Full wwPDB X-ray Structure Validation Report (i)

Dec 12, 2023 – 10:42 pm GMT

PDB ID	:	4BL3
Title	:	Crystal structure of PBP2a clinical mutant N146K from MRSA
Authors	:	Otero, L.H.; Rojas-Altuve, A.; Carrasco-Lopez, C.; Hermoso, J.A.
Deposited on	:	2013-04-30
Resolution	:	3.00 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

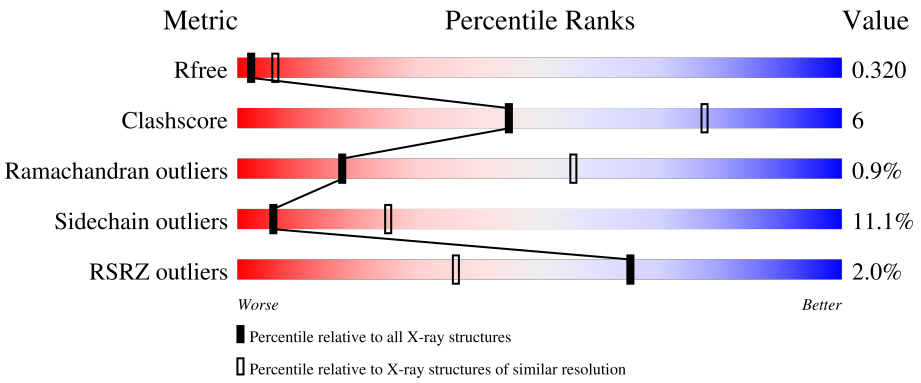
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

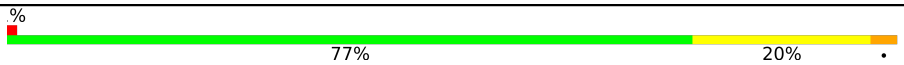
The reported resolution of this entry is 3.00 Å.

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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	640	
1	B	640	

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
4	MUR	A	1677	-	-	X	X
4	MUR	B	1677	-	-	X	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10427 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 PENICILLIN BINDING PROTEIN 2 PRIME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	640	5141	3243	869	1013	16	0	0	0
1	B	639	5132	3238	867	1011	16	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	146	LYS	ASN	engineered mutation	UNP Q54113
A	?	-	GLU	deletion	UNP Q54113
A	?	-	THR	deletion	UNP Q54113
A	?	-	GLY	deletion	UNP Q54113
B	146	LYS	ASN	engineered mutation	UNP Q54113
B	?	-	GLU	deletion	UNP Q54113
B	?	-	THR	deletion	UNP Q54113
B	?	-	GLY	deletion	UNP Q54113

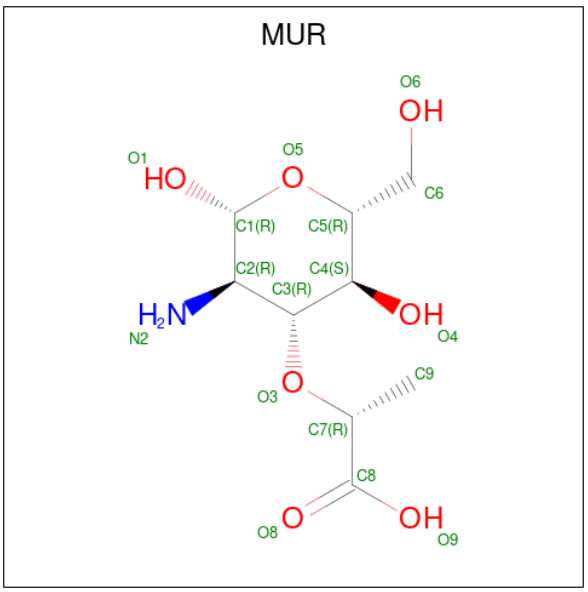
- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cd		
2	A	4	4	4	0	0
2	B	3	3	3	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
3	A	2	2	2	0	0
3	B	2	2	2	0	0

- Molecule 4 is beta-muramic acid (three-letter code: MUR) (formula: $C_9H_{17}NO_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	17	9	1	7	0	0
4	B	1	17	9	1	7	0	0

- Molecule 5 is water.

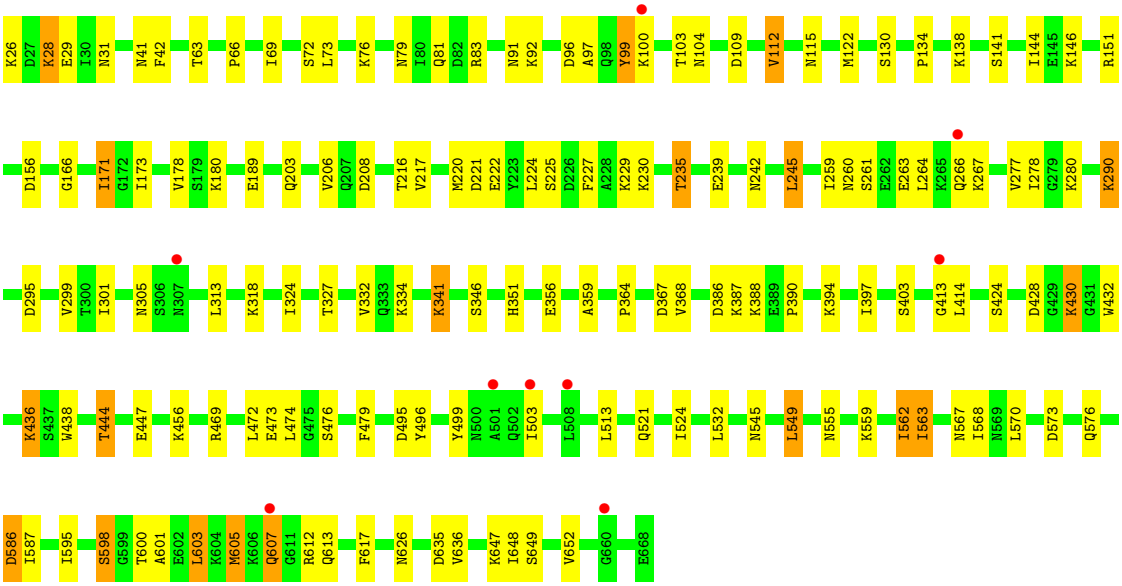
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	58	58	58	0	0
5	B	51	51	51	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

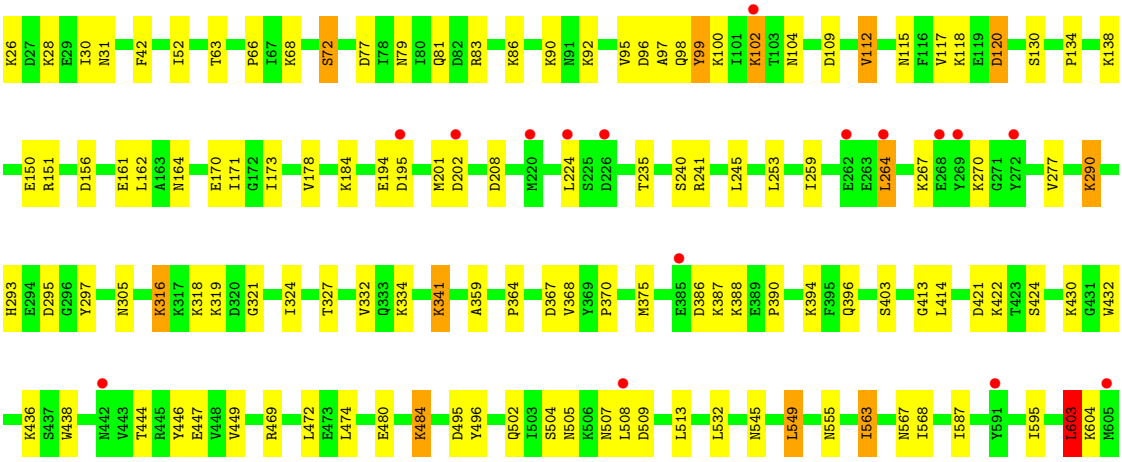
• Molecule 1: PENICILLIN BINDING PROTEIN 2 PRIME

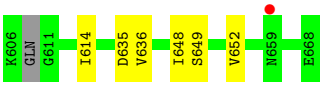
Chain A:



• Molecule 1: PENICILLIN BINDING PROTEIN 2 PRIME

Chain B:




K606
GLN
G611
I614
D635
V636
I648
S649
V652
N653
E668

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.79Å 102.39Å 187.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.74 – 3.00 46.78 – 3.00	Depositor EDS
% Data completeness (in resolution range)	81.9 (48.74-3.00) 81.9 (46.78-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.235 , 0.304 0.241 , 0.320	Depositor DCC
R_{free} test set	1866 reflections (7.07%)	wwPDB-VP
Wilson B-factor (Å^2)	58.2	Xtriage
Anisotropy	0.843	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 93.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	10427	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: MUR, CD, CL

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	0.50	0/5226	0.70	0/7022
1	B	0.49	0/5217	0.70	0/7010
All	All	0.50	0/10443	0.70	0/14032

There are no bond length outliers.

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	5141	0	5153	66	0
1	B	5132	0	5145	72	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	17	0	16	9	0
4	B	17	0	16	15	0
5	A	58	0	0	1	0
5	B	51	0	0	1	0
All	All	10427	0	10330	134	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 6.

All (134) 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:241:ARG:HD3	4:B:1677:MUR:H61	1.21	1.17
1:B:151:ARG:HB2	4:B:1677:MUR:O9	1.52	1.09
1:B:241:ARG:CD	4:B:1677:MUR:H61	2.00	0.92
1:B:151:ARG:HA	1:B:293:HIS:HD2	1.35	0.92
1:A:277:VAL:CB	4:A:1677:MUR:H7	2.04	0.87
1:A:277:VAL:HB	4:A:1677:MUR:H7	1.59	0.84
1:B:241:ARG:HD3	4:B:1677:MUR:C6	2.06	0.84
1:B:277:VAL:HB	4:B:1677:MUR:C9	2.12	0.79
1:B:151:ARG:HA	1:B:293:HIS:CD2	2.19	0.77
1:B:414:LEU:HD13	1:B:567:ASN:HB3	1.68	0.76
1:A:277:VAL:HB	4:A:1677:MUR:C7	2.21	0.71
1:B:277:VAL:HB	4:B:1677:MUR:H91	1.73	0.71
1:B:151:ARG:CB	4:B:1677:MUR:O9	2.35	0.70
1:B:77:ASP:HB3	1:B:102:LYS:HD2	1.74	0.70
1:B:151:ARG:CA	1:B:293:HIS:CD2	2.75	0.69
1:A:277:VAL:HB	4:A:1677:MUR:C8	2.24	0.67
1:B:293:HIS:HB2	1:B:319:LYS:O	1.94	0.67
1:B:277:VAL:CG1	4:B:1677:MUR:H7	2.25	0.66
1:A:277:VAL:CG1	4:A:1677:MUR:H7	2.24	0.66
1:B:151:ARG:N	1:B:293:HIS:CD2	2.65	0.65
4:B:1677:MUR:O9	4:B:1677:MUR:H4	1.96	0.64
1:A:414:LEU:HD13	1:A:567:ASN:HB3	1.80	0.63
1:A:397:ILE:HA	1:A:499:TYR:HD2	1.63	0.63
1:B:99:TYR:HD2	1:B:112:VAL:HG21	1.62	0.63
1:A:562:ILE:HG22	1:A:563:ILE:HG22	1.79	0.63
1:A:277:VAL:HG11	4:A:1677:MUR:H7	1.81	0.62
1:B:297:TYR:CE2	1:B:316:LYS:HD3	2.35	0.62
1:A:603:LEU:HD23	1:A:612:ARG:HB2	1.81	0.60
1:B:267:LYS:HA	1:B:270:LYS:HD2	1.83	0.60
1:B:396:GLN:HG3	1:B:496:TYR:HE2	1.66	0.60
1:B:173:ILE:HG12	1:B:178:VAL:HG21	1.82	0.60
1:A:503:ILE:O	1:A:524:ILE:HG12	2.04	0.58
1:B:161:GLU:HB3	1:B:164:ASN:HD22	1.69	0.58
1:A:259:ILE:HG12	1:A:264:LEU:HG	1.86	0.57
1:A:586:ASP:HB3	1:A:647:LYS:HG3	1.85	0.57
1:A:28:LYS:HA	1:A:31:ASN:HD22	1.70	0.57
1:B:290:LYS:HB3	1:B:324:ILE:HD11	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ILE:HG13	1:B:305:ASN:HD21	1.72	0.55
1:A:220:MET:HA	1:A:224:LEU:HD23	1.89	0.55
1:B:83:ARG:HA	1:B:97:ALA:HB2	1.89	0.55
1:A:305:ASN:HB3	1:B:72:SER:HB2	1.88	0.55
1:A:563:ILE:HG12	1:A:568:ILE:HG13	1.89	0.55
1:A:144:ILE:HG12	1:A:299:VAL:HG13	1.89	0.54
1:B:99:TYR:HB2	1:B:112:VAL:CG2	2.39	0.53
1:B:150:GLU:C	1:B:293:HIS:CD2	2.81	0.53
1:B:504:SER:HB2	1:B:507:ASN:HB2	1.91	0.53
1:B:28:LYS:HA	1:B:31:ASN:HD22	1.73	0.53
1:B:563:ILE:HG12	1:B:568:ILE:HG13	1.90	0.53
1:A:83:ARG:HA	1:A:97:ALA:HB2	1.91	0.52
1:B:370:PRO:HB2	1:B:375:MET:HE2	1.93	0.51
1:A:290:LYS:HB3	1:A:324:ILE:HD11	1.92	0.51
1:B:432:TRP:CZ2	1:B:469:ARG:HD3	2.46	0.51
1:A:327:THR:OG1	1:A:549:LEU:HA	2.11	0.50
1:B:436:LYS:C	1:B:438:TRP:H	2.14	0.50
1:A:189:GLU:HG2	1:A:227:PHE:CE1	2.46	0.50
1:A:151:ARG:HB3	4:A:1677:MUR:O4	2.11	0.50
1:A:72:SER:HB2	1:B:305:ASN:O	2.12	0.50
1:A:364:PRO:HG3	1:A:388:LYS:HB3	1.94	0.50
1:A:79:ASN:HB3	1:A:81:GLN:HE21	1.77	0.50
1:B:277:VAL:HG12	4:B:1677:MUR:H7	1.93	0.50
1:B:396:GLN:HG3	1:B:496:TYR:CE2	2.45	0.49
1:B:277:VAL:HB	4:B:1677:MUR:C7	2.42	0.49
1:A:173:ILE:HG23	1:A:178:VAL:HB	1.95	0.49
1:A:263:GLU:OE2	1:A:280:LYS:NZ	2.42	0.49
1:B:327:THR:OG1	1:B:549:LEU:HA	2.13	0.49
1:A:469:ARG:HA	1:A:472:LEU:HD12	1.94	0.49
1:A:239:GLU:HB3	4:A:1677:MUR:O1	2.13	0.49
1:A:430:LYS:O	1:A:444:THR:HA	2.12	0.49
1:A:432:TRP:CZ2	1:A:469:ARG:HD3	2.48	0.49
1:A:277:VAL:CG2	4:A:1677:MUR:H7	2.43	0.48
1:A:386:ASP:HB3	1:A:390:PRO:HD3	1.96	0.48
1:B:151:ARG:HB3	4:B:1677:MUR:H62	1.95	0.48
1:B:364:PRO:HG3	1:B:388:LYS:HB3	1.95	0.48
1:B:259:ILE:HG12	1:B:264:LEU:HG	1.96	0.48
1:B:386:ASP:HB3	1:B:390:PRO:HD3	1.96	0.48
1:B:469:ARG:HA	1:B:472:LEU:HD12	1.96	0.47
1:A:203:GLN:HB2	1:A:206:VAL:HG23	1.96	0.46
1:B:277:VAL:HB	4:B:1677:MUR:H7	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ASN:HB3	1:B:81:GLN:HE21	1.80	0.46
1:A:648:ILE:O	1:A:652:VAL:HG23	2.15	0.46
1:A:171:ILE:HG23	1:A:235:THR:HG23	1.98	0.46
1:B:502:GLN:HB2	5:B:2035:HOH:O	2.15	0.46
1:A:496:TYR:HB2	1:A:549:LEU:HD21	1.97	0.46
1:A:76:LYS:NZ	5:A:2003:HOH:O	2.49	0.45
1:A:601:ALA:O	1:A:613:GLN:HA	2.16	0.45
1:B:99:TYR:HB2	1:B:112:VAL:HG21	1.98	0.45
1:B:293:HIS:HB3	1:B:321:GLY:N	2.32	0.45
1:B:332:VAL:HG12	1:B:359:ALA:HB2	1.99	0.45
1:A:605:MET:HG3	1:A:607:GLN:CG	2.46	0.45
1:B:648:ILE:O	1:B:652:VAL:HG23	2.16	0.45
1:A:327:THR:HB	1:A:356:GLU:HB3	1.98	0.44
1:B:99:TYR:CD2	1:B:112:VAL:HG21	2.46	0.44
1:A:413:GLY:HA2	1:A:474:LEU:HD21	1.99	0.44
1:A:99:TYR:HD2	1:A:112:VAL:HG21	1.82	0.44
1:A:332:VAL:HG12	1:A:359:ALA:HB2	1.99	0.44
1:A:263:GLU:OE2	1:A:278:ILE:HD11	2.17	0.44
1:B:413:GLY:HA2	1:B:474:LEU:HD21	2.00	0.44
1:A:559:LYS:HB3	1:A:562:ILE:HD13	2.00	0.43
1:B:173:ILE:HB	1:B:201:MET:HE1	2.00	0.43
1:A:42:PHE:CE1	1:A:66:PRO:HB2	2.53	0.43
1:A:573:ASP:O	1:A:576:GLN:HB3	2.18	0.43
1:B:240:SER:HA	4:B:1677:MUR:O1	2.18	0.43
1:B:447:GLU:HG2	1:B:449:VAL:HG23	2.00	0.43
1:A:259:ILE:HG13	1:A:263:GLU:HG3	2.00	0.43
1:B:603:LEU:HD23	1:B:614:ILE:HD11	2.01	0.43
1:B:184:LYS:HG3	1:B:194:GLU:OE1	2.17	0.43
1:B:151:ARG:N	1:B:293:HIS:NE2	2.67	0.43
1:A:99:TYR:HB3	1:A:134:PRO:HG3	2.00	0.42
1:A:144:ILE:HG23	1:A:299:VAL:HG22	2.00	0.42
1:B:68:LYS:O	1:B:72:SER:HB3	2.19	0.42
1:A:73:LEU:HD21	1:A:299:VAL:HG11	2.02	0.42
1:A:42:PHE:HB3	1:A:63:THR:HA	2.01	0.42
1:B:484:LYS:HD3	1:B:484:LYS:HA	1.91	0.42
1:B:496:TYR:HB2	1:B:549:LEU:HD21	2.01	0.42
1:A:305:ASN:OD1	1:B:68:LYS:HB3	2.20	0.41
1:B:92:LYS:HG3	1:B:117:VAL:HG13	2.02	0.41
1:B:98:GLN:HE21	1:B:109:ASP:CG	2.23	0.41
1:B:42:PHE:CE1	1:B:66:PRO:HB2	2.55	0.41
1:A:69:ILE:HG13	1:B:305:ASN:ND2	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:LYS:C	1:A:438:TRP:H	2.24	0.41
1:A:245:LEU:HD22	1:A:245:LEU:HA	1.93	0.41
1:B:30:ILE:HG21	1:B:95:VAL:HG21	2.02	0.41
1:B:99:TYR:HB3	1:B:134:PRO:HG3	2.02	0.41
1:A:100:LYS:HG3	1:A:109:ASP:OD1	2.21	0.41
1:A:171:ILE:HG12	1:A:224:LEU:HD11	2.02	0.41
1:A:351:HIS:HD2	1:A:626:ASN:O	2.04	0.41
1:A:598:SER:HB2	1:A:617:PHE:CD2	2.56	0.41
1:B:364:PRO:HD2	1:B:394:LYS:NZ	2.36	0.41
1:A:166:GLY:HA3	1:A:242:ASN:HB2	2.02	0.40
1:A:301:ILE:HD11	1:A:313:LEU:HD21	2.03	0.40
1:B:42:PHE:HB3	1:B:63:THR:HA	2.03	0.40
1:A:346:SER:HB3	1:A:394:LYS:HB3	2.03	0.40
1:B:277:VAL:CB	4:B:1677:MUR:H7	2.52	0.40
1:B:162:LEU:HB3	1:B:253:LEU:HD11	2.04	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	636/640 (99%)	596 (94%)	34 (5%)	6 (1%)	17	55
1	B	635/640 (99%)	598 (94%)	31 (5%)	6 (1%)	17	55
All	All	1271/1280 (99%)	1194 (94%)	65 (5%)	12 (1%)	17	55

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	ASP
1	B	604	LYS
1	A	28	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	264	LEU
1	A	341	LYS
1	B	341	LYS
1	B	120	ASP
1	A	261	SER
1	A	476	SER
1	A	635	ASP
1	B	603	LEU
1	B	635	ASP

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	571/571 (100%)	502 (88%)	69 (12%)	5 21
1	B	570/571 (100%)	512 (90%)	58 (10%)	7 28
All	All	1141/1142 (100%)	1014 (89%)	127 (11%)	6 25

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LYS
1	A	29	GLU
1	A	41	ASN
1	A	91	ASN
1	A	92	LYS
1	A	96	ASP
1	A	99	TYR
1	A	103	THR
1	A	104	ASN
1	A	112	VAL
1	A	115	ASN
1	A	122	MET
1	A	130	SER
1	A	138	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	141	SER
1	A	146	LYS
1	A	156	ASP
1	A	171	ILE
1	A	180	LYS
1	A	208	ASP
1	A	216	THR
1	A	217	VAL
1	A	222	GLU
1	A	225	SER
1	A	229	LYS
1	A	230	LYS
1	A	235	THR
1	A	245	LEU
1	A	260	ASN
1	A	266	GLN
1	A	267	LYS
1	A	290	LYS
1	A	295	ASP
1	A	318	LYS
1	A	334	LYS
1	A	341	LYS
1	A	367	ASP
1	A	368	VAL
1	A	387	LYS
1	A	403	SER
1	A	424	SER
1	A	428	ASP
1	A	430	LYS
1	A	436	LYS
1	A	444	THR
1	A	447	GLU
1	A	456	LYS
1	A	473	GLU
1	A	479	PHE
1	A	495	ASP
1	A	513	LEU
1	A	521	GLN
1	A	532	LEU
1	A	545	ASN
1	A	549	LEU
1	A	555	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	562	ILE
1	A	563	ILE
1	A	570	LEU
1	A	586	ASP
1	A	587	ILE
1	A	595	ILE
1	A	598	SER
1	A	600	THR
1	A	603	LEU
1	A	605	MET
1	A	607	GLN
1	A	636	VAL
1	A	649	SER
1	B	26	LYS
1	B	52	ILE
1	B	72	SER
1	B	86	LYS
1	B	90	LYS
1	B	96	ASP
1	B	99	TYR
1	B	100	LYS
1	B	102	LYS
1	B	104	ASN
1	B	112	VAL
1	B	115	ASN
1	B	118	LYS
1	B	120	ASP
1	B	130	SER
1	B	138	LYS
1	B	156	ASP
1	B	170	GLU
1	B	171	ILE
1	B	195	ASP
1	B	202	ASP
1	B	208	ASP
1	B	224	LEU
1	B	235	THR
1	B	245	LEU
1	B	290	LYS
1	B	295	ASP
1	B	316	LYS
1	B	318	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	334	LYS
1	B	341	LYS
1	B	367	ASP
1	B	368	VAL
1	B	387	LYS
1	B	403	SER
1	B	421	ASP
1	B	422	LYS
1	B	424	SER
1	B	430	LYS
1	B	444	THR
1	B	446	TYR
1	B	480	GLU
1	B	484	LYS
1	B	495	ASP
1	B	505	ASN
1	B	508	LEU
1	B	509	ASP
1	B	513	LEU
1	B	532	LEU
1	B	545	ASN
1	B	549	LEU
1	B	555	ASN
1	B	563	ILE
1	B	587	ILE
1	B	595	ILE
1	B	603	LEU
1	B	636	VAL
1	B	649	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	177	ASN
1	A	232	HIS
1	A	457	GLN
1	A	500	ASN
1	A	505	ASN
1	A	521	GLN
1	A	541	ASN
1	A	569	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	580	ASN
1	B	31	ASN
1	B	81	GLN
1	B	98	GLN
1	B	111	ASN
1	B	305	ASN
1	B	457	GLN
1	B	500	ASN
1	B	505	ASN
1	B	507	ASN
1	B	541	ASN
1	B	567	ASN
1	B	576	GLN
1	B	580	ASN
1	B	613	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 11 are monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
4	MUR	B	1677	-	17,17,17	0.74	0	21,24,24	1.09	1 (4%)
4	MUR	A	1677	-	17,17,17	0.72	0	21,24,24	0.66	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
4	MUR	B	1677	-	-	5/10/30/30	0/1/1/1
4	MUR	A	1677	-	-	5/10/30/30	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1677	MUR	O5-C1-C2	2.62	112.57	109.51

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1677	MUR	C9-C7-C8-O8
4	A	1677	MUR	C9-C7-C8-O9
4	B	1677	MUR	C9-C7-C8-O8
4	B	1677	MUR	C9-C7-C8-O9
4	A	1677	MUR	O5-C5-C6-O6
4	B	1677	MUR	O5-C5-C6-O6
4	A	1677	MUR	C4-C5-C6-O6
4	B	1677	MUR	C4-C5-C6-O6
4	A	1677	MUR	C9-C7-O3-C3
4	B	1677	MUR	C9-C7-O3-C3

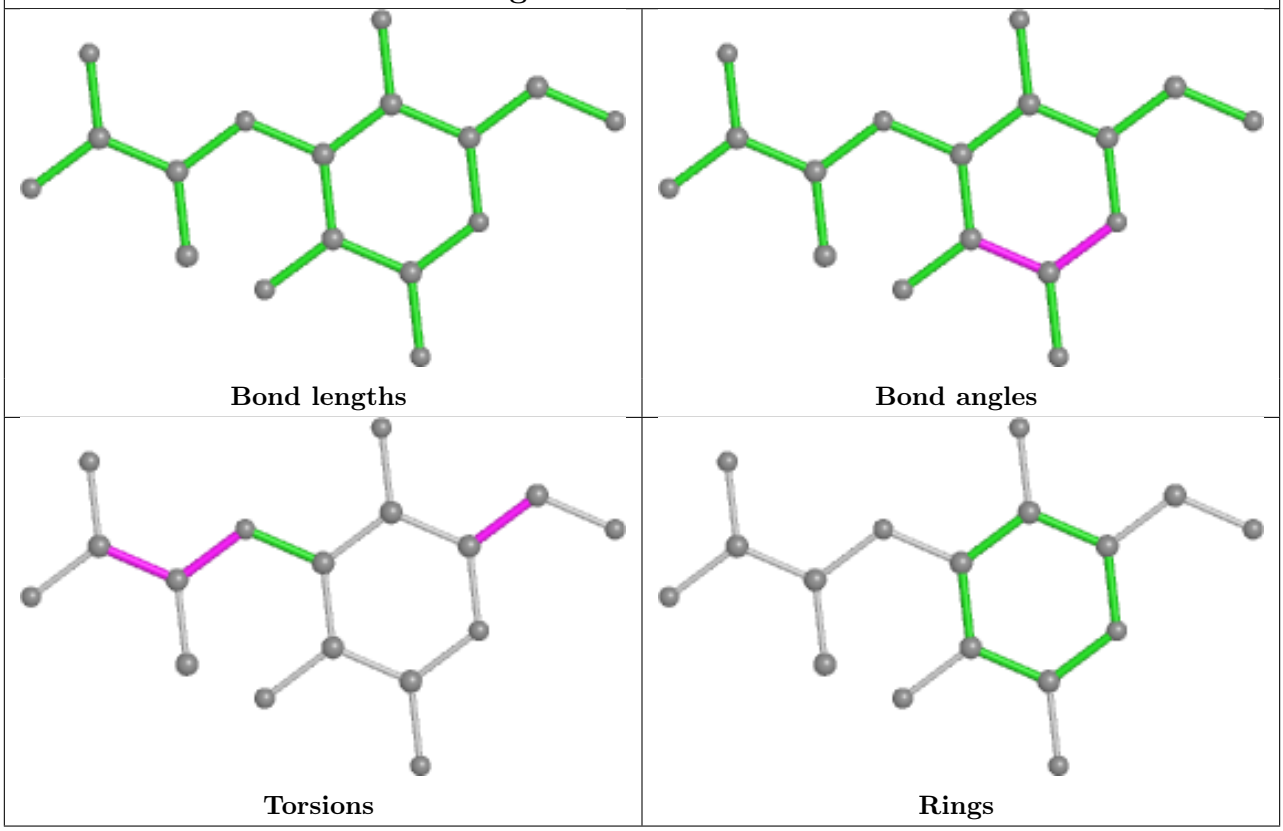
There are no ring outliers.

2 monomers are involved in 24 short contacts:

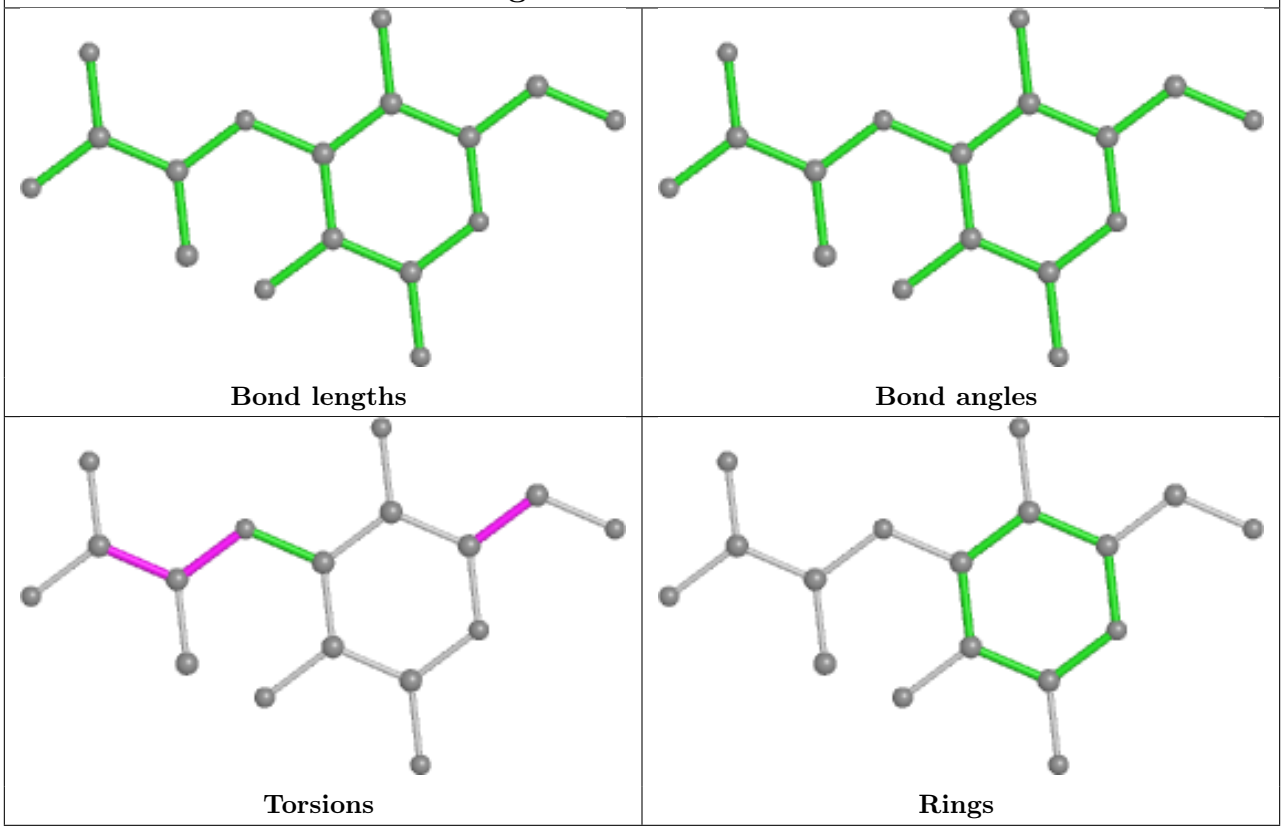
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1677	MUR	15	0
4	A	1677	MUR	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand MUR B 1677



Ligand MUR A 1677



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	607:GLN	C	611:GLY	N	13.17

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	640/640 (100%)	-0.02	9 (1%)	75	49	25, 74, 114, 145	0
1	B	639/640 (99%)	0.04	17 (2%)	54	26	44, 71, 111, 151	0
All	All	1279/1280 (99%)	0.01	26 (2%)	65	36	25, 72, 113, 151	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	ASN	4.6
1	B	272	TYR	4.3
1	A	508	LEU	4.3
1	B	269	TYR	3.4
1	A	503	ILE	3.2
1	A	607	GLN	2.8
1	B	224	LEU	2.8
1	B	442	ASN	2.8
1	B	195	ASP	2.7
1	A	266	GLN	2.7
1	B	226	ASP	2.5
1	A	100	LYS	2.5
1	A	660	GLY	2.4
1	B	268	GLU	2.4
1	B	264	LEU	2.3
1	B	659	ASN	2.3
1	A	413	GLY	2.3
1	B	202	ASP	2.3
1	A	501	ALA	2.3
1	B	605	MET	2.2
1	B	385	GLU	2.2
1	B	220	MET	2.1
1	B	508	LEU	2.1
1	B	102	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	262	GLU	2.1
1	B	591	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

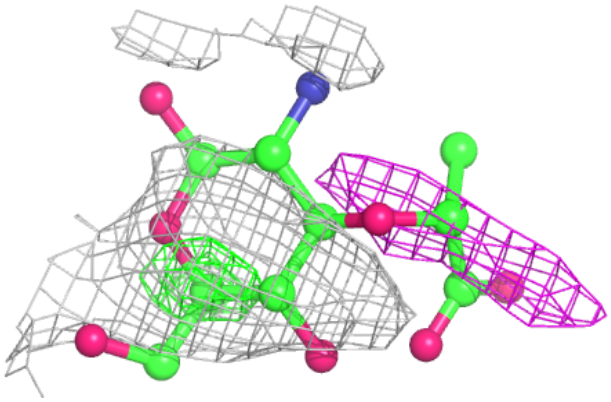
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

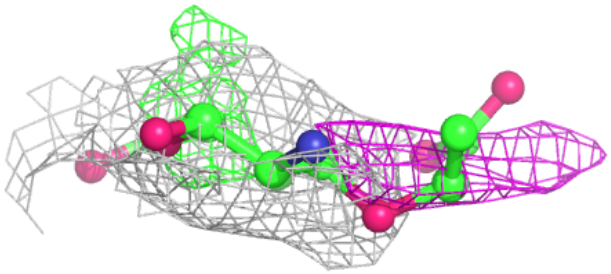
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MUR	A	1677	17/17	0.64	0.60	130,132,136,136	0
4	MUR	B	1677	17/17	0.68	0.56	115,118,121,121	0
2	CD	B	1007	1/1	0.93	0.20	132,132,132,132	0
2	CD	B	1006	1/1	0.98	0.07	140,140,140,140	0
3	CL	B	1009	1/1	0.98	0.23	50,50,50,50	0
2	CD	A	1004	1/1	0.99	0.12	116,116,116,116	0
2	CD	A	1005	1/1	0.99	0.12	80,80,80,80	0
2	CD	B	1002	1/1	0.99	0.11	64,64,64,64	0
2	CD	A	1001	1/1	0.99	0.12	63,63,63,63	0
2	CD	A	1003	1/1	1.00	0.17	70,70,70,70	0
3	CL	B	1012	1/1	1.00	0.17	60,60,60,60	0
3	CL	A	1010	1/1	1.00	0.14	57,57,57,57	0
3	CL	A	1011	1/1	1.00	0.15	73,73,73,73	0

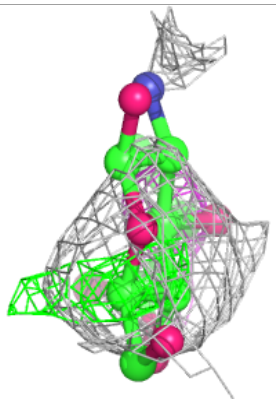
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around MUR A 1677:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

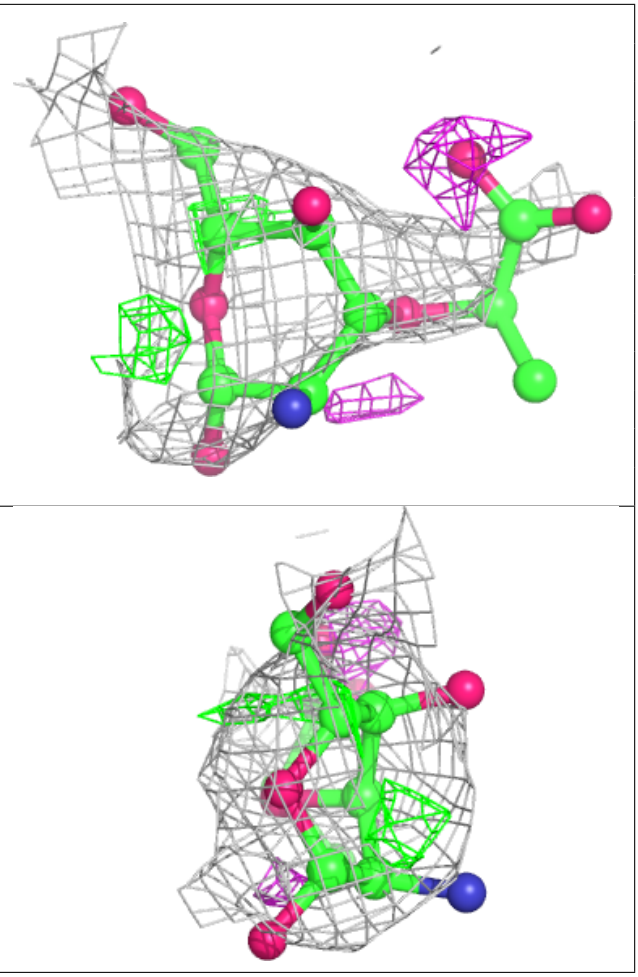






Electron density around MUR B 1677:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.