



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:18 AM 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 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

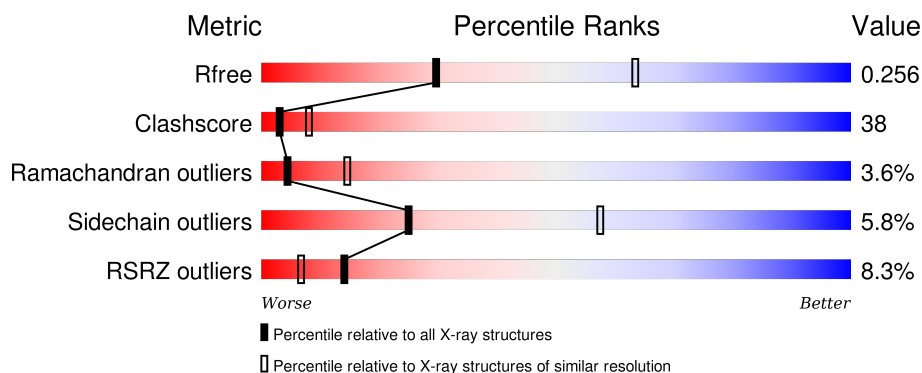
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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. 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	
1	B	291	

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	707	-	-	X	-

2 Entry composition

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
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		

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 ($\text{RSRZ} > 2$). 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.

- Chain A:

Residue Type	Count
GLY	1
PRO	1
LEU	1
VAL	1
ASP	1
GLY	1
SER	1
ILE	1
ALA	1
PRO	1
THR	1
VAL	1
PHE	1
SER	1
GLN	1
Met	1
L440	1
L444	1
K445	1
R450	1
E451	1
D452	1
E453	1
V454	1
T455	1
T456	1
H457	1
Y462	1
P463	1
V464	1
R465	1
S468	1
D469	1
V470	1
K471	1
T472	1
D475	1
K478	1
F483	1
M484	1
D559	1
I560	1
P487	1
S488	1
F489	1
K493	1
D494	1
E495	1
Q496	1
N500	1
M501	1
L502	1
R503	1
L504	1
S505	1
V506	1
E507	1
V508	1
T509	1
E510	1
K511	1
S512	1
F513	1
Y514	1
ALA	1
PRO	1
GLN	1
ASN	1
D519	1
I520	1
L521	1
K522	1
S523	1
D524	1
I525	1
E526	1
L526	1
Q527	1
A528	1
M529	1
M530	1
K531	1
D532	1
Y533	1
M534	1
Q535	1
V538	1
S541	1
S544	1
L545	1
T554	1
P555	1
A556	1
T557	1
R558	1
D559	1
I560	1
Y561	1
L562	1
Y563	1
M564	1
L570	1
V575	1
M582	1
LEU	1
ASP	1
THR	1
GLY	1
VAL	1
LEU	1
ASP	1
V590	1
P591	1
T592	1
F593	1
T596	1
A597	1
Y598	1
V602	1
K603	1
L604	1
G605	1
E606	1
L607	1
V608	1
V613	1
V614	1
L615	1
F619	1
R620	1
S621	1
G622	1
K623	1
I624	1
G625	1
V628	1
V629	1
S630	1
V631	1
M632	1
G633	1
I634	1
V635	1
E636	1
L637	1
N638	1
S639	1
I640	1
K641	1
Q642	1
G643	1
E644	1
I647	1
T648	1
P649	1
I650	1
D651	1
D652	1
K653	1
A654	1
D655	1

- [illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.80 Å)	Xtriage
Refinement program	REFMAC 5.5.0104	Depositor
R, R_{free}	0.245 , 0.260 0.243 , 0.256	Depositor DCC
R_{free} test set	1276 reflections (8.35%)	DCC
Wilson B-factor (Å ²)	61.7	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.4	EDS
Estimated twinning fraction	0.041 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 16592 reflections	Xtriage
F_o, F_c correlation	0.91	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.

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: 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

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: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
1:A:624:ILE:O	1:A:624:ILE:HG22	1.85	0.75

Continued on next page...

Continued from previous page...

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: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

Continued on next page...

Continued from previous page...

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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:698:ASP:O	1:B:700:VAL:HG13	2.07	0.54
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

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:B:592:PHE:HA	1:B:675:ASP:OD1	2.15	0.46
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

Continued on next page...

Continued from previous page...

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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 [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%)	7	24
1	B	207/291 (71%)	159 (77%)	38 (18%)	10 (5%)	3	9
All	All	446/582 (77%)	368 (82%)	62 (14%)	16 (4%)	4	14

All (16) Ramachandran outliers are listed below:

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

Continued on next page...

Continued from previous page...

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 ⓘ

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%)	29	63
1	B	182/228 (80%)	170 (93%)	12 (7%)	21	51
All	All	397/456 (87%)	374 (94%)	23 (6%)	25	57

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

Continued on next page...

Continued from previous page...

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 ⓘ

There are no RNA molecules 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	9,10,11	0.50	0	9,11,13	0.91	0
1	MLY	A	471	1	9,10,11	0.48	0	9,11,13	0.92	0
1	MLY	A	478	1	9,10,11	0.54	0	9,11,13	0.92	0
1	MLY	A	482	1	7,8,11	0.45	0	6,8,13	0.82	0
1	MLY	A	493	1	9,10,11	0.50	0	9,11,13	0.85	0
1	MLY	A	511	1	9,10,11	0.50	0	9,11,13	0.91	0
1	MLY	A	522	1	7,8,11	0.44	0	6,8,13	0.82	0
1	MLY	A	531	1	7,8,11	0.45	0	6,8,13	0.83	0
1	MLY	A	547	1	7,8,11	0.43	0	6,8,13	0.86	0
1	MLY	A	551	1	3,4,11	0.57	0	0,4,13	0.00	-
1	MLY	A	556	1	9,10,11	0.52	0	9,11,13	0.87	0
1	MLY	A	590	1	3,4,11	0.57	0	0,4,13	0.00	-
1	MLY	A	603	1	9,10,11	0.50	0	9,11,13	0.90	0
1	MLY	A	623	1	7,8,11	0.42	0	6,8,13	0.87	0
1	MLY	A	641	1	9,10,11	0.52	0	9,11,13	0.94	0
1	MLY	A	646	1	4,5,11	0.82	0	3,5,13	1.16	0
1	MLY	A	653	1	4,5,11	0.81	0	3,5,13	1.16	0
1	MLY	A	662	1	9,10,11	0.48	0	9,11,13	0.91	0
1	MLY	A	676	1	9,10,11	0.50	0	9,11,13	0.82	0
1	MLY	A	694	1	9,10,11	0.53	0	9,11,13	0.87	0
1	MLY	A	707	1	9,10,11	0.51	0	9,11,13	0.96	0
1	MLY	A	710	1	9,10,11	0.57	0	9,11,13	1.00	0
1	MLY	A	712	1	9,10,11	0.58	0	9,11,13	1.02	0
1	MLY	B	445	1	3,4,11	0.57	0	0,4,13	0.00	-
1	MLY	B	471	1	7,8,11	0.44	0	6,8,13	0.80	0
1	MLY	B	478	1	3,4,11	0.56	0	0,4,13	0.00	-
1	MLY	B	482	1	4,5,11	0.81	0	3,5,13	1.18	0
1	MLY	B	493	1	7,8,11	0.44	0	6,8,13	0.82	0
1	MLY	B	511	1	7,8,11	0.44	0	6,8,13	0.79	0
1	MLY	B	547	1	7,8,11	0.43	0	6,8,13	0.85	0
1	MLY	B	551	1	3,4,11	0.57	0	0,4,13	0.00	-
1	MLY	B	556	1	7,8,11	0.42	0	6,8,13	0.82	0
1	MLY	B	603	1	9,10,11	0.56	0	9,11,13	0.94	0
1	MLY	B	623	1	9,10,11	0.50	0	9,11,13	0.88	0
1	MLY	B	641	1	7,8,11	0.43	0	6,8,13	0.79	0
1	MLY	B	646	1	4,5,11	0.81	0	3,5,13	1.17	0
1	MLY	B	653	1	3,4,11	0.55	0	0,4,13	0.00	-
1	MLY	B	662	1	3,4,11	0.57	0	0,4,13	0.00	-
1	MLY	B	676	1	9,10,11	0.55	0	9,11,13	0.96	0
1	MLY	B	707	1	7,8,11	0.44	0	6,8,13	0.82	0
1	MLY	B	710	1	4,5,11	0.82	0	3,5,13	1.17	0
1	MLY	B	712	1	4,5,11	0.81	0	3,5,13	1.17	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	-	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
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

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.

24 monomers are involved in 47 short contacts:

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

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.

No monomer is involved in short contacts.

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	236/291 (81%)	0.03	10 (4%) 40 28	2, 20, 52, 59	0
1	B	211/291 (72%)	0.71	27 (12%) 5 2	6, 46, 71, 74	0
All	All	447/582 (76%)	0.35	37 (8%) 14 7	2, 35, 63, 74	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	622	PHE	4.8
1	A	624	ILE	4.7
1	A	521	LEU	4.5
1	A	628	VAL	4.4
1	B	683	TYR	4.2
1	B	453	TYR	4.1
1	B	580	PHE	4.0
1	B	655	GLN	3.6
1	B	508	TYR	3.5
1	B	550	PHE	3.3
1	B	443	GLN	3.3
1	B	456	THR	3.3
1	B	490	ALA	3.3
1	B	491	LEU	3.2
1	B	546	SER	3.2
1	B	561	TYR	3.1
1	B	479	HIS	3.1
1	B	548	PRO	2.9
1	B	565	PRO	2.8
1	B	477	GLY	2.7
1	B	699	LEU	2.7
1	A	629	VAL	2.6
1	B	507	GLU	2.6
1	B	708	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	474	VAL	2.5
1	A	524	ASP	2.5
1	B	476	GLY	2.5
1	B	642	GLN	2.4
1	B	447	ILE	2.4
1	B	557	THR	2.4
1	A	631	VAL	2.3
1	B	684	VAL	2.2
1	A	625	GLY	2.2
1	A	591	PRO	2.1
1	B	492	SER	2.1
1	A	514	TYR	2.1
1	B	702	ASN	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. 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
1	MLY	A	493	11/12	0.96	0.19	-	7,7,10,10	0
1	MLY	A	662	11/12	0.94	0.25	-	29,29,29,29	0
1	MLY	B	662	5/12	0.88	0.17	-	35,35,35,36	0
1	MLY	B	547	9/12	0.85	0.33	-	72,73,73,73	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	547	9/12	0.91	0.12	-	26,27,27,27	0
1	MLY	B	603	11/12	0.92	0.16	-	9,10,13,14	0
1	MLY	A	707	11/12	0.96	0.15	-	14,15,17,17	0
1	MLY	B	511	9/12	0.86	0.28	-	63,63,63,63	0
1	MLY	B	482	6/12	0.85	0.35	-	57,57,57,58	0
1	MLY	A	694	11/12	0.86	0.32	-	16,17,20,20	0
1	MLY	A	556	11/12	0.91	0.20	-	21,23,26,26	0
1	MLY	B	710	6/12	0.96	0.34	-	60,60,61,61	0
1	MLY	A	471	11/12	0.93	0.22	-	2,2,7,7	0
1	MLY	B	471	9/12	0.70	0.33	-	57,57,57,57	0
1	MLY	A	590	5/12	0.41	0.80	-	35,35,35,35	0
1	MLY	B	641	9/12	0.78	0.55	-	43,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	MLY	B	493	9/12	0.86	0.27	-	53,53,54,54	0
1	MLY	A	482	9/12	0.92	0.23	-	10,10,12,12	0
1	MLY	A	531	9/12	0.91	0.20	-	32,32,33,33	0
1	MLY	A	603	11/12	0.88	0.24	-	40,40,41,41	0
1	MLY	B	707	9/12	0.85	0.42	-	58,59,59,59	0
1	MLY	B	445	5/12	0.90	0.16	-	59,59,59,60	0
1	MLY	A	641	11/12	0.88	0.22	-	45,45,45,45	0
1	MLY	A	551	5/12	0.94	0.12	-	28,28,29,29	0
1	MLY	A	712	11/12	0.88	0.25	-	15,16,19,19	0
1	MLY	A	522	9/12	0.86	0.32	-	37,37,38,38	0
1	MLY	B	646	6/12	0.87	0.15	-	41,41,41,42	0
1	MLY	A	478	11/12	0.92	0.15	-	9,10,14,15	0
1	MLY	A	623	9/12	0.74	0.39	-	57,57,57,58	0
1	MLY	B	556	9/12	0.78	0.33	-	67,67,67,68	0
1	MLY	B	653	5/12	0.94	0.28	-	36,36,37,37	0
1	MLY	A	653	6/12	0.74	0.27	-	41,41,42,42	0
1	MLY	B	551	5/12	0.92	0.23	-	72,72,72,73	0
1	MLY	A	676	11/12	0.89	0.40	-	25,26,27,27	0
1	MLY	B	478	5/12	0.56	0.29	-	61,61,61,61	0
1	MLY	B	712	6/12	0.82	0.20	-	61,61,61,61	0
1	MLY	A	511	11/12	0.89	0.25	-	22,23,25,25	0
1	MLY	B	676	11/12	0.85	0.27	-	36,36,37,37	0
1	MLY	A	646	6/12	0.92	0.13	-	46,46,46,46	0
1	MLY	B	623	11/12	0.89	0.39	-	25,26,28,28	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
2	CA	A	1	1/1	0.91	0.10	-	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.