



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:11 pm BST

PDB ID : 3AAG  
Title : Crystal structure of *C. jejuni* pglb C-terminal domain  
Authors : Maita, N.; Kohda, D.  
Deposited on : 2009-11-16  
Resolution : 2.80 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](mailto: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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

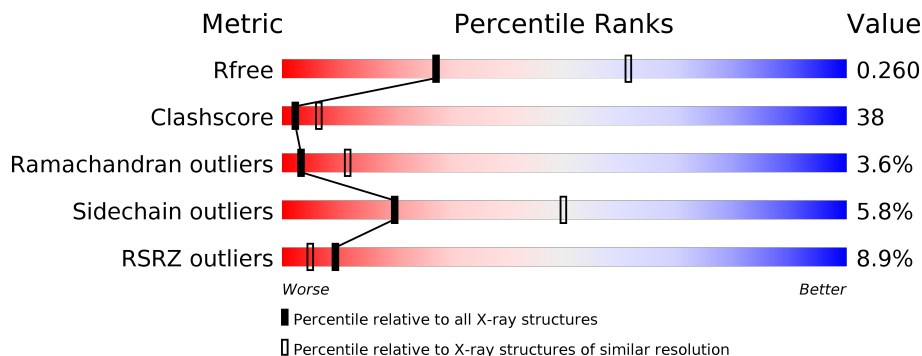
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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	291	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 48%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 39%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div>
1	B	291	<div style="display: flex; align-items: center;"> <div style="width: 11%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 34%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 41%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: grey;"></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
1	MLY	A	590	-	-	-	X
1	MLY	A	707	-	-	X	-
1	MLY	B	641	-	-	-	X

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 4036 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 General glycosylation pathway protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	267	2176	1426	336	406	8	0	0	0
1	B	236	1859	1221	286	346	6	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	423	GLY	-	EXPRESSION TAG	UNP Q5HTX9
A	424	PRO	-	EXPRESSION TAG	UNP Q5HTX9
A	425	LEU	-	EXPRESSION TAG	UNP Q5HTX9
A	426	GLY	-	EXPRESSION TAG	UNP Q5HTX9
A	427	SER	-	EXPRESSION TAG	UNP Q5HTX9
B	423	GLY	-	EXPRESSION TAG	UNP Q5HTX9
B	424	PRO	-	EXPRESSION TAG	UNP Q5HTX9
B	425	LEU	-	EXPRESSION TAG	UNP Q5HTX9
B	426	GLY	-	EXPRESSION TAG	UNP Q5HTX9
B	427	SER	-	EXPRESSION TAG	UNP Q5HTX9

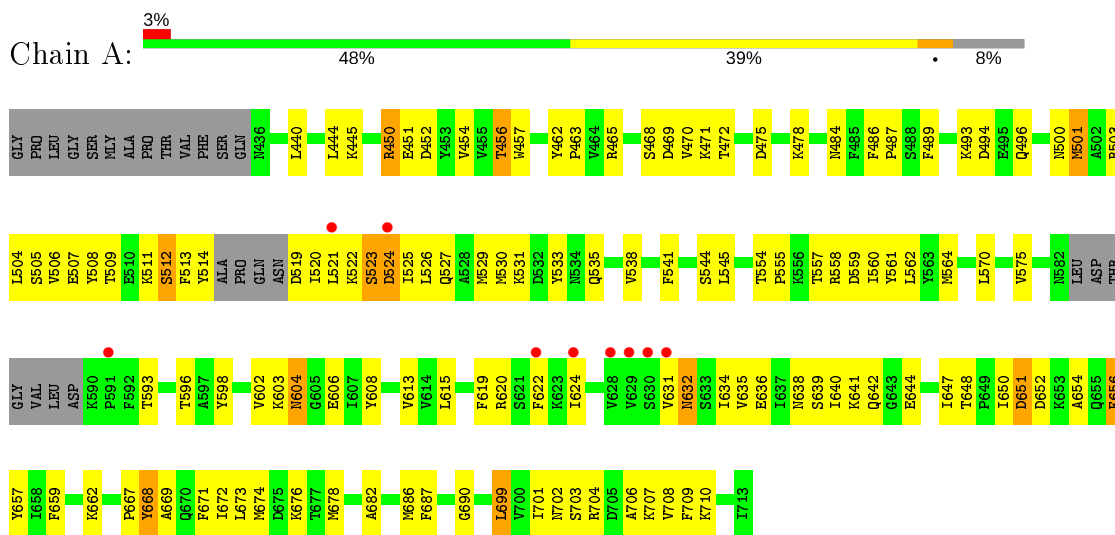
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

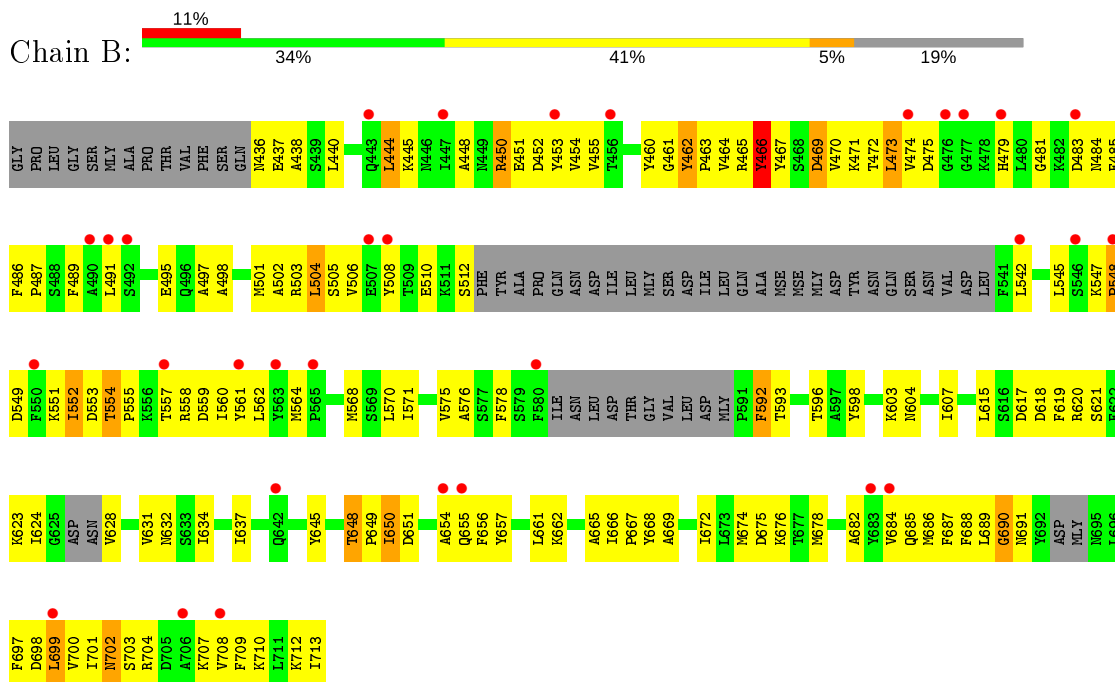
### 3 Residue-property plots

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: General glycosylation pathway protein



- Molecule 1: General glycosylation pathway protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.26 Å 115.26 Å 88.88 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.80 28.81 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.80) 99.9 (28.81-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.83 (at 2.80 Å)	Xtrriage
Refinement program	REFMAC 5.5.0104	Depositor
R, $R_{free}$	0.245 , 0.260 0.244 , 0.260	Depositor DCC
$R_{free}$ test set	1281 reflections (7.72%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.7	Xtrriage
Anisotropy	0.002	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 57.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.041 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4036	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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: CA, MLY

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.29	2/1997 (0.1%)	0.34	0/2711
1	B	0.26	0/1753	0.33	0/2379
All	All	0.28	2/3750 (0.1%)	0.34	0/5090

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	608	TYR	CB-CG	-6.29	1.42	1.51
1	A	636	GLU	CB-CG	-5.29	1.42	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2176	0	2114	141	0
1	B	1859	0	1728	161	0
2	A	1	0	0	0	0
All	All	4036	0	3842	302	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 38.

All (302) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:LEU:O	1:B:504:LEU:HD23	1.45	1.15
1:A:501:MSE:HA	1:A:501:MSE:HE3	1.18	1.13
1:B:682:ALA:HB1	1:B:686:MSE:HE2	1.14	1.11
1:A:501:MSE:HA	1:A:501:MSE:CE	1.81	1.10
1:A:501:MSE:HE2	1:A:501:MSE:O	1.55	1.04
1:A:678:MSE:HE2	1:A:678:MSE:HA	1.38	1.00
1:A:687:PHE:O	1:A:707:MLY:HH13	1.61	1.00
1:A:541:PHE:O	1:A:544:SER:HB3	1.63	0.98
1:B:553:ASP:O	1:B:554:THR:HG23	1.65	0.97
1:A:501:MSE:CA	1:A:501:MSE:CE	2.44	0.94
1:B:564:MSE:HE3	1:B:687:PHE:HB2	1.51	0.91
1:B:454:VAL:HG22	1:B:561:TYR:HB2	1.53	0.90
1:A:501:MSE:HE3	1:A:504:LEU:HB2	1.53	0.90
1:B:682:ALA:CB	1:B:686:MSE:HE2	2.03	0.87
1:B:502:ALA:O	1:B:506:VAL:HG23	1.75	0.86
1:B:436:ASN:ND2	1:B:438:ALA:H	1.74	0.85
1:B:484:ASN:O	1:B:487:PRO:HD2	1.77	0.85
1:B:657:TYR:HE1	1:B:676:MLY:HG3	1.38	0.84
1:A:501:MSE:HE3	1:A:501:MSE:CA	2.04	0.84
1:A:501:MSE:O	1:A:501:MSE:CE	2.26	0.83
1:A:650:ILE:HG22	1:A:650:ILE:O	1.78	0.83
1:B:682:ALA:HB1	1:B:686:MSE:CE	2.05	0.83
1:B:665:ALA:HB2	1:B:704:ARG:NH2	1.93	0.82
1:A:501:MSE:C	1:A:501:MSE:HE2	2.00	0.81
1:B:450:ARG:N	1:B:450:ARG:HE	1.77	0.81
1:A:667:PRO:O	1:A:668:TYR:HB2	1.79	0.80
1:A:501:MSE:CE	1:A:504:LEU:HB2	2.11	0.80
1:B:473:LEU:N	1:B:473:LEU:HD12	1.97	0.80
1:B:678:MSE:HA	1:B:678:MSE:HE2	1.64	0.80
1:A:650:ILE:O	1:A:651:ASP:HB3	1.82	0.79
1:A:526:LEU:HG	1:A:530:MSE:HE2	1.64	0.78
1:B:649:PRO:O	1:B:650:ILE:HD12	1.83	0.78
1:B:455:VAL:HG13	1:B:562:LEU:HD12	1.66	0.78
1:A:602:VAL:HG12	1:A:602:VAL:O	1.85	0.77
1:A:690:GLY:HA2	1:A:707:MLY:HH11	1.66	0.77
1:B:553:ASP:O	1:B:554:THR:CG2	2.31	0.77
1:B:462:TYR:N	1:B:463:PRO:HD2	2.01	0.76
1:B:700:VAL:HG23	1:B:701:ILE:HG13	1.67	0.75
1:A:682:ALA:O	1:A:686:MSE:HB2	1.85	0.75
1:A:624:ILE:O	1:A:624:ILE:HG22	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:PHE:CD2	1:A:501:MSE:HG3	2.22	0.74
1:A:678:MSE:CE	1:A:678:MSE:HA	2.16	0.74
1:A:690:GLY:CA	1:A:707:MLY:HH11	2.17	0.74
1:A:622:PHE:HE2	1:A:631:VAL:HG12	1.53	0.72
1:A:634:ILE:HG12	1:A:648:THR:HB	1.71	0.71
1:B:618:ASP:OD1	1:B:620:ARG:HB2	1.91	0.71
1:A:678:MSE:CA	1:A:678:MSE:HE2	2.20	0.70
1:B:649:PRO:C	1:B:650:ILE:HD12	2.12	0.70
1:B:666:ILE:HG23	1:B:669:ALA:HB3	1.72	0.70
1:B:506:VAL:HG21	1:B:560:ILE:HD13	1.73	0.69
1:B:632:ASN:HA	1:B:654:ALA:HB3	1.74	0.68
1:B:699:LEU:HD21	1:B:702:ASN:HB2	1.75	0.68
1:B:634:ILE:HB	1:B:648:THR:HG23	1.75	0.68
1:B:665:ALA:HB2	1:B:704:ARG:HH22	1.57	0.67
1:A:511:MLY:HA	1:A:514:TYR:CE2	2.29	0.67
1:A:620:ARG:HG2	1:A:650:ILE:HD13	1.77	0.67
1:B:657:TYR:CE1	1:B:676:MLY:HG3	2.28	0.66
1:B:455:VAL:HG13	1:B:562:LEU:CD1	2.26	0.66
1:A:501:MSE:HE2	1:A:501:MSE:CA	2.21	0.66
1:A:656:PHE:HD2	1:A:656:PHE:N	1.94	0.66
1:B:553:ASP:O	1:B:554:THR:CB	2.44	0.66
1:B:571:ILE:HG22	1:B:571:ILE:O	1.95	0.66
1:B:655:GLN:HG2	1:B:656:PHE:CD1	2.31	0.65
1:A:667:PRO:O	1:A:668:TYR:CB	2.44	0.65
1:B:553:ASP:O	1:B:554:THR:OG1	2.14	0.64
1:A:622:PHE:CE2	1:A:631:VAL:HG12	2.32	0.64
1:A:596:THR:HG22	1:A:672:ILE:HG12	1.79	0.64
1:A:613:VAL:HG22	1:A:624:ILE:HG12	1.78	0.64
1:A:450:ARG:NH1	1:A:469:ASP:O	2.29	0.64
1:B:462:TYR:N	1:B:463:PRO:CD	2.60	0.64
1:B:469:ASP:CG	1:B:469:ASP:O	2.36	0.64
1:B:545:LEU:HD12	1:B:545:LEU:H	1.62	0.63
1:A:523:SER:O	1:A:524:ASP:CB	2.46	0.63
1:A:656:PHE:CD2	1:A:656:PHE:N	2.66	0.62
1:B:689:LEU:C	1:B:691:ASN:H	2.02	0.62
1:A:529:MSE:O	1:A:533:TYR:HD1	1.83	0.61
1:A:564:MSE:HE2	1:A:709:PHE:CD2	2.36	0.60
1:A:699:LEU:HG	1:A:709:PHE:CE1	2.36	0.60
1:B:547:MLY:HD2	1:B:548:PRO:HD2	1.84	0.59
1:B:699:LEU:HD21	1:B:702:ASN:OD1	2.02	0.59
1:B:712:MLY:CG	1:B:713:ILE:H	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:699:LEU:HD13	1:B:709:PHE:HE2	1.68	0.59
1:A:511:MLY:C	1:A:513:PHE:H	2.15	0.59
1:B:461:GLY:C	1:B:463:PRO:HD2	2.23	0.58
1:B:460:TYR:O	1:B:463:PRO:HG2	2.02	0.58
1:A:640:ILE:H	1:A:704:ARG:NH1	2.01	0.58
1:B:473:LEU:N	1:B:473:LEU:CD1	2.67	0.58
1:A:650:ILE:O	1:A:650:ILE:CG2	2.51	0.58
1:A:603:MLY:O	1:A:604:ASN:HB2	2.02	0.58
1:B:450:ARG:HE	1:B:450:ARG:CA	2.16	0.58
1:A:527:GLN:HA	1:A:530:MSE:HE3	1.86	0.58
1:A:639:SER:O	1:A:642:GLN:O	2.22	0.57
1:A:564:MSE:HE2	1:A:709:PHE:CE2	2.38	0.57
1:B:504:LEU:O	1:B:504:LEU:CD2	2.37	0.57
1:B:555:PRO:O	1:B:557:THR:HG23	2.04	0.57
1:B:454:VAL:HG23	1:B:470:VAL:HG21	1.87	0.57
1:B:547:MLY:C	1:B:549:ASP:H	2.16	0.57
1:A:520:ILE:HG23	1:A:521:LEU:N	2.18	0.57
1:B:504:LEU:C	1:B:504:LEU:HD23	2.23	0.56
1:B:689:LEU:O	1:B:691:ASN:N	2.38	0.56
1:A:650:ILE:O	1:A:651:ASP:CB	2.50	0.56
1:A:638:ASN:HB2	1:A:644:GLU:HB3	1.87	0.56
1:A:657:TYR:O	1:A:673:LEU:HD12	2.06	0.56
1:B:667:PRO:C	1:B:669:ALA:H	2.09	0.56
1:A:523:SER:O	1:A:524:ASP:HB2	2.05	0.56
1:B:491:LEU:HD13	1:B:568:MSE:HE1	1.88	0.56
1:A:452:ASP:CG	1:A:559:ASP:HB2	2.27	0.56
1:A:454:VAL:HG23	1:A:470:VAL:HG21	1.86	0.56
1:A:519:ASP:CG	1:A:520:ILE:H	2.08	0.55
1:B:648:THR:O	1:B:650:ILE:HD12	2.06	0.55
1:A:484:ASN:O	1:A:487:PRO:HD2	2.06	0.55
1:B:452:ASP:O	1:B:470:VAL:HB	2.05	0.55
1:A:619:PHE:O	1:A:634:ILE:HG22	2.07	0.55
1:B:685:GLN:HA	1:B:689:LEU:HD13	1.87	0.55
1:A:445:MLY:HG2	1:A:468:SER:O	2.08	0.54
1:B:436:ASN:CG	1:B:437:GLU:H	2.10	0.54
1:A:471:MLY:HH22	1:A:471:MLY:HG2	1.89	0.54
1:B:551:MLY:O	1:B:552:ILE:O	2.25	0.54
1:A:501:MSE:C	1:A:501:MSE:CE	2.67	0.54
1:A:501:MSE:HG2	1:A:545:LEU:HD13	1.90	0.54
1:A:519:ASP:CG	1:A:520:ILE:N	2.61	0.54
1:A:531:MLY:C	1:A:533:TYR:H	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:ILE:O	1:A:642:GLN:O	2.25	0.54
1:B:570:LEU:C	1:B:571:ILE:HD12	2.29	0.54
1:B:698:ASP:O	1:B:700:VAL:HG13	2.07	0.54
1:B:699:LEU:HD21	1:B:702:ASN:CB	2.37	0.53
1:B:576:ALA:C	1:B:578:PHE:H	2.11	0.53
1:B:452:ASP:HB3	1:B:559:ASP:O	2.08	0.53
1:B:486:PHE:CD2	1:B:501:MSE:HE1	2.44	0.53
1:B:623:MLY:HG3	1:B:628:VAL:HG22	1.90	0.53
1:B:545:LEU:N	1:B:545:LEU:HD12	2.24	0.53
1:B:466:TYR:CD2	1:B:466:TYR:C	2.82	0.53
1:B:452:ASP:CG	1:B:559:ASP:HB3	2.29	0.53
1:B:453:TYR:O	1:B:561:TYR:N	2.41	0.53
1:A:640:ILE:O	1:A:641:MLY:C	2.57	0.52
1:B:596:THR:HG22	1:B:672:ILE:HG12	1.90	0.52
1:B:454:VAL:HG12	1:B:454:VAL:O	2.08	0.52
1:A:519:ASP:OD2	1:A:520:ILE:HG22	2.08	0.52
1:B:436:ASN:CG	1:B:437:GLU:N	2.63	0.52
1:B:460:TYR:O	1:B:464:VAL:HG23	2.09	0.52
1:A:478:MLY:O	1:A:478:MLY:HG3	2.10	0.51
1:A:486:PHE:HB2	1:A:487:PRO:HD3	1.91	0.51
1:B:438:ALA:HA	1:B:467:TYR:CD1	2.46	0.51
1:B:637:ILE:O	1:B:637:ILE:HG22	2.10	0.51
1:B:682:ALA:O	1:B:686:MSE:HG3	2.10	0.51
1:B:593:THR:HG1	1:B:656:PHE:HE2	1.56	0.51
1:B:655:GLN:OE1	1:B:655:GLN:N	2.33	0.51
1:B:684:VAL:O	1:B:688:PHE:HB2	2.11	0.51
1:B:486:PHE:HB2	1:B:487:PRO:HD3	1.93	0.51
1:B:687:PHE:HA	1:B:707:MLY:NZ	2.25	0.51
1:A:522:MLY:HD2	1:A:523:SER:N	2.26	0.50
1:A:501:MSE:HE1	1:A:505:SER:N	2.26	0.50
1:B:701:ILE:HB	1:B:708:VAL:HB	1.94	0.50
1:A:634:ILE:CG1	1:A:648:THR:HB	2.42	0.50
1:B:666:ILE:HG23	1:B:666:ILE:O	2.12	0.50
1:A:564:MSE:CE	1:A:709:PHE:CE2	2.94	0.49
1:B:645:TYR:HE2	1:B:689:LEU:O	1.95	0.49
1:B:678:MSE:HA	1:B:678:MSE:CE	2.39	0.49
1:B:489:PHE:HE2	1:B:497:ALA:HB1	1.77	0.49
1:B:454:VAL:HG22	1:B:561:TYR:CB	2.34	0.49
1:A:530:MSE:HE1	1:A:538:VAL:HG22	1.95	0.49
1:B:450:ARG:N	1:B:450:ARG:NE	2.55	0.49
1:B:489:PHE:CE2	1:B:497:ALA:HB1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:TYR:N	1:B:508:TYR:HD1	2.10	0.49
1:B:448:ALA:HB2	1:B:561:TYR:CZ	2.47	0.49
1:B:571:ILE:CG2	1:B:571:ILE:O	2.60	0.49
1:B:675:ASP:OD2	1:B:678:MSE:HB2	2.12	0.49
1:B:700:VAL:CG1	1:B:710:MLY:HB3	2.43	0.49
1:B:712:MLY:CG	1:B:713:ILE:N	2.74	0.49
1:A:690:GLY:HA2	1:A:707:MLY:CH1	2.41	0.49
1:B:503:ARG:C	1:B:505:SER:N	2.66	0.48
1:B:667:PRO:O	1:B:668:TYR:HB2	2.13	0.48
1:A:508:TYR:HB3	1:A:525:ILE:HG23	1.95	0.48
1:A:659:PHE:O	1:A:671:PHE:HD1	1.96	0.48
1:B:472:THR:C	1:B:473:LEU:HD12	2.34	0.48
1:A:520:ILE:CG2	1:A:521:LEU:N	2.77	0.48
1:B:436:ASN:HD22	1:B:438:ALA:CB	2.27	0.48
1:B:503:ARG:C	1:B:505:SER:H	2.17	0.48
1:B:699:LEU:CD2	1:B:702:ASN:HB2	2.41	0.48
1:B:471:MLY:NZ	1:B:510:GLU:OE2	2.47	0.48
1:B:436:ASN:HD22	1:B:438:ALA:H	1.56	0.48
1:B:542:LEU:HD12	1:B:542:LEU:N	2.29	0.47
1:A:451:GLU:HA	1:A:471:MLY:CH2	2.44	0.47
1:B:699:LEU:HD21	1:B:702:ASN:CG	2.34	0.47
1:A:465:ARG:NH1	1:A:475:ASP:OD2	2.47	0.47
1:A:531:MLY:C	1:A:533:TYR:N	2.78	0.47
1:A:659:PHE:HB2	1:A:672:ILE:HB	1.95	0.47
1:A:564:MSE:CE	1:A:709:PHE:HE2	2.27	0.47
1:B:689:LEU:C	1:B:691:ASN:N	2.68	0.47
1:A:445:MLY:O	1:A:450:ARG:NH2	2.47	0.47
1:A:507:GLU:OE1	1:A:557:THR:OG1	2.31	0.47
1:A:634:ILE:O	1:A:647:ILE:HA	2.15	0.47
1:B:508:TYR:N	1:B:508:TYR:CD1	2.81	0.47
1:A:656:PHE:HD2	1:A:656:PHE:H	1.58	0.47
1:B:466:TYR:C	1:B:466:TYR:HD2	2.18	0.47
1:A:507:GLU:OE1	1:A:507:GLU:HA	2.14	0.47
1:A:440:LEU:HG	1:A:701:ILE:HG21	1.97	0.47
1:A:690:GLY:HA3	1:A:707:MLY:HH11	1.96	0.47
1:B:553:ASP:C	1:B:554:THR:OG1	2.53	0.47
1:B:510:GLU:OE1	1:B:510:GLU:HA	2.14	0.47
1:A:508:TYR:CE1	1:A:554:THR:HG21	2.50	0.47
1:B:598:TYR:CE2	1:B:668:TYR:HD1	2.33	0.47
1:A:619:PHE:O	1:A:634:ILE:CG2	2.63	0.46
1:A:642:GLN:HB2	1:A:644:GLU:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:661:LEU:O	1:B:662:MLY:C	2.62	0.46
1:A:501:MSE:HE1	1:A:504:LEU:HB2	1.97	0.46
1:A:562:LEU:O	1:A:708:VAL:HA	2.15	0.46
1:B:592:PHE:HA	1:B:675:ASP:OD1	2.15	0.46
1:A:508:TYR:O	1:A:512:SER:HB3	2.16	0.46
1:A:506:VAL:HG21	1:A:560:ILE:HD13	1.97	0.46
1:A:511:MLY:C	1:A:513:PHE:N	2.79	0.46
1:B:454:VAL:CG2	1:B:470:VAL:HG21	2.45	0.46
1:B:651:ASP:HB3	1:B:654:ALA:HB2	1.97	0.46
1:B:703:SER:OG	1:B:704:ARG:N	2.49	0.46
1:B:466:TYR:HD2	1:B:467:TYR:N	2.14	0.46
1:B:510:GLU:C	1:B:512:SER:H	2.18	0.46
1:A:686:MSE:O	1:A:690:GLY:HA2	2.16	0.45
1:B:484:ASN:HB3	1:B:578:PHE:CD2	2.51	0.45
1:A:710:MLY:HD3	1:A:710:MLY:HH12	1.73	0.45
1:A:570:LEU:HD21	1:A:669:ALA:HB2	1.99	0.45
1:B:547:MLY:O	1:B:549:ASP:N	2.47	0.45
1:B:645:TYR:CE2	1:B:689:LEU:O	2.70	0.45
1:A:564:MSE:HE1	1:A:686:MSE:HB3	1.99	0.45
1:B:440:LEU:HD23	1:B:440:LEU:O	2.17	0.45
1:B:618:ASP:CG	1:B:620:ARG:HB2	2.38	0.45
1:B:697:PHE:HA	1:B:710:MLY:O	2.17	0.44
1:B:700:VAL:HG11	1:B:710:MLY:HB3	2.00	0.44
1:A:496:GLN:HE21	1:A:500:ASN:ND2	2.15	0.44
1:A:639:SER:HB3	1:A:644:GLU:HB2	1.98	0.44
1:A:642:GLN:OE1	1:A:644:GLU:OE1	2.35	0.44
1:B:593:THR:O	1:B:674:MSE:HA	2.18	0.44
1:B:547:MLY:C	1:B:549:ASP:N	2.81	0.44
1:B:699:LEU:CG	1:B:702:ASN:HB2	2.48	0.44
1:B:687:PHE:HD1	1:B:707:MLY:CB	2.31	0.44
1:B:503:ARG:O	1:B:505:SER:N	2.51	0.44
1:A:703:SER:HB3	1:A:706:ALA:O	2.17	0.44
1:B:687:PHE:CD1	1:B:707:MLY:HB3	2.53	0.44
1:B:564:MSE:CE	1:B:687:PHE:HB2	2.35	0.44
1:B:554:THR:HB	1:B:555:PRO:HD2	2.00	0.44
1:B:460:TYR:C	1:B:463:PRO:HD2	2.38	0.43
1:B:479:HIS:CG	1:B:479:HIS:O	2.71	0.43
1:B:615:LEU:HD12	1:B:621:SER:O	2.17	0.43
1:B:620:ARG:O	1:B:631:VAL:HG22	2.19	0.43
1:A:489:PHE:CZ	1:A:493:MLY:HG2	2.53	0.43
1:A:639:SER:N	1:A:644:GLU:HB2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:THR:O	1:A:674:MSE:HA	2.18	0.43
1:A:527:GLN:OE1	1:A:527:GLN:HA	2.19	0.43
1:B:452:ASP:OD1	1:B:559:ASP:HB3	2.19	0.43
1:A:457:TRP:CD2	1:A:575:VAL:HG22	2.54	0.43
1:A:615:LEU:HD21	1:A:619:PHE:CD2	2.54	0.43
1:B:510:GLU:O	1:B:512:SER:N	2.44	0.43
1:B:607:ILE:N	1:B:615:LEU:O	2.48	0.43
1:A:512:SER:HA	1:A:521:LEU:HG	2.01	0.42
1:B:648:THR:O	1:B:650:ILE:CD1	2.67	0.42
1:A:561:TYR:HA	1:A:709:PHE:O	2.19	0.42
1:B:448:ALA:O	1:B:450:ARG:NH2	2.52	0.42
1:A:522:MLY:C	1:A:522:MLY:HD2	2.50	0.42
1:A:632:ASN:HD22	1:A:632:ASN:C	2.23	0.42
1:A:657:TYR:HE1	1:A:676:MLY:HG3	1.83	0.42
1:B:619:PHE:CD2	1:B:619:PHE:N	2.86	0.42
1:A:632:ASN:HA	1:A:654:ALA:HB3	2.02	0.42
1:A:558:ARG:HG2	1:A:558:ARG:HH11	1.84	0.42
1:B:465:ARG:HD3	1:B:475:ASP:OD1	2.20	0.42
1:B:495:GLU:O	1:B:498:ALA:HB3	2.20	0.42
1:A:465:ARG:HG3	1:A:472:THR:CG2	2.50	0.42
1:B:498:ALA:O	1:B:502:ALA:HB2	2.20	0.42
1:B:484:ASN:C	1:B:487:PRO:HD2	2.37	0.42
1:A:624:ILE:O	1:A:624:ILE:CG2	2.57	0.42
1:A:686:MSE:O	1:A:707:MLY:CH1	2.68	0.42
1:B:506:VAL:HG21	1:B:560:ILE:CD1	2.47	0.42
1:A:686:MSE:HE2	1:A:709:PHE:CD2	2.55	0.41
1:A:503:ARG:O	1:A:507:GLU:HG2	2.20	0.41
1:B:444:LEU:O	1:B:445:MLY:C	2.68	0.41
1:B:508:TYR:HD1	1:B:508:TYR:H	1.68	0.41
1:B:702:ASN:C	1:B:702:ASN:HD22	2.22	0.41
1:B:542:LEU:CD1	1:B:542:LEU:N	2.83	0.41
1:B:575:VAL:O	1:B:575:VAL:HG12	2.21	0.41
1:A:456:THR:HG23	1:A:457:TRP:O	2.20	0.41
1:A:440:LEU:C	1:A:440:LEU:HD23	2.40	0.41
1:A:541:PHE:C	1:A:544:SER:HB3	2.38	0.41
1:A:554:THR:HA	1:A:555:PRO:HD3	1.84	0.41
1:A:525:ILE:HG22	1:A:529:MSE:HE3	2.02	0.41
1:B:436:ASN:HD22	1:B:438:ALA:HB3	1.85	0.41
1:B:440:LEU:HD23	1:B:440:LEU:C	2.41	0.41
1:A:452:ASP:OD1	1:A:559:ASP:HB2	2.19	0.41
1:A:635:VAL:O	1:A:659:PHE:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:TYR:CE2	1:B:475:ASP:HB3	2.55	0.41
1:A:501:MSE:CE	1:A:505:SER:H	2.33	0.41
1:A:478:MLY:HH11	1:A:509:THR:HG23	2.02	0.41
1:A:457:TRP:CE2	1:A:575:VAL:HG22	2.56	0.41
1:A:678:MSE:CE	1:A:678:MSE:CA	2.91	0.41
1:A:462:TYR:HB2	1:A:463:PRO:HD3	2.03	0.41
1:A:702:ASN:OD1	1:A:707:MLY:HH22	2.21	0.41
1:A:489:PHE:CE1	1:A:493:MLY:HG2	2.57	0.40
1:A:598:TYR:CD2	1:A:598:TYR:N	2.89	0.40
1:B:451:GLU:O	1:B:558:ARG:HB3	2.22	0.40
1:B:603:MLY:HB2	1:B:604:ASN:H	1.55	0.40
1:B:686:MSE:O	1:B:690:GLY:HA2	2.22	0.40
1:A:662:MLY:HH12	1:A:662:MLY:HD3	1.67	0.40
1:A:682:ALA:O	1:A:686:MSE:CB	2.63	0.40
1:A:632:ASN:ND2	1:A:632:ASN:C	2.75	0.40
1:B:485:PHE:CD1	1:B:485:PHE:C	2.94	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	239/291 (82%)	209 (87%)	24 (10%)	6 (2%)	<b>5</b>   <b>19</b>
1	B	207/291 (71%)	159 (77%)	38 (18%)	10 (5%)	<b>2</b>   <b>7</b>
All	All	446/582 (77%)	368 (82%)	62 (14%)	16 (4%)	<b>3</b>   <b>11</b>

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	524	ASP
1	B	554	THR

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Mol	Chain	Res	Type
1	B	466	TYR
1	B	552	ILE
1	B	690	GLY
1	A	668	TYR
1	B	481	GLY
1	B	504	LEU
1	A	512	SER
1	A	651	ASP
1	A	523	SER
1	B	624	ILE
1	B	699	LEU
1	A	604	ASN
1	B	548	PRO
1	B	650	ILE

### 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	215/228 (94%)	204 (95%)	11 (5%)	24	55
1	B	182/228 (80%)	170 (93%)	12 (7%)	16	44
All	All	397/456 (87%)	374 (94%)	23 (6%)	20	50

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	444	LEU
1	A	450	ARG
1	A	456	THR
1	A	494	ASP
1	A	501	MSE
1	A	535	GLN
1	A	606	GLU
1	A	632	ASN
1	A	652	ASP

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Mol	Chain	Res	Type
1	A	656	PHE
1	A	699	LEU
1	B	444	LEU
1	B	450	ARG
1	B	462	TYR
1	B	466	TYR
1	B	469	ASP
1	B	473	LEU
1	B	474	VAL
1	B	483	ASP
1	B	592	PHE
1	B	617	ASP
1	B	648	THR
1	B	702	ASN

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

Mol	Chain	Res	Type
1	A	496	GLN
1	A	535	GLN
1	A	632	ASN
1	A	655	GLN
1	B	436	ASN
1	B	604	ASN
1	B	702	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

42 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	445	1	9,10,11	0.48	0	6,11,13	0.70	0
1	MLY	A	493	1	9,10,11	0.49	0	6,11,13	0.64	0
1	MLY	A	707	1	9,10,11	0.48	0	6,11,13	0.80	0
1	MLY	A	662	1	9,10,11	0.47	0	6,11,13	0.70	0
1	MLY	B	662	1	3,4,11	0.65	0	2,4,13	0.80	0
1	MLY	B	547	1	7,8,11	0.46	0	3,8,13	0.42	0
1	MLY	A	710	1	9,10,11	0.52	0	6,11,13	0.87	0
1	MLY	B	603	1	9,10,11	0.52	0	6,11,13	0.76	0
1	MLY	A	556	1	9,10,11	0.50	0	6,11,13	0.69	0
1	MLY	B	511	1	7,8,11	0.47	0	3,8,13	0.42	0
1	MLY	B	482	1	4,5,11	0.92	0	1,5,13	1.03	0
1	MLY	A	694	1	9,10,11	0.50	0	6,11,13	0.65	0
1	MLY	B	710	1	4,5,11	0.92	0	1,5,13	1.03	0
1	MLY	A	471	1	9,10,11	0.48	0	6,11,13	0.77	0
1	MLY	B	471	1	7,8,11	0.47	0	3,8,13	0.39	0
1	MLY	A	590	1	3,4,11	0.64	0	2,4,13	0.84	0
1	MLY	B	641	1	7,8,11	0.46	0	3,8,13	0.40	0
1	MLY	B	493	1	7,8,11	0.47	0	3,8,13	0.43	0
1	MLY	A	482	1	7,8,11	0.48	0	3,8,13	0.38	0
1	MLY	A	531	1	7,8,11	0.47	0	3,8,13	0.44	0
1	MLY	A	603	1	9,10,11	0.48	0	6,11,13	0.74	0
1	MLY	B	707	1	7,8,11	0.47	0	3,8,13	0.42	0
1	MLY	B	556	1	7,8,11	0.45	0	3,8,13	0.45	0
1	MLY	A	547	1	7,8,11	0.46	0	3,8,13	0.43	0
1	MLY	A	551	1	3,4,11	0.65	0	2,4,13	0.75	0
1	MLY	A	712	1	9,10,11	0.52	0	6,11,13	0.89	0
1	MLY	A	522	1	7,8,11	0.48	0	3,8,13	0.43	0
1	MLY	B	646	1	4,5,11	0.92	0	1,5,13	1.06	0
1	MLY	A	478	1	9,10,11	0.51	0	6,11,13	0.76	0
1	MLY	A	623	1	7,8,11	0.45	0	3,8,13	0.49	0
1	MLY	A	641	1	9,10,11	0.49	0	6,11,13	0.80	0
1	MLY	B	653	1	3,4,11	0.62	0	2,4,13	0.78	0
1	MLY	B	445	1	3,4,11	0.65	0	2,4,13	0.78	0
1	MLY	A	646	1	4,5,11	0.92	0	1,5,13	1.03	0
1	MLY	A	653	1	4,5,11	0.92	0	1,5,13	0.97	0
1	MLY	A	676	1	9,10,11	0.49	0	6,11,13	0.58	0
1	MLY	B	478	1	3,4,11	0.63	0	2,4,13	0.80	0
1	MLY	B	712	1	4,5,11	0.92	0	1,5,13	1.03	0
1	MLY	A	511	1	9,10,11	0.48	0	6,11,13	0.72	0
1	MLY	B	676	1	9,10,11	0.50	0	6,11,13	0.78	0
1	MLY	B	551	1	3,4,11	0.65	0	2,4,13	0.78	0
1	MLY	B	623	1	9,10,11	0.49	0	6,11,13	0.72	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	445	1	-	2/8/9/11	-
1	MLY	A	493	1	-	1/8/9/11	-
1	MLY	A	707	1	-	1/8/9/11	-
1	MLY	A	662	1	-	0/8/9/11	-
1	MLY	B	662	1	-	0/0/2/11	-
1	MLY	B	547	1	-	2/6/7/11	-
1	MLY	A	710	1	-	0/8/9/11	-
1	MLY	B	603	1	-	4/8/9/11	-
1	MLY	A	556	1	-	0/8/9/11	-
1	MLY	B	511	1	-	0/6/7/11	-
1	MLY	B	482	1	-	2/3/4/11	-
1	MLY	A	694	1	-	2/8/9/11	-
1	MLY	B	710	1	-	0/3/4/11	-
1	MLY	A	471	1	-	1/8/9/11	-
1	MLY	B	471	1	-	0/6/7/11	-
1	MLY	A	590	1	-	0/0/2/11	-
1	MLY	B	641	1	-	0/6/7/11	-
1	MLY	B	493	1	-	1/6/7/11	-
1	MLY	A	482	1	-	2/6/7/11	-
1	MLY	A	531	1	-	0/6/7/11	-
1	MLY	A	603	1	-	1/8/9/11	-
1	MLY	B	707	1	-	1/6/7/11	-
1	MLY	B	556	1	-	0/6/7/11	-
1	MLY	A	547	1	-	0/6/7/11	-
1	MLY	A	551	1	-	0/0/2/11	-
1	MLY	A	712	1	-	4/8/9/11	-
1	MLY	A	522	1	-	0/6/7/11	-
1	MLY	B	646	1	-	0/3/4/11	-
1	MLY	A	478	1	-	0/8/9/11	-
1	MLY	A	623	1	-	1/6/7/11	-
1	MLY	A	641	1	-	0/8/9/11	-
1	MLY	B	653	1	-	0/0/2/11	-
1	MLY	B	445	1	-	0/0/2/11	-
1	MLY	A	646	1	-	0/3/4/11	-
1	MLY	A	653	1	-	0/3/4/11	-
1	MLY	A	676	1	-	1/8/9/11	-
1	MLY	B	478	1	-	0/0/2/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	B	712	1	-	0/3/4/11	-
1	MLY	A	511	1	-	2/8/9/11	-
1	MLY	B	676	1	-	2/8/9/11	-
1	MLY	B	551	1	-	0/0/2/11	-
1	MLY	B	623	1	-	1/8/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	547	MLY	N-CA-CB-CG
1	B	547	MLY	C-CA-CB-CG
1	B	603	MLY	C-CA-CB-CG
1	B	603	MLY	O-C-CA-CB
1	A	707	MLY	O-C-CA-CB
1	A	694	MLY	C-CA-CB-CG
1	A	482	MLY	O-C-CA-CB
1	A	712	MLY	C-CA-CB-CG
1	A	712	MLY	O-C-CA-CB
1	A	623	MLY	O-C-CA-CB
1	A	511	MLY	O-C-CA-CB
1	B	623	MLY	O-C-CA-CB
1	A	445	MLY	CG-CD-CE-NZ
1	A	676	MLY	CD-CE-NZ-CH2
1	A	471	MLY	CG-CD-CE-NZ
1	B	707	MLY	CA-CB-CG-CD
1	B	676	MLY	CG-CD-CE-NZ
1	A	603	MLY	CG-CD-CE-NZ
1	B	482	MLY	N-CA-CB-CG
1	B	493	MLY	CG-CD-CE-NZ
1	A	493	MLY	CA-CB-CG-CD
1	A	445	MLY	N-CA-CB-CG
1	A	712	MLY	N-CA-CB-CG
1	B	603	MLY	CA-CB-CG-CD
1	A	712	MLY	CD-CE-NZ-CH2
1	B	676	MLY	C-CA-CB-CG
1	A	482	MLY	CA-CB-CG-CD
1	A	511	MLY	CA-CB-CG-CD

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Mol	Chain	Res	Type	Atoms
1	B	482	MLY	C-CA-CB-CG
1	B	603	MLY	N-CA-CB-CG
1	A	694	MLY	N-CA-CB-CG

There are no ring outliers.

24 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	445	MLY	2	0
1	A	493	MLY	2	0
1	A	707	MLY	7	0
1	A	662	MLY	1	0
1	B	662	MLY	1	0
1	B	547	MLY	4	0
1	A	710	MLY	1	0
1	B	603	MLY	1	0
1	B	710	MLY	3	0
1	A	471	MLY	2	0
1	B	471	MLY	1	0
1	A	531	MLY	2	0
1	A	603	MLY	1	0
1	B	707	MLY	3	0
1	A	522	MLY	2	0
1	A	478	MLY	2	0
1	A	641	MLY	1	0
1	B	445	MLY	1	0
1	A	676	MLY	1	0
1	B	712	MLY	2	0
1	A	511	MLY	3	0
1	B	676	MLY	2	0
1	B	551	MLY	1	0
1	B	623	MLY	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	236/291 (81%)	0.03	9 (3%) 40 30	2, 20, 52, 59	0
1	B	211/291 (72%)	0.77	31 (14%) 2 1	6, 46, 71, 74	0
All	All	447/582 (76%)	0.38	40 (8%) 9 5	2, 35, 63, 74	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	622	PHE	5.1
1	B	683	TYR	4.5
1	A	628	VAL	4.4
1	A	521	LEU	4.4
1	A	624	ILE	4.3
1	B	453	TYR	4.1
1	B	580	PHE	4.1
1	B	655	GLN	3.8
1	B	550	PHE	3.7
1	B	491	LEU	3.6
1	B	546	SER	3.4
1	B	479	HIS	3.4
1	B	508	TYR	3.4
1	B	443	GLN	3.3
1	B	456	THR	3.2
1	B	490	ALA	3.2
1	B	565	PRO	3.1
1	B	642	GLN	2.9
1	B	561	TYR	2.8
1	B	548	PRO	2.8
1	B	708	VAL	2.8
1	B	474	VAL	2.8
1	A	629	VAL	2.7
1	B	477	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	699	LEU	2.6
1	A	631	VAL	2.6
1	A	524	ASP	2.5
1	B	447	ILE	2.5
1	B	684	VAL	2.4
1	B	476	GLY	2.4
1	A	630	SER	2.2
1	B	542	LEU	2.2
1	B	507	GLU	2.2
1	B	483	ASP	2.2
1	B	563	TYR	2.2
1	B	706	ALA	2.1
1	B	492	SER	2.1
1	A	591	PRO	2.1
1	B	557	THR	2.0
1	B	654	ALA	2.0

## 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
1	MLY	A	590	5/12	0.42	0.82	35,35,35,35	0
1	MLY	B	478	5/12	0.56	0.30	61,61,61,61	0
1	MLY	B	471	9/12	0.69	0.35	57,57,57,57	0
1	MLY	A	653	6/12	0.74	0.27	41,41,42,42	0
1	MLY	A	623	9/12	0.75	0.38	57,57,57,58	0
1	MLY	B	641	9/12	0.77	0.60	43,44,44,44	0
1	MLY	B	556	9/12	0.79	0.30	67,67,67,68	0
1	MLY	B	712	6/12	0.83	0.20	61,61,61,61	0
1	MLY	B	482	6/12	0.85	0.37	57,57,57,58	0
1	MLY	B	547	9/12	0.85	0.34	72,73,73,73	0
1	MLY	B	511	9/12	0.85	0.28	63,63,63,63	0
1	MLY	B	676	11/12	0.85	0.28	36,36,37,37	0
1	MLY	B	493	9/12	0.86	0.27	53,53,54,54	0
1	MLY	B	707	9/12	0.86	0.43	58,59,59,59	0
1	MLY	A	522	9/12	0.86	0.33	37,37,38,38	0
1	MLY	B	646	6/12	0.86	0.15	41,41,41,42	0
1	MLY	A	694	11/12	0.86	0.32	16,17,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MLY	A	603	11/12	0.88	0.24	40,40,41,41	0
1	MLY	B	662	5/12	0.88	0.17	35,35,35,36	0
1	MLY	A	641	11/12	0.88	0.23	45,45,45,45	0
1	MLY	A	712	11/12	0.88	0.25	15,16,19,19	0
1	MLY	A	511	11/12	0.89	0.24	22,23,25,25	0
1	MLY	A	676	11/12	0.89	0.37	25,26,27,27	0
1	MLY	B	623	11/12	0.89	0.38	25,26,28,28	0
1	MLY	B	445	5/12	0.90	0.16	59,59,59,60	0
1	MLY	A	547	9/12	0.90	0.12	26,27,27,27	0
1	MLY	A	482	9/12	0.91	0.25	10,10,12,12	0
1	MLY	A	531	9/12	0.91	0.20	32,32,33,33	0
1	MLY	A	556	11/12	0.91	0.19	21,23,26,26	0
1	MLY	A	478	11/12	0.92	0.15	9,10,14,15	0
1	MLY	B	603	11/12	0.92	0.16	9,10,13,14	0
1	MLY	A	646	6/12	0.92	0.14	46,46,46,46	0
1	MLY	B	551	5/12	0.92	0.26	72,72,72,73	0
1	MLY	A	471	11/12	0.93	0.22	2,2,7,7	0
1	MLY	A	662	11/12	0.94	0.22	29,29,29,29	0
1	MLY	A	551	5/12	0.94	0.15	28,28,29,29	0
1	MLY	B	653	5/12	0.94	0.28	36,36,37,37	0
1	MLY	A	445	11/12	0.94	0.19	7,7,11,11	0
1	MLY	A	710	11/12	0.95	0.17	13,14,15,15	0
1	MLY	A	707	11/12	0.95	0.15	14,15,17,17	0
1	MLY	A	493	11/12	0.96	0.19	7,7,10,10	0
1	MLY	B	710	6/12	0.96	0.34	60,60,61,61	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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	A	1	1/1	0.91	0.10	34,34,34,34	0

## 6.5 Other polymers

There are no such residues in this entry.