



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 05:59 AM BST

PDB ID : 4ARA
Title : Mus musculus Acetylcholinesterase in complex with (R)-C5685 at 2.5 Å resolution.
Authors : Berg, L.; Niemiec, M.S.; Qian, W.; Andersson, C.D.; WittungStafshede, P.; Ekstrom, F.; Linusson, A.
Deposited on : 2012-04-23
Resolution : 2.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

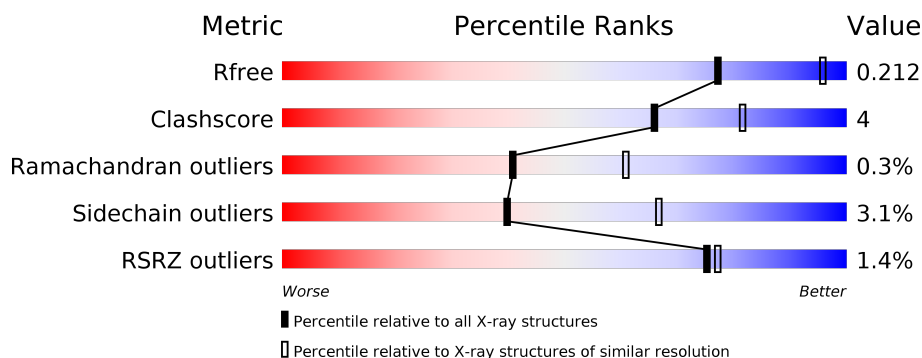
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	548	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 88% 9% .. </div> </div>
1	B	548	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 85% 11% .. </div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9217 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.

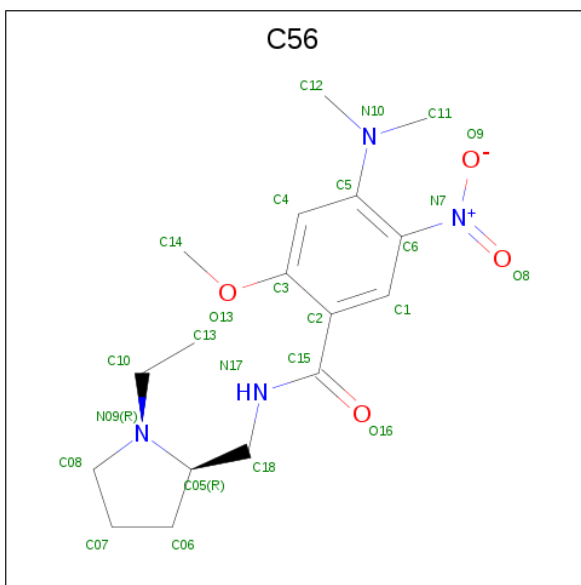
- Molecule 1 is a protein called ACETYLCHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	2	0
			4173	2680	722	757	14			
1	B	533	Total	C	N	O	S	0	2	0
			4162	2675	718	755	14			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	544	ALA	-	expression tag	UNP P21836
A	545	THR	-	expression tag	UNP P21836
A	546	GLU	-	expression tag	UNP P21836
A	547	ALA	-	expression tag	UNP P21836
A	548	PRO	-	expression tag	UNP P21836
B	544	ALA	-	expression tag	UNP P21836
B	545	THR	-	expression tag	UNP P21836
B	546	GLU	-	expression tag	UNP P21836
B	547	ALA	-	expression tag	UNP P21836
B	548	PRO	-	expression tag	UNP P21836

- Molecule 2 is 4-(DIMETHYLAMINO)-N-{|(2R)-1-ETHYLPYRROLIDIN-2-YL|METHYL}-2-METHOXY-5-NITROBENZAMIDE (three-letter code: C56) (formula: C₁₇H₂₆N₄O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	1
			50	34	8	8		
2	B	1	Total	C	N	O	0	1
			50	34	8	8		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



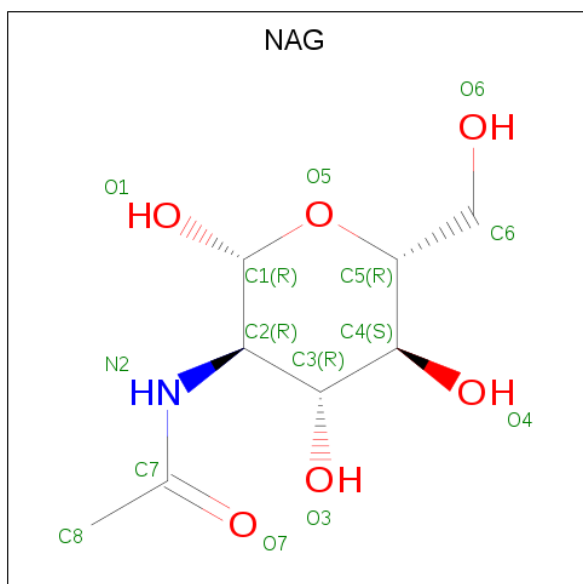
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

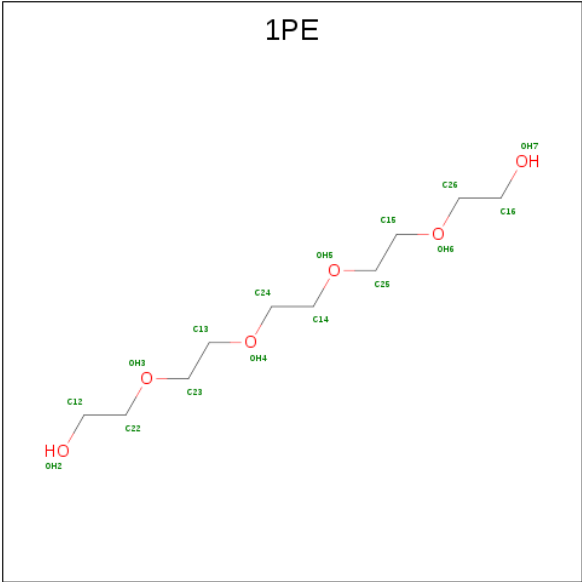
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	C O	0	0
			16	10 6		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cl	0	0
			1	1		

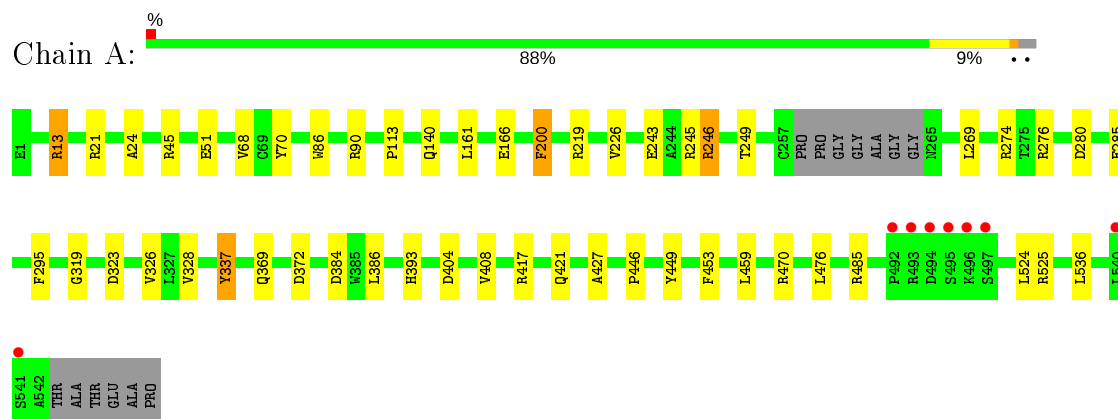
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	349	Total	O	0	0
			349	349		
8	B	279	Total	O	0	0
			279	279		

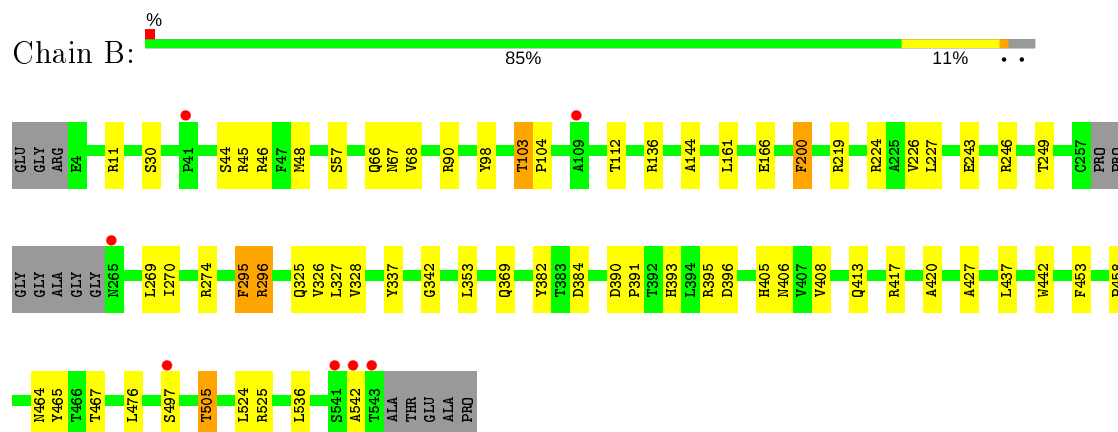
3 Residue-property plots [i](#)

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: ACETYLCHOLINESTERASE



• Molecule 1: ACETYLCHOLINESTERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.76Å 112.01Å 227.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.86 – 2.50 28.86 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (28.86-2.50) 99.8 (28.86-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.79 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.183 , 0.222 0.175 , 0.212	Depositor DCC
R_{free} test set	1416 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	40.5	Xtriage
Anisotropy	0.808	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9217	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: C56, NAG, CL, EDO, 1PE, PEG

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	0.26	0/4300	0.45	0/5880
1	B	0.26	0/4287	0.45	0/5863
All	All	0.26	0/8587	0.45	0/11743

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4173	0	4043	23	1
1	B	4162	0	4029	41	1
2	A	50	0	52	3	0
2	B	50	0	52	6	0
3	A	21	0	30	1	0
3	B	42	0	60	3	0
4	A	20	0	30	0	0
4	B	12	0	18	1	0
5	A	28	0	26	1	0
5	B	14	0	13	0	0
6	B	16	0	22	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	1	0	0	0	0
8	A	349	0	0	3	0
8	B	279	0	0	4	0
All	All	9217	0	8375	67	1

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 (67) 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:1553:NAG:O4	8:A:2349:HOH:O	2.00	0.72
1:B:390:ASP:OD2	1:B:393[A]:HIS:ND1	2.26	0.68
1:A:276[A]:ARG:NH2	1:A:280:ASP:OD2	2.28	0.67
1:B:296:ARG:NH2	1:B:406:ASN:OD1	2.29	0.65
1:B:30:SER:HB2	1:B:103:THR:HG22	1.79	0.65
1:A:219:ARG:NH2	8:A:2188:HOH:O	2.29	0.64
1:A:459:LEU:HD12	1:A:470:ARG:HG2	1.79	0.63
1:B:382:TYR:HA	3:B:1548:PEG:H12	1.81	0.62
6:B:1546:1PE:OH7	8:B:2266:HOH:O	2.15	0.61
1:B:295:PHE:N	2:B:600[B]:C56:O8	2.32	0.59
1:B:44:SER:HA	1:B:274:ARG:HD2	1.84	0.58
1:B:295:PHE:N	2:B:600[A]:C56:O8	2.33	0.58
1:B:161:LEU:HD11	1:B:269:LEU:HD23	1.85	0.58
1:B:68:VAL:HG23	1:B:90:ARG:HB2	1.86	0.58
1:B:112:THR:HG23	3:B:1545:PEG:H32	1.86	0.57
1:A:45:ARG:NH1	1:A:51:GLU:OE1	2.36	0.57
1:B:408:VAL:HG11	1:B:525:ARG:HG3	1.89	0.55
1:A:319:GLY:O	1:A:421:GLN:NE2	2.39	0.55
1:B:337[A]:TYR:OH	2:B:600[A]:C56:H081	2.07	0.54
1:B:353:LEU:HB3	1:B:391:PRO:HB2	1.89	0.54
1:B:464:ASN:ND2	8:B:2233:HOH:O	2.40	0.54
1:B:243:GLU:OE2	1:B:246:ARG:NH1	2.41	0.53
1:A:285:GLU:OE2	8:A:2223:HOH:O	2.19	0.51
1:A:68:VAL:HG23	1:A:90:ARG:HB2	1.93	0.51
1:B:161:LEU:HD12	1:B:270:ILE:HD11	1.92	0.51
1:B:337[A]:TYR:HE1	2:B:600[A]:C56:H181	1.78	0.48
1:A:245:ARG:O	1:A:249:THR:HG23	2.14	0.47
1:B:337[B]:TYR:CE1	2:B:600[B]:C56:H182	2.50	0.47
1:A:24:ALA:HB3	1:A:140:GLN:HG3	1.96	0.47
1:A:243:GLU:OE2	1:A:246:ARG:NH1	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:ARG:NH1	1:B:396:ASP:OD1	2.42	0.47
1:B:525:ARG:NH2	8:B:2187:HOH:O	2.48	0.47
1:B:67:ASN:ND2	8:B:2058:HOH:O	2.45	0.47
1:A:446:PRO:HG2	1:A:449:TYR:CD2	2.50	0.47
1:A:113:PRO:HG2	1:A:485:ARG:HG2	1.96	0.46
1:B:369:GLN:HE22	1:B:405:HIS:CE1	2.33	0.46
1:B:226:VAL:HG22	1:B:327:LEU:HB3	1.98	0.45
1:B:413:GLN:O	1:B:417:ARG:HG2	2.16	0.45
1:B:48:MET:SD	1:B:166:GLU:HA	2.56	0.45
1:B:144:ALA:HA	3:B:1545:PEG:H41	1.99	0.45
1:A:323:ASP:HB2	3:A:1547:PEG:H22	1.99	0.45
1:B:453:PHE:HB3	1:B:476:LEU:HD12	1.99	0.44
1:A:417:ARG:HA	1:A:417:ARG:HD2	1.81	0.44
1:B:66:GLN:HG3	1:B:98:TYR:CD2	2.52	0.44
1:A:161:LEU:HD11	1:A:269:LEU:HD22	1.99	0.44
1:B:536:LEU:HD23	1:B:536:LEU:HA	1.84	0.43
1:B:328:VAL:O	1:B:427:ALA:HA	2.19	0.43
1:B:337[A]:TYR:CE1	2:B:600[A]:C56:H181	2.54	0.43
1:A:328:VAL:O	1:A:427:ALA:HA	2.18	0.43
1:B:200:PHE:CB	1:B:226:VAL:HB	2.48	0.42
1:A:166:GLU:HB3	1:A:274:ARG:HH22	1.83	0.42
1:A:86:TRP:CG	2:A:600[B]:C56:H062	2.54	0.42
1:B:224:ARG:HG2	1:B:325:GLN:HB2	2.01	0.42
1:A:384:ASP:HB2	1:A:393:HIS:CE1	2.54	0.42
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.55	0.42
1:A:404:ASP:HA	1:A:408:VAL:HB	2.01	0.42
1:B:103:THR:HG23	1:B:104:PRO:O	2.19	0.42
2:A:600[B]:C56:H102	2:A:600[B]:C56:C15	2.50	0.42
1:A:337[A]:TYR:OH	2:A:600[A]:C56:H061	2.20	0.41
1:B:219:ARG:HD3	4:B:1549:EDO:H21	2.00	0.41
1:B:384:ASP:HB2	1:B:393[B]:HIS:NE2	2.36	0.41
1:B:420:ALA:HB2	1:B:505:THR:HG21	2.01	0.41
1:B:46:ARG:HB3	1:B:274:ARG:HG2	2.03	0.40
1:A:200:PHE:CB	1:A:226:VAL:HB	2.51	0.40
1:B:227:LEU:HB2	1:B:328:VAL:HG12	2.03	0.40
1:B:395:ARG:CZ	1:B:442:TRP:HB2	2.52	0.40
1:A:453:PHE:HB3	1:A:476:LEU:HD12	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ARG:NH1	1:B:57:SER:O[2_555]	2.16	0.04

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	533/548 (97%)	515 (97%)	18 (3%)	0	100	100
1	B	531/548 (97%)	512 (96%)	16 (3%)	3 (1%)	25	43
All	All	1064/1096 (97%)	1027 (96%)	34 (3%)	3 (0%)	41	61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	497	SER
1	B	542	ALA
1	B	342	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	436/446 (98%)	421 (97%)	15 (3%)	37	63
1	B	436/446 (98%)	423 (97%)	13 (3%)	41	68
All	All	872/892 (98%)	844 (97%)	28 (3%)	40	65

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	21	ARG
1	A	70	TYR
1	A	200	PHE
1	A	246	ARG
1	A	295	PHE
1	A	326	VAL
1	A	337[A]	TYR
1	A	337[B]	TYR
1	A	369	GLN
1	A	372	ASP
1	A	386	LEU
1	A	524	LEU
1	A	525	ARG
1	A	536	LEU
1	B	11	ARG
1	B	45	ARG
1	B	103	THR
1	B	136	ARG
1	B	200	PHE
1	B	249	THR
1	B	295	PHE
1	B	296	ARG
1	B	326	VAL
1	B	437	LEU
1	B	467	THR
1	B	505	THR
1	B	524	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 1 is monoatomic - leaving 25 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	C56	A	600[A]	-	25,26,26	1.48	4 (16%)	32,36,36	2.39	13 (40%)
3	PEG	B	1547	-	6,6,6	0.64	0	5,5,5	1.38	0
2	C56	A	600[B]	-	25,26,26	1.46	4 (16%)	32,36,36	2.33	13 (40%)
3	PEG	B	1548	-	6,6,6	0.63	0	5,5,5	1.46	0
3	PEG	B	1554	-	6,6,6	0.63	0	5,5,5	1.45	0
4	EDO	A	1550	-	3,3,3	0.56	0	2,2,2	0.81	0
2	C56	B	600[B]	-	25,26,26	1.45	4 (16%)	32,36,36	2.40	12 (37%)
2	C56	B	600[A]	-	25,26,26	1.47	3 (12%)	32,36,36	2.49	13 (40%)
4	EDO	A	1552	-	3,3,3	0.59	0	2,2,2	0.73	0
3	PEG	B	1551	-	6,6,6	0.64	0	5,5,5	1.37	0
6	1PE	B	1546	-	15,15,15	0.65	0	14,14,14	0.97	0
4	EDO	B	1549	-	3,3,3	0.57	0	2,2,2	0.84	0
5	NAG	A	1553	1	14,14,15	1.36	1 (7%)	17,19,21	1.17	2 (11%)
5	NAG	B	1552	1	14,14,15	1.37	1 (7%)	17,19,21	1.23	3 (17%)
3	PEG	B	1550	-	6,6,6	0.63	0	5,5,5	1.45	0
4	EDO	A	1551	-	3,3,3	0.57	0	2,2,2	0.77	0
5	NAG	A	1549	1	14,14,15	1.37	1 (7%)	17,19,21	1.12	2 (11%)
4	EDO	A	1545	-	3,3,3	0.58	0	2,2,2	0.77	0
3	PEG	B	1545	-	6,6,6	0.65	0	5,5,5	1.37	0
3	PEG	A	1544	-	6,6,6	0.63	0	5,5,5	1.40	0
3	PEG	A	1547	-	6,6,6	0.64	0	5,5,5	1.31	0
4	EDO	A	1548	-	3,3,3	0.55	0	2,2,2	0.85	0
4	EDO	B	1556	-	3,3,3	0.59	0	2,2,2	0.76	0
4	EDO	B	1553	-	3,3,3	0.55	0	2,2,2	0.80	0
3	PEG	A	1546	-	6,6,6	0.63	0	5,5,5	1.43	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
2	C56	A	600[A]	-	-	2/19/31/31	0/2/2/2
3	PEG	B	1547	-	-	2/4/4/4	-
2	C56	A	600[B]	-	-	4/19/31/31	0/2/2/2
3	PEG	B	1548	-	-	1/4/4/4	-
3	PEG	B	1554	-	-	1/4/4/4	-
4	EDO	A	1550	-	-	1/1/1/1	-
2	C56	B	600[B]	-	-	5/19/31/31	0/2/2/2
2	C56	B	600[A]	-	-	5/19/31/31	0/2/2/2
4	EDO	A	1552	-	-	1/1/1/1	-
3	PEG	B	1551	-	-	1/4/4/4	-
6	1PE	B	1546	-	-	5/13/13/13	-
4	EDO	B	1549	-	-	1/1/1/1	-
5	NAG	A	1553	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1552	1	-	2/6/23/26	0/1/1/1
3	PEG	B	1550	-	-	1/4/4/4	-
4	EDO	A	1551	-	-	1/1/1/1	-
5	NAG	A	1549	1	-	2/6/23/26	0/1/1/1
4	EDO	A	1545	-	-	1/1/1/1	-
3	PEG	B	1545	-	-	2/4/4/4	-
3	PEG	A	1544	-	-	0/4/4/4	-
3	PEG	A	1547	-	-	2/4/4/4	-
4	EDO	A	1548	-	-	1/1/1/1	-
4	EDO	B	1556	-	-	1/1/1/1	-
4	EDO	B	1553	-	-	1/1/1/1	-
3	PEG	A	1546	-	-	2/4/4/4	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600[A]	C56	C15-N17	3.97	1.42	1.33
2	B	600[A]	C56	C15-N17	3.96	1.42	1.33
2	A	600[B]	C56	C15-N17	3.82	1.42	1.33
2	B	600[B]	C56	C15-N17	3.80	1.42	1.33
5	A	1549	NAG	C7-N2	3.77	1.47	1.34
5	B	1552	NAG	C7-N2	3.72	1.47	1.34
5	A	1553	NAG	C7-N2	3.70	1.47	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600[B]	C56	C4-C5	2.58	1.43	1.39
2	A	600[B]	C56	C4-C5	2.56	1.43	1.39
2	A	600[A]	C56	C4-C5	2.46	1.43	1.39
2	B	600[A]	C56	C4-C5	2.45	1.43	1.39
2	B	600[A]	C56	C6-C5	2.16	1.44	1.40
2	A	600[B]	C56	C6-C5	2.15	1.44	1.40
2	B	600[B]	C56	C6-C5	2.11	1.44	1.40
2	A	600[A]	C56	C6-C5	2.07	1.43	1.40
2	B	600[B]	C56	C2-C3	2.06	1.44	1.40
2	A	600[B]	C56	C2-C3	2.06	1.44	1.40
2	A	600[A]	C56	C2-C3	2.03	1.44	1.40

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600[A]	C56	C11-N10-C5	5.56	132.43	115.17
2	B	600[A]	C56	C6-C5-N10	5.45	131.97	121.38
2	B	600[B]	C56	C11-N10-C5	5.44	132.05	115.17
2	B	600[B]	C56	C6-C5-N10	5.28	131.64	121.38
2	A	600[A]	C56	C11-N10-C5	5.10	130.99	115.17
2	A	600[A]	C56	C6-C5-N10	5.05	131.19	121.38
2	A	600[B]	C56	C11-N10-C5	5.04	130.81	115.17
2	A	600[B]	C56	C6-C5-N10	4.89	130.89	121.38
2	A	600[B]	C56	C2-C15-N17	4.11	125.43	117.36
2	B	600[A]	C56	C07-C08-N09	4.07	110.78	104.15
2	B	600[B]	C56	C2-C1-C6	4.03	126.05	118.20
2	A	600[A]	C56	C07-C08-N09	3.95	110.59	104.15
2	A	600[B]	C56	C2-C1-C6	3.90	125.79	118.20
2	B	600[B]	C56	C2-C15-N17	3.83	124.88	117.36
2	B	600[A]	C56	C2-C1-C6	3.81	125.61	118.20
2	B	600[A]	C56	C4-C5-N10	-3.76	115.87	120.91
2	A	600[A]	C56	C2-C1-C6	3.73	125.45	118.20
2	A	600[A]	C56	C4-C5-N10	-3.55	116.15	120.91
2	B	600[B]	C56	C4-C5-N10	-3.48	116.24	120.91
2	B	600[B]	C56	C1-C2-C3	-3.44	113.47	118.29
2	B	600[A]	C56	C1-C2-C3	-3.41	113.51	118.29
2	A	600[A]	C56	C1-C2-C3	-3.39	113.54	118.29
2	A	600[B]	C56	C4-C5-N10	-3.37	116.39	120.91
2	B	600[B]	C56	C5-C4-C3	3.33	125.00	117.91
2	B	600[A]	C56	C5-C4-C3	3.23	124.80	117.91
2	A	600[B]	C56	C1-C2-C3	-3.20	113.81	118.29
2	A	600[A]	C56	C2-C15-N17	3.15	123.55	117.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600[B]	C56	C5-C4-C3	3.13	124.58	117.91
5	B	1552	NAG	C1-O5-C5	3.04	116.31	112.19
2	A	600[A]	C56	C5-C4-C3	3.04	124.38	117.91
5	A	1553	NAG	C1-O5-C5	3.00	116.25	112.19
2	A	600[B]	C56	O16-C15-N17	-2.95	116.73	122.61
2	B	600[A]	C56	C11-N10-C12	-2.93	106.68	116.12
2	A	600[A]	C56	C14-O13-C3	2.92	121.93	117.53
2	B	600[A]	C56	C1-C6-C5	2.90	121.94	118.69
2	B	600[B]	C56	C11-N10-C12	-2.89	106.81	116.12
5	A	1549	NAG	C1-O5-C5	2.88	116.10	112.19
2	A	600[B]	C56	C14-O13-C3	2.88	121.88	117.53
2	B	600[A]	C56	C14-O13-C3	2.78	121.73	117.53
2	B	600[B]	C56	C4-C5-C6	-2.76	112.10	117.70
2	B	600[A]	C56	C4-C5-C6	-2.75	112.11	117.70
2	A	600[B]	C56	C11-N10-C12	-2.75	107.25	116.12
2	A	600[A]	C56	C1-C6-C5	2.75	121.78	118.69
2	B	600[B]	C56	C14-O13-C3	2.75	121.68	117.53
2	B	600[B]	C56	C1-C6-C5	2.71	121.73	118.69
2	A	600[A]	C56	C11-N10-C12	-2.71	107.40	116.12
2	B	600[A]	C56	C2-C15-N17	2.66	122.59	117.36
2	B	600[B]	C56	O16-C15-N17	-2.60	117.43	122.61
2	A	600[A]	C56	C4-C5-C6	-2.50	112.63	117.70
2	A	600[A]	C56	O16-C15-N17	-2.48	117.66	122.61
2	A	600[B]	C56	C1-C6-C5	2.48	121.47	118.69
2	A	600[B]	C56	C4-C5-C6	-2.47	112.69	117.70
5	B	1552	NAG	C8-C7-N2	2.29	119.98	116.10
5	A	1553	NAG	C8-C7-N2	2.17	119.78	116.10
5	B	1552	NAG	C2-N2-C7	-2.17	119.81	122.90
5	A	1549	NAG	C8-C7-N2	2.12	119.69	116.10
2	B	600[A]	C56	O16-C15-N17	-2.11	118.40	122.61
2	A	600[B]	C56	C05-C18-N17	2.04	117.22	111.96

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600[B]	C56	C13-C10-N09-C08
2	B	600[B]	C56	C06-C05-C18-N17
2	B	600[B]	C56	N09-C05-C18-N17
2	B	600[B]	C56	C13-C10-N09-C08
2	B	600[A]	C56	C06-C05-C18-N17
2	B	600[A]	C56	N09-C05-C18-N17

Continued on next page...

Continued from previous page...

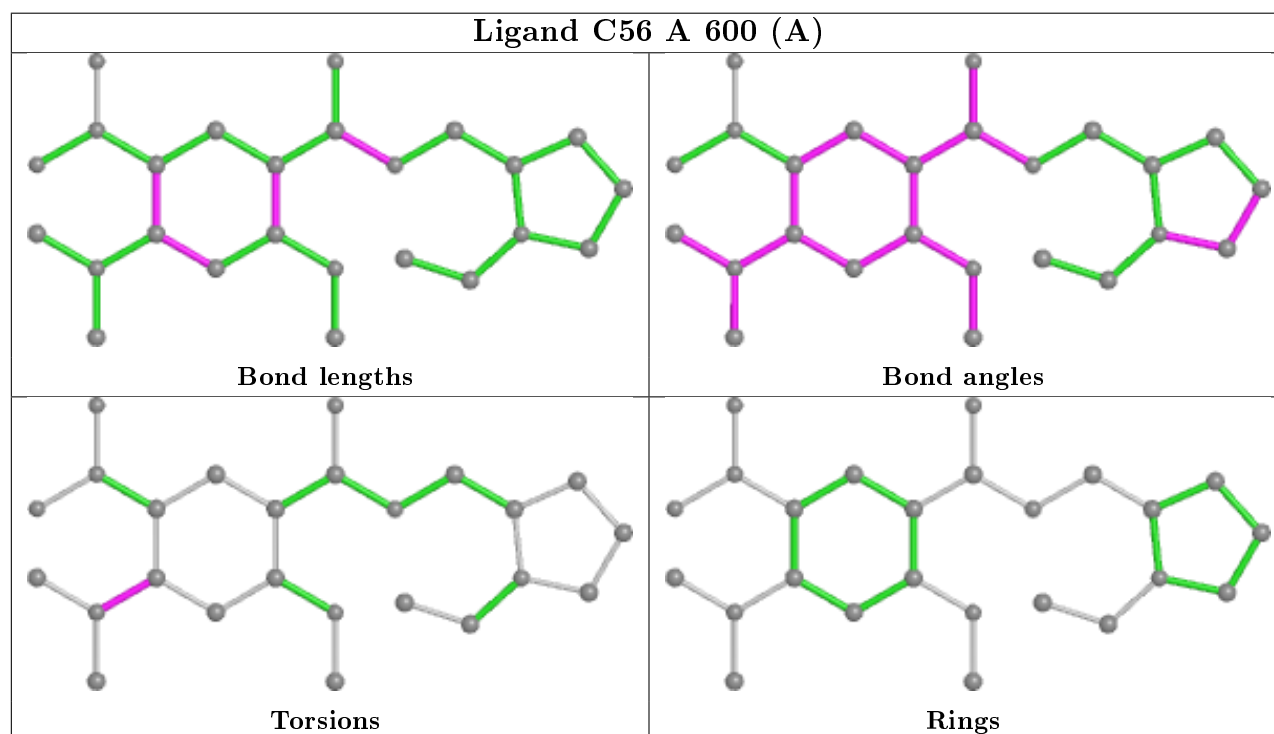
Mol	Chain	Res	Type	Atoms
2	B	600[A]	C56	C13-C10-N09-C08
5	B	1552	NAG	O5-C5-C6-O6
5	B	1552	NAG	C4-C5-C6-O6
3	B	1545	PEG	O2-C3-C4-O4
2	A	600[A]	C56	C6-C5-N10-C11
2	A	600[B]	C56	C6-C5-N10-C11
2	A	600[A]	C56	C4-C5-N10-C11
2	A	600[B]	C56	C4-C5-N10-C11
5	A	1549	NAG	C4-C5-C6-O6
3	A	1547	PEG	O1-C1-C2-O2
4	A	1550	EDO	O1-C1-C2-O2
4	A	1545	EDO	O1-C1-C2-O2
5	A	1549	NAG	O5-C5-C6-O6
2	B	600[A]	C56	C4-C5-N10-C11
4	A	1552	EDO	O1-C1-C2-O2
2	B	600[B]	C56	C4-C5-N10-C11
3	B	1550	PEG	O1-C1-C2-O2
4	B	1556	EDO	O1-C1-C2-O2
4	B	1553	EDO	O1-C1-C2-O2
2	A	600[B]	C56	C13-C10-N09-C05
3	A	1546	PEG	O2-C3-C4-O4
6	B	1546	1PE	C12-C22-OH3-C23
6	B	1546	1PE	C14-C24-OH4-C13
3	B	1547	PEG	C4-C3-O2-C2
3	A	1547	PEG	C1-C2-O2-C3
6	B	1546	1PE	OH6-C15-C25-OH5
3	B	1547	PEG	O1-C1-C2-O2
3	B	1554	PEG	O2-C3-C4-O4
3	B	1548	PEG	O1-C1-C2-O2
5	A	1553	NAG	O5-C5-C6-O6
4	A	1548	EDO	O1-C1-C2-O2
3	A	1546	PEG	C1-C2-O2-C3
3	B	1545	PEG	O1-C1-C2-O2
3	B	1551	PEG	O1-C1-C2-O2
2	B	600[A]	C56	C6-C5-N10-C11
4	B	1549	EDO	O1-C1-C2-O2
5	A	1553	NAG	C4-C5-C6-O6
4	A	1551	EDO	O1-C1-C2-O2
6	B	1546	1PE	C23-C13-OH4-C24
6	B	1546	1PE	C25-C15-OH6-C26
2	B	600[B]	C56	C6-C5-N10-C11

There are no ring outliers.

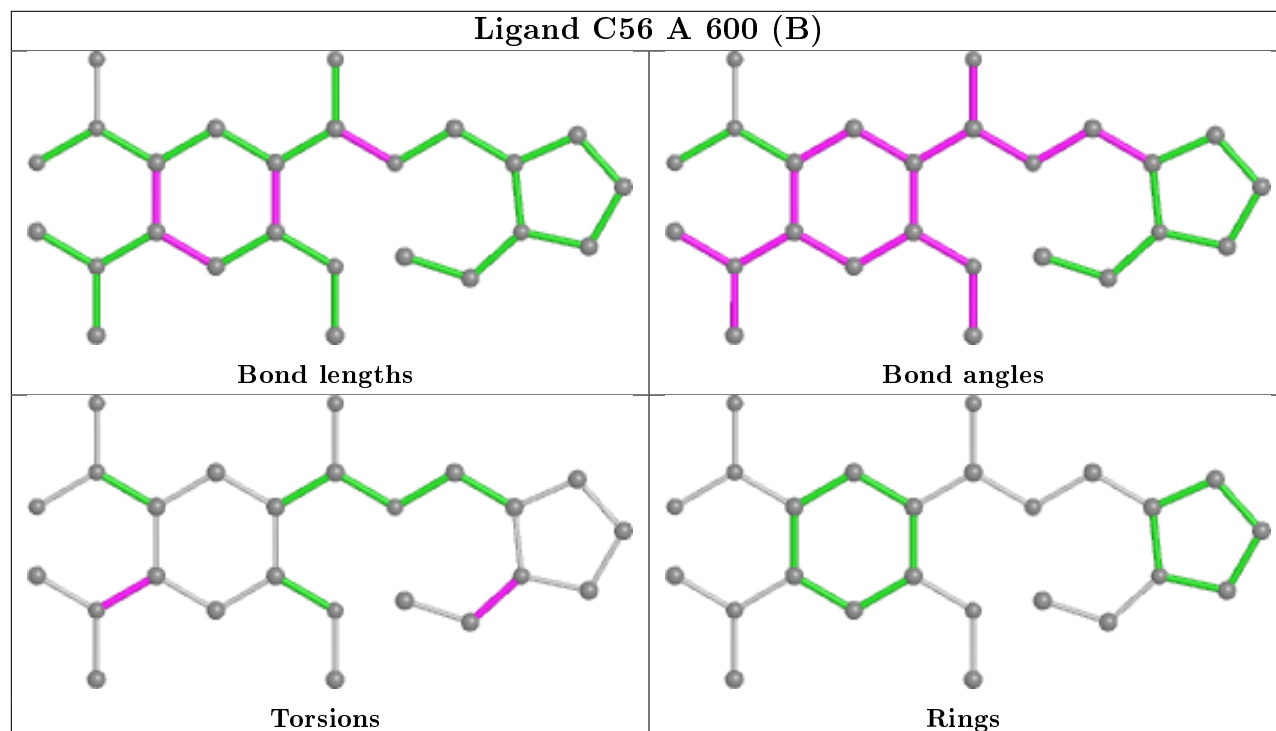
10 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600[A]	C56	1	0
2	A	600[B]	C56	2	0
3	B	1548	PEG	1	0
2	B	600[B]	C56	2	0
2	B	600[A]	C56	4	0
6	B	1546	1PE	1	0
4	B	1549	EDO	1	0
5	A	1553	NAG	1	0
3	B	1545	PEG	2	0
3	A	1547	PEG	1	0

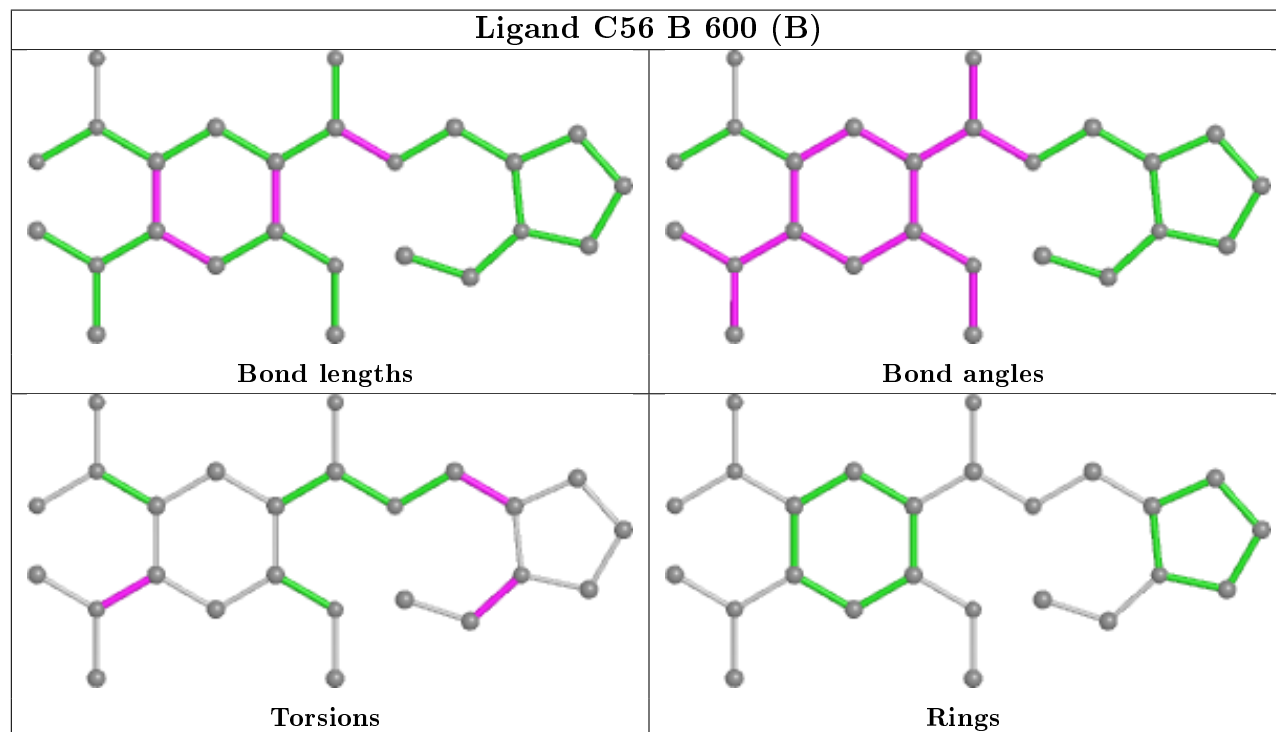
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

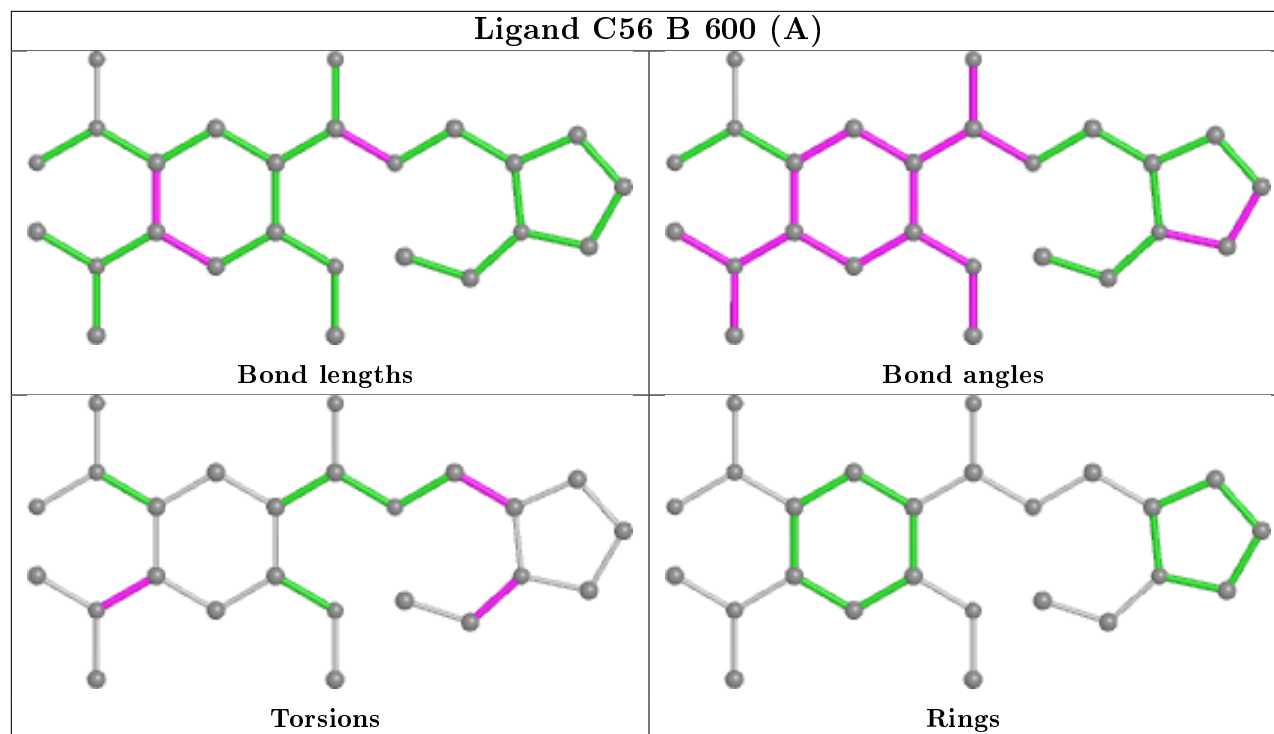


Ligand C56 A 600 (B)



Ligand C56 B 600 (B)





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 [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	535/548 (97%)	-0.38	8 (1%) 73 75	26, 43, 70, 124	0
1	B	533/548 (97%)	-0.25	7 (1%) 77 79	30, 49, 75, 123	0
All	All	1068/1096 (97%)	-0.31	15 (1%) 75 77	26, 46, 73, 124	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	495	SER	4.9
1	A	496	LYS	4.5
1	B	543	THR	4.1
1	B	541	SER	3.7
1	A	494	ASP	3.7
1	A	493	ARG	3.6
1	A	497	SER	3.3
1	B	542	ALA	2.8
1	A	492	PRO	2.8
1	B	265	ASN	2.6
1	A	541	SER	2.5
1	B	497	SER	2.2
1	B	41	PRO	2.2
1	B	109	ALA	2.1
1	A	540	LEU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

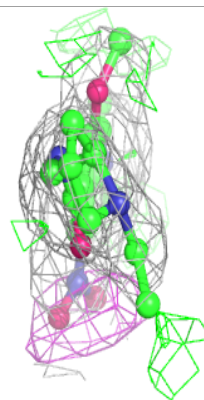
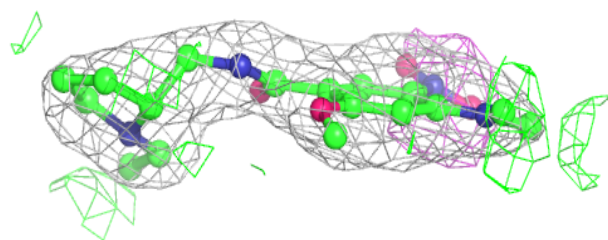
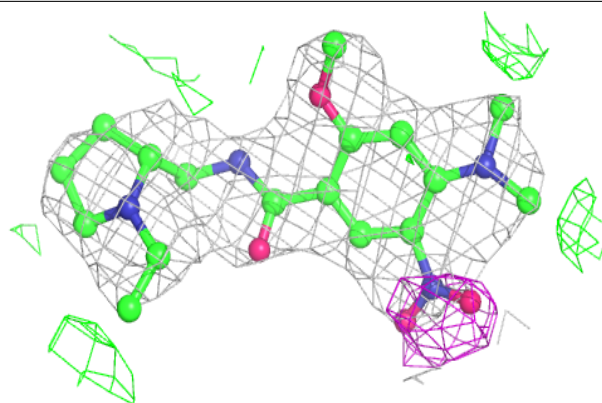
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	NAG	B	1552	14/15	0.69	0.40	68,98,104,104	0
3	PEG	B	1547	7/7	0.73	0.21	82,90,97,98	0
5	NAG	A	1553	14/15	0.76	0.29	71,99,108,109	0
3	PEG	B	1554	7/7	0.79	0.15	71,75,82,84	0
5	NAG	A	1549	14/15	0.81	0.35	82,91,95,99	0
3	PEG	B	1545	7/7	0.81	0.20	68,72,89,94	0
3	PEG	B	1550	7/7	0.84	0.22	65,72,80,81	0
3	PEG	A	1546	7/7	0.84	0.17	91,101,105,106	0
4	EDO	B	1549	4/4	0.85	0.17	77,83,84,85	0
2	C56	B	600[B]	25/25	0.86	0.20	73,78,82,84	25
2	C56	B	600[A]	25/25	0.86	0.20	73,78,82,85	25
4	EDO	A	1548	4/4	0.86	0.18	69,71,81,86	0
4	EDO	A	1551	4/4	0.86	0.15	70,72,73,75	0
4	EDO	A	1545	4/4	0.87	0.18	69,74,79,80	0
2	C56	A	600[B]	25/25	0.91	0.19	61,67,73,74	25
3	PEG	B	1548	7/7	0.91	0.14	51,58,67,69	0
4	EDO	B	1553	4/4	0.91	0.13	49,61,70,72	0
2	C56	A	600[A]	25/25	0.91	0.19	60,68,74,75	25
3	PEG	A	1547	7/7	0.92	0.18	89,93,95,98	0
4	EDO	A	1552	4/4	0.92	0.12	78,78,80,82	0
3	PEG	B	1551	7/7	0.92	0.12	58,61,74,76	0
3	PEG	A	1544	7/7	0.92	0.16	57,61,76,81	0
7	CL	B	1555	1/1	0.93	0.07	80,80,80,80	0
4	EDO	A	1550	4/4	0.93	0.16	65,67,69,70	0
6	1PE	B	1546	16/16	0.94	0.21	38,62,70,74	0
4	EDO	B	1556	4/4	0.94	0.15	85,86,86,87	0

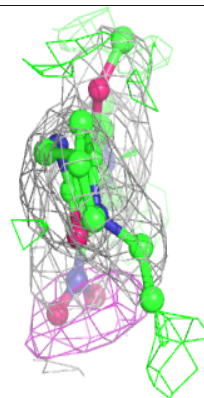
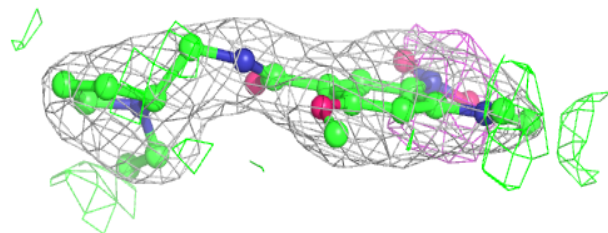
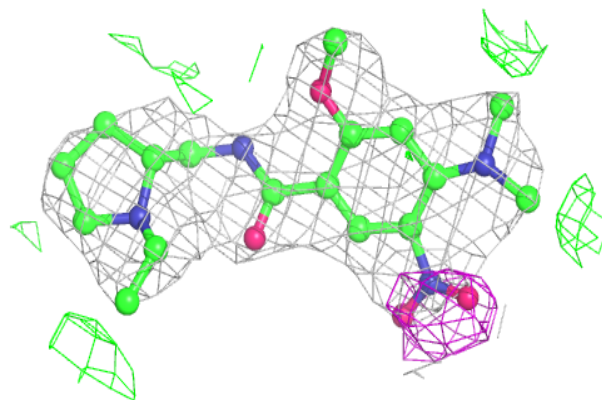
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around C56 B 600 (B):

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

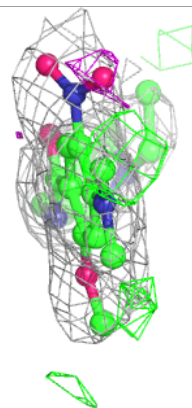
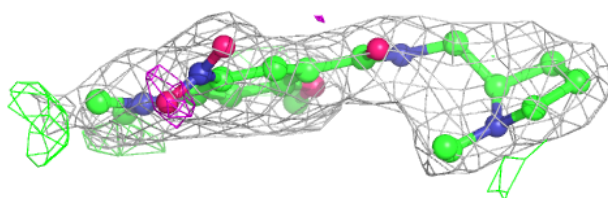
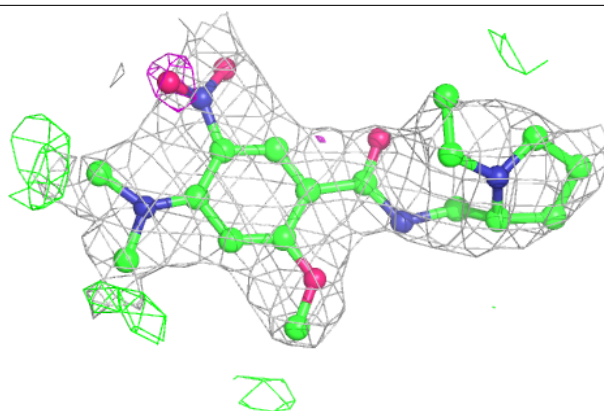
**Electron density around C56 B 600 (A):**

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

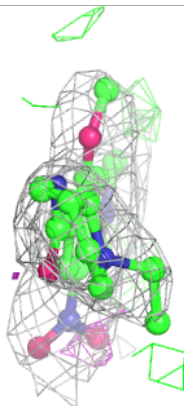
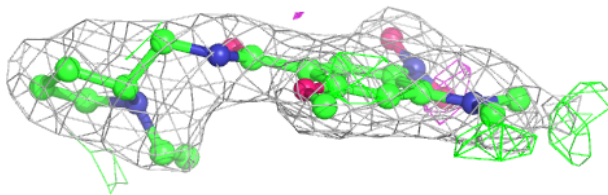
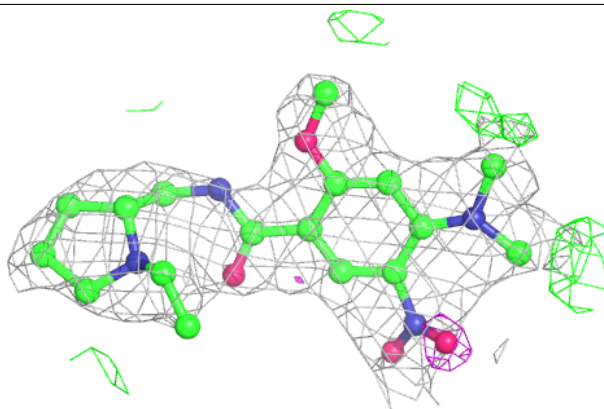


Electron density around C56 A 600 (B):

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

**Electron density around C56 A 600 (A):**

$2mF_o-DF_c$ (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.