	CG-CD-CE	-2.61	100.96	113.27
4	D	474	M3L	O-C-CA	-2.57	118.79	125.49
1	A	400	MLY	O-C-CA	-2.48	119.03	125.49
1	A	518	MLZ	O-C-CA	-2.46	119.09	125.49
3	C	474	M3L	O-C-CA	-2.45	119.10	125.49
2	B	364	MLY	O-C-CA	-2.45	119.11	125.49
4	D	498	M3L	CM2-NZ-CM1	-2.35	102.93	108.98
1	A	498	M3L	O-C-CA	-2.34	119.39	125.49
3	C	518	MLY	O-C-CA	-2.33	119.41	125.49
3	C	364	MLY	O-C-CA	-2.33	119.42	125.49
2	B	402	MLY	CD-CG-CB	-2.32	105.43	113.66
4	D	402	MLY	O-C-CA	-2.31	119.47	125.49
4	D	400	M3L	O-C-CA	-2.31	119.47	125.49
3	C	150	MLZ	O-C-CA	-2.30	119.50	125.49
2	B	150	M3L	O-C-CA	-2.29	119.52	125.49
3	C	402	MLY	O-C-CA	-2.27	119.59	125.49
1	A	390	M3L	O-C-CA	-2.18	119.80	125.49
2	B	235	MLY	CD-CG-CB	-2.17	105.96	113.66
1	A	364	M3L	O-C-CA	-2.16	119.86	125.49
2	B	235	MLY	CD-CE-NZ	-2.13	108.45	113.92
2	B	474	M3L	O-C-CA	-2.12	119.97	125.49
4	D	498	M3L	CM3-NZ-CM2	-2.12	103.53	108.98
3	C	213	MLY	O-C-CA	-2.09	120.05	125.49
2	B	210	MLY	O-C-CA	-2.03	120.20	125.49
1	A	405	MLZ	O-C-CA	-2.03	120.20	125.49
1	A	210	MLY	C-CA-CB	-2.01	107.58	112.33
4	D	498	M3L	CM3-NZ-CM1	2.24	114.74	108.98
1	A	210	MLY	CH1-NZ-CE	2.27	119.83	110.79
4	D	474	M3L	CM3-NZ-CM1	2.36	115.06	108.98
2	B	210	MLY	CH2-NZ-CH1	2.45	116.29	109.72
1	A	390	M3L	CM1-NZ-CE	2.47	119.71	109.90
2	B	374	MLY	CH2-NZ-CE	2.47	120.63	110.79
1	A	210	MLY	CH2-NZ-CH1	2.49	116.39	109.72
1	A	290	MLY	CH2-NZ-CE	2.59	121.11	110.79
2	B	374	MLY	CH2-NZ-CH1	2.60	116.67	109.72
4	D	402	MLY	CH2-NZ-CH1	2.63	116.76	109.72
3	C	150	MLZ	CM-NZ-CE	2.64	119.94	112.23
3	C	121	MLY	CH2-NZ-CE	2.66	121.39	110.79
3	C	210	MLY	CH2-NZ-CE	2.68	121.45	110.79
1	A	565	MLY	CH2-NZ-CE	2.69	121.51	110.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	405	MLZ	CM-NZ-CE	2.71	120.17	112.23
2	B	400	M3L	CB-CA-N	2.72	118.26	110.52
2	B	498	MLY	CH2-NZ-CE	2.77	121.80	110.79
1	A	210	MLY	CH2-NZ-CE	2.78	121.86	110.79
1	A	400	MLY	CH1-NZ-CE	2.80	121.95	110.79
1	A	518	MLZ	CM-NZ-CE	2.82	120.49	112.23
3	C	213	MLY	CH1-NZ-CE	2.84	122.08	110.79
3	C	620	MLZ	CM-NZ-CE	2.88	120.65	112.23
2	B	402	MLY	CH2-NZ-CH1	2.93	117.55	109.72
2	B	374	MLY	CH1-NZ-CE	2.96	122.56	110.79
3	C	518	MLY	CH2-NZ-CH1	2.96	117.64	109.72
1	A	625	MLZ	CM-NZ-CE	2.98	120.94	112.23
3	C	402	MLY	CH2-NZ-CH1	2.99	117.72	109.72
1	A	93	MLY	CH1-NZ-CE	2.99	122.70	110.79
1	A	402	MLY	CH2-NZ-CH1	3.01	117.76	109.72
3	C	402	MLY	CH2-NZ-CE	3.08	123.05	110.79
3	C	552	MLY	CH2-NZ-CH1	3.10	118.01	109.72
3	C	364	MLY	CH2-NZ-CE	3.10	123.13	110.79
1	A	390	M3L	CM2-NZ-CE	3.11	122.28	109.90
2	B	235	MLY	CH1-NZ-CE	3.11	123.19	110.79
3	C	552	MLY	CH2-NZ-CE	3.12	123.21	110.79
4	D	210	MLY	CH2-NZ-CH1	3.15	118.14	109.72
2	B	364	MLY	CH2-NZ-CE	3.18	123.45	110.79
1	A	390	M3L	CM2-NZ-CM1	3.19	117.19	108.98
3	C	364	MLY	CH2-NZ-CH1	3.31	118.58	109.72
2	B	390	MLY	CH2-NZ-CH1	3.36	118.71	109.72
2	B	210	MLY	CH1-NZ-CE	3.39	124.28	110.79
2	B	390	MLY	CH2-NZ-CE	3.42	124.41	110.79
2	B	364	MLY	CH2-NZ-CH1	3.43	118.89	109.72
4	D	210	MLY	CH1-NZ-CE	3.46	124.58	110.79
4	D	390	MLY	CH2-NZ-CE	3.50	124.74	110.79
3	C	210	MLY	CH2-NZ-CH1	3.63	119.44	109.72
1	A	402	MLY	CH1-NZ-CE	3.69	125.49	110.79
3	C	213	MLY	CH2-NZ-CH1	3.75	119.76	109.72
4	D	402	MLY	CH2-NZ-CE	3.82	126.00	110.79
3	C	518	MLY	CH1-NZ-CE	3.88	126.25	110.79
2	B	402	MLY	CH2-NZ-CE	3.92	126.39	110.79
1	A	565	MLY	CH2-NZ-CH1	3.92	120.20	109.72
3	C	390	MLY	CH1-NZ-CE	3.98	126.62	110.79
1	A	552	MLY	CH2-NZ-CE	4.01	126.75	110.79
2	B	498	MLY	CH2-NZ-CH1	4.06	120.57	109.72
2	B	235	MLY	CH2-NZ-CH1	4.12	120.75	109.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	MLY	CH2-NZ-CH1	4.17	120.87	109.72
1	A	93	MLY	CH2-NZ-CH1	4.17	120.88	109.72
1	A	400	MLY	CH2-NZ-CH1	4.20	120.96	109.72
3	C	121	MLY	CH2-NZ-CH1	4.25	121.08	109.72
4	D	390	MLY	CH2-NZ-CH1	4.93	122.91	109.72
3	C	390	MLY	CH2-NZ-CH1	5.35	124.03	109.72

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	0.32	0	5,5,5	0.50	0
5	GOL	B	701	-	5,5,5	0.34	0	5,5,5	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	D	701	-	5,5,5	0.23	0	5,5,5	0.71	0
5	GOL	D	702	-	5,5,5	0.48	0	5,5,5	1.16	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
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 ⓘ

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	526/546 (96%)	-0.47	2 (0%) 93 91	5, 12, 23, 39	0
2	B	527/546 (96%)	-0.20	6 (1%) 82 80	8, 18, 30, 43	0
3	C	526/546 (96%)	-0.55	4 (0%) 87 85	4, 9, 21, 46	0
4	D	532/546 (97%)	-0.42	8 (1%) 76 72	5, 13, 24, 48	0
All	All	2111/2184 (96%)	-0.41	20 (0%) 85 83	4, 13, 27, 48	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	605	SER	6.7
4	D	386[A]	TYR	5.4
3	C	605	SER	4.9
3	C	604	ASP	4.5
3	C	607	GLN	3.8
4	D	606	ASN	3.6
4	D	387[A]	SER	3.6
3	C	606	ASN	3.3
2	B	605	SER	3.2
1	A	632	SER	3.2
2	B	294	ALA	2.8
4	D	607	GLN	2.8
4	D	388[A]	ASN	2.8
2	B	602	VAL	2.7
2	B	229	GLY	2.7
4	D	94	PRO	2.6
2	B	632	SER	2.5
2	B	604	ASP	2.4
1	A	209[A]	ASN	2.3
4	D	97	ASN	2.3

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. 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, 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	LLDF	B-factors(Å ²)	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
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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, 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	LLDF	B-factors(\AA^2)	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.