



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:51 PM UTC

PDB ID : 3ZG0 / pdb_00003zg0
Title : Crystal structure of ceftaroline acyl-PBP2a from MRSA with non-covalently bound ceftaroline and muramic acid at allosteric site obtained by cocrystallization
Authors : Otero, L.H.; Rojas-Altuve, A.; Hermoso, J.A.
Deposited on : 2012-12-13
Resolution : 2.60 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

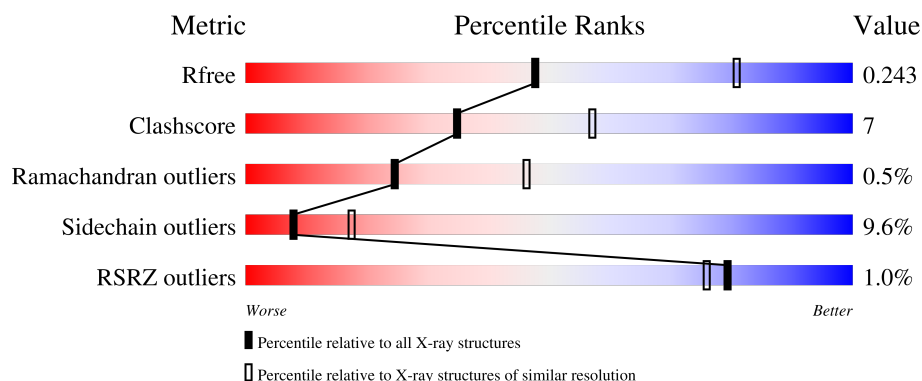
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	642	% 76% 20% .
1	B	642	% 75% 22% ..

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
2	AI8	B	1403	X	-	-	-

2 Entry composition [i](#)

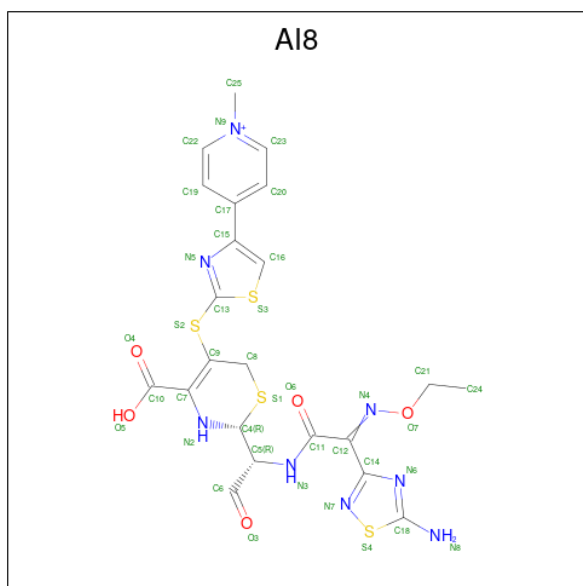
There are 7 unique types of molecules in this entry. The entry contains 10896 atoms, of which 32 are hydrogens and 0 are deuteriums.

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	642	Total	C	N	O	S	0	0	0
			5151	3246	870	1019	16			
1	B	635	Total	C	N	O	S	0	0	0
			5101	3217	861	1008	15			

- Molecule 2 is Ceftaroline, bound form (CCD ID: AI8) (formula: $C_{22}H_{23}N_8O_5S_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			39	22	8	5	4		
2	B	1	Total	C	N	O	S	0	0
			39	22	8	5	4		

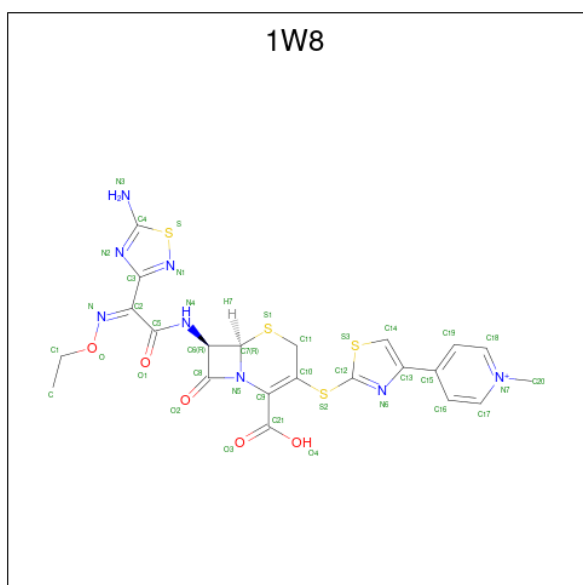
- Molecule 3 is CADMIUM ION (CCD ID: CD) (formula: Cd).

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

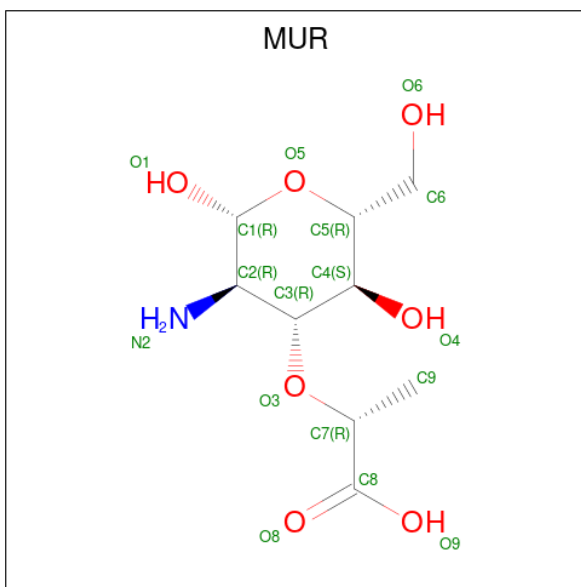
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Cl	0	0
			2	2		
4	B	2	Total	Cl	0	0
			2	2		

- Molecule 5 is Ceftaroline (CCD ID: 1W8) (formula: C₂₂H₂₁N₈O₅S₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			39	22	8	5	4		
5	B	1	Total	C	N	O	S	0	0
			39	22	8	5	4		

- Molecule 6 is beta-muramic acid (CCD ID: MUR) (formula: C₉H₁₇NO₇).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	0	0
			33	9	16	1	7		
6	B	1	Total	C	H	N	O	0	0
			33	9	16	1	7		

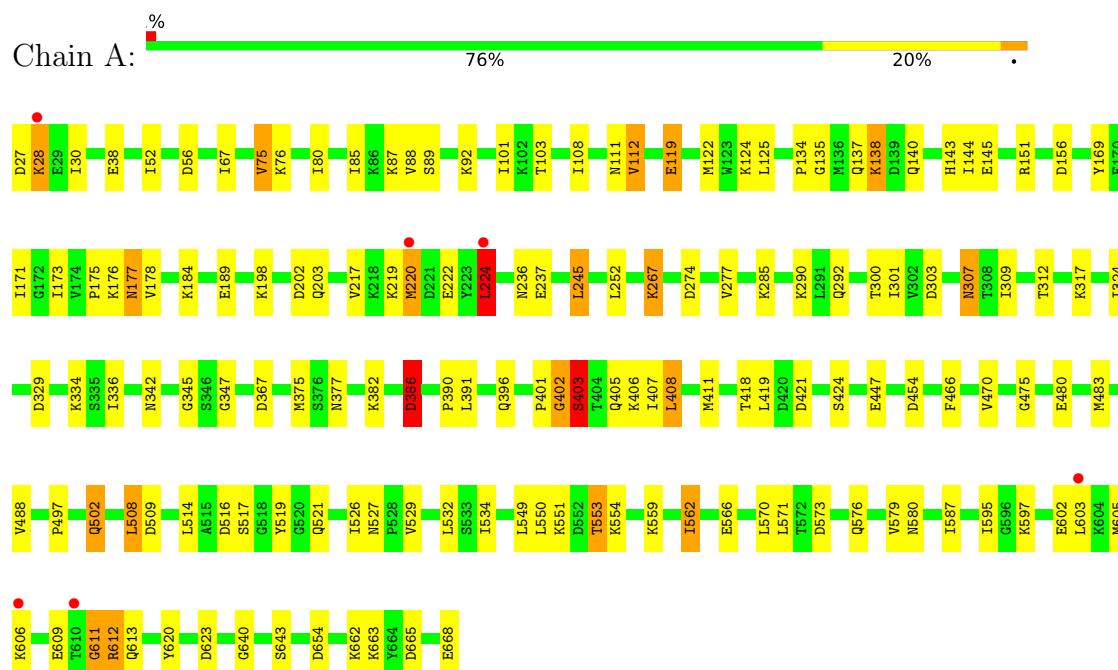
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	239	Total	O	0	0
			239	239		
7	B	171	Total	O	0	0
			171	171		

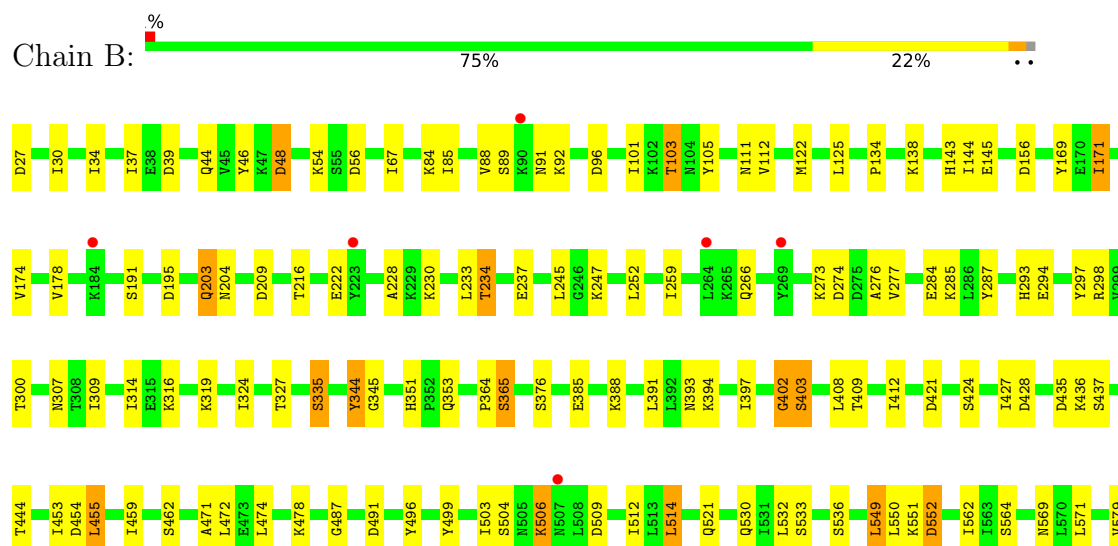
3 Residue-property plots

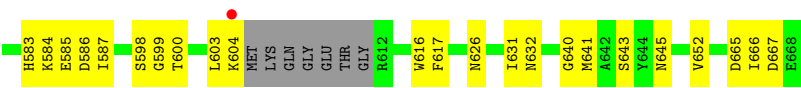
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	80.76Å 102.67Å 187.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.48 – 2.60 63.48 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (63.48-2.60) 100.0 (63.48-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.182 , 0.268 (Not available) , 0.243	Depositor DCC
R_{free} test set	3510 reflections (7.21%)	wwPDB-VP
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.765	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 75.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10896	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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: CD, 1W8, CL, AI8, 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	0.89	1/5236 (0.0%)	1.40	40/7038 (0.6%)
1	B	0.86	0/5186	1.38	41/6973 (0.6%)
All	All	0.87	1/10422 (0.0%)	1.39	81/14011 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	1
1	B	0	2
All	All	1	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	402	GLY	C-N	7.71	1.44	1.33

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	402	GLY	O-C-N	-32.95	85.06	122.95
1	B	402	GLY	O-C-N	-20.89	96.46	122.58
1	B	402	GLY	CA-C-N	9.15	153.51	122.20
1	B	402	GLY	C-N-CA	9.15	153.51	122.20
1	B	617	PHE	CA-CB-CG	-7.80	106.00	113.80
1	A	623	ASP	CA-CB-CG	7.16	119.76	112.60
1	A	573	ASP	CA-CB-CG	7.00	119.59	112.60
1	A	403	SER	CA-C-O	6.86	130.32	120.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	552	ASP	CA-CB-CG	6.77	119.37	112.60
1	A	75	VAL	N-CA-CB	6.57	117.69	110.53
1	B	454	ASP	CA-CB-CG	6.46	119.06	112.60
1	B	203	GLN	CA-C-N	6.44	133.84	121.54
1	B	203	GLN	C-N-CA	6.44	133.84	121.54
1	A	236	ASN	CA-CB-CG	6.36	118.96	112.60
1	A	345	GLY	N-CA-C	6.33	118.49	110.38
1	B	48	ASP	CA-CB-CG	6.26	118.86	112.60
1	A	377	ASN	CA-C-N	6.09	128.76	120.54
1	A	377	ASN	C-N-CA	6.09	128.76	120.54
1	B	171	ILE	N-CA-CB	6.05	117.32	110.72
1	A	329	ASP	CA-C-N	5.94	128.52	120.38
1	A	329	ASP	C-N-CA	5.94	128.52	120.38
1	A	177	ASN	CA-CB-CG	5.92	118.52	112.60
1	A	175	PRO	CA-C-N	5.87	128.42	120.38
1	A	175	PRO	C-N-CA	5.87	128.42	120.38
1	B	300	THR	CA-C-N	5.85	130.72	123.12
1	B	300	THR	C-N-CA	5.85	130.72	123.12
1	B	491	ASP	CA-CB-CG	5.71	118.31	112.60
1	B	56	ASP	CA-CB-CG	5.67	118.27	112.60
1	A	613	GLN	N-CA-C	5.65	118.68	109.59
1	B	284	GLU	CA-C-N	5.56	127.98	120.65
1	B	284	GLU	C-N-CA	5.56	127.98	120.65
1	A	67	ILE	CA-C-N	5.52	127.94	120.44
1	A	67	ILE	C-N-CA	5.52	127.94	120.44
1	A	611	GLY	CA-C-N	5.47	131.98	121.54
1	A	611	GLY	C-N-CA	5.47	131.98	121.54
1	B	665	ASP	CA-CB-CG	5.46	118.06	112.60
1	B	436	LYS	N-CA-C	-5.44	106.60	113.18
1	A	654	ASP	CA-CB-CG	5.44	118.04	112.60
1	B	459	ILE	N-CA-C	-5.43	105.80	110.74
1	B	436	LYS	CA-C-N	5.40	128.51	120.31
1	B	436	LYS	C-N-CA	5.40	128.51	120.31
1	A	502	GLN	CA-C-N	-5.39	117.64	123.08
1	A	502	GLN	C-N-CA	-5.39	117.64	123.08
1	B	44	GLN	CA-C-N	5.32	127.47	120.60
1	B	44	GLN	C-N-CA	5.32	127.47	120.60
1	B	412	ILE	CA-C-N	5.24	125.79	119.98
1	B	412	ILE	C-N-CA	5.24	125.79	119.98
1	A	508	LEU	CA-C-N	5.23	127.55	120.38
1	A	508	LEU	C-N-CA	5.23	127.55	120.38
1	B	564	SER	CA-C-N	5.23	127.29	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	564	SER	C-N-CA	5.23	127.29	120.28
1	A	203	GLN	CA-C-N	5.22	127.28	120.28
1	A	203	GLN	C-N-CA	5.22	127.28	120.28
1	B	39	ASP	CA-CB-CG	5.22	117.82	112.60
1	B	266	GLN	CA-C-N	5.20	127.19	120.44
1	B	266	GLN	C-N-CA	5.20	127.19	120.44
1	A	475	GLY	CA-C-N	5.19	127.55	120.54
1	A	475	GLY	C-N-CA	5.19	127.55	120.54
1	B	472	LEU	CA-C-N	5.19	127.23	120.28
1	B	472	LEU	C-N-CA	5.19	127.23	120.28
1	A	224	LEU	CA-C-N	5.18	127.23	120.28
1	A	224	LEU	C-N-CA	5.18	127.23	120.28
1	B	665	ASP	CA-C-N	5.17	127.17	120.56
1	B	665	ASP	C-N-CA	5.17	127.17	120.56
1	A	386	ASP	CA-C-N	5.16	127.91	120.38
1	A	386	ASP	C-N-CA	5.16	127.91	120.38
1	A	56	ASP	CA-CB-CG	5.15	117.75	112.60
1	A	454	ASP	CA-C-N	5.12	127.46	120.54
1	A	454	ASP	C-N-CA	5.12	127.46	120.54
1	A	301	ILE	N-CA-CB	5.12	117.80	111.41
1	B	626	ASN	CA-CB-CG	5.10	117.70	112.60
1	B	67	ILE	CA-C-N	5.08	127.51	120.29
1	B	67	ILE	C-N-CA	5.08	127.51	120.29
1	B	274	ASP	CA-C-N	5.06	128.00	120.31
1	B	274	ASP	C-N-CA	5.06	128.00	120.31
1	B	285	LYS	CA-C-N	5.05	127.30	120.38
1	B	285	LYS	C-N-CA	5.05	127.30	120.38
1	A	454	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	88	VAL	N-CA-C	-5.04	108.36	113.20
1	A	267	LYS	CA-C-N	5.01	126.99	120.28
1	A	267	LYS	C-N-CA	5.01	126.99	120.28

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	403	SER	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	402	GLY	Peptide
1	B	402	GLY	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	403	SER	Peptide

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	5151	0	5148	61	0
1	B	5101	0	5099	83	0
2	A	39	0	21	3	0
2	B	39	0	21	18	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	39	0	20	17	0
5	B	39	0	20	12	0
6	A	17	16	15	2	0
6	B	17	16	16	6	0
7	A	239	0	0	0	0
7	B	171	0	0	1	0
All	All	10864	32	10360	155	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 7.

All (155) 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)
5:A:1676:1W8:C20	1:B:298:ARG:HD2	1.62	1.28
1:B:643:SER:OG	2:B:1403:AI8:H22	1.12	1.28
5:A:1676:1W8:H201	1:B:298:ARG:CD	1.65	1.25
1:A:309:ILE:CD1	5:B:1676:1W8:H201	1.66	1.25
1:A:309:ILE:CD1	5:B:1676:1W8:C20	2.28	1.10
1:A:309:ILE:HD11	5:B:1676:1W8:C20	1.81	1.10
1:A:309:ILE:HD11	5:B:1676:1W8:H202	1.32	1.09
1:A:309:ILE:HD12	5:B:1676:1W8:H201	1.10	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:643:SER:OG	2:B:1403:AI8:C22	2.08	1.02
5:A:1676:1W8:H14	1:B:309:ILE:HD11	1.42	0.97
1:A:217:VAL:HG21	1:A:224:LEU:HD12	1.52	0.91
5:A:1676:1W8:H14	1:B:309:ILE:CD1	2.01	0.90
5:B:1676:1W8:S3	5:B:1676:1W8:H112	2.13	0.89
1:B:643:SER:HG	2:B:1403:AI8:H22	1.41	0.83
1:A:309:ILE:HD12	5:B:1676:1W8:C20	2.00	0.80
1:B:174:VAL:HG23	1:B:234:THR:HG21	1.64	0.80
1:B:521:GLN:HG2	2:B:1403:AI8:C18	2.14	0.76
1:B:277:VAL:HB	6:B:1677:MUR:H91	1.70	0.73
1:B:521:GLN:HA	2:B:1403:AI8:N8	2.05	0.72
2:B:1403:AI8:H121	2:B:1403:AI8:HN3	1.55	0.72
1:B:89:SER:HB3	1:B:92:LYS:HB2	1.73	0.69
2:B:1403:AI8:N6	7:B:2113:HOH:O	2.26	0.68
1:A:144:ILE:HG22	5:A:1676:1W8:S2	2.36	0.65
1:A:138:LYS:HD2	1:A:138:LYS:H	1.61	0.65
1:A:217:VAL:HG21	1:A:224:LEU:CD1	2.25	0.64
1:A:403:SER:O	1:A:597:LYS:HE3	1.98	0.63
1:B:293:HIS:CE1	6:B:1677:MUR:H93	2.33	0.63
1:B:144:ILE:O	5:B:1676:1W8:H18	1.97	0.63
1:A:89:SER:HB3	1:A:92:LYS:HB2	1.81	0.62
5:A:1676:1W8:C14	1:B:309:ILE:HD11	2.24	0.62
1:B:403:SER:HB2	1:B:599:GLY:HA2	1.83	0.61
1:B:504:SER:HB3	1:B:506:LYS:HG2	1.82	0.61
1:B:144:ILE:O	5:B:1676:1W8:H19	2.02	0.59
6:B:1677:MUR:H92	6:B:1677:MUR:HN22	1.66	0.59
5:A:1676:1W8:C19	1:B:309:ILE:HD11	2.34	0.58
1:A:138:LYS:H	1:A:138:LYS:CD	2.17	0.58
5:A:1676:1W8:H19	1:B:309:ILE:HD11	1.86	0.58
1:B:144:ILE:HG22	5:B:1676:1W8:H14	1.85	0.58
1:B:462:SER:OG	2:B:1403:AI8:N2	2.35	0.57
1:A:640:GLY:O	1:A:643:SER:HB2	2.05	0.56
1:A:576:GLN:HG2	1:A:580:ASN:HD21	1.69	0.56
5:A:1676:1W8:C21	5:A:1676:1W8:S3	2.94	0.56
1:A:550:LEU:HB2	1:A:553:THR:OG1	2.06	0.55
5:A:1676:1W8:H18	1:B:298:ARG:HH11	1.71	0.55
1:B:364:PRO:HG3	1:B:388:LYS:HB3	1.89	0.55
1:A:521:GLN:O	1:A:521:GLN:HG3	2.06	0.55
2:A:1403:AI8:HN3	2:A:1403:AI8:H18	1.71	0.55
1:B:144:ILE:O	5:B:1676:1W8:C18	2.54	0.55
1:A:151:ARG:HD2	6:A:1677:MUR:O9	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:583:HIS:CE1	2:B:1403:AI8:C19	2.91	0.54
1:B:351:HIS:CE1	1:B:353:GLN:HB2	2.41	0.54
1:B:144:ILE:O	5:B:1676:1W8:C19	2.55	0.54
1:A:396:GLN:HG3	1:A:497:PRO:O	2.07	0.54
1:B:474:LEU:O	1:B:478:LYS:HB2	2.07	0.54
1:A:602:GLU:O	2:A:1403:AI8:S4	2.66	0.54
1:B:598:SER:OG	2:B:1403:AI8:O5	2.25	0.53
1:A:143:HIS:HB3	1:A:145:GLU:OE2	2.08	0.53
1:B:247:LYS:HB3	1:B:365:SER:HB3	1.90	0.53
1:A:220:MET:HA	1:A:224:LEU:HD13	1.91	0.53
5:A:1676:1W8:C18	1:B:298:ARG:HH11	2.22	0.52
1:B:345:GLY:HA3	1:B:632:ASN:O	2.10	0.52
1:A:28:LYS:HE2	1:A:28:LYS:H	1.75	0.52
1:A:407:ILE:HG23	1:A:571:LEU:HD13	1.92	0.52
1:A:576:GLN:HG2	1:A:580:ASN:ND2	2.24	0.52
1:B:112:VAL:HG13	1:B:134:PRO:HB3	1.92	0.52
1:A:140:GLN:HG2	1:A:303:ASP:HA	1.92	0.51
5:A:1676:1W8:H14	1:B:309:ILE:HD12	1.91	0.51
1:B:583:HIS:HE1	2:B:1403:AI8:C19	2.24	0.51
1:A:112:VAL:HG13	1:A:134:PRO:HB3	1.92	0.51
1:B:228:ALA:HA	1:B:233:LEU:HD12	1.93	0.51
1:A:137:GLN:HB3	1:A:138:LYS:HD2	1.92	0.50
1:A:222:GLU:H	1:A:222:GLU:CD	2.19	0.50
1:B:600:THR:HG21	1:B:641:MET:HB3	1.93	0.50
1:B:393:ASN:C	1:B:393:ASN:HD22	2.20	0.49
1:A:605:MET:HE3	1:A:612:ARG:H	1.78	0.49
1:B:496:TYR:CD2	1:B:549:LEU:HD21	2.48	0.49
1:A:408:LEU:HD22	1:A:534:ILE:HG21	1.94	0.49
1:B:487:GLY:O	1:B:530:GLN:NE2	2.46	0.49
1:B:105:TYR:O	1:B:314:ILE:HG21	2.12	0.49
1:A:559:LYS:HB3	1:A:562:ILE:HD13	1.94	0.49
1:B:277:VAL:HB	6:B:1677:MUR:C9	2.39	0.49
1:B:532:LEU:O	1:B:536:SER:HB3	2.12	0.48
1:B:666:ILE:HG13	1:B:667:ASP:N	2.29	0.48
5:A:1676:1W8:N4	5:A:1676:1W8:O	2.46	0.48
1:A:403:SER:HB2	2:A:1403:AI8:HN2	1.79	0.48
1:A:101:ILE:HB	1:A:108:ILE:HB	1.95	0.47
1:A:300:THR:HG22	1:A:312:THR:HA	1.96	0.47
1:A:406:LYS:HE3	1:A:519:TYR:HB2	1.97	0.47
1:B:191:SER:HB3	1:B:376:SER:HB3	1.96	0.47
1:A:605:MET:HE2	1:A:609:GLU:HB3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:HIS:HB3	1:B:145:GLU:OE2	2.16	0.46
1:B:344:TYR:C	1:B:344:TYR:CD1	2.94	0.46
1:A:559:LYS:HB3	1:A:562:ILE:CD1	2.46	0.46
5:A:1676:1W8:C20	1:B:298:ARG:HH11	2.29	0.46
1:B:403:SER:HB2	1:B:599:GLY:CA	2.46	0.46
1:A:401:PRO:HG2	1:A:405:GLN:HB2	1.98	0.45
1:A:516:ASP:HA	1:A:519:TYR:CE1	2.52	0.45
1:B:335:SER:HB3	1:B:652:VAL:HG13	1.98	0.45
1:B:287:TYR:CZ	1:B:550:LEU:HD11	2.51	0.45
1:B:327:THR:OG1	1:B:549:LEU:HA	2.16	0.45
1:A:336:ILE:HG21	1:A:347:GLY:HA3	1.98	0.45
1:B:584:LYS:C	1:B:586:ASP:H	2.24	0.45
1:B:586:ASP:OD2	2:B:1403:AI8:H225	2.17	0.45
1:A:173:ILE:HG23	1:A:178:VAL:HB	1.98	0.45
1:A:277:VAL:HB	6:A:1677:MUR:C8	2.46	0.45
1:A:290:LYS:HB2	1:A:324:ILE:HD11	1.99	0.45
1:A:386:ASP:HB3	1:A:390:PRO:HD3	1.98	0.45
1:A:579:VAL:HG13	1:A:587:ILE:HG23	1.99	0.45
1:B:427:ILE:HD12	1:B:453:ILE:HG13	1.98	0.44
5:A:1676:1W8:H201	1:B:298:ARG:HD2	0.69	0.44
1:B:169:TYR:CE1	1:B:237:GLU:HG2	2.53	0.44
1:B:583:HIS:HE1	2:B:1403:AI8:H19	1.83	0.44
1:B:640:GLY:O	1:B:643:SER:HB2	2.17	0.44
1:B:435:ASP:HB3	1:B:437:SER:H	1.83	0.44
6:B:1677:MUR:H92	6:B:1677:MUR:N2	2.30	0.44
1:B:600:THR:CG2	1:B:641:MET:HB3	2.48	0.43
1:A:27:ASP:HA	1:A:30:ILE:HD12	2.01	0.43
1:A:277:VAL:O	1:A:292:GLN:NE2	2.46	0.43
1:A:665:ASP:HB3	1:A:668:GLU:HB2	2.00	0.43
1:B:101:ILE:HG22	1:B:103:THR:HG22	2.00	0.43
1:B:169:TYR:O	1:B:216:THR:HA	2.18	0.43
2:B:1403:AI8:O6	2:B:1403:AI8:C6	2.67	0.43
1:B:471:ALA:HB1	1:B:514:LEU:HD22	2.00	0.43
1:B:579:VAL:HG13	1:B:587:ILE:HG23	2.01	0.42
1:A:38:GLU:HG3	1:A:80:ILE:HD12	2.02	0.42
1:A:527:ASN:OD1	1:A:529:VAL:HB	2.19	0.42
1:A:466:PHE:O	1:A:470:VAL:HG23	2.19	0.42
1:A:483:MET:HE3	1:A:488:VAL:HG11	2.01	0.42
1:A:605:MET:HG2	1:A:609:GLU:HB3	2.02	0.42
1:B:88:VAL:HG13	1:B:92:LYS:HB3	2.01	0.42
1:B:293:HIS:HE1	6:B:1677:MUR:O8	2.03	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:ILE:HG22	1:B:276:ALA:O	2.19	0.42
1:B:455:LEU:HD21	1:B:571:LEU:HD23	2.01	0.42
1:B:364:PRO:HD2	1:B:394:LYS:HZ3	1.84	0.41
1:B:521:GLN:HG2	2:B:1403:AI8:N8	2.33	0.41
1:B:616:TRP:HA	1:B:631:ILE:O	2.20	0.41
2:B:1403:AI8:O3	2:B:1403:AI8:C11	2.66	0.41
1:A:480:GLU:HG3	1:A:508:LEU:HD12	2.02	0.41
1:B:34:ILE:HA	1:B:37:ILE:HD12	2.03	0.41
1:B:643:SER:HG	2:B:1403:AI8:C22	2.16	0.41
1:A:595:ILE:HD11	1:A:620:TYR:CZ	2.55	0.41
1:B:397:ILE:HA	1:B:499:TYR:HD2	1.85	0.41
1:A:169:TYR:CE2	1:A:237:GLU:HG2	2.55	0.41
1:A:245:LEU:HD13	1:A:334:LYS:HG3	2.03	0.41
5:A:1676:1W8:S3	5:A:1676:1W8:O4	2.79	0.41
2:B:1403:AI8:H121	2:B:1403:AI8:N3	2.30	0.41
1:B:27:ASP:HB2	1:B:85:ILE:HD13	2.03	0.41
5:A:1676:1W8:S1	5:A:1676:1W8:O1	2.79	0.41
1:A:307:ASN:HD21	1:B:143:HIS:HA	1.86	0.41
1:B:273:LYS:HE2	1:B:294:GLU:HG3	2.03	0.41
1:A:119:GLU:HB2	1:A:124:LYS:HG3	2.03	0.41
1:A:135:GLY:HA2	1:B:209:ASP:OD2	2.20	0.41
1:B:297:TYR:CE2	1:B:316:LYS:HD2	2.56	0.41
1:B:631:ILE:HG22	1:B:645:ASN:HD22	1.86	0.40
1:B:46:TYR:O	1:B:54:LYS:HD3	2.22	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	638/642 (99%)	605 (95%)	30 (5%)	3 (0%)	24 46

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	631/642 (98%)	578 (92%)	50 (8%)	3 (0%)	24	46
All	All	1269/1284 (99%)	1183 (93%)	80 (6%)	6 (0%)	24	46

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	403	SER
1	A	612	ARG
1	B	91	ASN
1	B	204	ASN
1	B	203	GLN
1	A	611	GLY

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	572/572 (100%)	510 (89%)	62 (11%)	6	13
1	B	567/572 (99%)	520 (92%)	47 (8%)	10	23
All	All	1139/1144 (100%)	1030 (90%)	109 (10%)	8	17

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LYS
1	A	52	ILE
1	A	75	VAL
1	A	76	LYS
1	A	85	ILE
1	A	87	LYS
1	A	103	THR
1	A	111	ASN
1	A	112	VAL
1	A	119	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	122	MET
1	A	125	LEU
1	A	138	LYS
1	A	156	ASP
1	A	171	ILE
1	A	176	LYS
1	A	177	ASN
1	A	184	LYS
1	A	189	GLU
1	A	198	LYS
1	A	202	ASP
1	A	219	LYS
1	A	220	MET
1	A	224	LEU
1	A	245	LEU
1	A	252	LEU
1	A	267	LYS
1	A	274	ASP
1	A	285	LYS
1	A	307	ASN
1	A	317	LYS
1	A	342	ASN
1	A	367	ASP
1	A	375	MET
1	A	382	LYS
1	A	386	ASP
1	A	391	LEU
1	A	403	SER
1	A	408	LEU
1	A	411	MET
1	A	418	THR
1	A	419	LEU
1	A	421	ASP
1	A	424	SER
1	A	447	GLU
1	A	502	GLN
1	A	509	ASP
1	A	514	LEU
1	A	517	SER
1	A	526	ILE
1	A	532	LEU
1	A	549	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	551	LYS
1	A	553	THR
1	A	554	LYS
1	A	562	ILE
1	A	566	GLU
1	A	570	LEU
1	A	603	LEU
1	A	606	LYS
1	A	662	LYS
1	A	663	LYS
1	B	30	ILE
1	B	48	ASP
1	B	84	LYS
1	B	96	ASP
1	B	103	THR
1	B	111	ASN
1	B	122	MET
1	B	125	LEU
1	B	138	LYS
1	B	156	ASP
1	B	171	ILE
1	B	178	VAL
1	B	195	ASP
1	B	222	GLU
1	B	230	LYS
1	B	234	THR
1	B	245	LEU
1	B	252	LEU
1	B	307	ASN
1	B	319	LYS
1	B	324	ILE
1	B	335	SER
1	B	344	TYR
1	B	365	SER
1	B	385	GLU
1	B	391	LEU
1	B	408	LEU
1	B	409	THR
1	B	421	ASP
1	B	424	SER
1	B	428	ASP
1	B	444	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	455	LEU
1	B	503	ILE
1	B	506	LYS
1	B	509	ASP
1	B	512	ILE
1	B	514	LEU
1	B	533	SER
1	B	549	LEU
1	B	551	LYS
1	B	552	ASP
1	B	562	ILE
1	B	569	ASN
1	B	585	GLU
1	B	603	LEU
1	B	604	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	41	ASN
1	A	79	ASN
1	A	81	GLN
1	A	91	ASN
1	A	107	ASN
1	A	115	ASN
1	A	200	GLN
1	A	203	GLN
1	A	207	GLN
1	A	266	GLN
1	A	293	HIS
1	A	307	ASN
1	A	396	GLN
1	A	502	GLN
1	A	530	GLN
1	A	540	ASN
1	A	567	ASN
1	A	569	ASN
1	A	580	ASN
1	A	624	ASN
1	A	626	ASN
1	A	661	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	32	ASN
1	B	44	GLN
1	B	98	GLN
1	B	137	GLN
1	B	177	ASN
1	B	293	HIS
1	B	307	ASN
1	B	339	ASN
1	B	393	ASN
1	B	396	GLN
1	B	442	ASN
1	B	530	GLN
1	B	576	GLN
1	B	580	ASN
1	B	624	ASN
1	B	632	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 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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
6	MUR	A	1677	-	17,17,17	1.36	2 (11%)	21,24,24	2.35	5 (23%)
5	1W8	A	1676	-	43,43,43	2.23	3 (6%)	54,62,62	1.47	5 (9%)
2	AI8	A	1403	1	39,42,42	3.93	16 (41%)	43,58,58	4.23	19 (44%)
6	MUR	B	1677	-	17,17,17	1.37	3 (17%)	21,24,24	2.09	6 (28%)
2	AI8	B	1403	1	39,42,42	4.39	18 (46%)	43,58,58	5.17	22 (51%)
5	1W8	B	1676	-	43,43,43	0.99	3 (6%)	54,62,62	1.01	3 (5%)

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
6	MUR	A	1677	-	-	5/10/30/30	0/1/1/1
5	1W8	A	1676	-	-	15/24/57/57	0/5/5/5
2	AI8	A	1403	1	-	13/24/47/47	0/3/4/4
6	MUR	B	1677	-	-	7/10/30/30	0/1/1/1
2	AI8	B	1403	1	1/1/7/10	15/24/47/47	0/3/4/4
5	1W8	B	1676	-	-	7/24/57/57	0/5/5/5

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1403	AI8	C4-S1	-14.11	1.47	1.82
2	A	1403	AI8	C4-S1	-13.96	1.47	1.82
5	A	1676	1W8	C12-S2	-12.99	1.60	1.75
2	B	1403	AI8	C8-S1	-12.82	1.56	1.82
2	A	1403	AI8	C9-S2	7.65	1.89	1.77
2	A	1403	AI8	C11-N3	7.35	1.49	1.34
2	B	1403	AI8	C9-S2	6.99	1.88	1.77
2	B	1403	AI8	C11-N3	6.91	1.48	1.34
2	A	1403	AI8	C18-N8	6.58	1.47	1.34
2	A	1403	AI8	C8-S1	-6.57	1.69	1.82
2	B	1403	AI8	C18-N8	5.88	1.46	1.34
2	B	1403	AI8	C17-C15	5.85	1.56	1.47
2	B	1403	AI8	C13-S2	5.83	1.82	1.75
2	A	1403	AI8	C16-C15	5.82	1.43	1.36
2	B	1403	AI8	O7-N4	-5.60	1.32	1.42
2	A	1403	AI8	O7-N4	-5.51	1.32	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1403	AI8	C16-C15	4.96	1.42	1.36
2	A	1403	AI8	C13-S2	4.84	1.81	1.75
2	A	1403	AI8	C17-C15	4.84	1.54	1.47
2	B	1403	AI8	C18-N6	4.66	1.38	1.31
2	B	1403	AI8	C12-N4	-4.64	1.18	1.29
2	A	1403	AI8	C18-N6	4.62	1.38	1.31
5	B	1676	1W8	C4-S	4.14	1.80	1.73
5	A	1676	1W8	C4-S	4.10	1.80	1.73
2	B	1403	AI8	C18-S4	-4.09	1.66	1.73
2	A	1403	AI8	C7-N2	3.91	1.47	1.37
5	A	1676	1W8	C10-S2	-3.63	1.71	1.77
2	B	1403	AI8	C7-N2	3.42	1.45	1.37
2	B	1403	AI8	C13-S3	-3.28	1.68	1.73
2	B	1403	AI8	C13-N5	3.03	1.37	1.30
5	B	1676	1W8	C12-S2	-2.84	1.72	1.75
2	A	1403	AI8	O7-C21	-2.84	1.39	1.44
2	B	1403	AI8	O7-C21	-2.83	1.39	1.44
2	B	1403	AI8	C19-C17	2.79	1.43	1.39
2	A	1403	AI8	C12-C14	2.61	1.49	1.46
2	A	1403	AI8	C13-N5	2.56	1.36	1.30
2	A	1403	AI8	C7-C10	2.53	1.52	1.48
6	B	1677	MUR	O5-C5	-2.33	1.38	1.44
2	A	1403	AI8	C18-S4	-2.31	1.69	1.73
5	B	1676	1W8	C10-S2	-2.31	1.73	1.77
6	A	1677	MUR	O5-C5	-2.27	1.38	1.44
6	B	1677	MUR	O5-C1	-2.24	1.37	1.42
6	A	1677	MUR	O5-C1	-2.12	1.37	1.42
6	B	1677	MUR	O3-C7	-2.11	1.39	1.44
2	B	1403	AI8	S4-N7	-2.11	1.57	1.66

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1403	AI8	C21-O7-N4	16.32	119.60	108.30
2	A	1403	AI8	C21-O7-N4	16.27	119.57	108.30
2	B	1403	AI8	S3-C13-N5	-14.12	106.17	115.15
2	B	1403	AI8	C18-S4-N7	13.48	102.43	91.81
2	B	1403	AI8	C8-S1-C4	10.23	113.09	94.36
2	A	1403	AI8	C18-S4-N7	9.48	99.27	91.81
2	A	1403	AI8	S3-C13-N5	-9.44	109.14	115.15
6	A	1677	MUR	C1-O5-C5	8.08	129.29	113.65
2	B	1403	AI8	O5-C10-O4	7.68	142.19	123.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1403	AI8	C8-S1-C4	7.47	108.04	94.36
2	B	1403	AI8	C9-S2-C13	7.27	114.66	101.81
6	B	1677	MUR	C1-O5-C5	7.02	127.23	113.65
2	A	1403	AI8	O5-C10-O4	6.79	140.07	123.90
5	A	1676	1W8	C10-S2-C12	6.74	113.73	101.81
2	B	1403	AI8	C16-S3-C13	6.18	97.65	89.06
2	B	1403	AI8	O5-C10-C7	-6.02	107.19	116.73
2	B	1403	AI8	S4-C18-N6	-5.87	103.51	112.14
2	A	1403	AI8	O4-C10-C7	-5.73	110.22	120.20
2	B	1403	AI8	C4-C5-N3	5.57	121.73	109.93
2	B	1403	AI8	O4-C10-C7	-5.51	110.61	120.20
2	A	1403	AI8	C17-C15-C16	-5.02	120.58	126.54
5	A	1676	1W8	O-N-C2	4.84	118.35	111.59
5	B	1676	1W8	O-N-C2	4.83	118.33	111.59
2	A	1403	AI8	S4-C18-N6	-4.77	105.14	112.14
2	A	1403	AI8	C16-S3-C13	4.44	95.23	89.06
2	A	1403	AI8	O5-C10-C7	-4.43	109.71	116.73
2	A	1403	AI8	C17-C15-N5	4.25	126.45	119.95
2	B	1403	AI8	N8-C18-N6	4.09	128.81	124.05
5	A	1676	1W8	C10-C9-N5	-4.08	112.02	121.91
2	B	1403	AI8	C15-C16-S3	-4.02	106.29	111.16
6	A	1677	MUR	O3-C7-C9	3.84	118.23	107.54
2	A	1403	AI8	O7-N4-C12	3.74	116.81	111.59
2	A	1403	AI8	C15-C16-S3	-3.46	106.97	111.16
2	A	1403	AI8	O7-C21-C24	3.37	117.52	109.10
2	B	1403	AI8	O7-C21-C24	3.37	117.52	109.10
2	B	1403	AI8	O7-N4-C12	3.22	116.08	111.59
6	B	1677	MUR	O3-C3-C2	3.12	116.52	108.89
6	A	1677	MUR	C3-C4-C5	3.05	116.08	109.57
2	B	1403	AI8	C20-C17-C15	3.05	124.29	120.87
2	A	1403	AI8	N8-C18-N6	2.97	127.51	124.05
5	B	1676	1W8	C10-C9-N5	-2.86	114.96	121.91
6	A	1677	MUR	O9-C8-O8	-2.68	118.00	124.08
6	A	1677	MUR	C1-C2-C3	-2.63	105.41	110.10
5	A	1676	1W8	C2-C3-N2	-2.54	118.18	122.55
6	B	1677	MUR	C1-C2-C3	2.49	114.54	110.10
6	B	1677	MUR	O9-C8-O8	-2.47	118.47	124.08
2	A	1403	AI8	C4-C5-N3	2.45	115.12	109.93
2	A	1403	AI8	S2-C13-N5	2.40	129.91	121.39
6	B	1677	MUR	O3-C7-C9	2.31	113.96	107.54
2	B	1403	AI8	S4-C18-N8	2.28	127.67	119.00
2	A	1403	AI8	C18-N6-C14	2.24	112.82	106.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1676	1W8	C2-C3-N2	-2.24	118.70	122.55
2	B	1403	AI8	C16-C15-N5	-2.21	111.99	114.53
2	B	1403	AI8	C5-N3-C11	-2.21	117.60	121.97
2	A	1403	AI8	S4-C18-N8	2.19	127.36	119.00
2	B	1403	AI8	C19-C17-C15	-2.17	118.44	120.87
2	B	1403	AI8	S3-C13-S2	2.15	129.43	121.40
5	A	1676	1W8	C9-C10-S2	2.15	122.99	118.69
2	B	1403	AI8	C18-N6-C14	2.09	112.38	106.10
6	B	1677	MUR	C9-C7-C8	2.05	113.27	109.42

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1403	AI8	C5

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1403	AI8	C11-C12-N4-O7
2	A	1403	AI8	C14-C12-N4-O7
2	A	1403	AI8	O5-C10-C7-N2
2	A	1403	AI8	N5-C15-C17-C19
2	A	1403	AI8	N5-C15-C17-C20
2	A	1403	AI8	C16-C15-C17-C19
2	A	1403	AI8	C16-C15-C17-C20
2	B	1403	AI8	C6-C5-N3-C11
2	B	1403	AI8	C12-N4-O7-C21
2	B	1403	AI8	C11-C12-N4-O7
2	B	1403	AI8	C14-C12-N4-O7
2	B	1403	AI8	O5-C10-C7-N2
2	B	1403	AI8	O5-C10-C7-C9
2	B	1403	AI8	C24-C21-O7-N4
5	A	1676	1W8	O1-C5-N4-C6
5	A	1676	1W8	C2-C5-N4-C6
5	B	1676	1W8	C-C1-O-N
5	B	1676	1W8	O1-C5-N4-C6
5	B	1676	1W8	C2-C5-N4-C6
5	B	1676	1W8	C8-C6-N4-C5
5	B	1676	1W8	O4-C21-C9-C10
6	A	1677	MUR	C9-C7-O3-C3
6	A	1677	MUR	C9-C7-C8-O8
6	A	1677	MUR	C9-C7-C8-O9

Continued on next page...

Continued from previous page...

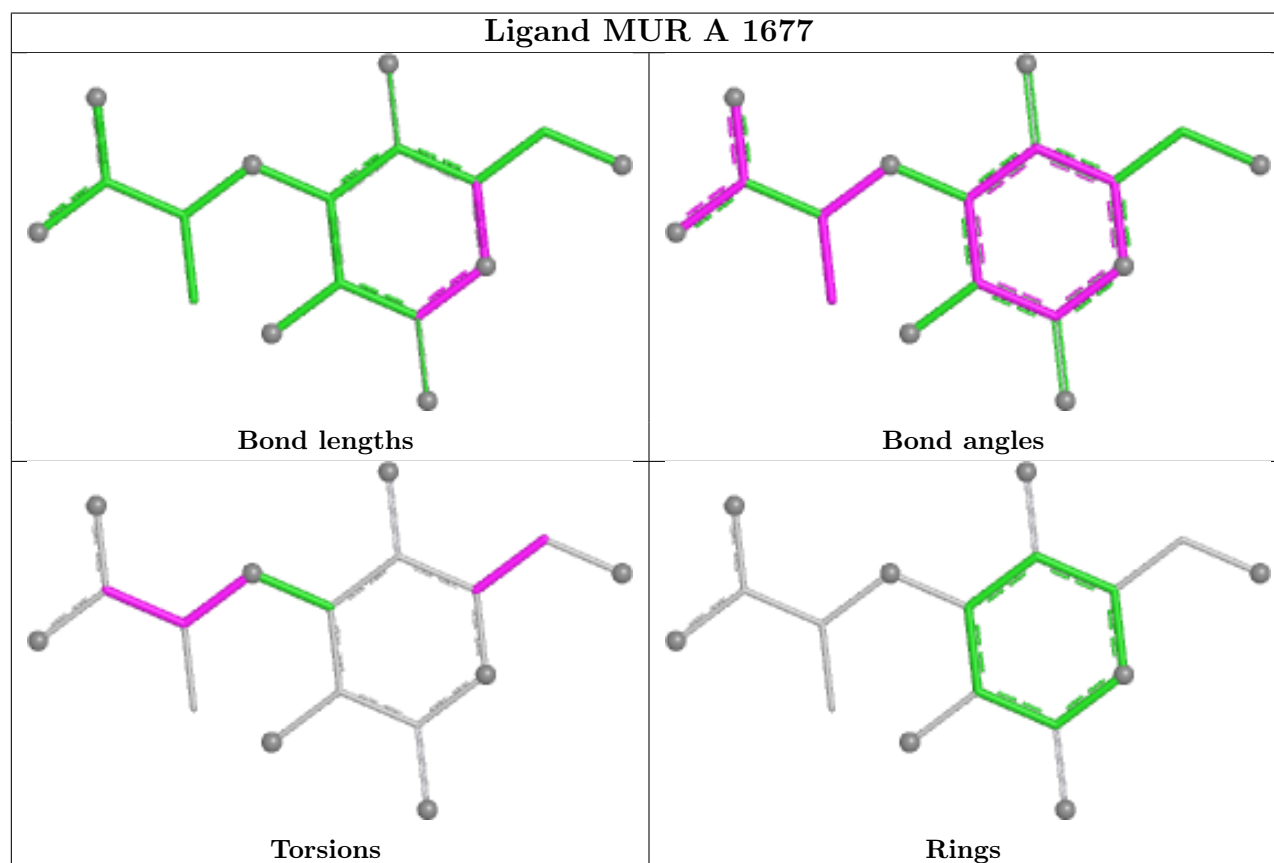
Mol	Chain	Res	Type	Atoms
6	B	1677	MUR	C2-C3-O3-C7
6	B	1677	MUR	C9-C7-O3-C3
6	B	1677	MUR	O3-C7-C8-O8
6	B	1677	MUR	O3-C7-C8-O9
6	A	1677	MUR	C4-C5-C6-O6
5	A	1676	1W8	C7-C6-N4-C5
6	A	1677	MUR	O5-C5-C6-O6
5	A	1676	1W8	N-C2-C5-N4
6	B	1677	MUR	C9-C7-C8-O9
5	A	1676	1W8	C3-C2-C5-O1
5	A	1676	1W8	C3-C2-C5-N4
6	B	1677	MUR	C9-C7-C8-O8
2	B	1403	AI8	C4-C5-N3-C11
5	A	1676	1W8	O3-C21-C9-C10
2	B	1403	AI8	N5-C13-S2-C9
5	A	1676	1W8	N-C2-C5-O1
5	A	1676	1W8	N6-C12-S2-C10
2	B	1403	AI8	O6-C11-C12-N4
6	B	1677	MUR	O5-C5-C6-O6
2	A	1403	AI8	N3-C11-C12-C14
2	A	1403	AI8	O6-C11-C12-C14
2	B	1403	AI8	N3-C11-C12-C14
2	B	1403	AI8	O6-C11-C12-C14
2	A	1403	AI8	O4-C10-C7-C9
5	A	1676	1W8	N6-C13-C15-C16
5	B	1676	1W8	N-C2-C5-O1
5	A	1676	1W8	O3-C21-C9-N5
5	A	1676	1W8	N6-C13-C15-C19
5	A	1676	1W8	C14-C13-C15-C16
5	A	1676	1W8	C14-C13-C15-C19
2	B	1403	AI8	S3-C13-S2-C9
5	A	1676	1W8	S3-C12-S2-C10
2	A	1403	AI8	N3-C11-C12-N4
2	B	1403	AI8	N3-C11-C12-N4
5	B	1676	1W8	N-C2-C5-N4
2	A	1403	AI8	O4-C10-C7-N2
2	A	1403	AI8	O6-C11-C12-N4
2	B	1403	AI8	O4-C10-C7-N2

There are no ring outliers.

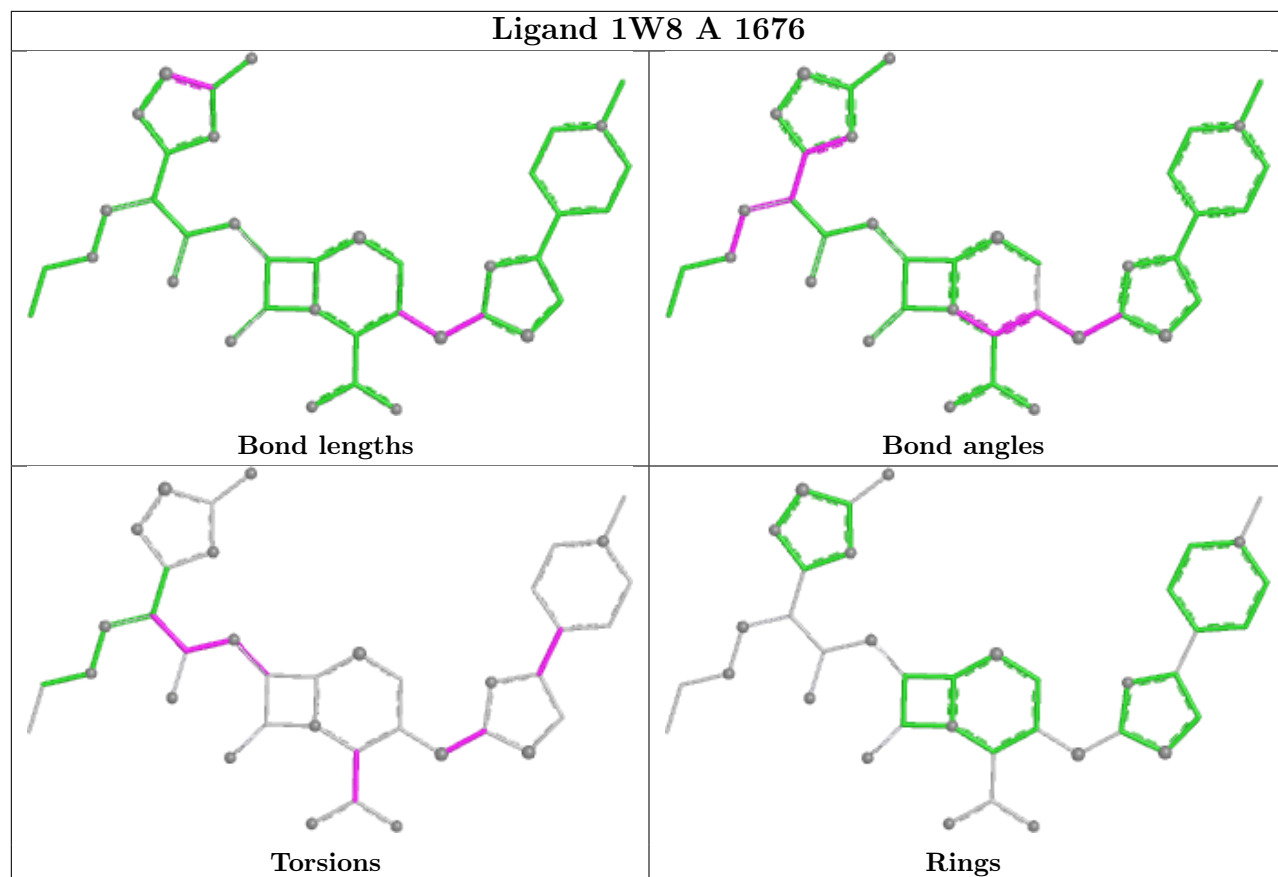
6 monomers are involved in 58 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1677	MUR	2	0
5	A	1676	1W8	17	0
2	A	1403	AI8	3	0
6	B	1677	MUR	6	0
2	B	1403	AI8	18	0
5	B	1676	1W8	12	0

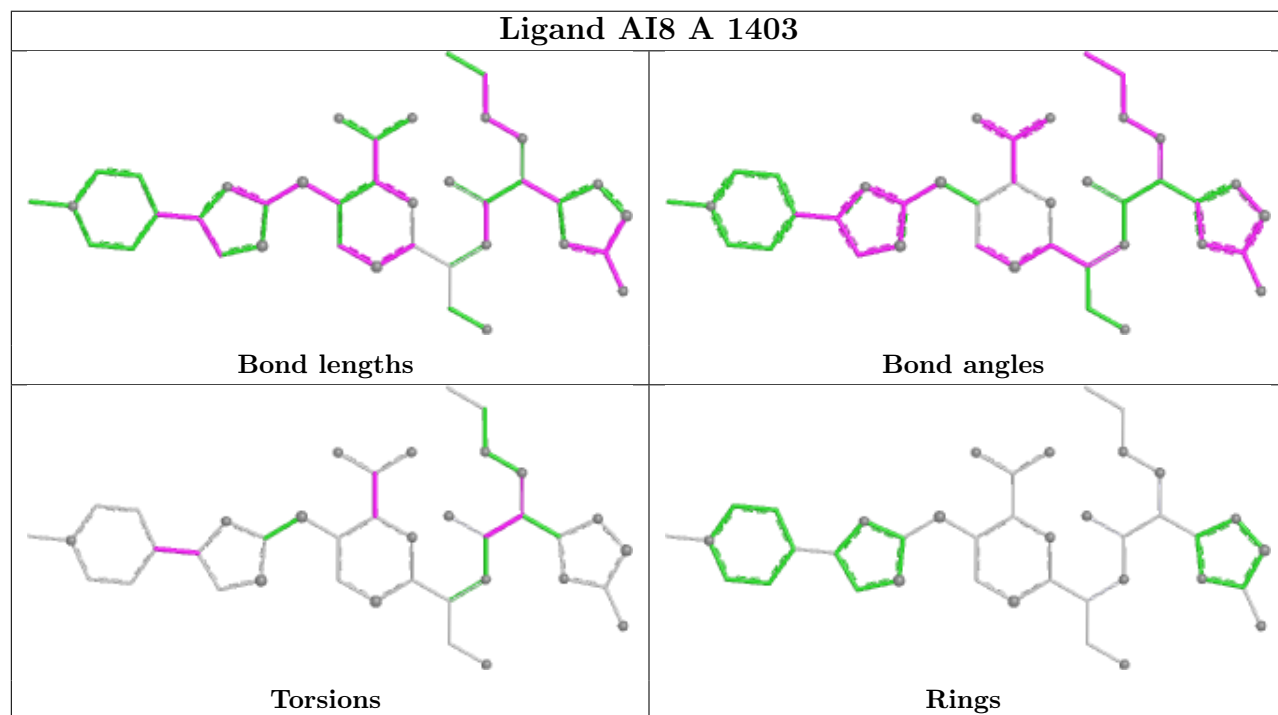
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



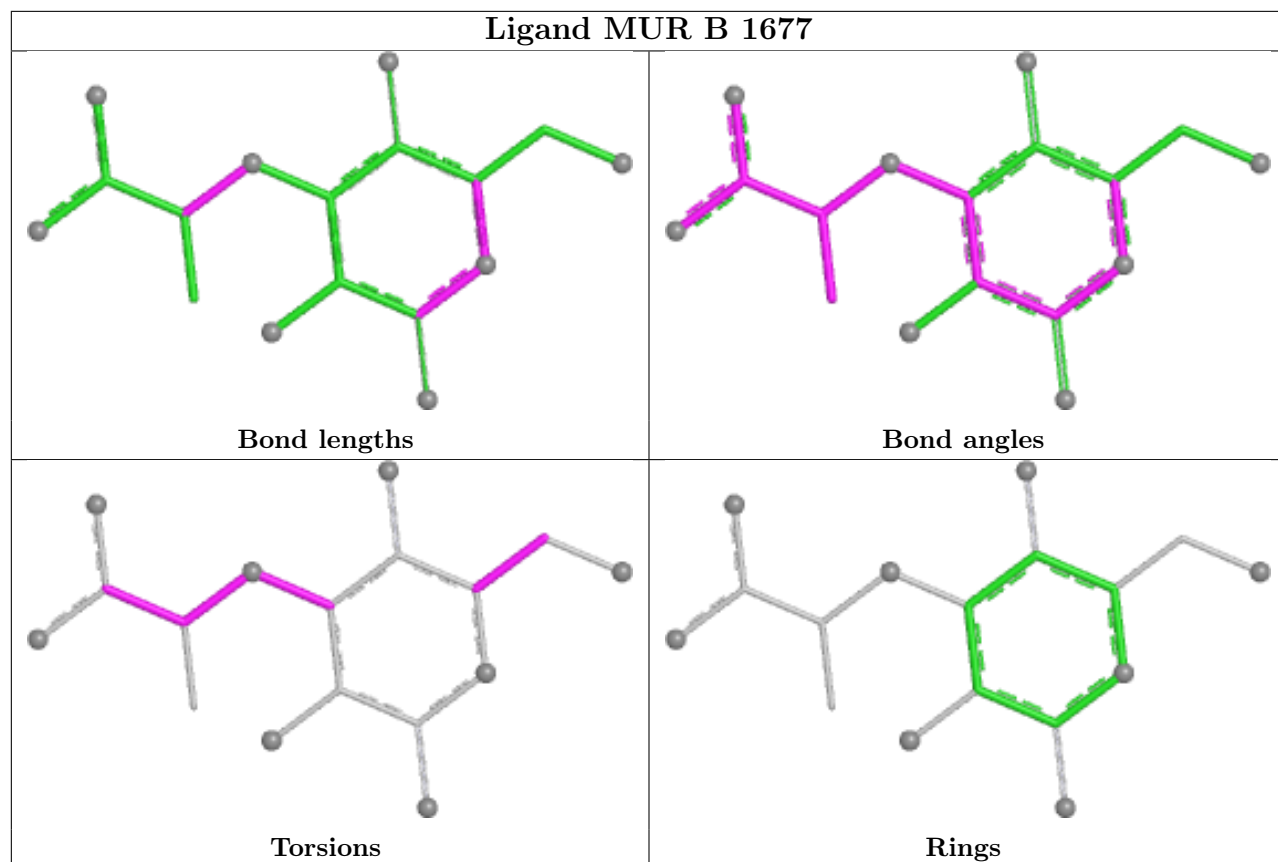
Ligand 1W8 A 1676



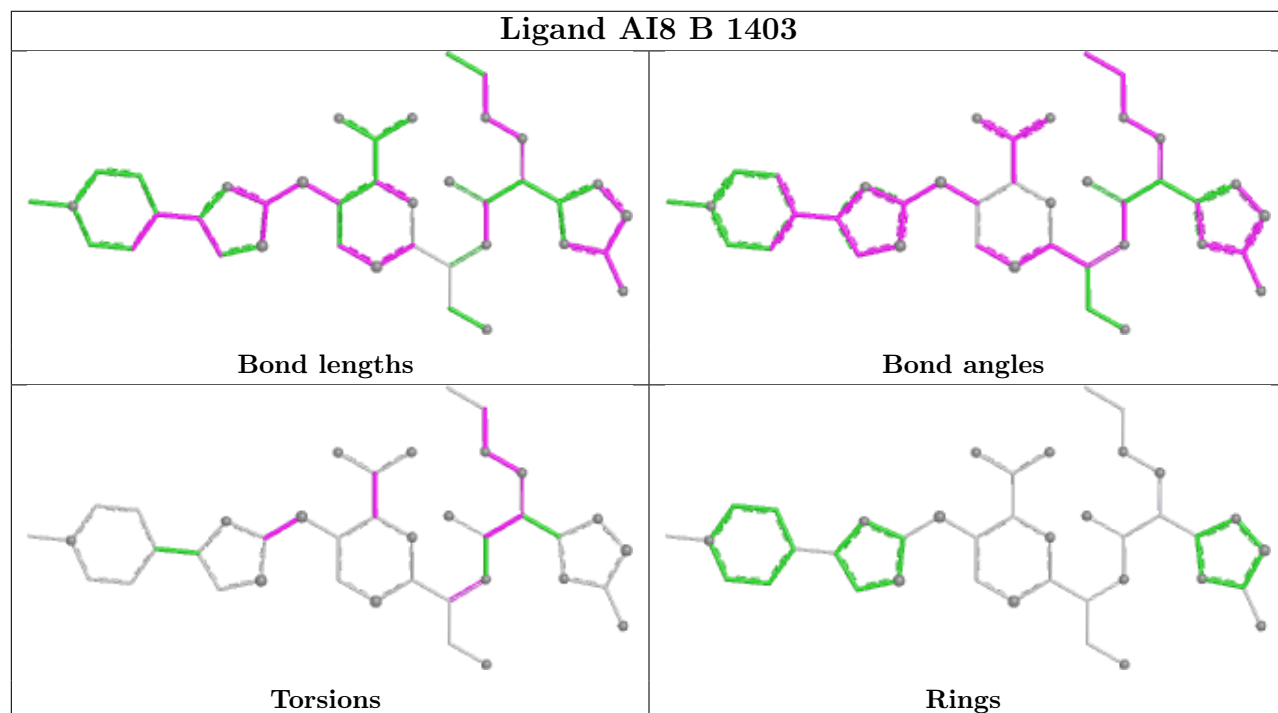
Ligand AI8 A 1403

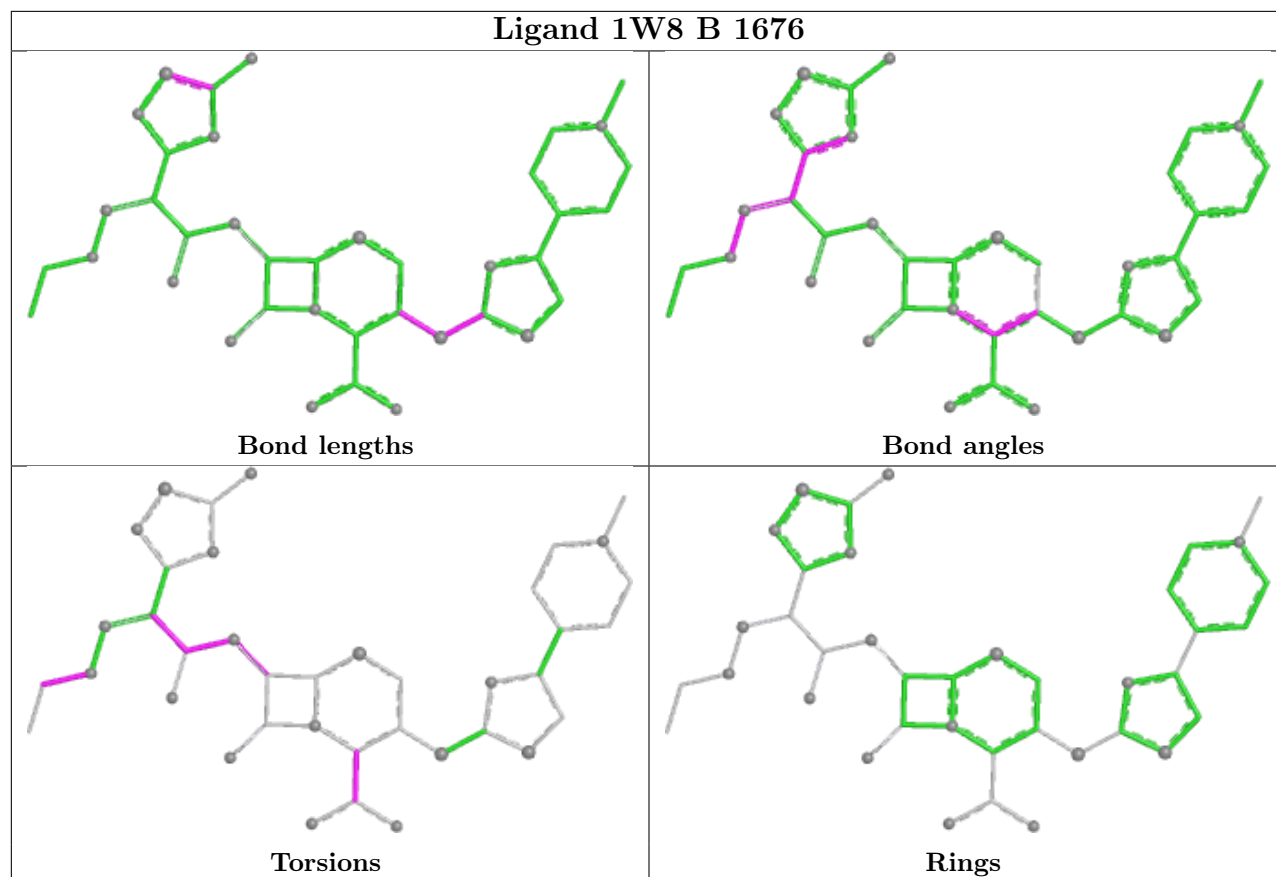


Ligand MUR B 1677



Ligand AI8 B 1403





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	272:TYR	C	273:LYS	N	3.32

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	642/642 (100%)	-0.14	6 (0%) 81 78	33, 66, 106, 148	0
1	B	635/642 (98%)	0.00	7 (1%) 78 74	35, 72, 115, 145	0
All	All	1277/1284 (99%)	-0.07	13 (1%) 79 76	33, 69, 113, 148	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	28	LYS	3.3
1	A	610	THR	3.0
1	A	603	LEU	2.7
1	B	223	TYR	2.4
1	B	507	ASN	2.4
1	B	184	LYS	2.3
1	B	604	LYS	2.2
1	A	220	MET	2.2
1	B	269	TYR	2.1
1	A	224	LEU	2.1
1	B	90	LYS	2.1
1	A	606	LYS	2.0
1	B	264	LEU	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 ⓘ

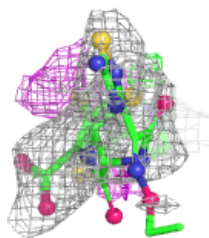
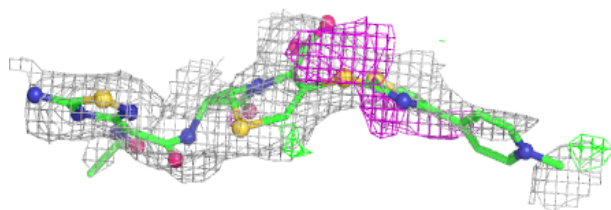
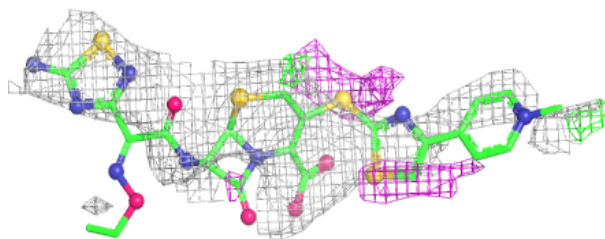
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	1W8	A	1676	39/39	0.69	0.20	149,154,160,161	0
3	CD	A	1673	1/1	0.76	0.12	265,265,265,265	0
5	1W8	B	1676	39/39	0.76	0.18	178,180,181,181	0
6	MUR	B	1677	17/17	0.77	0.22	146,150,152,153	0
6	MUR	A	1677	17/17	0.78	0.17	116,117,121,122	0
2	AI8	B	1403	39/39	0.80	0.15	81,99,125,125	0
3	CD	B	1672	1/1	0.87	0.11	193,193,193,193	0
2	AI8	A	1403	39/39	0.88	0.14	51,75,94,95	0
3	CD	A	1671	1/1	0.89	0.12	202,202,202,202	0
3	CD	B	1673	1/1	0.95	0.06	131,131,131,131	0
4	CL	B	1674	1/1	0.96	0.08	69,69,69,69	0
4	CL	B	1675	1/1	0.99	0.05	58,58,58,58	0
3	CD	B	1671	1/1	0.99	0.03	54,54,54,54	0
4	CL	A	1674	1/1	0.99	0.05	47,47,47,47	0
4	CL	A	1675	1/1	0.99	0.06	74,74,74,74	0
3	CD	A	1670	1/1	0.99	0.03	59,59,59,59	0
3	CD	B	1669	1/1	1.00	0.02	66,66,66,66	0
3	CD	A	1672	1/1	1.00	0.03	72,72,72,72	0

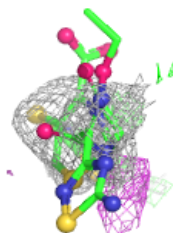
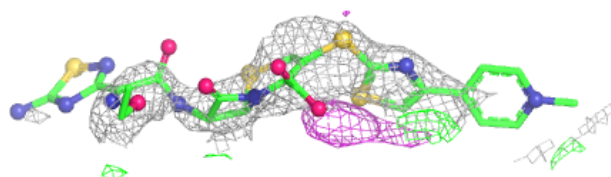
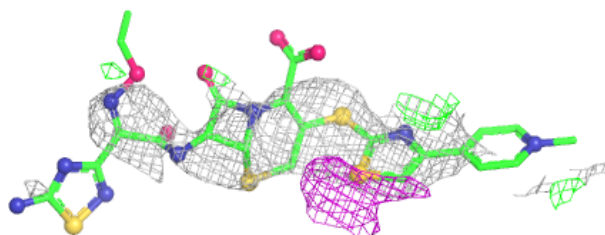
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 1W8 A 1676:

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

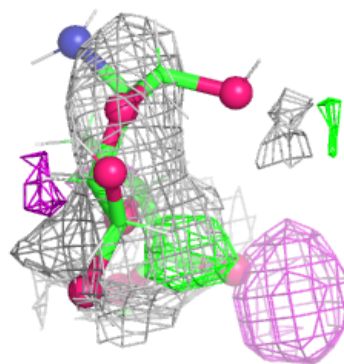
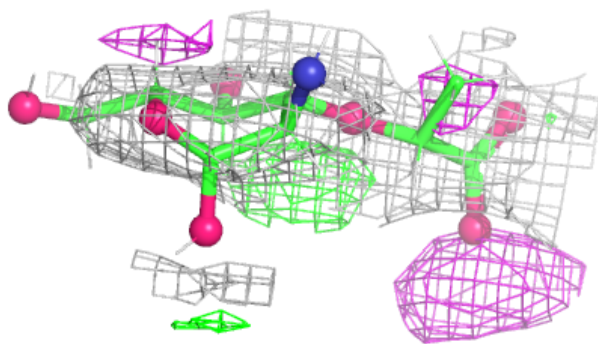
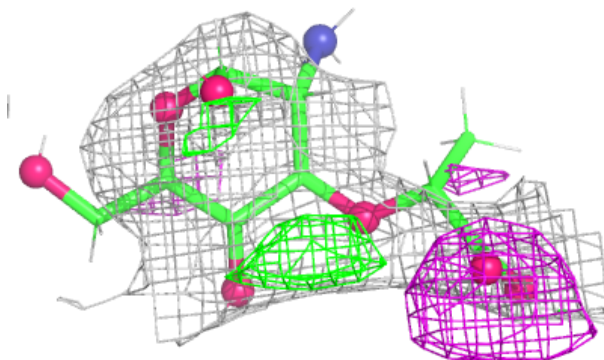
**Electron density around 1W8 B 1676:**

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



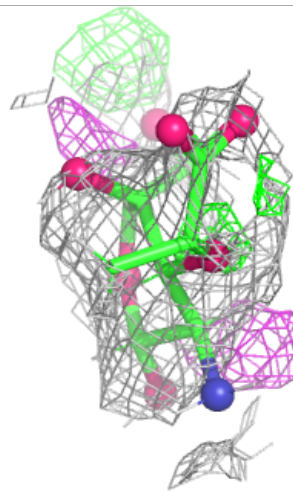
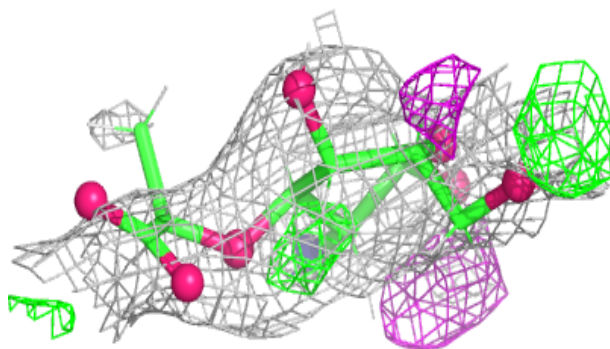
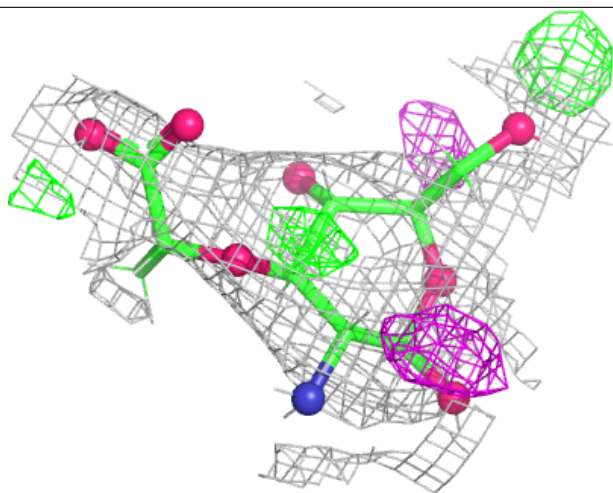
Electron density around MUR B 1677:

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



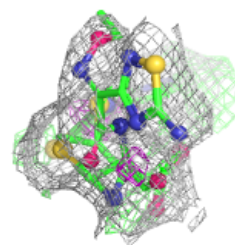
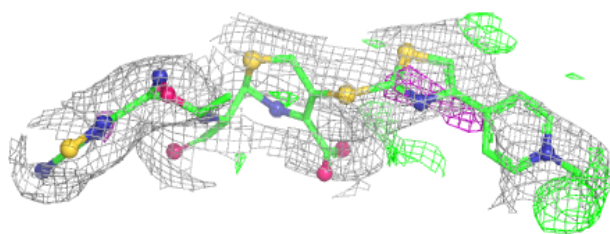
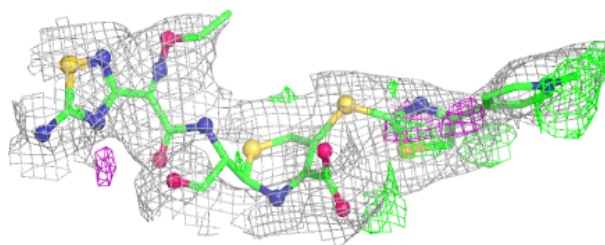
Electron density around MUR A 1677:

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

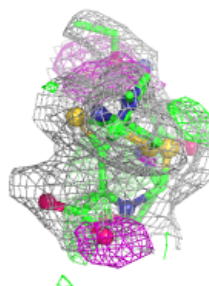
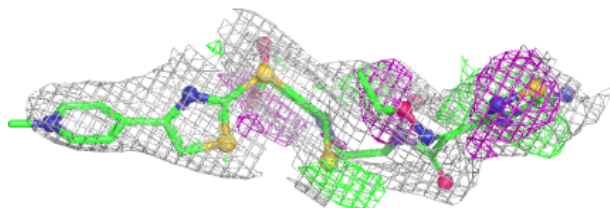
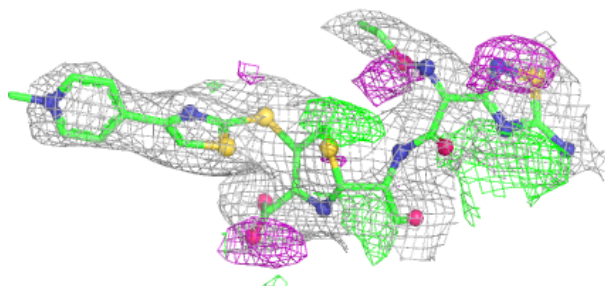


Electron density around AI8 B 1403:

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

**Electron density around AI8 A 1403:**

$2mF_o-DF_c$ (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.