



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:26 AM UTC

PDB ID : 7H7U / pdb_00007h7u
Title : Group deposition for crystallographic fragment screening of Chikungunya virus nsP3 macrodomain – Crystal structure of Chikungunya virus nsP3 macrodomain in complex with POB0112 (CHIKV_MacB-x0997)
Authors : Aschenbrenner, J.C.; Fairhead, M.; Godoy, A.S.; Balcomb, B.H.; Capkin, E.; Chandran, A.V.; Dolci, I.; Golding, M.; Koekemoer, L.; Lithgo, R.M.; Marples, P.G.; Ni, X.; Oliva, G.; Thompson, W.; Tomlinson, C.W.E.; Wild, C.; Winokan, M.; Xavier, M.-A.E.; Fearon, D.; von Delft, F.
Deposited on : 2024-04-26
Resolution : 1.40 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

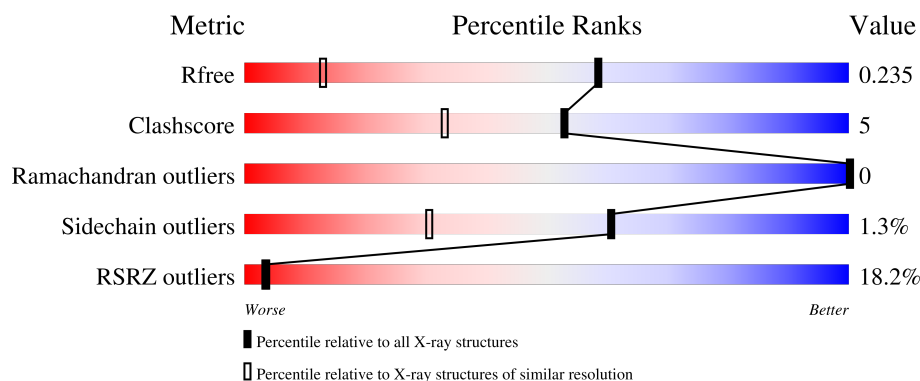
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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	163	8% 89% 10%
1	B	163	12% 90% 10%
1	C	163	35% 88% 11%

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Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	D	163	18% 90% 8%

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	DMS	A	202	-	-	X	-
2	DMS	B	201	-	-	-	X
2	DMS	C	303	-	-	-	X
3	TRS	D	202	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5859 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 Non-structural protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	163	Total	C	N	O	S	0	2	0
			1262	787	220	245	10			
1	B	163	Total	C	N	O	S	0	2	0
			1263	787	220	247	9			
1	C	163	Total	C	N	O	S	0	4	0
			1283	799	226	249	9			
1	D	159	Total	C	N	O	S	0	3	0
			1246	777	217	243	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q8JUX6
A	-1	ALA	-	expression tag	UNP Q8JUX6
A	0	MET	-	expression tag	UNP Q8JUX6
A	77	THR	SER	conflict	UNP Q8JUX6
B	-2	GLY	-	expression tag	UNP Q8JUX6
B	-1	ALA	-	expression tag	UNP Q8JUX6
B	0	MET	-	expression tag	UNP Q8JUX6
B	77	THR	SER	conflict	UNP Q8JUX6
C	-2	GLY	-	expression tag	UNP Q8JUX6
C	-1	ALA	-	expression tag	UNP Q8JUX6
C	0	MET	-	expression tag	UNP Q8JUX6
C	77	THR	SER	conflict	UNP Q8JUX6
D	-2	GLY	-	expression tag	UNP Q8JUX6
D	-1	ALA	-	expression tag	UNP Q8JUX6
D	0	MET	-	expression tag	UNP Q8JUX6
D	77	THR	SER	conflict	UNP Q8JUX6

- Molecule 2 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



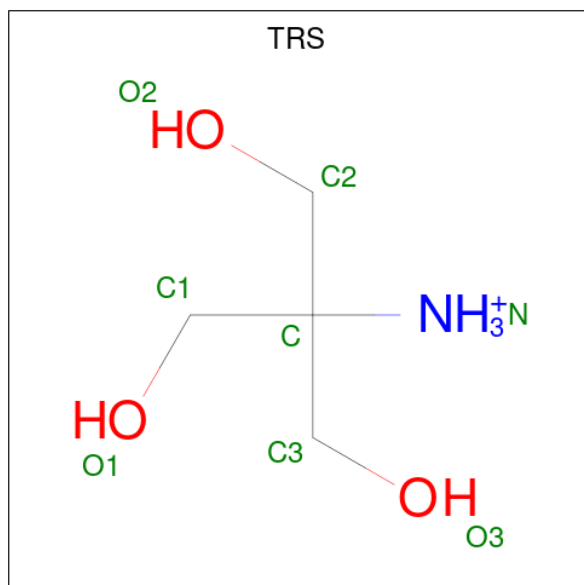
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		
2	C	1	Total	C	O	S	0	0
			4	2	1	1		
2	D	1	Total	C	O	S	0	0
			4	2	1	1		
2	D	1	Total	C	O	S	0	0
			4	2	1	1		
2	D	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).

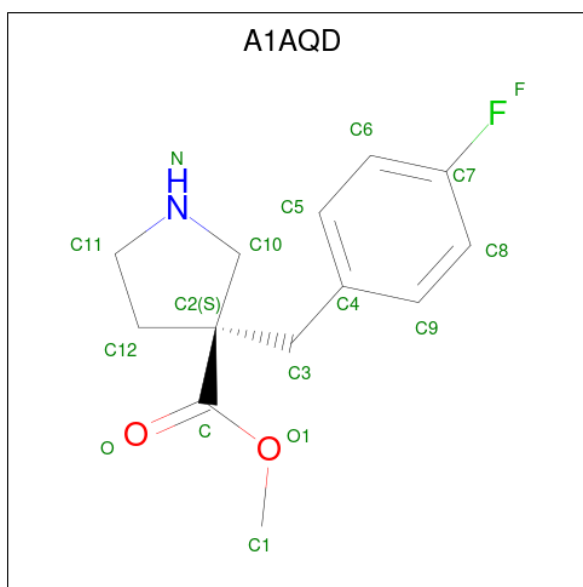


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		
3	D	1	Total	C	N	O	0	0
			8	4	1	3		

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

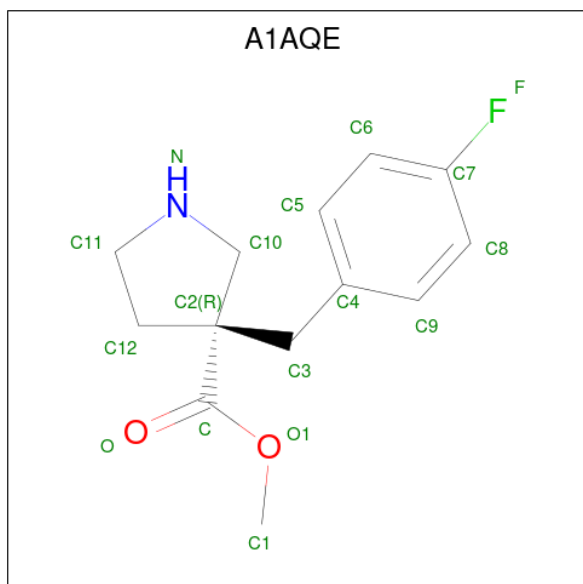
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Cl	0	0
			3	3		
4	B	2	Total	Cl	0	0
			2	2		
4	C	2	Total	Cl	0	0
			2	2		
4	D	2	Total	Cl	0	0
			2	2		

- Molecule 5 is methyl (3S)-3-[(4-fluorophenyl)methyl]pyrrolidine-3-carboxylate (CCD ID: A1AQD) (formula: $C_{13}H_{16}FNO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	F	N	O	0	0
			17	13	1	1	2		

- Molecule 6 is methyl (3R)-3-[(4-fluorophenyl)methyl]pyrrolidine-3-carboxylate (CCD ID: A1AQE) (formula: C₁₃H₁₆FNO₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	F	N	O	0	0
			17	13	1	1	2		

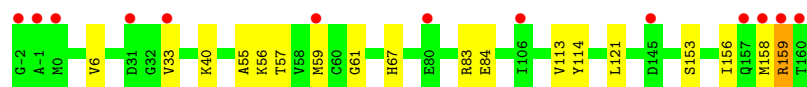
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	211	Total 211	O 211	0	0
7	B	165	Total 165	O 165	0	0
7	C	156	Total 156	O 156	0	0
7	D	154	Total 154	O 154	0	0

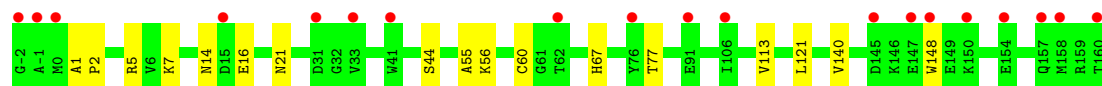
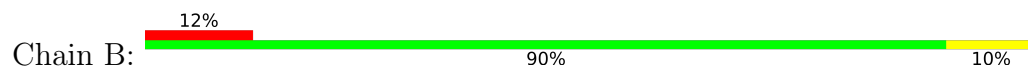
3 Residue-property plots [i](#)

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.

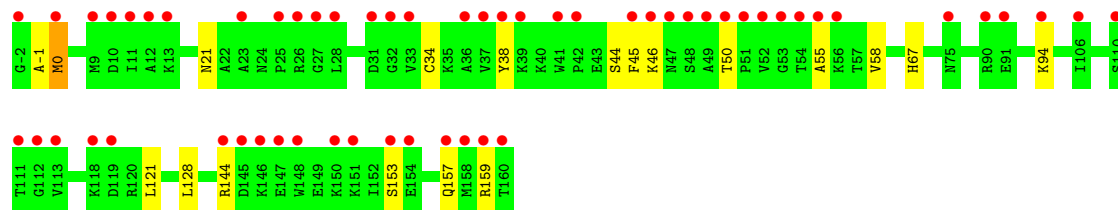
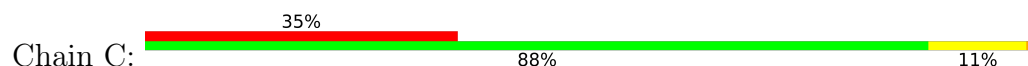
- Molecule 1: Non-structural protein 3



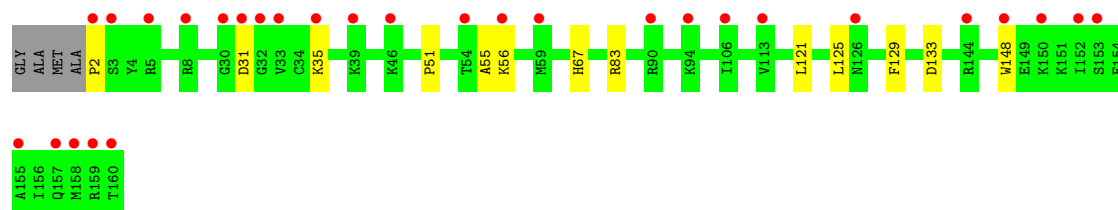
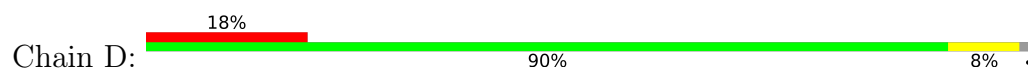
- Molecule 1: Non-structural protein 3



- Molecule 1: Non-structural protein 3



- Molecule 1: Non-structural protein 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	87.33Å 87.33Å 85.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	75.63 – 1.40 75.63 – 1.40	Depositor EDS
% Data completeness (in resolution range)	98.0 (75.63-1.40) 98.0 (75.63-1.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC5	Depositor
R, R_{free}	0.185 , 0.216 0.208 , 0.235	Depositor DCC
R_{free} test set	7115 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.028 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5859	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.30 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.9365e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, A1AQD, TRS, DMS, A1AQE

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	1.03	0/1285	1.14	0/1739
1	B	1.07	1/1286 (0.1%)	1.22	1/1741 (0.1%)
1	C	1.09	0/1306	1.27	1/1766 (0.1%)
1	D	1.06	0/1269	1.26	0/1717
All	All	1.06	1/5146 (0.0%)	1.23	2/6963 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	77	THR	C-O	5.62	1.31	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	50	THR	CB-CA-C	7.48	120.09	109.92
1	B	21	ASN	OD1-CG-ND2	5.22	127.82	122.60

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	1262	0	1256	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1263	0	1253	12	0
1	C	1283	0	1277	12	0
1	D	1246	0	1236	9	0
2	A	32	0	48	13	0
2	B	8	0	12	2	0
2	C	4	0	6	0	0
2	D	16	0	24	1	0
3	A	8	0	12	0	0
3	D	8	0	12	0	0
4	A	3	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	B	17	0	0	0	0
6	C	17	0	0	0	0
7	A	211	0	0	3	0
7	B	165	0	0	2	0
7	C	156	0	0	1	0
7	D	154	0	0	4	0
All	All	5859	0	5136	52	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 5.

All (52) 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:D:35:LYS:NZ	7:D:301:HOH:O	2.06	0.88
1:B:113:VAL:CG2	2:B:202:DMS:H21	2.16	0.75
1:A:113:VAL:CG2	2:A:202:DMS:H21	2.16	0.74
2:A:201:DMS:H13	7:A:458:HOH:O	1.94	0.67
1:D:121:LEU:HD12	1:D:148:TRP:CD2	2.31	0.66
1:A:6:VAL:HG12	2:A:207:DMS:S	2.36	0.65
1:A:59[A]:MET:HG2	2:A:205:DMS:H12	1.77	0.65
1:C:0:MET:HE1	7:D:378:HOH:O	1.96	0.65
1:B:5:ARG:HD3	7:B:377:HOH:O	1.98	0.62
1:A:113:VAL:HG23	2:A:202:DMS:H21	1.84	0.59
1:B:7:LYS:HE2	1:B:140:VAL:HG11	1.86	0.58
1:A:40:LYS:NZ	2:A:201:DMS:H12	2.18	0.57
1:A:40:LYS:CE	2:A:201:DMS:H12	2.35	0.57
1:A:113:VAL:CG2	2:A:202:DMS:C2	2.85	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:TYR:HA	1:C:45:PHE:CE1	2.43	0.53
1:C:121:LEU:C	1:C:121:LEU:HD23	2.33	0.53
1:D:56:LYS:NZ	7:D:302:HOH:O	2.39	0.53
1:B:121:LEU:HD12	1:B:148:TRP:CG	2.45	0.51
1:C:21:ASN:OD1	1:C:34:CYS:HA	2.11	0.51
1:B:113:VAL:HG23	2:B:202:DMS:H21	1.93	0.51
1:D:125:LEU:HG	1:D:129:PHE:CE2	2.46	0.50
1:A:56:LYS:HE2	7:A:416:HOH:O	2.12	0.50
1:B:121:LEU:C	1:B:121:LEU:HD23	2.38	0.49
1:A:61:GLY:N	2:A:212:DMS:H23	2.27	0.49
1:A:83:ARG:NH2	1:A:84:GLU:OE2	2.46	0.48
1:A:153:SER:OG	2:A:207:DMS:H11	2.14	0.47
1:C:58:VAL:HG22	7:C:483:HOH:O	2.13	0.47
1:D:121:LEU:C	1:D:121:LEU:HD23	2.39	0.47
1:C:44:SER:O	1:C:58:VAL:HB	2.15	0.46
1:C:153:SER:O	1:C:157:GLN:HG2	2.15	0.46
1:A:156:ILE:O	1:A:159:ARG:HG3	2.15	0.46
1:D:121:LEU:HD12	1:D:148:TRP:CG	2.50	0.46
1:C:157:GLN:NE2	1:C:157:GLN:HA	2.32	0.45
2:D:204:DMS:H13	7:D:382:HOH:O	2.17	0.45
1:B:44:SER:HB3	1:B:60:CYS:SG	2.57	0.44
1:D:2:PRO:HG3	1:D:133:ASP:HA	2.00	0.44
1:A:121:LEU:C	1:A:121:LEU:HD23	2.43	0.44
1:D:55:ALA:HA	1:D:67:HIS:O	2.18	0.43
1:A:158:MET:HB3	7:A:323:HOH:O	2.18	0.43
1:A:57:THR:O	2:A:205:DMS:H13	2.19	0.43
1:B:55:ALA:HA	1:B:67:HIS:O	2.18	0.43
1:B:121:LEU:HD12	1:B:148:TRP:CD2	2.53	0.43
1:C:94:LYS:HE3	1:C:94:LYS:HB3	1.76	0.43
1:C:55:ALA:HA	1:C:67:HIS:O	2.19	0.42
1:A:55:ALA:HA	1:A:67:HIS:O	2.19	0.42
1:B:56:LYS:NZ	7:B:305:HOH:O	2.52	0.42
1:A:114:TYR:CZ	2:A:202:DMS:H13	2.55	0.41
1:B:14:ASN:HB2	1:B:16:GLU:OE2	2.21	0.41
1:C:128:LEU:C	1:C:128:LEU:HD23	2.46	0.41
1:B:1:ALA:O	1:B:2:PRO:C	2.64	0.41
1:A:33:VAL:HG23	2:A:206:DMS:H13	2.03	0.40
1:C:-1:ALA:O	1:D:51:PRO:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	163/163 (100%)	162 (99%)	1 (1%)	0	100	100
1	B	163/163 (100%)	162 (99%)	1 (1%)	0	100	100
1	C	165/163 (101%)	164 (99%)	1 (1%)	0	100	100
1	D	160/163 (98%)	159 (99%)	1 (1%)	0	100	100
All	All	651/652 (100%)	647 (99%)	4 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	136/134 (102%)	135 (99%)	1 (1%)	76	52
1	B	136/134 (102%)	136 (100%)	0	100	100
1	C	138/134 (103%)	134 (97%)	4 (3%)	37	9
1	D	136/134 (102%)	134 (98%)	2 (2%)	57	26
All	All	546/536 (102%)	539 (99%)	7 (1%)	61	30

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	ARG
1	C	0	MET

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Mol	Chain	Res	Type
1	C	46	LYS
1	C	144	ARG
1	C	159	ARG
1	D	31	ASP
1	D	83	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	GLN
1	B	47	ASN
1	C	157	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 9 are monoatomic - leaving 19 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	$\# Z > 2$
2	DMS	C	303	-	3,3,3	0.21	0	3,3,3	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DMS	D	204	-	3,3,3	0.21	0	3,3,3	0.11	0
3	TRS	A	204	-	7,7,7	0.35	0	9,9,9	0.57	0
2	DMS	A	203	-	3,3,3	0.18	0	3,3,3	0.09	0
2	DMS	A	207	-	3,3,3	0.56	0	3,3,3	0.28	0
5	A1AQD	B	205	-	18,18,18	0.24	0	17,25,25	0.50	0
2	DMS	B	201	-	3,3,3	0.21	0	3,3,3	0.10	0
2	DMS	A	202	-	3,3,3	0.28	0	3,3,3	0.40	0
2	DMS	D	205	-	3,3,3	0.22	0	3,3,3	0.04	0
2	DMS	B	202	-	3,3,3	0.25	0	3,3,3	0.48	0
2	DMS	A	205	-	3,3,3	0.27	0	3,3,3	0.15	0
2	DMS	D	201	-	3,3,3	0.26	0	3,3,3	0.12	0
2	DMS	A	206	-	3,3,3	0.26	0	3,3,3	0.04	0
2	DMS	A	201	-	3,3,3	0.64	0	3,3,3	0.31	0
2	DMS	A	212	-	3,3,3	0.26	0	3,3,3	0.25	0
2	DMS	A	211	-	3,3,3	0.23	0	3,3,3	0.11	0
3	TRS	D	202	-	7,7,7	0.17	0	9,9,9	0.26	0
6	A1AQE	C	304	-	18,18,18	0.17	0	17,25,25	0.35	0
2	DMS	D	203	-	3,3,3	0.48	0	3,3,3	0.19	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
5	A1AQD	B	205	-	-	2/13/22/22	0/2/2/2
6	A1AQE	C	304	-	-	0/13/22/22	0/2/2/2
3	TRS	D	202	-	-	2/9/9/9	-
3	TRS	A	204	-	-	0/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	205	A1AQD	C2-C-O1-C1
5	B	205	A1AQD	O-C-O1-C1
3	D	202	TRS	C1-C-C3-O3
3	D	202	TRS	N-C-C3-O3

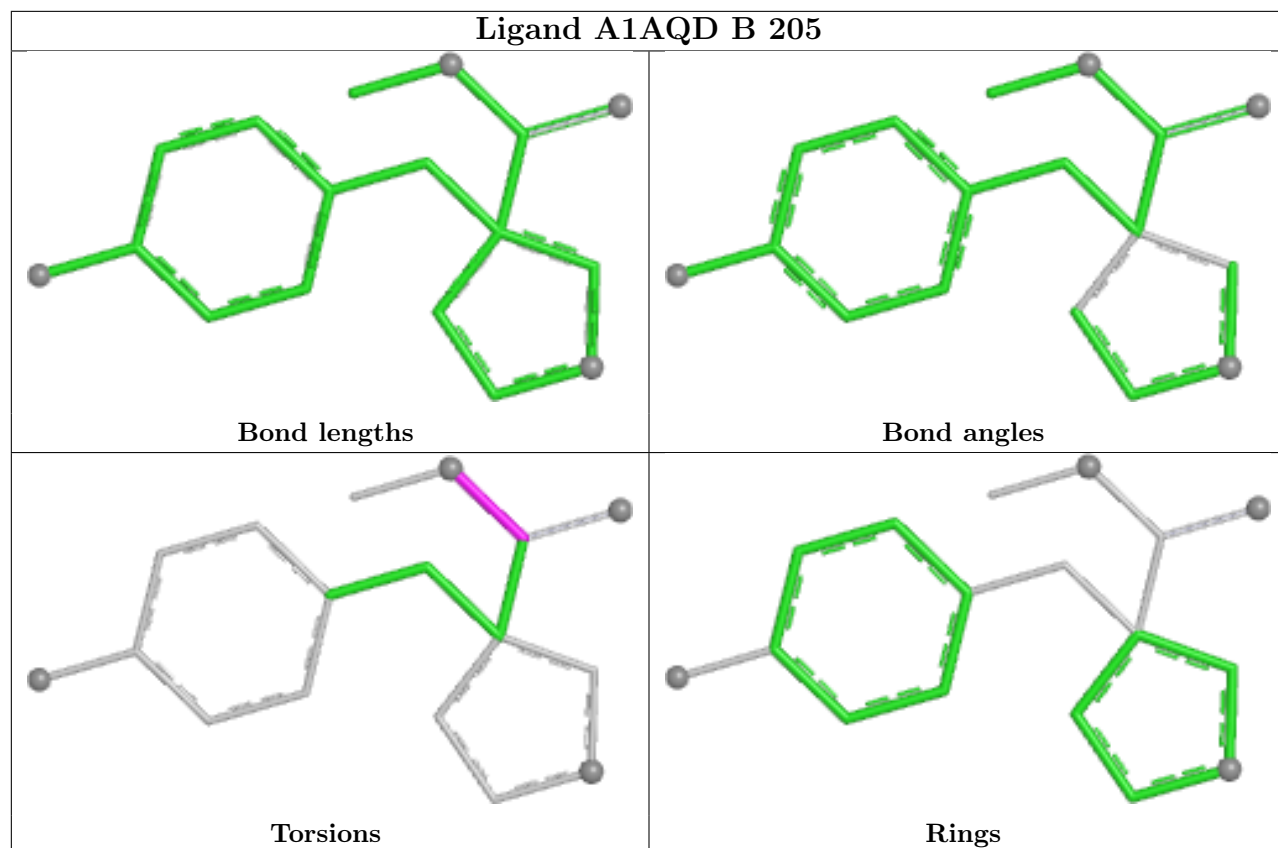
There are no ring outliers.

8 monomers are involved in 16 short contacts:

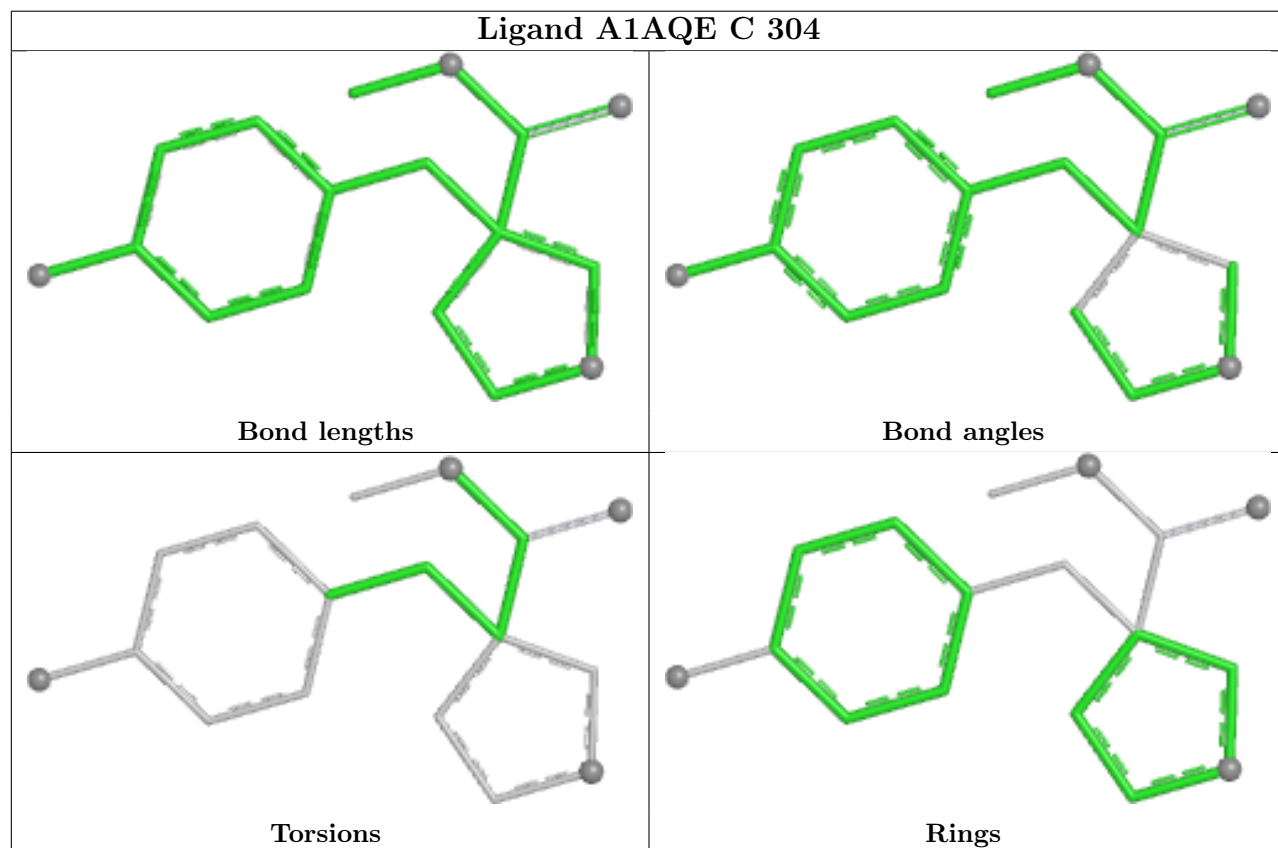
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	204	DMS	1	0
2	A	207	DMS	2	0
2	A	202	DMS	4	0
2	B	202	DMS	2	0
2	A	205	DMS	2	0
2	A	206	DMS	1	0
2	A	201	DMS	3	0
2	A	212	DMS	1	0

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 A1AQD B 205



Ligand A1AQE C 304



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	163/163 (100%)	0.40	13 (7%)	18 18	4, 19, 32, 41	9 (5%)
1	B	163/163 (100%)	0.88	19 (11%)	9 9	5, 21, 33, 49	14 (8%)
1	C	163/163 (100%)	1.83	57 (34%)	1 1	7, 22, 38, 52	35 (21%)
1	D	159/163 (97%)	1.25	29 (18%)	3 3	5, 23, 42, 59	15 (9%)
All	All	648/652 (99%)	1.09	118 (18%)	3 3	4, 21, 36, 59	73 (11%)

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	106[A]	ILE	11.5
1	A	106[A]	ILE	10.5
1	D	160	THR	10.4
1	B	76	TYR	9.8
1	D	106[A]	ILE	9.4
1	B	148	TRP	9.3
1	D	3[A]	SER	9.1
1	D	158	MET	9.0
1	D	159	ARG	8.4
1	B	160	THR	8.1
1	A	160	THR	8.0
1	C	113	VAL	7.5
1	A	158	MET	7.4
1	A	145	ASP	7.2
1	B	158	MET	6.8
1	A	159	ARG	6.8
1	D	113	VAL	6.7
1	C	46	LYS	6.6
1	C	158	MET	6.4
1	B	33	VAL	6.3
1	C	112	GLY	6.3

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Mol	Chain	Res	Type	RSRZ
1	C	33	VAL	6.1
1	C	147[A]	GLU	6.0
1	A	80	GLU	5.9
1	C	111	THR	5.8
1	C	0	MET	5.7
1	D	54	THR	5.7
1	C	47	ASN	5.7
1	A	157	GLN	5.7
1	A	31	ASP	5.6
1	C	144	ARG	5.6
1	C	153	SER	5.5
1	D	56	LYS	5.5
1	C	151	LYS	5.5
1	C	55	ALA	5.5
1	B	145	ASP	5.4
1	C	145	ASP	5.4
1	D	59[A]	MET	5.3
1	C	54	THR	5.2
1	D	46	LYS	5.2
1	C	106[A]	ILE	5.2
1	C	42	PRO	5.1
1	C	38	TYR	5.1
1	C	48	SER	5.0
1	D	39	LYS	5.0
1	C	9	MET	5.0
1	C	53	GLY	5.0
1	C	13[A]	LYS	4.9
1	D	35	LYS	4.9
1	C	160	THR	4.8
1	C	150	LYS	4.8
1	C	118	LYS	4.7
1	C	32	GLY	4.7
1	D	90	ARG	4.6
1	D	31	ASP	4.6
1	B	91[A]	GLU	4.6
1	B	147	GLU	4.6
1	B	31	ASP	4.4
1	A	59[A]	MET	4.4
1	B	150	LYS	4.3
1	C	10	ASP	4.3
1	C	157	GLN	4.3
1	C	119	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	56	LYS	4.1
1	C	159	ARG	4.1
1	C	154	GLU	4.1
1	B	15	ASP	4.0
1	C	36	ALA	4.0
1	D	94	LYS	4.0
1	C	90[A]	ARG	3.8
1	C	110	SER	3.7
1	B	157	GLN	3.7
1	B	154	GLU	3.6
1	C	-2	GLY	3.6
1	C	51	PRO	3.5
1	C	12	ALA	3.4
1	C	31	ASP	3.4
1	C	52	VAL	3.3
1	C	25	PRO	3.3
1	C	75	ASN	3.3
1	B	-2	GLY	3.2
1	D	2	PRO	3.2
1	C	49	ALA	3.1
1	B	0	MET	3.1
1	C	39	LYS	3.0
1	C	94	LYS	3.0
1	C	26	ARG	2.9
1	D	157	GLN	2.9
1	C	45	PHE	2.9
1	D	155	ALA	2.8
1	C	28	LEU	2.8
1	C	23	ALA	2.6
1	C	37	VAL	2.6
1	D	148	TRP	2.6
1	A	-2	GLY	2.6
1	A	0	MET	2.6
1	B	-1	ALA	2.3
1	C	41	TRP	2.3
1	D	144	ARG	2.3
1	C	91	GLU	2.3
1	D	32	GLY	2.2
1	A	33	VAL	2.2
1	D	152	ILE	2.2
1	B	62	THR	2.2
1	D	153	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	-1	ALA	2.1
1	C	27	GLY	2.1
1	D	150	LYS	2.1
1	C	148	TRP	2.1
1	B	41	TRP	2.1
1	D	30	GLY	2.1
1	C	50	THR	2.0
1	C	146	LYS	2.0
1	C	11	ILE	2.0
1	D	126	ASN	2.0
1	D	5	ARG	2.0
1	D	8	ARG	2.0
1	D	33	VAL	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(Å ²)	Q<0.9
2	DMS	C	303	4/4	0.49	0.67	129,132,133,134	4
5	A1AQD	B	205	17/17	0.59	0.30	41,47,51,52	17
2	DMS	D	201	4/4	0.69	0.28	42,44,45,46	4
3	TRS	D	202	8/8	0.70	0.60	178,181,183,183	8
2	DMS	A	207	4/4	0.72	0.22	27,43,45,58	0
2	DMS	A	206	4/4	0.73	0.31	78,85,88,88	0
6	A1AQE	C	304	17/17	0.74	0.23	38,42,43,46	17
2	DMS	B	201	4/4	0.75	0.56	77,79,79,80	4
3	TRS	A	204	8/8	0.78	0.15	38,46,51,57	0
2	DMS	A	201	4/4	0.79	0.20	42,44,52,57	0

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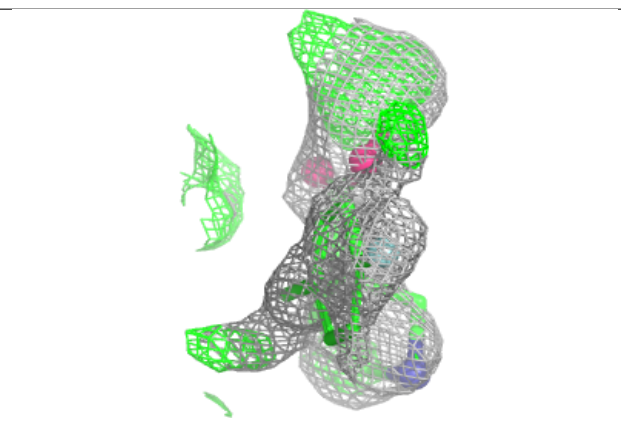
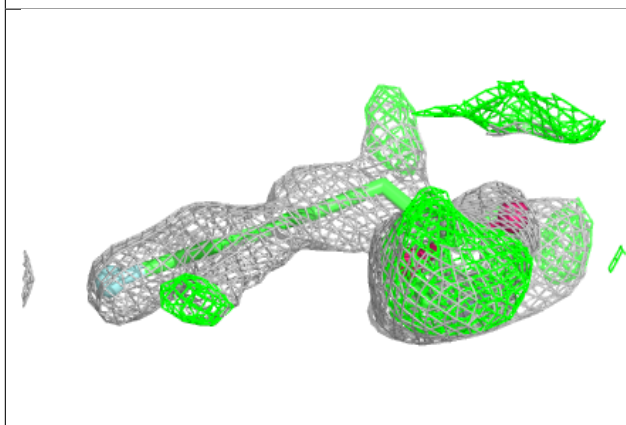
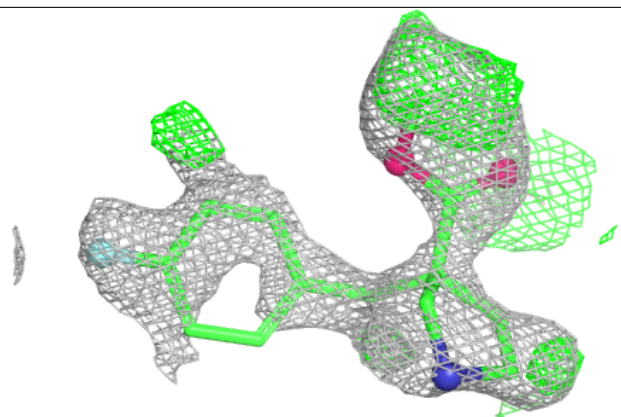
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DMS	A	212	4/4	0.81	0.22	64,70,74,74	0
2	DMS	A	203	4/4	0.83	0.19	51,55,64,64	0
2	DMS	D	205	4/4	0.84	0.26	43,53,53,56	4
2	DMS	D	204	4/4	0.86	0.49	69,73,74,75	4
2	DMS	A	205	4/4	0.86	0.17	46,58,60,69	0
2	DMS	D	203	4/4	0.87	0.16	37,38,41,43	0
2	DMS	A	211	4/4	0.90	0.16	26,30,30,32	4
4	CL	C	302	1/1	0.90	0.15	48,48,48,48	0
4	CL	C	301	1/1	0.91	0.12	41,41,41,41	0
2	DMS	A	202	4/4	0.91	0.15	36,37,39,44	0
2	DMS	B	202	4/4	0.93	0.15	46,46,49,51	0
4	CL	D	206	1/1	0.95	0.08	39,39,39,39	0
4	CL	A	210	1/1	0.97	0.10	27,27,27,27	0
4	CL	D	207	1/1	0.98	0.07	26,26,26,26	0
4	CL	B	203	1/1	0.98	0.05	27,27,27,27	0
4	CL	A	209	1/1	0.98	0.05	22,22,22,22	0
4	CL	A	208	1/1	0.99	0.03	20,20,20,20	0
4	CL	B	204	1/1	0.99	0.03	19,19,19,19	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.

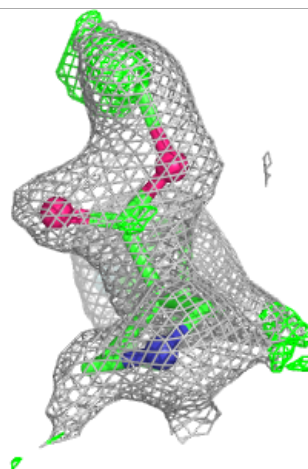
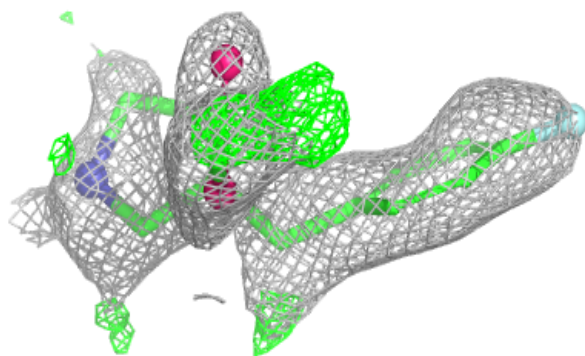
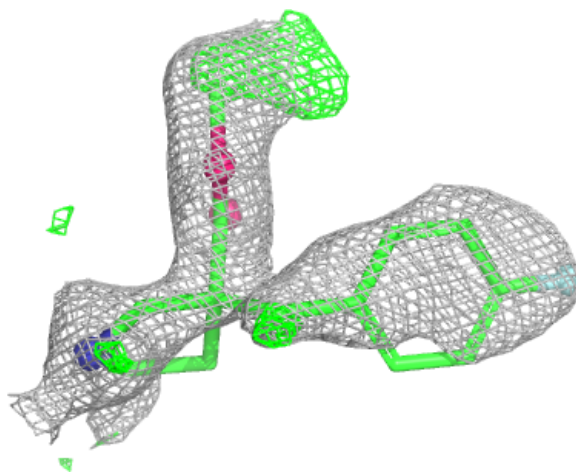
Electron density around A1AQD B 205:

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



Electron density around A1AQE C 304:

$2mF_o-DF_c$ (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.