



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:57 PM GMT

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 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/ValidationPDFNotes.html>

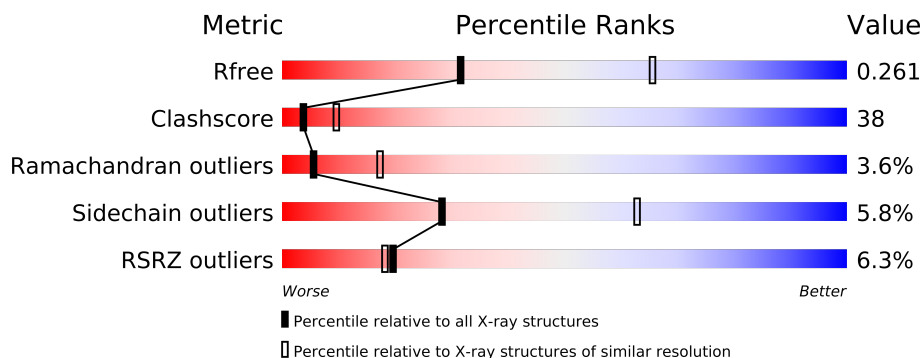
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	291	
1	B	291	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	CA	A	1	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4036 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	A	267	Total	C	N	O	Se	0	0	0
			2176	1426	336	406	8			
1	B	236	Total	C	N	O	Se	0	0	0
			1859	1221	286	346	6			

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		

4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α , β , γ	115.26Å 115.26Å 88.88Å 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
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.5.0104	Depositor
R, R_{free}	0.245 , 0.260 0.246 , 0.261	Depositor DCC
R_{free} test set	1281 reflections (8.37%)	DCC
Wilson B-factor (Å ²)	61.7	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 13.1	EDS
Estimated twinning fraction	0.041 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 16592 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4036	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 38.

All (302) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:690:GLY:HA2	1:A:707:MLY:HH11	1.66	0.77
1:A:602:VAL:HG12	1:A:602:VAL:O	1.85	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:624:ILE:O	1:A:624:ILE:HG22	1.85	0.75
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:620:ARG:HG2	1:A:650:ILE:HD13	1.77	0.67
1:A:511:MLY:HA	1:A:514:TYR:CE2	2.29	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:B:553:ASP:O	1:B:554:THR:CB	2.44	0.66
1:A:656:PHE:N	1:A:656:PHE:HD2	1.94	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:613:VAL:HG22	1:A:624:ILE:HG12	1.78	0.64
1:A:596:THR:HG22	1:A:672:ILE:HG12	1.79	0.64
1:B:462:TYR:N	1:B:463:PRO:CD	2.60	0.64
1:A:450:ARG:NH1	1:A:469:ASP:O	2.29	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:699:LEU:HD21	1:B:702:ASN:OD1	2.02	0.59
1:B:547:MLY:HD2	1:B:548:PRO:HD2	1.84	0.59
1:B:712:MLY:CG	1:B:713:ILE:H	2.15	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(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:B:473:LEU:N	1:B:473:LEU:CD1	2.67	0.58
1:A:640:ILE:H	1:A:704:ARG:NH1	2.01	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:B:504:LEU:O	1:B:504:LEU:CD2	2.37	0.57
1:A:564:MSE:HE2	1:A:709:PHE:CE2	2.38	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:B:667:PRO:C	1:B:669:ALA:H	2.09	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: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:B:648:THR:O	1:B:650:ILE:HD12	2.06	0.55
1:A:519:ASP:CG	1:A:520:ILE:H	2.08	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:B:436:ASN:CG	1:B:437:GLU:H	2.10	0.54
1:A:445:MLY:HG2	1:A:468:SER:O	2.08	0.54
1:A:471:MLY:HG2	1:A:471:MLY:HH22	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
1:B:698:ASP:O	1:B:700:VAL:HG13	2.07	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:570:LEU:C	1:B:571:ILE:HD12	2.29	0.54
1:A:640:ILE:O	1:A:642:GLN:O	2.25	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:452:ASP:CG	1:B:559:ASP:HB3	2.29	0.53
1:B:466:TYR:CD2	1:B:466:TYR:C	2.82	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:486:PHE:HB2	1:A:487:PRO:HD3	1.91	0.51
1:A:478:MLY:O	1:A:478:MLY:HG3	2.10	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:687:PHE:HA	1:B:707:MLY:NZ	2.25	0.51
1:B:486:PHE:HB2	1:B:487:PRO:HD3	1.93	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: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:489:PHE:CE2	1:B:497:ALA:HB1	2.47	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:508:TYR:N	1:B:508:TYR:HD1	2.10	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:B:472:THR:C	1:B:473:LEU:HD12	2.34	0.48
1:A:659:PHE:O	1:A:671:PHE:HD1	1.96	0.48
1:A:508:TYR:HB3	1:A:525:ILE:HG23	1.95	0.48
1:B:436:ASN:HD22	1:B:438:ALA:CB	2.27	0.48
1:B:699:LEU:CD2	1:B:702:ASN:HB2	2.41	0.48
1:A:520:ILE:CG2	1:A:521:LEU:N	2.77	0.48
1:B:503:ARG:C	1:B:505:SER:H	2.17	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:N	1:B:542:LEU:HD12	2.29	0.47
1:B:699:LEU:HD21	1:B:702:ASN:CG	2.34	0.47
1:A:451:GLU:HA	1:A:471:MLY:CH2	2.44	0.47
1:A:564:MSE:CE	1:A:709:PHE:HE2	2.27	0.47
1:A:659:PHE:HB2	1:A:672:ILE:HB	1.95	0.47
1:B:689:LEU:C	1:B:691:ASN:N	2.68	0.47
1:A:531:MLY:C	1:A:533:TYR:N	2.78	0.47
1:A:465:ARG:NH1	1:A:475:ASP:OD2	2.47	0.47
1:A:634:ILE:O	1:A:647:ILE:HA	2.15	0.47
1:A:445:MLY:O	1:A:450:ARG:NH2	2.47	0.47
1:B:508:TYR:N	1:B:508:TYR:CD1	2.81	0.47
1:A:507:GLU:OE1	1:A:557:THR:OG1	2.31	0.47
1:B:466:TYR:C	1:B:466:TYR:HD2	2.18	0.47
1:A:656:PHE:H	1:A:656:PHE:HD2	1.58	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: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: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
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:B:592:PHE:HA	1:B:675:ASP:OD1	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:562:LEU:O	1:A:708:VAL:HA	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:B:454:VAL:CG2	1:B:470:VAL:HG21	2.45	0.46
1:B:703:SER:OG	1:B:704:ARG:N	2.49	0.46
1:B:651:ASP:HB3	1:B:654:ALA:HB2	1.97	0.46
1:A:511:MLY:C	1:A:513:PHE:N	2.79	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:B:547:MLY:O	1:B:549:ASP:N	2.47	0.45
1:A:570:LEU:HD21	1:A:669:ALA:HB2	1.99	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:618:ASP:CG	1:B:620:ARG:HB2	2.38	0.45
1:B:440:LEU:HD23	1:B:440:LEU:O	2.17	0.45
1:B:700:VAL:HG11	1:B:710:MLY:HB3	2.00	0.44
1:B:697:PHE:HA	1:B:710:MLY:O	2.17	0.44
1:A:496:GLN:HE21	1:A:500:ASN:ND2	2.15	0.44
1:B:593:THR:O	1:B:674:MSE:HA	2.18	0.44
1:A:642:GLN:OE1	1:A:644:GLU:OE1	2.35	0.44
1:A:639:SER:HB3	1:A:644:GLU:HB2	1.98	0.44
1:B:547:MLY:C	1:B:549:ASP:N	2.81	0.44
1:B:687:PHE:HD1	1:B:707:MLY:CB	2.31	0.44
1:B:699:LEU:CG	1:B:702:ASN:HB2	2.48	0.44
1:B:503:ARG:O	1:B:505:SER:N	2.51	0.44
1:B:564:MSE:CE	1:B:687:PHE:HB2	2.35	0.44
1:B:687:PHE:CD1	1:B:707:MLY:HB3	2.53	0.44
1:A:703:SER:HB3	1:A:706:ALA:O	2.17	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:620:ARG:O	1:B:631:VAL:HG22	2.19	0.43
1:B:615:LEU:HD12	1:B:621:SER:O	2.17	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
1:A:593:THR:O	1:A:674:MSE:HA	2.18	0.43
1:B:452:ASP:OD1	1:B:559:ASP:HB3	2.19	0.43
1:A:527:GLN:OE1	1:A:527:GLN:HA	2.19	0.43
1:A:615:LEU:HD21	1:A:619:PHE:CD2	2.54	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:457:TRP:CD2	1:A:575:VAL:HG22	2.54	0.43
1:B:648:THR:O	1:B:650:ILE:CD1	2.67	0.42
1:A:512:SER:HA	1:A:521:LEU:HG	2.01	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:657:TYR:HE1	1:A:676:MLY:HG3	1.83	0.42
1:A:632:ASN:HD22	1:A:632:ASN:C	2.23	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:B:495:GLU:O	1:B:498:ALA:HB3	2.20	0.42
1:B:465:ARG:HD3	1:B:475:ASP:OD1	2.20	0.42
1:A:558:ARG:HG2	1:A:558:ARG:HH11	1.84	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: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:624:ILE:O	1:A:624:ILE:CG2	2.57	0.42
1:A:686:MSE:HE2	1:A:709:PHE:CD2	2.55	0.41
1:B:702:ASN:C	1:B:702:ASN:HD22	2.22	0.41
1:B:508:TYR:HD1	1:B:508:TYR:H	1.68	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: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: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:440:LEU:C	1:A:440:LEU:HD23	2.40	0.41
1:B:436:ASN:HD22	1:B:438:ALA:HB3	1.85	0.41
1:A:525:ILE:HG22	1:A:529:MSE:HE3	2.02	0.41
1:B:440:LEU:HD23	1:B:440:LEU:C	2.41	0.41
1:A:635:VAL:O	1:A:659:PHE:HA	2.20	0.41
1:A:452:ASP:OD1	1:A:559:ASP:HB2	2.19	0.41
1:A:501:MSE:CE	1:A:505:SER:H	2.33	0.41
1:A:678:MSE:CE	1:A:678:MSE:CA	2.91	0.41
1:B:462:TYR:CE2	1:B:475:ASP:HB3	2.55	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:702:ASN:OD1	1:A:707:MLY:HH22	2.21	0.41
1:A:462:TYR:HB2	1:A:463:PRO:HD3	2.03	0.41
1:A:489:PHE:CE1	1:A:493:MLY:HG2	2.57	0.40
1:B:603:MLY:HB2	1:B:604:ASN:H	1.55	0.40
1:B:451:GLU:O	1:B:558:ARG:HB3	2.22	0.40
1:A:598:TYR:CD2	1:A:598:TYR:N	2.89	0.40
1:B:686:MSE:O	1:B:690:GLY:HA2	2.22	0.40
1:A:682:ALA:O	1:A:686:MSE:CB	2.63	0.40
1:A:662:MLY:HH12	1:A:662:MLY:HD3	1.67	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

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	239/291 (82%)	209 (87%)	24 (10%)	6 (2%)	9	28
1	B	207/291 (71%)	159 (77%)	38 (18%)	10 (5%)	4	10
All	All	446/582 (77%)	368 (82%)	62 (14%)	16 (4%)	5	17

All (16) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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 ⓘ

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%)	33	69
1	B	182/228 (80%)	170 (93%)	12 (7%)	24	56
All	All	397/456 (87%)	374 (94%)	23 (6%)	28	63

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
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

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Mol	Chain	Res	Type
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 ⓘ

There are no RNA chains in this entry.

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

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	10,10,11	5.57	1 (10%)	9,11,13	0.96	1 (11%)
1	MLY	A	471	1	10,10,11	5.59	1 (10%)	9,11,13	1.00	1 (11%)
1	MLY	A	478	1	10,10,11	5.70	1 (10%)	9,11,13	1.16	1 (11%)
1	MLY	A	482	1	7,8,11	6.80	2 (28%)	5,8,13	1.08	1 (20%)
1	MLY	A	493	1	10,10,11	5.51	1 (10%)	9,11,13	0.99	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	A	511	1	10,10,11	5.61	1 (10%)	9,11,13	0.89	0
1	MLY	A	522	1	7,8,11	6.82	2 (28%)	5,8,13	1.64	1 (20%)
1	MLY	A	531	1	7,8,11	6.73	2 (28%)	5,8,13	1.22	1 (20%)
1	MLY	A	547	1	7,8,11	6.72	2 (28%)	5,8,13	1.17	1 (20%)
1	MLY	A	551	1	3,4,11	10.32	2 (66%)	1,4,13	2.08	1 (100%)
1	MLY	A	556	1	10,10,11	5.58	1 (10%)	9,11,13	1.08	1 (11%)
1	MLY	A	590	1	3,4,11	10.36	2 (66%)	1,4,13	2.37	1 (100%)
1	MLY	A	603	1	10,10,11	5.59	1 (10%)	9,11,13	0.76	0
1	MLY	A	623	1	7,8,11	6.72	2 (28%)	5,8,13	0.43	0
1	MLY	A	641	1	10,10,11	5.59	1 (10%)	9,11,13	1.39	1 (11%)
1	MLY	A	646	1	5,5,11	16.69	3 (60%)	2,5,13	1.57	1 (50%)
1	MLY	A	653	1	5,5,11	16.47	3 (60%)	2,5,13	1.70	1 (50%)
1	MLY	A	662	1	10,10,11	5.60	1 (10%)	9,11,13	0.64	0
1	MLY	A	676	1	10,10,11	5.61	1 (10%)	9,11,13	0.84	1 (11%)
1	MLY	A	694	1	10,10,11	5.55	1 (10%)	9,11,13	0.92	1 (11%)
1	MLY	A	707	1	10,10,11	5.61	1 (10%)	9,11,13	1.22	1 (11%)
1	MLY	A	710	1	10,10,11	5.63	1 (10%)	9,11,13	1.18	1 (11%)
1	MLY	A	712	1	10,10,11	5.55	1 (10%)	9,11,13	1.23	1 (11%)
1	MLY	B	445	1	3,4,11	10.38	2 (66%)	1,4,13	2.98	1 (100%)
1	MLY	B	471	1	7,8,11	6.76	2 (28%)	5,8,13	1.20	1 (20%)
1	MLY	B	478	1	3,4,11	10.38	2 (66%)	1,4,13	2.54	1 (100%)
1	MLY	B	482	1	5,5,11	16.50	3 (60%)	2,5,13	1.79	1 (50%)
1	MLY	B	493	1	7,8,11	6.75	2 (28%)	5,8,13	1.18	1 (20%)
1	MLY	B	511	1	7,8,11	6.84	2 (28%)	5,8,13	1.44	1 (20%)
1	MLY	B	547	1	7,8,11	6.74	2 (28%)	5,8,13	1.28	1 (20%)
1	MLY	B	551	1	3,4,11	10.35	2 (66%)	1,4,13	2.98	1 (100%)
1	MLY	B	556	1	7,8,11	6.76	2 (28%)	5,8,13	1.41	1 (20%)
1	MLY	B	603	1	10,10,11	5.71	1 (10%)	9,11,13	0.73	0
1	MLY	B	623	1	10,10,11	5.65	1 (10%)	9,11,13	1.18	1 (11%)
1	MLY	B	641	1	7,8,11	6.73	2 (28%)	5,8,13	1.56	1 (20%)
1	MLY	B	646	1	5,5,11	16.59	3 (60%)	2,5,13	1.18	0
1	MLY	B	653	1	3,4,11	10.24	2 (66%)	1,4,13	2.14	1 (100%)
1	MLY	B	662	1	3,4,11	10.32	2 (66%)	1,4,13	3.46	1 (100%)
1	MLY	B	676	1	10,10,11	5.60	1 (10%)	9,11,13	0.97	1 (11%)
1	MLY	B	707	1	7,8,11	6.74	2 (28%)	5,8,13	1.32	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	B	710	1	5,5,11	16.65	3 (60%)	2,5,13	1.74	1 (50%)
1	MLY	B	712	1	5,5,11	16.61	3 (60%)	2,5,13	1.96	1 (50%)

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	-	0/7/9/11	0/0/0/0
1	MLY	A	471	1	-	0/7/9/11	0/0/0/0
1	MLY	A	478	1	-	0/7/9/11	0/0/0/0
1	MLY	A	482	1	-	0/5/7/11	0/0/0/0
1	MLY	A	493	1	-	0/7/9/11	0/0/0/0
1	MLY	A	511	1	-	0/7/9/11	0/0/0/0
1	MLY	A	522	1	-	0/5/7/11	0/0/0/0
1	MLY	A	531	1	-	0/5/7/11	0/0/0/0
1	MLY	A	547	1	-	0/5/7/11	0/0/0/0
1	MLY	A	551	1	-	0/0/2/11	0/0/0/0
1	MLY	A	556	1	-	0/7/9/11	0/0/0/0
1	MLY	A	590	1	-	0/0/2/11	0/0/0/0
1	MLY	A	603	1	-	0/7/9/11	0/0/0/0
1	MLY	A	623	1	-	0/5/7/11	0/0/0/0
1	MLY	A	641	1	-	0/7/9/11	0/0/0/0
1	MLY	A	646	1	-	0/2/4/11	0/0/0/0
1	MLY	A	653	1	-	0/2/4/11	0/0/0/0
1	MLY	A	662	1	-	0/7/9/11	0/0/0/0
1	MLY	A	676	1	-	0/7/9/11	0/0/0/0
1	MLY	A	694	1	-	0/7/9/11	0/0/0/0
1	MLY	A	707	1	-	0/7/9/11	0/0/0/0
1	MLY	A	710	1	-	0/7/9/11	0/0/0/0
1	MLY	A	712	1	-	0/7/9/11	0/0/0/0
1	MLY	B	445	1	-	0/0/2/11	0/0/0/0
1	MLY	B	471	1	-	0/5/7/11	0/0/0/0
1	MLY	B	478	1	-	0/0/2/11	0/0/0/0
1	MLY	B	482	1	-	0/2/4/11	0/0/0/0
1	MLY	B	493	1	-	0/5/7/11	0/0/0/0
1	MLY	B	511	1	-	0/5/7/11	0/0/0/0
1	MLY	B	547	1	-	0/5/7/11	0/0/0/0
1	MLY	B	551	1	-	0/0/2/11	0/0/0/0
1	MLY	B	556	1	-	0/5/7/11	0/0/0/0
1	MLY	B	603	1	-	0/7/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	B	623	1	-	0/7/9/11	0/0/0/0
1	MLY	B	641	1	-	0/5/7/11	0/0/0/0
1	MLY	B	646	1	-	0/2/4/11	0/0/0/0
1	MLY	B	653	1	-	0/0/2/11	0/0/0/0
1	MLY	B	662	1	-	0/0/2/11	0/0/0/0
1	MLY	B	676	1	-	0/7/9/11	0/0/0/0
1	MLY	B	707	1	-	0/5/7/11	0/0/0/0
1	MLY	B	710	1	-	0/2/4/11	0/0/0/0
1	MLY	B	712	1	-	0/2/4/11	0/0/0/0

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	646	MLY	CG-CB	-32.77	1.42	1.55
1	B	710	MLY	CG-CB	-32.71	1.42	1.55
1	B	712	MLY	CG-CB	-32.63	1.42	1.55
1	B	646	MLY	CG-CB	-32.52	1.42	1.55
1	B	482	MLY	CG-CB	-32.36	1.42	1.55
1	A	653	MLY	CG-CB	-32.15	1.42	1.55
1	B	603	MLY	O-C	17.96	1.23	1.11
1	A	478	MLY	O-C	17.95	1.23	1.11
1	B	511	MLY	O-C	17.91	1.23	1.11
1	A	522	MLY	O-C	17.86	1.23	1.11
1	B	445	MLY	O-C	17.81	1.23	1.11
1	A	482	MLY	O-C	17.79	1.23	1.11
1	B	623	MLY	O-C	17.78	1.23	1.11
1	A	653	MLY	O-C	17.78	1.23	1.11
1	B	478	MLY	O-C	17.78	1.23	1.11
1	B	551	MLY	O-C	17.75	1.23	1.11
1	A	590	MLY	O-C	17.74	1.23	1.11
1	A	710	MLY	O-C	17.71	1.23	1.11
1	B	662	MLY	O-C	17.71	1.23	1.11
1	B	471	MLY	O-C	17.70	1.23	1.11
1	B	646	MLY	O-C	17.70	1.23	1.11
1	B	556	MLY	O-C	17.70	1.23	1.11
1	A	551	MLY	O-C	17.69	1.23	1.11
1	A	646	MLY	O-C	17.69	1.23	1.11
1	B	493	MLY	O-C	17.68	1.23	1.11
1	A	676	MLY	O-C	17.67	1.23	1.11
1	A	707	MLY	O-C	17.67	1.23	1.11
1	A	511	MLY	O-C	17.66	1.23	1.11
1	B	547	MLY	O-C	17.65	1.23	1.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	707	MLY	O-C	17.65	1.23	1.11
1	A	662	MLY	O-C	17.63	1.23	1.11
1	A	531	MLY	O-C	17.63	1.23	1.11
1	B	641	MLY	O-C	17.62	1.23	1.11
1	B	676	MLY	O-C	17.62	1.23	1.11
1	A	603	MLY	O-C	17.61	1.23	1.11
1	A	471	MLY	O-C	17.60	1.23	1.11
1	A	547	MLY	O-C	17.59	1.23	1.11
1	A	641	MLY	O-C	17.59	1.23	1.11
1	A	623	MLY	O-C	17.59	1.23	1.11
1	B	710	MLY	O-C	17.58	1.23	1.11
1	B	712	MLY	O-C	17.57	1.23	1.11
1	A	556	MLY	O-C	17.57	1.23	1.11
1	B	482	MLY	O-C	17.54	1.23	1.11
1	B	653	MLY	O-C	17.54	1.23	1.11
1	A	445	MLY	O-C	17.53	1.23	1.11
1	A	694	MLY	O-C	17.46	1.23	1.11
1	A	712	MLY	O-C	17.45	1.23	1.11
1	A	493	MLY	O-C	17.36	1.23	1.11
1	A	590	MLY	CA-C	2.67	1.53	1.48
1	A	482	MLY	CA-C	2.63	1.53	1.48
1	B	653	MLY	CA-C	2.59	1.53	1.48
1	A	551	MLY	CA-C	2.58	1.53	1.48
1	A	623	MLY	CA-C	2.58	1.53	1.48
1	B	478	MLY	CA-C	2.58	1.53	1.48
1	B	471	MLY	CA-C	2.54	1.53	1.48
1	B	712	MLY	CA-C	2.53	1.53	1.48
1	B	547	MLY	CA-C	2.52	1.53	1.48
1	B	710	MLY	CA-C	2.52	1.53	1.48
1	A	522	MLY	CA-C	2.51	1.53	1.48
1	B	511	MLY	CA-C	2.50	1.53	1.48
1	B	493	MLY	CA-C	2.50	1.52	1.48
1	B	646	MLY	CA-C	2.50	1.52	1.48
1	A	547	MLY	CA-C	2.48	1.52	1.48
1	B	445	MLY	CA-C	2.48	1.52	1.48
1	B	707	MLY	CA-C	2.48	1.52	1.48
1	B	641	MLY	CA-C	2.46	1.52	1.48
1	A	646	MLY	CA-C	2.46	1.52	1.48
1	B	556	MLY	CA-C	2.46	1.52	1.48
1	B	482	MLY	CA-C	2.46	1.52	1.48
1	B	551	MLY	CA-C	2.46	1.52	1.48
1	A	653	MLY	CA-C	2.45	1.52	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	531	MLY	CA-C	2.43	1.52	1.48
1	B	662	MLY	CA-C	2.38	1.52	1.48

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	641	MLY	C-CA-N	-3.65	110.19	113.83
1	A	522	MLY	C-CA-N	-3.58	110.26	113.83
1	B	662	MLY	C-CA-N	-3.46	110.37	113.83
1	B	641	MLY	C-CA-N	-3.40	110.43	113.83
1	B	511	MLY	C-CA-N	-3.13	110.71	113.83
1	B	623	MLY	C-CA-N	-3.06	110.78	113.83
1	A	707	MLY	C-CA-N	-3.05	110.78	113.83
1	B	556	MLY	C-CA-N	-3.04	110.79	113.83
1	B	551	MLY	C-CA-N	-2.98	110.85	113.83
1	B	445	MLY	C-CA-N	-2.98	110.86	113.83
1	A	478	MLY	C-CA-N	-2.91	110.92	113.83
1	A	712	MLY	C-CA-N	-2.89	110.94	113.83
1	B	707	MLY	C-CA-N	-2.83	111.00	113.83
1	B	712	MLY	C-CA-N	-2.77	111.06	113.83
1	A	710	MLY	C-CA-N	-2.75	111.08	113.83
1	A	556	MLY	C-CA-N	-2.75	111.09	113.83
1	B	547	MLY	C-CA-N	-2.74	111.09	113.83
1	A	531	MLY	C-CA-N	-2.59	111.24	113.83
1	B	471	MLY	C-CA-N	-2.58	111.25	113.83
1	B	478	MLY	C-CA-N	-2.54	111.30	113.83
1	B	482	MLY	C-CA-N	-2.53	111.30	113.83
1	B	493	MLY	C-CA-N	-2.51	111.32	113.83
1	A	493	MLY	C-CA-N	-2.48	111.35	113.83
1	A	547	MLY	C-CA-N	-2.47	111.36	113.83
1	B	710	MLY	C-CA-N	-2.46	111.37	113.83
1	A	653	MLY	C-CA-N	-2.40	111.43	113.83
1	A	590	MLY	C-CA-N	-2.37	111.47	113.83
1	A	471	MLY	C-CA-N	-2.34	111.49	113.83
1	A	482	MLY	C-CA-N	-2.31	111.52	113.83
1	A	646	MLY	C-CA-N	-2.23	111.61	113.83
1	A	445	MLY	C-CA-N	-2.17	111.67	113.83
1	A	694	MLY	C-CA-N	-2.17	111.67	113.83
1	B	653	MLY	C-CA-N	-2.14	111.69	113.83
1	A	551	MLY	C-CA-N	-2.08	111.75	113.83
1	B	676	MLY	C-CA-N	-2.05	111.78	113.83
1	A	676	MLY	C-CA-N	-2.03	111.81	113.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	267/291 (91%)	0.05	10 (3%) 39 39	2, 21, 51, 59	0
1	B	236/291 (81%)	0.54	22 (9%) 9 7	6, 49, 72, 74	0
All	All	503/582 (86%)	0.28	32 (6%) 19 17	2, 35, 63, 74	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	447	ILE	5.1
1	B	561	TYR	5.0
1	B	548	PRO	4.9
1	A	624	ILE	4.9
1	A	625	GLY	4.8
1	B	550	PHE	4.6
1	A	628	VAL	4.3
1	A	521	LEU	4.1
1	B	546	SER	3.7
1	B	580	PHE	3.3
1	B	699	LEU	3.1
1	A	590	MLY	3.0
1	B	542	LEU	3.0
1	B	443	GLN	2.9
1	B	476	GLY	2.8
1	A	514	TYR	2.8
1	B	549	ASP	2.8
1	A	622	PHE	2.8
1	B	474	VAL	2.7
1	B	683	TYR	2.7
1	A	549	ASP	2.7
1	B	655	GLN	2.6
1	B	559	ASP	2.5
1	B	623	MLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	641	MLY	2.5
1	B	456	THR	2.3
1	A	623	MLY	2.3
1	A	502	ALA	2.3
1	B	709	PHE	2.2
1	B	569	SER	2.1
1	B	477	GLY	2.1
1	B	673	LEU	2.0

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	MLY	A	590	5/12	0.56	6.61	35,35,35,35	0
1	MLY	B	641	9/12	0.52	4.21	43,44,44,44	0
1	MLY	B	623	11/12	0.52	3.65	25,26,28,28	0
1	MLY	A	676	11/12	0.34	3.33	25,26,27,27	0
1	MLY	A	653	6/12	0.26	2.83	41,41,42,42	0
1	MLY	A	493	11/12	0.28	2.68	7,7,10,10	0
1	MLY	A	445	11/12	0.21	2.28	7,7,11,11	0
1	MLY	A	694	11/12	0.39	2.14	16,17,20,20	0
1	MLY	A	482	9/12	0.29	1.64	10,10,12,12	0
1	MLY	A	662	11/12	0.21	1.50	29,29,29,29	0
1	MLY	B	511	9/12	0.31	1.16	63,63,63,63	0
1	MLY	A	603	11/12	0.23	1.12	40,40,41,41	0
1	MLY	A	712	11/12	0.25	1.03	15,16,19,19	0
1	MLY	A	623	9/12	0.50	0.93	57,57,57,58	0
1	MLY	B	471	9/12	0.27	0.89	57,57,57,57	0
1	MLY	A	531	9/12	0.22	0.88	32,32,33,33	0
1	MLY	A	471	11/12	0.22	0.84	2,2,7,7	0
1	MLY	B	676	11/12	0.27	0.79	36,36,37,37	0
1	MLY	B	493	9/12	0.32	0.76	53,53,54,54	0
1	MLY	B	710	6/12	0.34	0.45	60,60,61,61	0
1	MLY	A	641	11/12	0.22	0.44	45,45,45,45	0
1	MLY	A	478	11/12	0.17	0.43	9,10,14,15	0
1	MLY	A	522	9/12	0.31	0.31	37,37,38,38	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	MLY	B	547	9/12	0.39	0.23	72,73,73,73	0
1	MLY	B	707	9/12	0.29	0.21	58,59,59,59	0
1	MLY	B	556	9/12	0.21	0.13	67,67,67,68	0
1	MLY	A	511	11/12	0.23	-0.05	22,23,25,25	0
1	MLY	B	603	11/12	0.18	-0.10	9,10,13,14	0
1	MLY	B	482	6/12	0.23	-0.19	57,57,57,58	0
1	MLY	A	707	11/12	0.17	-0.49	14,15,17,17	0
1	MLY	B	662	5/12	0.17	-0.68	35,35,35,36	0
1	MLY	A	556	11/12	0.15	-0.69	21,23,26,26	0
1	MLY	A	710	11/12	0.18	-0.74	13,14,15,15	0
1	MLY	B	653	5/12	0.12	-0.80	36,36,37,37	0
1	MLY	A	551	5/12	0.14	-0.99	28,28,29,29	0
1	MLY	B	445	5/12	0.13	-1.01	59,59,59,60	0
1	MLY	B	551	5/12	0.19	-1.03	72,72,72,73	0
1	MLY	A	547	9/12	0.12	-1.12	26,27,27,27	0
1	MLY	A	646	6/12	0.18	-1.18	46,46,46,46	0
1	MLY	B	478	5/12	0.21	-1.36	61,61,61,61	0
1	MLY	B	646	6/12	0.14	-2.35	41,41,41,42	0
1	MLY	B	712	6/12	0.15	-3.28	61,61,61,61	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CA	A	1	1/1	0.22	3.93	34,34,34,34	0

6.5 Other polymers ⓘ

There are no such residues in this entry.