



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 03:55 PM UTC

PDB ID : 4CPK / pdb_00004cpk
Title : Crystal structure of PBP2a double clinical mutant N146K-E150K from MRSA
Authors : Otero, L.H.; Rojas-Altuve, A.; Hermoso, J.A.
Deposited on : 2014-02-07
Resolution : 2.35 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

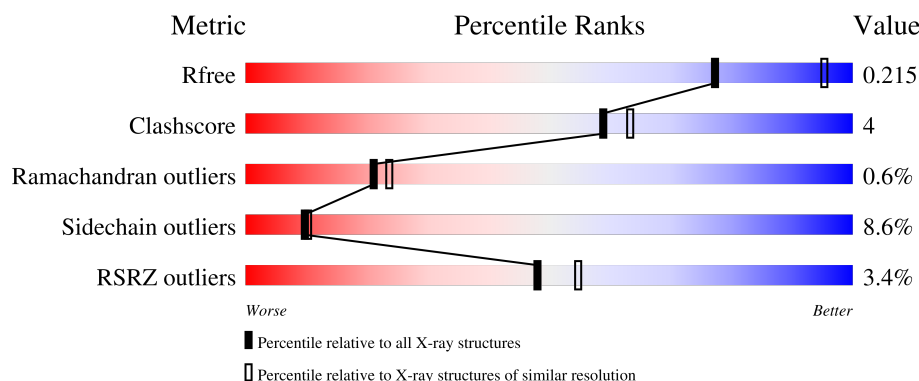
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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 $\leq 5\%$. 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	643	 3% 83% 15% ..
1	B	643	 4% 82% 14% ..

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	1679	-	-	X	-
4	MUR	B	1677	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11030 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
1	A	637	Total	C	N	O	S	0	0	0
			5113	3226	864	1008	15			
1	B	636	Total	C	N	O	S	0	0	0
			5104	3220	862	1007	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	146	LYS	ASN	engineered mutation	UNP A0A0H3JPA5
A	150	LYS	GLU	engineered mutation	UNP A0A0H3JPA5
B	146	LYS	ASN	engineered mutation	UNP A0A0H3JPA5
B	150	LYS	GLU	engineered mutation	UNP A0A0H3JPA5

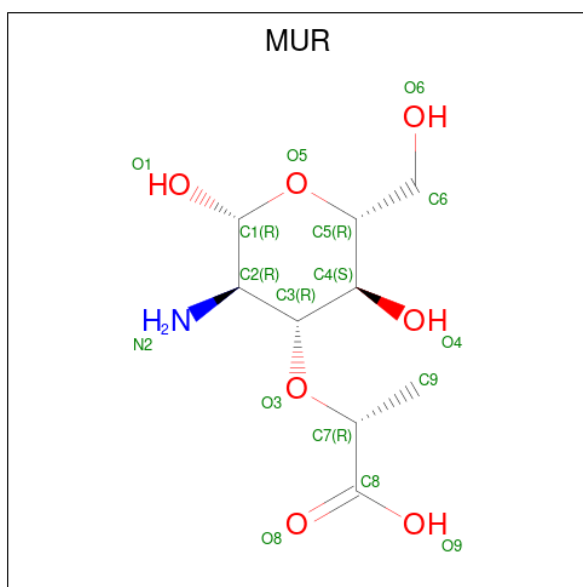
- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total	Cd	0	0
			7	7		
2	B	4	Total	Cd	0	0
			4	4		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 4 is beta-muramic acid (CCD ID: MUR) (formula: C₉H₁₇NO₇).



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

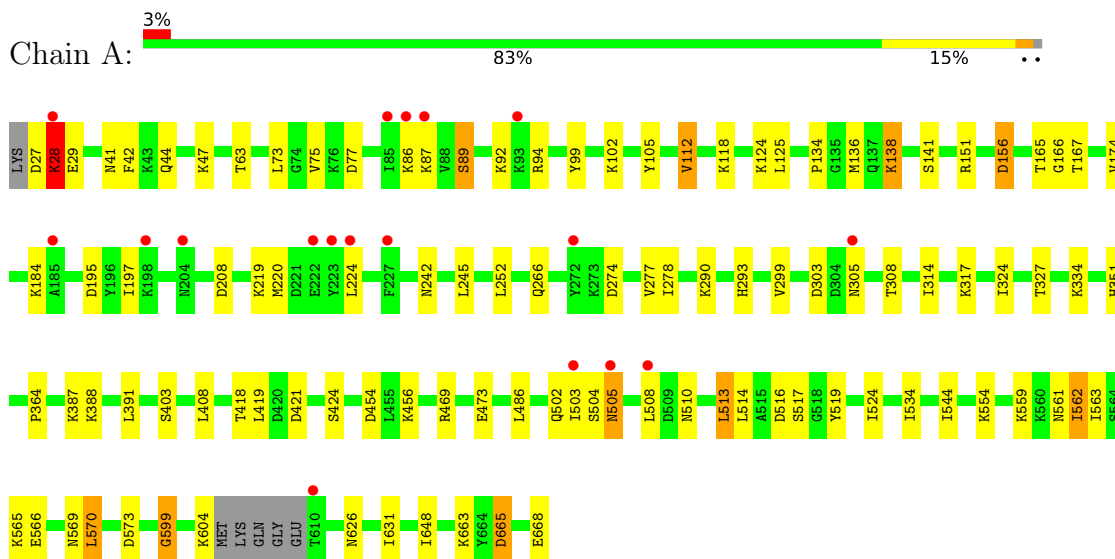
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	406	Total	O	0	0
			406	406		
5	B	358	Total	O	0	0
			358	358		

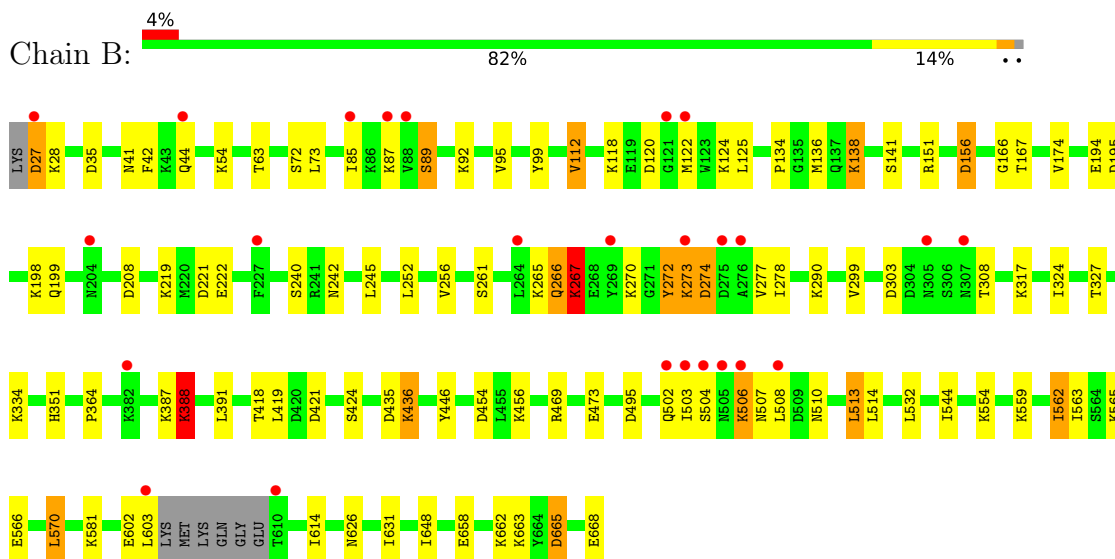
3 Residue-property plots [i](#)

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



- Molecule 1: Penicillin binding protein 2 prime



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.44Å 101.64Å 186.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.64 – 2.35 46.64 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.64-2.35) 99.9 (46.64-2.35)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.34Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.182 , 0.231 (Not available) , 0.215	Depositor DCC
R_{free} test set	3324 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.819	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11030	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: CL, CD, MUR

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	0.84	0/5198	1.25	16/6987 (0.2%)
1	B	0.84	0/5189	1.28	22/6976 (0.3%)
All	All	0.84	0/10387	1.27	38/13963 (0.3%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	505	ASN	CA-CB-CG	7.02	119.62	112.60
1	A	454	ASP	CA-CB-CG	6.80	119.40	112.60
1	B	174	VAL	N-CA-C	-6.78	100.00	107.73
1	A	174	VAL	N-CA-C	-6.73	100.06	107.73
1	B	602	GLU	CA-C-N	6.73	133.81	121.70
1	B	602	GLU	C-N-CA	6.73	133.81	121.70
1	B	454	ASP	CA-CB-CG	6.45	119.05	112.60
1	B	495	ASP	CA-CB-CG	6.37	118.97	112.60
1	B	665	ASP	CA-CB-CG	6.30	118.90	112.60
1	A	197	ILE	CA-C-N	6.15	128.84	120.54
1	A	197	ILE	C-N-CA	6.15	128.84	120.54
1	B	27	ASP	CA-CB-CG	6.07	118.67	112.60
1	A	665	ASP	CA-CB-CG	5.97	118.58	112.60
1	A	156	ASP	CA-CB-CG	5.97	118.57	112.60
1	B	388	LYS	CA-C-N	5.96	129.27	122.83
1	B	388	LYS	C-N-CA	5.96	129.27	122.83
1	B	156	ASP	CA-CB-CG	5.85	118.45	112.60
1	A	327	THR	CA-C-N	5.85	128.56	120.49
1	A	327	THR	C-N-CA	5.85	128.56	120.49
1	A	599	GLY	N-CA-C	5.68	118.70	111.37
1	B	435	ASP	CA-CB-CG	5.64	118.24	112.60
1	B	327	THR	CA-C-N	5.63	128.04	120.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	327	THR	C-N-CA	5.63	128.04	120.50
1	B	28	LYS	CA-C-N	5.60	128.09	120.54
1	B	28	LYS	C-N-CA	5.60	128.09	120.54
1	B	510	ASN	CA-C-N	5.52	127.68	120.28
1	B	510	ASN	C-N-CA	5.52	127.68	120.28
1	A	510	ASN	CA-C-N	5.48	127.63	120.28
1	A	510	ASN	C-N-CA	5.48	127.63	120.28
1	B	54	LYS	CA-C-N	5.35	127.45	120.28
1	B	54	LYS	C-N-CA	5.35	127.45	120.28
1	A	28	LYS	CA-C-N	5.34	128.84	120.82
1	A	28	LYS	C-N-CA	5.34	128.84	120.82
1	B	222	GLU	CA-C-N	5.31	127.70	120.54
1	B	222	GLU	C-N-CA	5.31	127.70	120.54
1	B	418	THR	N-CA-C	-5.26	106.86	113.28
1	A	418	THR	N-CA-C	-5.23	106.90	113.28
1	A	219	LYS	N-CA-C	5.07	117.50	109.50

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	5113	0	5124	46	0
1	B	5104	0	5111	42	0
2	A	7	0	0	0	0
2	B	4	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	406	0	0	1	0
5	B	358	0	0	0	0
All	All	11030	0	10267	90	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 4.

All (90) 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:277:VAL:CG1	4:B:1677:MUR:H91	1.67	1.25
1:B:277:VAL:HG11	4:B:1677:MUR:H91	1.32	1.11
1:B:277:VAL:HG11	4:B:1677:MUR:C9	1.91	0.98
1:B:256:VAL:HG21	4:B:1677:MUR:H92	1.55	0.86
1:B:277:VAL:HG12	4:B:1677:MUR:H91	1.59	0.84
1:A:277:VAL:HB	4:A:1679:MUR:H91	1.65	0.78
1:A:220:MET:HA	1:A:224:LEU:HD23	1.67	0.77
1:B:277:VAL:CG1	4:B:1677:MUR:C9	2.54	0.75
1:B:138:LYS:HD2	1:B:138:LYS:H	1.51	0.74
1:A:277:VAL:HB	4:A:1679:MUR:C9	2.17	0.74
1:A:138:LYS:HD2	1:A:138:LYS:H	1.53	0.73
1:B:256:VAL:CG2	4:B:1677:MUR:H92	2.18	0.72
1:A:293:HIS:NE2	4:A:1679:MUR:O9	2.24	0.70
4:B:1677:MUR:H93	4:B:1677:MUR:N2	2.11	0.66
1:A:28:LYS:HG2	1:A:29:GLU:H	1.61	0.65
1:B:89:SER:HB3	1:B:92:LYS:HB2	1.80	0.64
1:A:559:LYS:HB3	1:A:562:ILE:HD13	1.80	0.63
4:B:1677:MUR:O8	4:B:1677:MUR:H3	1.98	0.63
1:B:559:LYS:HB3	1:B:562:ILE:HD13	1.81	0.62
1:A:305:ASN:HB3	1:B:72:SER:HB3	1.84	0.59
1:B:112:VAL:HG13	1:B:134:PRO:HB3	1.87	0.57
1:A:112:VAL:HG13	1:A:134:PRO:HB3	1.88	0.56
1:B:138:LYS:H	1:B:138:LYS:CD	2.19	0.56
1:A:165:THR:OG1	4:A:1679:MUR:O6	2.14	0.56
1:A:364:PRO:HG2	1:A:388:LYS:HB3	1.89	0.55
1:B:277:VAL:CB	4:B:1677:MUR:H91	2.35	0.54
1:A:73:LEU:HD21	1:A:299:VAL:HG11	1.90	0.54
1:A:138:LYS:H	1:A:138:LYS:CD	2.20	0.53
1:A:86:LYS:HE3	1:A:94:ARG:HD3	1.91	0.52
1:A:502:GLN:HE22	1:A:505:ASN:ND2	2.08	0.52
1:B:256:VAL:HG21	4:B:1677:MUR:C9	2.32	0.52
4:B:1677:MUR:C9	4:B:1677:MUR:HN22	2.24	0.51
4:B:1677:MUR:C9	4:B:1677:MUR:N2	2.72	0.51
1:A:151:ARG:HB2	4:A:1679:MUR:O9	2.11	0.51
1:B:151:ARG:HD2	4:B:1677:MUR:H7	1.92	0.51
1:A:166:GLY:HA3	1:A:242:ASN:HB2	1.94	0.50
1:B:166:GLY:HA3	1:B:242:ASN:HB2	1.93	0.50
1:A:504:SER:O	1:A:505:ASN:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:SER:HB3	1:A:524:ILE:HD11	1.93	0.50
1:A:508:LEU:HD23	1:A:513:LEU:HD23	1.94	0.49
1:B:73:LEU:HD21	1:B:299:VAL:HG11	1.94	0.49
1:A:277:VAL:HB	4:A:1679:MUR:C7	2.42	0.49
1:A:42:PHE:HB3	1:A:63:THR:HA	1.96	0.48
1:B:194:GLU:O	1:B:198:LYS:HD3	2.13	0.48
1:B:42:PHE:HB3	1:B:63:THR:HA	1.97	0.47
1:B:272:TYR:O	1:B:273:LYS:HB2	2.14	0.47
1:B:290:LYS:HB2	1:B:324:ILE:HD11	1.96	0.47
1:B:508:LEU:HD23	1:B:513:LEU:HD23	1.97	0.47
1:B:506:LYS:HD2	1:B:507:ASN:HB2	1.97	0.47
1:B:544:ILE:HB	1:B:559:LYS:HB2	1.97	0.46
1:B:240:SER:HA	4:B:1677:MUR:O1	2.15	0.46
1:B:436:LYS:HE3	1:B:436:LYS:H	1.81	0.46
1:A:99:TYR:HB2	1:A:112:VAL:HG22	1.98	0.45
1:B:41:ASN:ND2	1:B:44:GLN:HB2	2.32	0.45
1:B:99:TYR:HD2	1:B:112:VAL:HG11	1.82	0.45
1:A:277:VAL:CB	4:A:1679:MUR:C9	2.92	0.45
1:B:99:TYR:HB2	1:B:112:VAL:HG22	1.99	0.44
1:A:403:SER:CB	1:A:599:GLY:HA3	2.47	0.44
1:A:99:TYR:HD2	1:A:112:VAL:HG11	1.82	0.44
1:A:516:ASP:HA	1:A:519:TYR:CE1	2.53	0.44
1:A:665:ASP:HB3	1:A:668:GLU:HB2	2.00	0.44
1:A:277:VAL:O	4:A:1679:MUR:O8	2.36	0.43
1:A:503:ILE:O	1:A:524:ILE:HG12	2.17	0.43
1:B:658:GLU:HB2	1:B:662:LYS:HG2	2.00	0.43
1:A:486:LEU:HD23	1:A:562:ILE:HG13	2.00	0.43
1:B:665:ASP:HB3	1:B:668:GLU:HB2	1.99	0.43
1:A:290:LYS:HB2	1:A:324:ILE:HD11	2.00	0.43
1:A:561:ASN:ND2	5:A:2330:HOH:O	2.48	0.43
1:A:77:ASP:HB2	1:A:102:LYS:HD3	2.00	0.43
1:B:562:ILE:HG22	1:B:563:ILE:HG22	2.01	0.43
1:B:421:ASP:HB3	1:B:570:LEU:HD11	2.01	0.43
1:A:544:ILE:HB	1:A:559:LYS:HB2	2.00	0.43
1:B:85:ILE:HG12	1:B:95:VAL:HG22	2.00	0.43
1:A:351:HIS:HD2	1:A:626:ASN:O	2.02	0.43
1:A:41:ASN:ND2	1:A:44:GLN:HB2	2.33	0.42
1:A:245:LEU:HD13	1:A:334:LYS:HG3	2.01	0.42
1:A:421:ASP:HB3	1:A:570:LEU:HD11	2.00	0.42
1:A:562:ILE:HG22	1:A:563:ILE:HG22	2.02	0.42
1:A:305:ASN:C	1:B:72:SER:HB2	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:PRO:HG2	1:B:388:LYS:HB3	2.02	0.42
1:B:245:LEU:HD13	1:B:334:LYS:HG3	2.01	0.42
1:B:99:TYR:HB2	1:B:112:VAL:CG2	2.50	0.41
1:A:89:SER:HB3	1:A:92:LYS:HB2	2.02	0.41
1:A:631:ILE:HD13	1:A:648:ILE:HG22	2.02	0.41
1:B:631:ILE:HD13	1:B:648:ILE:HG22	2.03	0.41
1:A:277:VAL:CG1	4:A:1679:MUR:H7	2.51	0.41
1:B:266:GLN:HB3	1:B:267:LYS:H	1.65	0.41
1:A:105:TYR:O	1:A:314:ILE:HG21	2.22	0.40
1:A:408:LEU:HD22	1:A:534:ILE:HG21	2.02	0.40
1:B:351:HIS:HD2	1:B:626:ASN:O	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	633/643 (98%)	612 (97%)	20 (3%)	1 (0%)	43	52
1	B	632/643 (98%)	607 (96%)	19 (3%)	6 (1%)	14	14
All	All	1265/1286 (98%)	1219 (96%)	39 (3%)	7 (1%)	21	24

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	265	LYS
1	B	273	LYS
1	B	504	SER
1	B	267	LYS
1	B	506	LYS
1	A	28	LYS
1	B	274	ASP

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	568/573 (99%)	525 (92%)	43 (8%)	12	13
1	B	567/573 (99%)	512 (90%)	55 (10%)	8	7
All	All	1135/1146 (99%)	1037 (91%)	98 (9%)	10	10

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASP
1	A	28	LYS
1	A	47	LYS
1	A	75	VAL
1	A	87	LYS
1	A	89	SER
1	A	112	VAL
1	A	118	LYS
1	A	124	LYS
1	A	125	LEU
1	A	136	MET
1	A	138	LYS
1	A	141	SER
1	A	156	ASP
1	A	167	THR
1	A	184	LYS
1	A	195	ASP
1	A	208	ASP
1	A	252	LEU
1	A	266	GLN
1	A	274	ASP
1	A	278	ILE
1	A	303	ASP
1	A	308	THR
1	A	317	LYS
1	A	387	LYS
1	A	391	LEU

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Mol	Chain	Res	Type
1	A	419	LEU
1	A	424	SER
1	A	456	LYS
1	A	469	ARG
1	A	473	GLU
1	A	513	LEU
1	A	514	LEU
1	A	554	LYS
1	A	562	ILE
1	A	565	LYS
1	A	566	GLU
1	A	569	ASN
1	A	570	LEU
1	A	573	ASP
1	A	604	LYS
1	A	663	LYS
1	B	27	ASP
1	B	35	ASP
1	B	87	LYS
1	B	89	SER
1	B	112	VAL
1	B	118	LYS
1	B	120	ASP
1	B	122	MET
1	B	124	LYS
1	B	125	LEU
1	B	136	MET
1	B	138	LYS
1	B	141	SER
1	B	156	ASP
1	B	167	THR
1	B	195	ASP
1	B	199	GLN
1	B	208	ASP
1	B	219	LYS
1	B	221	ASP
1	B	252	LEU
1	B	261	SER
1	B	266	GLN
1	B	267	LYS
1	B	270	LYS
1	B	272	TYR

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Mol	Chain	Res	Type
1	B	274	ASP
1	B	278	ILE
1	B	303	ASP
1	B	308	THR
1	B	317	LYS
1	B	387	LYS
1	B	388	LYS
1	B	391	LEU
1	B	419	LEU
1	B	424	SER
1	B	436	LYS
1	B	446	TYR
1	B	456	LYS
1	B	469	ARG
1	B	473	GLU
1	B	502	GLN
1	B	503	ILE
1	B	513	LEU
1	B	514	LEU
1	B	532	LEU
1	B	554	LYS
1	B	562	ILE
1	B	565	LYS
1	B	566	GLU
1	B	570	LEU
1	B	581	LYS
1	B	603	LEU
1	B	614	ILE
1	B	663	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	41	ASN
1	A	107	ASN
1	A	113	GLN
1	A	115	ASN
1	A	177	ASN
1	A	203	GLN
1	A	502	GLN
1	A	505	ASN

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Mol	Chain	Res	Type
1	A	540	ASN
1	A	555	ASN
1	A	567	ASN
1	A	624	ASN
1	A	632	ASN
1	A	661	ASN
1	B	57	ASN
1	B	107	ASN
1	B	111	ASN
1	B	113	GLN
1	B	115	ASN
1	B	177	ASN
1	B	203	GLN
1	B	305	ASN
1	B	545	ASN
1	B	555	ASN
1	B	613	GLN
1	B	624	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 15 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	A	1679	-	17,17,17	1.44	4 (23%)	21,24,24	3.06	12 (57%)
4	MUR	B	1677	-	17,17,17	1.09	2 (11%)	21,24,24	2.86	9 (42%)

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	A	1679	-	-	5/10/30/30	0/1/1/1
4	MUR	B	1677	-	-	8/10/30/30	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1679	MUR	O5-C5	-2.46	1.38	1.44
4	A	1679	MUR	O9-C8	-2.33	1.23	1.30
4	A	1679	MUR	C4-C5	-2.28	1.48	1.53
4	A	1679	MUR	O3-C7	2.23	1.49	1.44
4	B	1677	MUR	O3-C3	-2.13	1.38	1.43
4	B	1677	MUR	C4-C5	-2.12	1.48	1.53

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1679	MUR	O5-C1-C2	-6.89	101.47	109.51
4	B	1677	MUR	O5-C1-C2	-6.21	102.26	109.51
4	B	1677	MUR	C6-C5-C4	-5.52	99.46	113.02
4	A	1679	MUR	C9-C7-C8	-4.99	100.07	109.42
4	A	1679	MUR	O3-C3-C2	4.50	119.91	108.89
4	B	1677	MUR	C1-C2-C3	-4.29	102.45	110.10
4	B	1677	MUR	C1-O5-C5	4.26	121.90	113.65
4	A	1679	MUR	C4-C3-C2	3.94	119.16	111.37
4	A	1679	MUR	O3-C7-C9	3.88	118.33	107.54
4	B	1677	MUR	C4-C3-C2	3.83	118.94	111.37
4	A	1679	MUR	O5-C5-C4	3.83	116.60	109.70
4	B	1677	MUR	C3-C2-N2	3.83	118.84	110.92
4	B	1677	MUR	O5-C5-C4	3.70	116.36	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1679	MUR	O4-C4-C3	-3.30	101.48	109.94
4	A	1679	MUR	O6-C6-C5	-3.12	100.73	111.33
4	A	1679	MUR	O1-C1-C2	3.09	115.33	108.96
4	B	1677	MUR	C9-C7-C8	-3.06	103.70	109.42
4	A	1679	MUR	O9-C8-O8	-2.75	117.85	124.08
4	A	1679	MUR	O4-C4-C5	-2.67	102.74	109.32
4	A	1679	MUR	C1-O5-C5	2.63	118.73	113.65
4	B	1677	MUR	O1-C1-C2	2.04	113.15	108.96

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1679	MUR	C9-C7-O3-C3
4	A	1679	MUR	O3-C7-C8-O8
4	A	1679	MUR	O3-C7-C8-O9
4	B	1677	MUR	C8-C7-O3-C3
4	B	1677	MUR	O3-C7-C8-O9
4	A	1679	MUR	C4-C5-C6-O6
4	A	1679	MUR	O5-C5-C6-O6
4	B	1677	MUR	O5-C5-C6-O6
4	B	1677	MUR	O3-C7-C8-O8
4	B	1677	MUR	C4-C5-C6-O6
4	B	1677	MUR	C9-C7-C8-O9
4	B	1677	MUR	C9-C7-C8-O8
4	B	1677	MUR	C9-C7-O3-C3

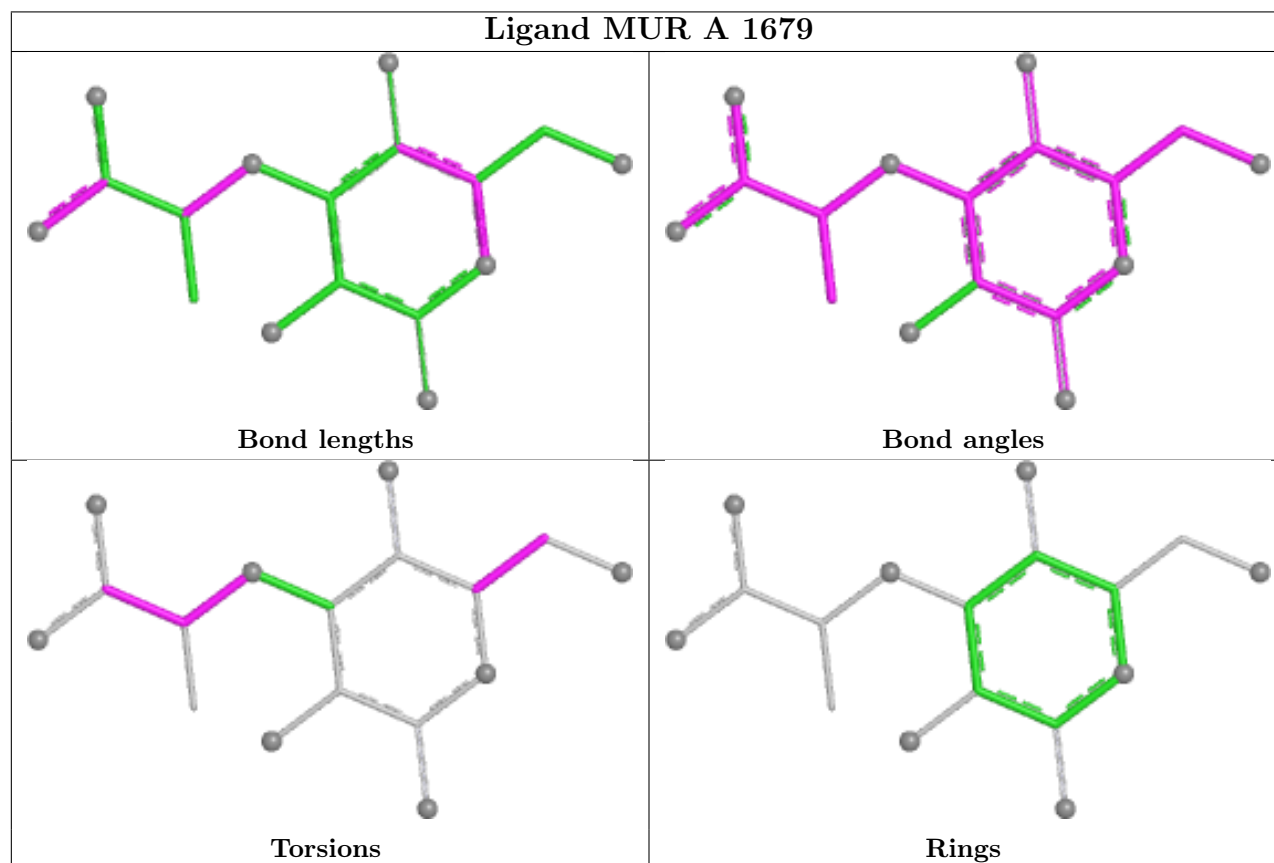
There are no ring outliers.

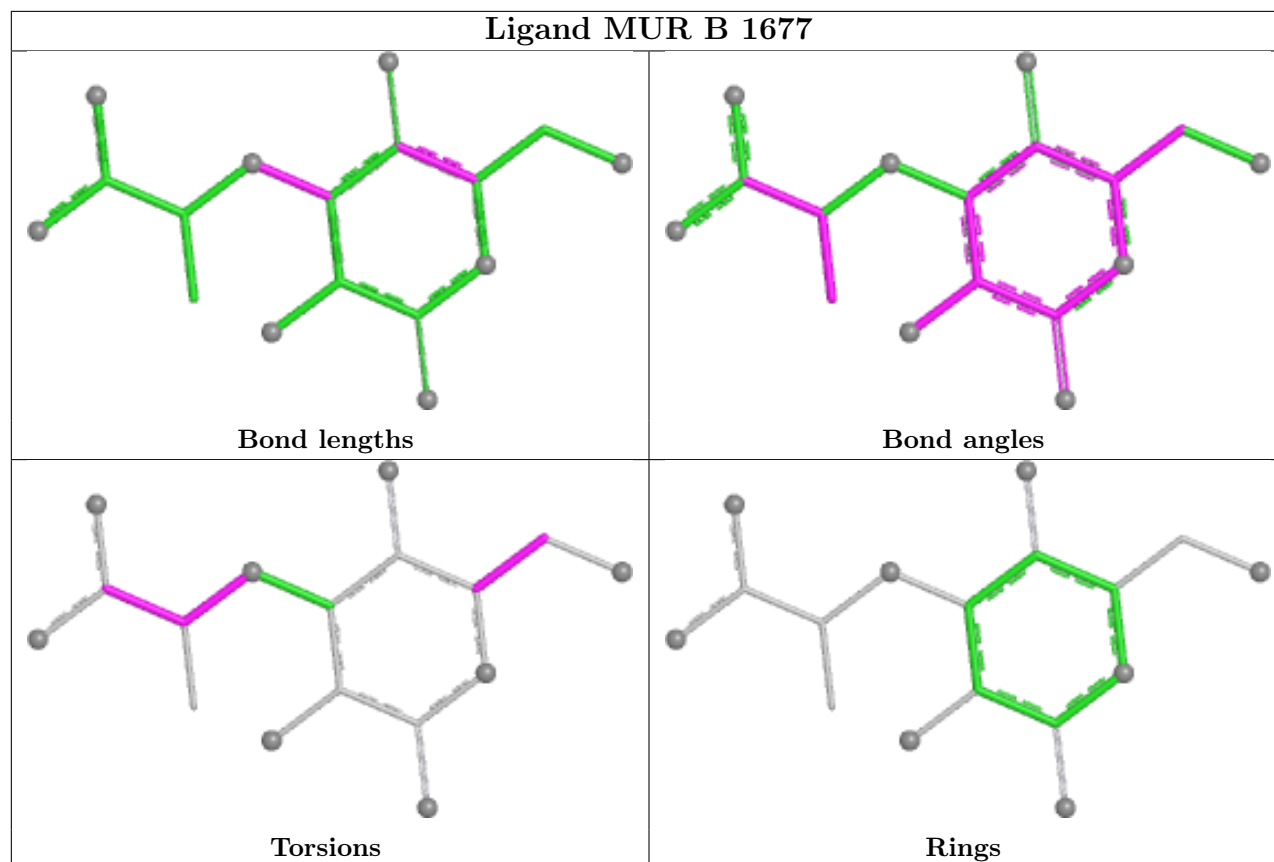
2 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1679	MUR	9	0
4	B	1677	MUR	15	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 than 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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	637/643 (99%)	0.15	18 (2%) 55 61	19, 42, 77, 106	0
1	B	636/643 (98%)	0.27	25 (3%) 43 49	25, 43, 87, 128	0
All	All	1273/1286 (98%)	0.21	43 (3%) 48 55	19, 43, 82, 128	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	603	LEU	5.2
1	A	223	TYR	4.4
1	B	503	ILE	4.3
1	B	122	MET	3.8
1	A	610	THR	3.6
1	B	121	GLY	3.4
1	B	273	LYS	3.3
1	B	502	GLN	3.2
1	A	204	ASN	3.2
1	B	506	LYS	3.0
1	B	610	THR	3.0
1	B	88	VAL	2.9
1	B	227	PHE	2.9
1	A	85	ILE	2.7
1	B	27	ASP	2.7
1	B	307	ASN	2.7
1	A	224	LEU	2.7
1	B	505	ASN	2.6
1	B	504	SER	2.6
1	B	305	ASN	2.5
1	B	204	ASN	2.5
1	A	198	LYS	2.5
1	A	222	GLU	2.4
1	B	87	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	382	LYS	2.3
1	B	508	LEU	2.3
1	A	93	LYS	2.3
1	B	44	GLN	2.3
1	B	269	TYR	2.2
1	A	87	LYS	2.2
1	A	508	LEU	2.2
1	A	185	ALA	2.2
1	B	276	ALA	2.2
1	A	503	ILE	2.1
1	A	28	LYS	2.1
1	A	86	LYS	2.1
1	B	264	LEU	2.1
1	A	505	ASN	2.1
1	B	275	ASP	2.1
1	A	227	PHE	2.1
1	A	272	TYR	2.0
1	A	305	ASN	2.0
1	B	85	ILE	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
4	MUR	A	1679	17/17	0.84	0.18	20,33,61,63	0
4	MUR	B	1677	17/17	0.84	0.17	22,43,64,72	0
2	CD	A	1674	1/1	0.91	0.10	160,160,160,160	0
2	CD	A	1675	1/1	0.93	0.09	123,123,123,123	0

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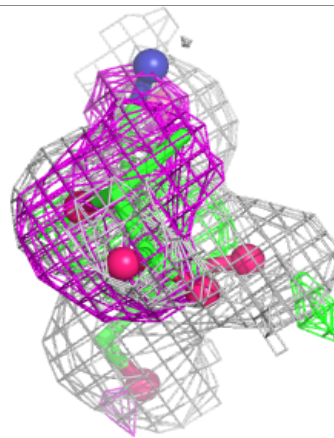
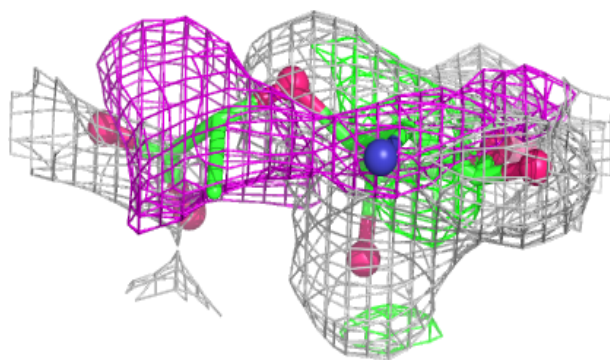
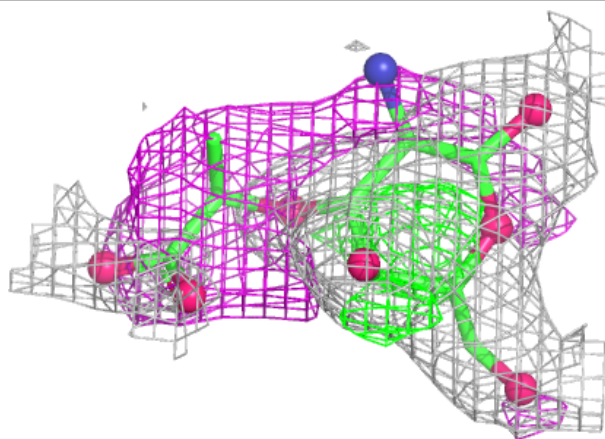
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CD	B	1669	1/1	0.95	0.05	35,35,35,35	0
3	CL	A	1678	1/1	0.95	0.09	35,35,35,35	0
3	CL	B	1674	1/1	0.95	0.10	36,36,36,36	0
2	CD	A	1672	1/1	0.95	0.05	39,39,39,39	0
2	CD	A	1673	1/1	0.95	0.12	123,123,123,123	0
2	CD	A	1671	1/1	0.96	0.06	84,84,84,84	0
2	CD	B	1671	1/1	0.96	0.05	33,33,33,33	0
2	CD	A	1676	1/1	0.97	0.10	122,122,122,122	0
2	CD	B	1672	1/1	0.97	0.05	86,86,86,86	0
3	CL	B	1675	1/1	0.98	0.07	33,33,33,33	0
2	CD	A	1670	1/1	0.98	0.04	34,34,34,34	0
3	CL	A	1677	1/1	0.98	0.06	35,35,35,35	0
2	CD	B	1673	1/1	0.99	0.02	47,47,47,47	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.

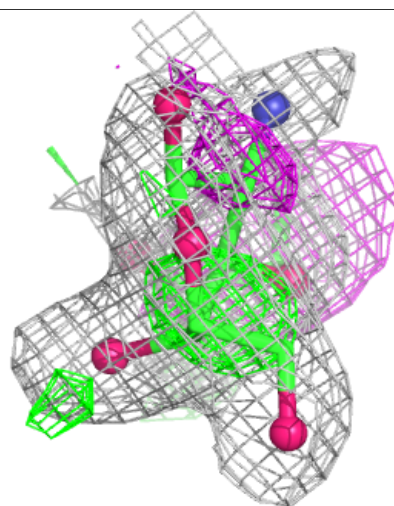
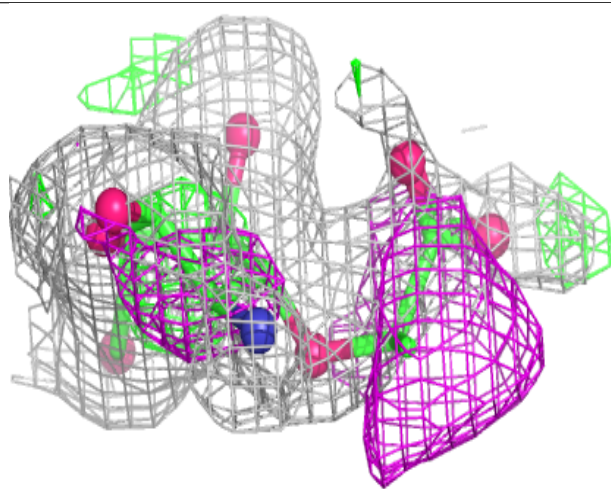
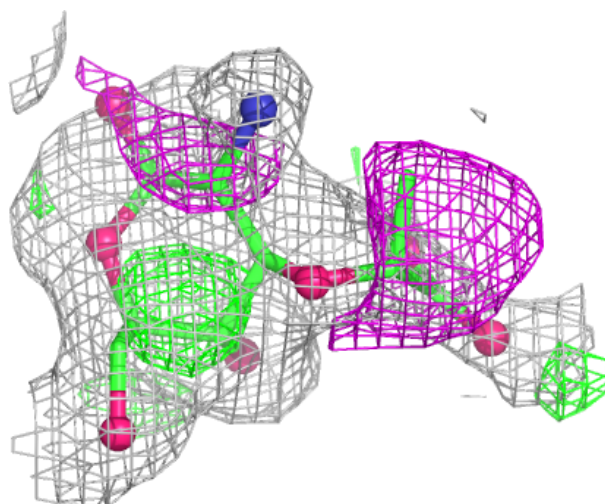
Electron density around MUR A 1679:

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 ⓘ

There are no such residues in this entry.