



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 12:29 PM BST

PDB ID : 4B7Z  
Title : Mus musculus Acetylcholinesterase in complex with N-(2-Diethylamino-ethyl)-1-(4-methylphenyl)-methanesulfonamide  
Authors : Andersson, C.D.; Forsgren, N.; Akfur, C.; Allgardsson, A.; Berg, L.; Qian, W.; Ekstrom, F.; Linusson, A.  
Deposited on : 2012-08-24  
Resolution : 2.30 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](mailto: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.

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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

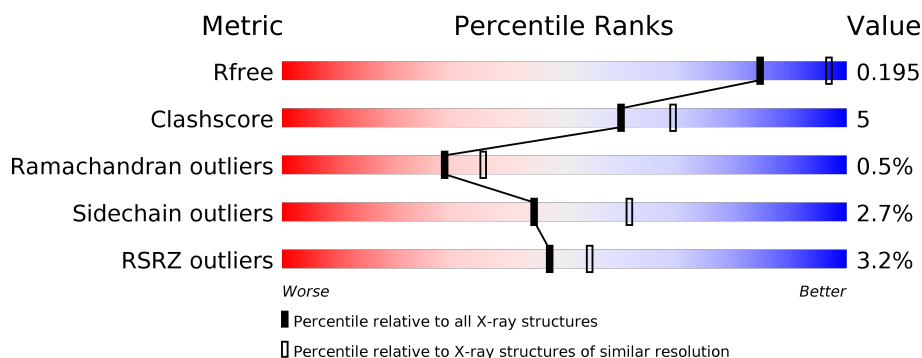
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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  $\geq 3$ , 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>3%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div>..</div> </div> </div>
1	B	548	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>..</div> </div> </div>

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
5	NAG	A	1548	X	-	-	X
5	NAG	B	1547	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 9292 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.

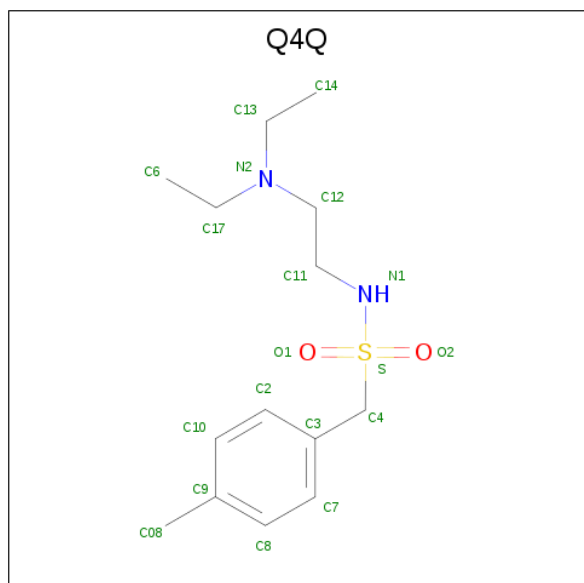
- Molecule 1 is a protein called ACETYLCHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	1	0
			4185	2684	728	759	14			
1	B	534	Total	C	N	O	S	0	0	1
			4159	2670	719	756	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	546	GLU	-	expression tag	UNP P21836
A	547	ALA	-	expression tag	UNP P21836
A	548	PRO	-	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 N-[2-(diethylamino)ethyl]-1-(4-methylphenyl)methanesulfonamide (three-letter code: Q4Q) (formula: C<sub>14</sub>H<sub>24</sub>N<sub>2</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			19	14	2	2	1		
2	B	1	Total	C	N	O	S	0	0
			19	14	2	2	1		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



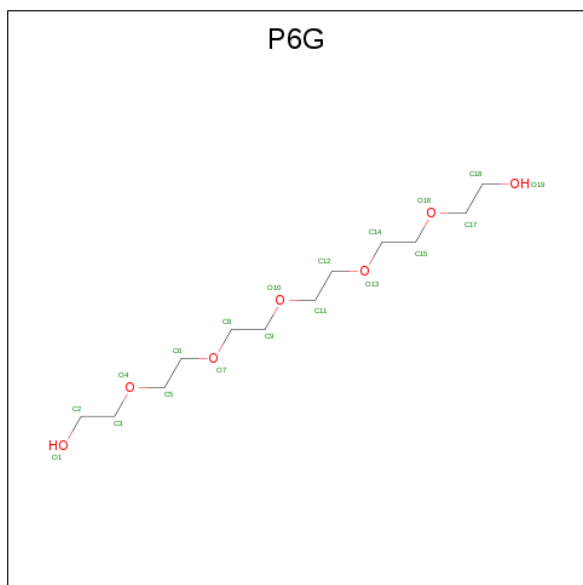
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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 HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula:  $C_{12}H_{26}O_7$ ).



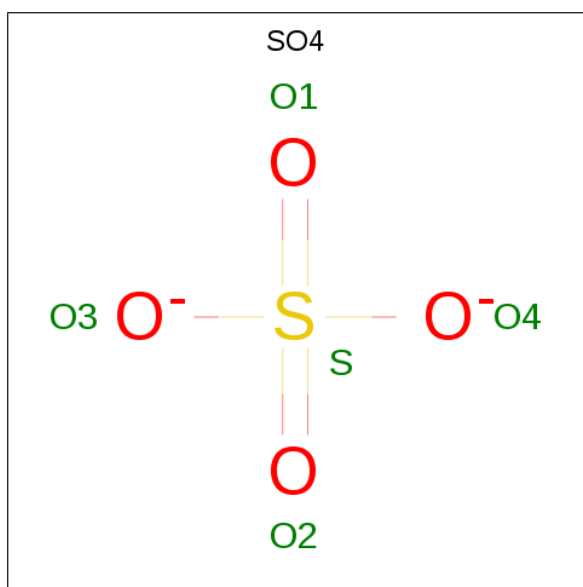
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			19	12	7		

- 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 SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is water.

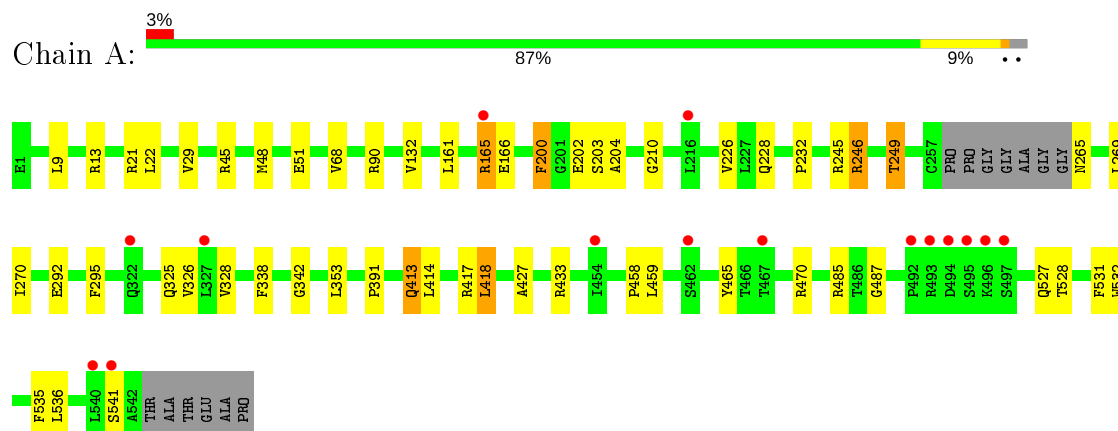
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	413	Total	O	0	0
			413	413		
7	B	335	Total	O	0	0
			335	335		



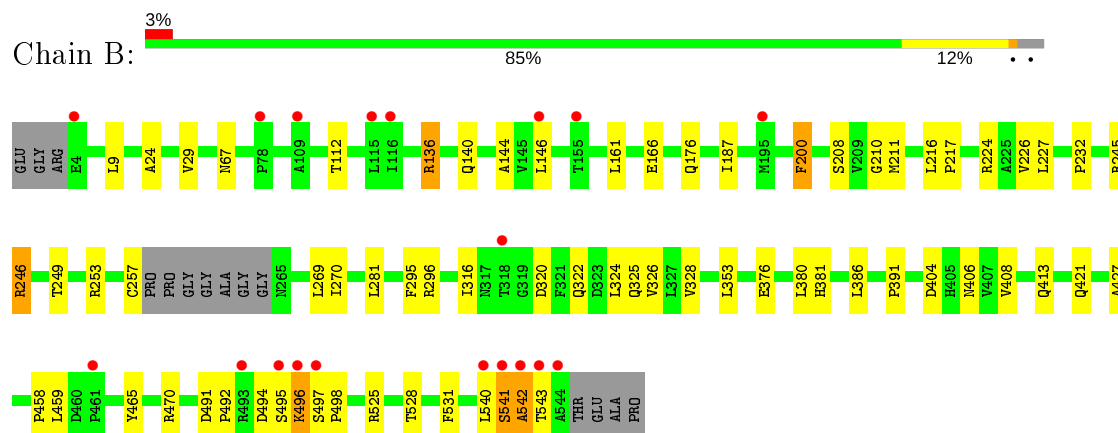
### 3 Residue-property plots

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: ACETYLCHOLINESTERASE



#### • Molecule 1: ACETYLCHOLINESTERASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.31Å 111.83Å 226.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.80 – 2.30 29.12 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (28.80-2.30) 99.9 (29.12-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.44 (at 2.31Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, $R_{free}$	0.171 , 0.201 0.164 , 0.195	Depositor DCC
$R_{free}$ test set	1786 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.0	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 56.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9292	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: SO4, PEG, NAG, P6G, Q4Q

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	0.42	0/4311	0.53	0/5889
1	B	0.39	0/4282	0.55	0/5853
All	All	0.41	0/8593	0.54	0/11742

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	4185	0	4076	37	0
1	B	4159	0	4046	40	0
2	A	19	0	24	1	0
2	B	19	0	24	0	0
3	A	49	0	70	4	0
3	B	42	0	60	3	0
4	A	19	0	26	4	0
5	A	28	0	26	0	0
5	B	14	0	13	0	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	413	0	0	7	0
7	B	335	0	0	4	0
All	All	9292	0	8365	77	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 (77) 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:A:45:ARG:NH1	1:A:51:GLU:OE1	2.12	0.82
1:A:245:ARG:O	1:A:249:THR:HG23	1.88	0.72
1:A:433:ARG:NH1	7:A:2358:HOH:O	2.20	0.72
1:A:203:SER:OG	7:A:2151:HOH:O	2.08	0.71
1:B:257:CYS:O	7:B:2193:HOH:O	2.10	0.68
1:A:161:LEU:HD11	1:A:269:LEU:HD22	1.76	0.67
1:A:353:LEU:HB3	1:A:391:PRO:HB2	1.78	0.66
1:A:161:LEU:HD12	1:A:270:ILE:HD11	1.76	0.66
1:A:246:ARG:NH2	7:A:2247:HOH:O	2.31	0.63
1:B:496:LYS:HD3	1:B:498:PRO:HA	1.82	0.62
1:B:245:ARG:O	1:B:249:THR:HG23	2.00	0.61
1:A:413:GLN:NE2	3:A:1551:PEG:H32	2.16	0.61
1:B:296:ARG:NH2	1:B:406:ASN:OD1	2.35	0.60
1:A:203:SER:OG	1:A:204:ALA:N	2.35	0.59
1:B:246:ARG:NH2	7:B:2184:HOH:O	2.35	0.59
1:B:161:LEU:HD12	1:B:270:ILE:HD11	1.85	0.59
1:A:265:ASN:N	7:A:2253:HOH:O	2.36	0.58
4:A:1544:P6G:H181	3:B:1546:PEG:H11	1.85	0.56
1:A:417:ARG:HD3	3:A:1551:PEG:H31	1.87	0.55
1:B:161:LEU:HD11	1:B:269:LEU:HD22	1.89	0.54
1:B:324:LEU:HG	1:B:326:VAL:HG23	1.91	0.53
1:B:67:ASN:ND2	7:B:2058:HOH:O	2.35	0.53
1:B:328:VAL:O	1:B:427:ALA:HA	2.09	0.52
1:A:527:GLN:HE21	4:A:1544:P6G:H152	1.75	0.51
1:A:48:MET:HE1	1:A:165:ARG:O	2.11	0.51
1:A:48:MET:HE1	1:A:166:GLU:HA	1.92	0.51
4:A:1544:P6G:H122	1:B:381:HIS:HA	1.93	0.51
1:A:338:PHE:CE2	2:A:600:Q4Q:H42C	2.47	0.49
1:A:458:PRO:HA	1:A:465:TYR:CD2	2.47	0.49
1:B:29:VAL:HG21	1:B:136:ARG:HB2	1.95	0.49
1:B:459:LEU:HD12	1:B:470:ARG:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:ARG:HG2	1:B:325:GLN:HB2	1.94	0.49
1:B:458:PRO:HA	1:B:465:TYR:CD1	2.48	0.48
1:A:433:ARG:NE	7:A:2357:HOH:O	2.34	0.48
1:A:535:PHE:HB2	1:B:380:LEU:HD12	1.95	0.48
1:B:408:VAL:HG11	1:B:525:ARG:HG3	1.95	0.47
1:A:328:VAL:O	1:A:427:ALA:HA	2.14	0.47
1:B:540:LEU:C	1:B:542:ALA:H	2.19	0.47
1:A:292:GLU:HA	3:A:1550:PEG:H42	1.96	0.46
1:B:211:MET:HG3	1:B:232:PRO:HB3	1.97	0.46
1:B:112:THR:HG23	3:B:1545:PEG:H32	1.98	0.45
1:A:210:GLY:HA3	1:A:232:PRO:HD3	1.97	0.45
1:A:459:LEU:HD12	1:A:470:ARG:HG2	1.99	0.45
1:A:165:ARG:NH2	7:A:2062:HOH:O	2.48	0.45
1:A:325:GLN:OE1	1:A:487:GLY:HA3	2.17	0.45
1:B:316:ILE:O	1:B:421:GLN:NE2	2.41	0.45
1:B:320:ASP:OD1	1:B:322:GLN:HG2	2.17	0.45
1:B:227:LEU:HB2	1:B:328:VAL:HG12	1.98	0.44
1:B:528:THR:O	1:B:531:PHE:HB3	2.17	0.44
1:B:24:ALA:HB3	1:B:140:GLN:HG3	1.99	0.43
1:B:495:SER:OG	1:B:496:LYS:N	2.49	0.43
1:B:216:LEU:HB3	1:B:217:PRO:HD3	2.01	0.43
1:B:541:SER:OG	1:B:541:SER:O	2.36	0.43
1:B:353:LEU:HB3	1:B:391:PRO:HB2	2.00	0.43
1:B:253:ARG:NH1	7:B:2191:HOH:O	2.51	0.43
1:B:326:VAL:HG12	1:B:328:VAL:HG13	2.01	0.43
4:A:1544:P6G:H182	1:B:381:HIS:CE1	2.54	0.42
1:A:200:PHE:CB	1:A:226:VAL:HB	2.49	0.42
1:A:414:LEU:HG	1:A:418:LEU:HD22	2.02	0.42
1:B:144:ALA:HA	3:B:1545:PEG:H41	2.01	0.42
1:A:22:LEU:HB2	1:A:29:VAL:HG22	2.01	0.42
1:B:376:GLU:O	1:B:380:LEU:HG	2.20	0.42
1:A:202:GLU:HA	1:A:228:GLN:O	2.20	0.42
1:B:210:GLY:HA3	1:B:232:PRO:HD3	2.01	0.42
1:A:485:ARG:HH11	3:A:1543:PEG:H22	1.84	0.42
1:A:9:LEU:HB3	7:A:2029:HOH:O	2.19	0.42
1:A:166:GLU:HB2	1:A:270:ILE:HD13	2.02	0.41
1:A:68:VAL:HG23	1:A:90[B]:ARG:HB2	2.02	0.41
1:B:200:PHE:CB	1:B:226:VAL:HB	2.50	0.41
1:A:536:LEU:HA	1:A:536:LEU:HD23	1.78	0.41
1:B:404:ASP:HA	1:B:408:VAL:HB	2.02	0.41
1:B:491:ASP:HA	1:B:492:PRO:HD3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:TRP:CE3	1:A:536:LEU:HD12	2.56	0.40
1:B:187:ILE:HA	1:B:187:ILE:HD12	1.94	0.40
1:A:528:THR:O	1:A:531:PHE:HB3	2.22	0.40
1:A:418:LEU:HA	1:A:418:LEU:HD12	1.95	0.40
1:B:176:GLN:OE1	1:B:208:SER:HB3	2.21	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	532/548 (97%)	516 (97%)	15 (3%)	1 (0%)	47	58
1	B	530/548 (97%)	511 (96%)	15 (3%)	4 (1%)	19	23
All	All	1062/1096 (97%)	1027 (97%)	30 (3%)	5 (0%)	29	35

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	543	THR
1	B	542	ALA
1	A	342	GLY
1	B	496	LYS
1	B	497	SER

### 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	440/446 (99%)	428 (97%)	12 (3%)	44	61
1	B	438/446 (98%)	426 (97%)	12 (3%)	44	61
All	All	878/892 (98%)	854 (97%)	24 (3%)	44	61

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	21	ARG
1	A	132	VAL
1	A	165	ARG
1	A	200	PHE
1	A	246	ARG
1	A	249	THR
1	A	295	PHE
1	A	326	VAL
1	A	413	GLN
1	A	418	LEU
1	A	541	SER
1	B	9	LEU
1	B	136	ARG
1	B	146	LEU
1	B	166	GLU
1	B	200	PHE
1	B	246	ARG
1	B	281	LEU
1	B	295	PHE
1	B	386	LEU
1	B	413	GLN
1	B	494	ASP
1	B	541	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	413	GLN

### 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 ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

21 ligands are modelled in this entry.

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	$\# Z  > 2$
3	PEG	A	1543	-	6,6,6	0.64	0	5,5,5	1.33	0
3	PEG	A	1545	-	6,6,6	0.60	0	5,5,5	1.50	0
2	Q4Q	B	600	-	18,19,19	1.11	1 (5%)	24,25,25	1.24	3 (12%)
3	PEG	A	1550	-	6,6,6	0.63	0	5,5,5	1.41	0
5	NAG	A	1548	1	14,14,15	0.49	0	17,19,21	1.01	2 (11%)
3	PEG	A	1552	-	6,6,6	0.56	0	5,5,5	1.53	0
3	PEG	B	1548	-	6,6,6	0.61	0	5,5,5	1.47	0
3	PEG	B	1545	-	6,6,6	0.63	0	5,5,5	1.40	0
4	P6G	A	1544	-	18,18,18	0.49	0	17,17,17	1.77	5 (29%)
5	NAG	B	1547	1	14,14,15	0.45	0	17,19,21	1.29	1 (5%)
3	PEG	B	1544	-	6,6,6	0.62	0	5,5,5	1.46	0
3	PEG	A	1551	-	6,6,6	0.60	0	5,5,5	1.60	1 (20%)
3	PEG	A	1549	-	6,6,6	0.59	0	5,5,5	1.59	0
5	NAG	A	1546	1	14,14,15	0.41	0	17,19,21	1.35	1 (5%)
2	Q4Q	A	600	-	18,19,19	1.28	2 (11%)	24,25,25	1.28	2 (8%)
6	SO4	A	1553	-	4,4,4	0.24	0	6,6,6	0.31	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PEG	B	1546	-	6,6,6	0.62	0	5,5,5	1.52	1 (20%)
3	PEG	B	1550	-	6,6,6	0.60	0	5,5,5	1.53	0
3	PEG	A	1547	-	6,6,6	0.64	0	5,5,5	1.43	0
6	SO4	B	1549	-	4,4,4	0.22	0	6,6,6	0.19	0
3	PEG	B	1551	-	6,6,6	0.58	0	5,5,5	1.55	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
3	PEG	A	1543	-	-	4/4/4/4	-
3	PEG	A	1545	-	-	0/4/4/4	-
2	Q4Q	B	600	-	-	4/16/16/16	0/1/1/1
3	PEG	A	1550	-	-	2/4/4/4	-
5	NAG	A	1548	1	1/1/5/7	2/6/23/26	0/1/1/1
3	PEG	A	1552	-	-	1/4/4/4	-
3	PEG	B	1548	-	-	1/4/4/4	-
3	PEG	B	1545	-	-	2/4/4/4	-
4	P6G	A	1544	-	-	7/16/16/16	-
5	NAG	B	1547	1	-	4/6/23/26	0/1/1/1
3	PEG	B	1544	-	-	1/4/4/4	-
3	PEG	A	1551	-	-	2/4/4/4	-
3	PEG	A	1549	-	-	3/4/4/4	-
5	NAG	A	1546	1	-	2/6/23/26	0/1/1/1
2	Q4Q	A	600	-	-	5/16/16/16	0/1/1/1
3	PEG	B	1546	-	-	2/4/4/4	-
3	PEG	B	1550	-	-	1/4/4/4	-
3	PEG	A	1547	-	-	2/4/4/4	-
3	PEG	B	1551	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	Q4Q	S-N1	2.85	1.68	1.61
2	A	600	Q4Q	C4-C3	2.83	1.55	1.50
2	B	600	Q4Q	S-N1	2.47	1.67	1.61

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1547	NAG	C1-O5-C5	4.57	118.39	112.19
5	A	1546	NAG	C1-O5-C5	4.48	118.26	112.19
2	A	600	Q4Q	C12-C11-N1	4.04	117.91	110.20
2	B	600	Q4Q	C12-C11-N1	3.29	116.48	110.20
2	A	600	Q4Q	C3-C4-S	3.14	119.06	112.34
5	A	1548	NAG	O5-C5-C6	2.64	111.34	107.20
5	A	1548	NAG	C1-O5-C5	2.54	115.63	112.19
4	A	1544	P6G	O10-C9-C8	2.28	120.69	110.39
2	B	600	Q4Q	C3-C4-S	2.24	117.12	112.34
2	B	600	Q4Q	O2-S-O1	2.22	122.57	119.35
4	A	1544	P6G	O7-C6-C5	2.11	119.93	110.39
4	A	1544	P6G	C5-O4-C3	2.09	122.36	113.29
3	A	1551	PEG	O2-C3-C4	2.07	119.16	110.07
4	A	1544	P6G	O4-C3-C2	2.06	119.10	110.07
4	A	1544	P6G	O13-C12-C11	2.02	119.48	110.39
3	B	1546	PEG	O2-C3-C4	2.01	118.90	110.07

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1548	NAG	C1

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	600	Q4Q	N1-C11-C12-N2
5	B	1547	NAG	C8-C7-N2-C2
5	B	1547	NAG	O7-C7-N2-C2
2	A	600	Q4Q	N1-C11-C12-N2
5	B	1547	NAG	O5-C5-C6-O6
5	B	1547	NAG	C4-C5-C6-O6
5	A	1546	NAG	C8-C7-N2-C2
3	B	1544	PEG	O1-C1-C2-O2
4	A	1544	P6G	O1-C2-C3-O4
3	A	1551	PEG	O2-C3-C4-O4
3	A	1549	PEG	O1-C1-C2-O2
3	A	1543	PEG	O1-C1-C2-O2
3	A	1543	PEG	O2-C3-C4-O4
3	B	1551	PEG	O2-C3-C4-O4
5	A	1546	NAG	O7-C7-N2-C2
3	A	1550	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
3	B	1545	PEG	O2-C3-C4-O4
3	B	1546	PEG	O1-C1-C2-O2
5	A	1548	NAG	C8-C7-N2-C2
3	B	1545	PEG	O1-C1-C2-O2
3	A	1549	PEG	O2-C3-C4-O4
4	A	1544	P6G	O13-C14-C15-O16
2	A	600	Q4Q	C14-C13-N2-C12
3	B	1548	PEG	O2-C3-C4-O4
3	A	1547	PEG	O2-C3-C4-O4
5	A	1548	NAG	O7-C7-N2-C2
3	A	1551	PEG	O1-C1-C2-O2
2	A	600	Q4Q	C11-C12-N2-C17
2	B	600	Q4Q	C11-C12-N2-C17
4	A	1544	P6G	O10-C11-C12-O13
4	A	1544	P6G	C15-C14-O13-C12
3	B	1550	PEG	O2-C3-C4-O4
2	B	600	Q4Q	C14-C13-N2-C12
4	A	1544	P6G	C14-C15-O16-C17
3	A	1552	PEG	C4-C3-O2-C2
3	B	1551	PEG	C1-C2-O2-C3
2	A	600	Q4Q	C14-C13-N2-C17
2	B	600	Q4Q	C11-C12-N2-C13
3	A	1543	PEG	C4-C3-O2-C2
3	A	1547	PEG	C4-C3-O2-C2
4	A	1544	P6G	C11-C12-O13-C14
3	B	1546	PEG	C4-C3-O2-C2
4	A	1544	P6G	C8-C9-O10-C11
3	A	1549	PEG	C4-C3-O2-C2
3	A	1550	PEG	O1-C1-C2-O2
2	A	600	Q4Q	C11-C12-N2-C13
3	A	1543	PEG	C1-C2-O2-C3

There are no ring outliers.

7 monomers are involved in 11 short contacts:

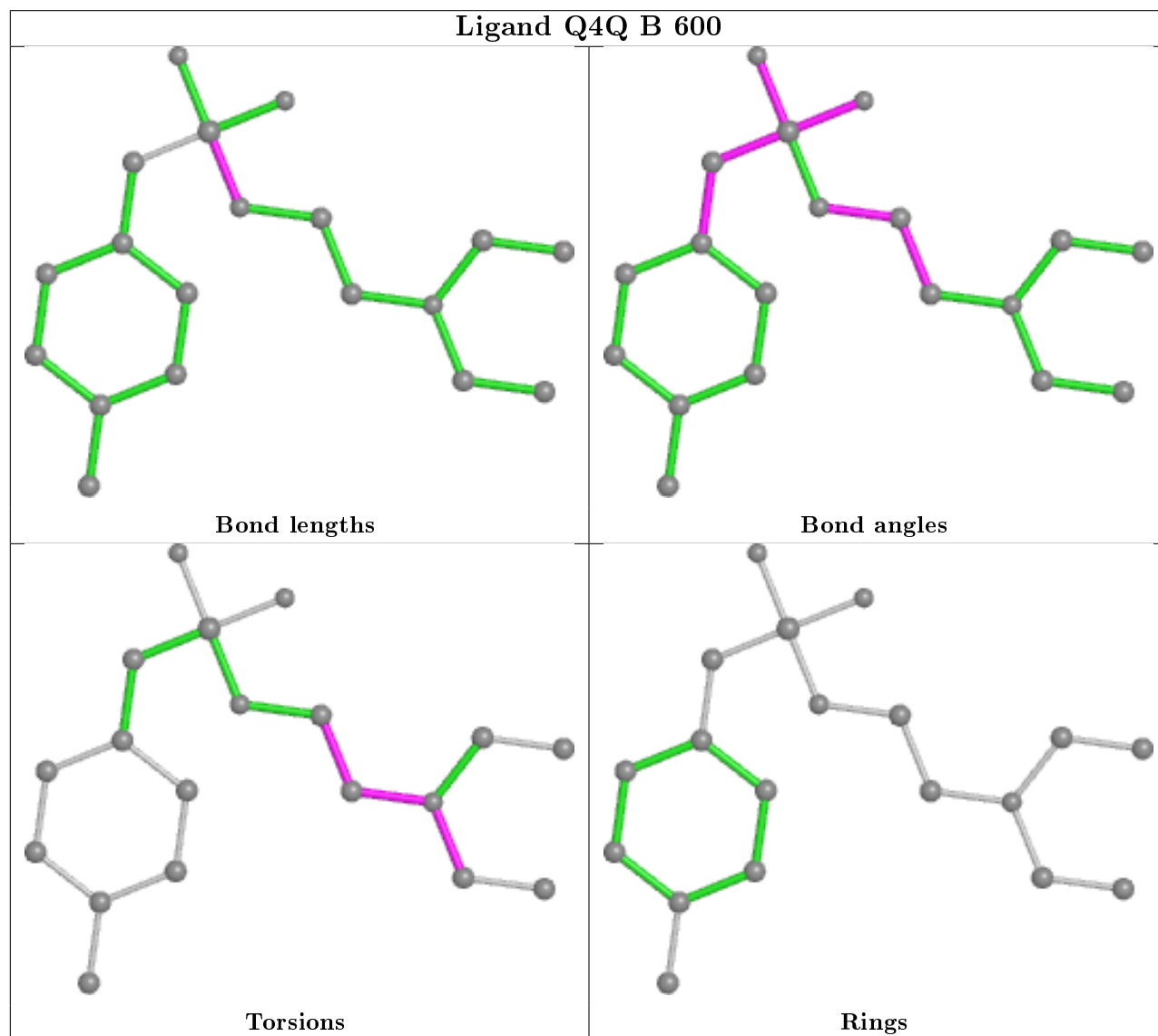
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1543	PEG	1	0
3	A	1550	PEG	1	0
3	B	1545	PEG	2	0
4	A	1544	P6G	4	0
3	A	1551	PEG	2	0
2	A	600	Q4Q	1	0

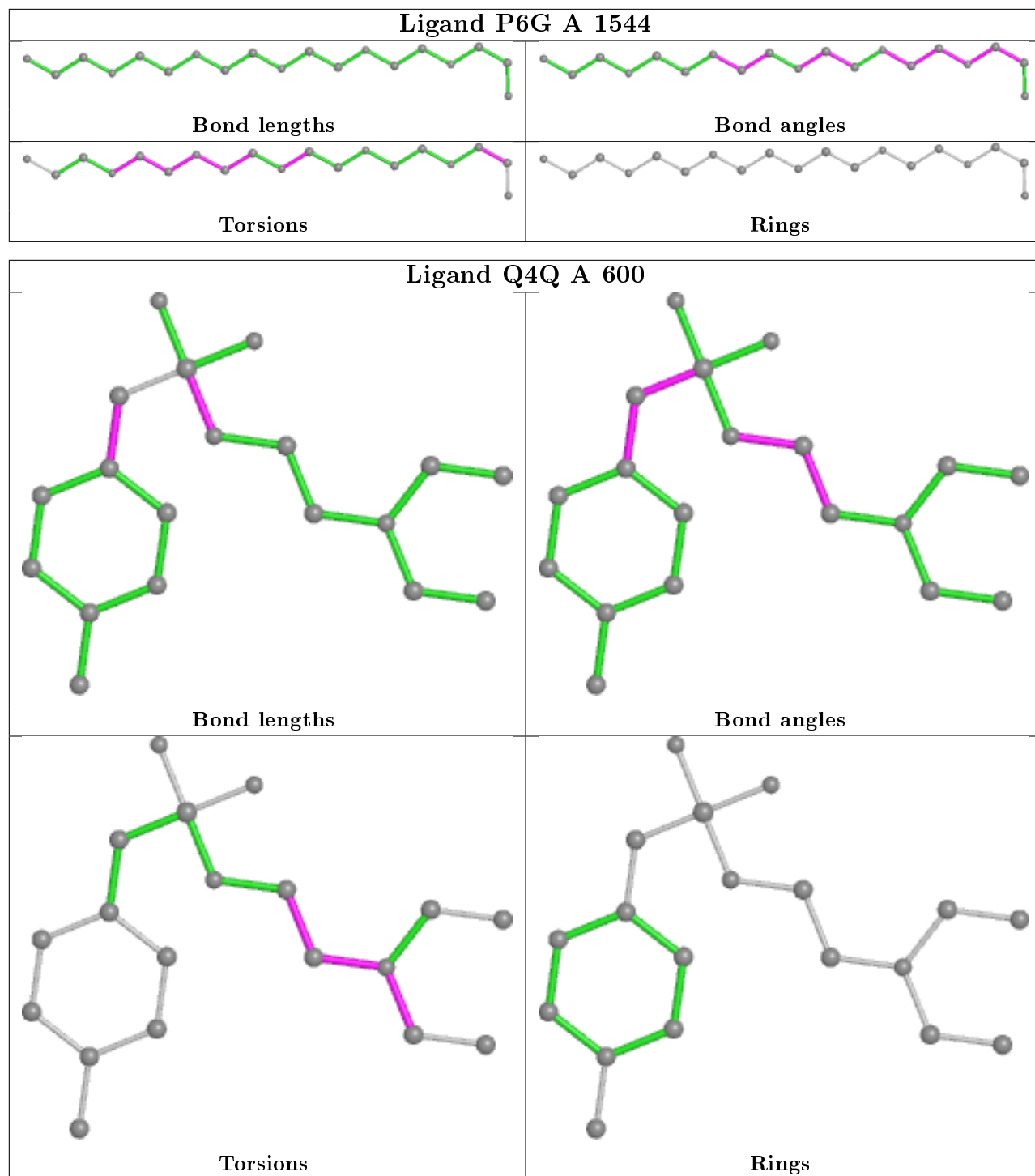
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1546	PEG	1	0

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.





## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	535/548 (97%)	-0.23	15 (2%)	53 60	28, 40, 68, 136	0
1	B	534/548 (97%)	-0.13	19 (3%)	42 49	29, 44, 74, 129	0
All	All	1069/1096 (97%)	-0.18	34 (3%)	47 54	28, 42, 71, 136	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	544	ALA	11.3
1	B	543	THR	6.7
1	A	493	ARG	5.8
1	B	497	SER	5.8
1	A	495	SER	5.7
1	A	496	LYS	4.5
1	A	494	ASP	4.5
1	B	541	SER	3.9
1	A	497	SER	3.2
1	B	109	ALA	3.2
1	B	542	ALA	3.2
1	A	541	SER	3.2
1	B	146	LEU	3.0
1	A	467	THR	2.7
1	B	496	LYS	2.7
1	A	492	PRO	2.5
1	B	318	THR	2.5
1	A	462	SER	2.4
1	B	4	GLU	2.4
1	A	540	LEU	2.3
1	B	540	LEU	2.2
1	B	495	SER	2.2
1	B	78	PRO	2.2
1	A	322	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	454	ILE	2.2
1	B	116	ILE	2.2
1	A	216	LEU	2.1
1	B	115	LEU	2.1
1	A	165	ARG	2.1
1	B	493	ARG	2.1
1	B	461	PRO	2.1
1	A	327	LEU	2.0
1	B	155	THR	2.0
1	B	195	MET	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	PEG	A	1551	7/7	0.67	0.25	73,86,90,91	0
5	NAG	B	1547	14/15	0.72	0.42	74,87,99,106	0
5	NAG	A	1548	14/15	0.76	0.46	93,105,108,111	0
3	PEG	B	1548	7/7	0.77	0.33	59,71,75,80	0
3	PEG	A	1552	7/7	0.80	0.22	53,64,69,72	0
3	PEG	B	1545	7/7	0.87	0.15	57,60,65,66	0
3	PEG	B	1544	7/7	0.88	0.13	74,78,85,89	0
3	PEG	B	1546	7/7	0.88	0.18	63,64,71,75	0
3	PEG	A	1547	7/7	0.88	0.21	72,75,88,90	0
3	PEG	A	1550	7/7	0.89	0.11	71,76,78,79	0
3	PEG	B	1550	7/7	0.89	0.17	74,76,87,89	0
3	PEG	A	1549	7/7	0.89	0.13	70,73,80,82	0
3	PEG	A	1545	7/7	0.91	0.15	63,64,73,74	0

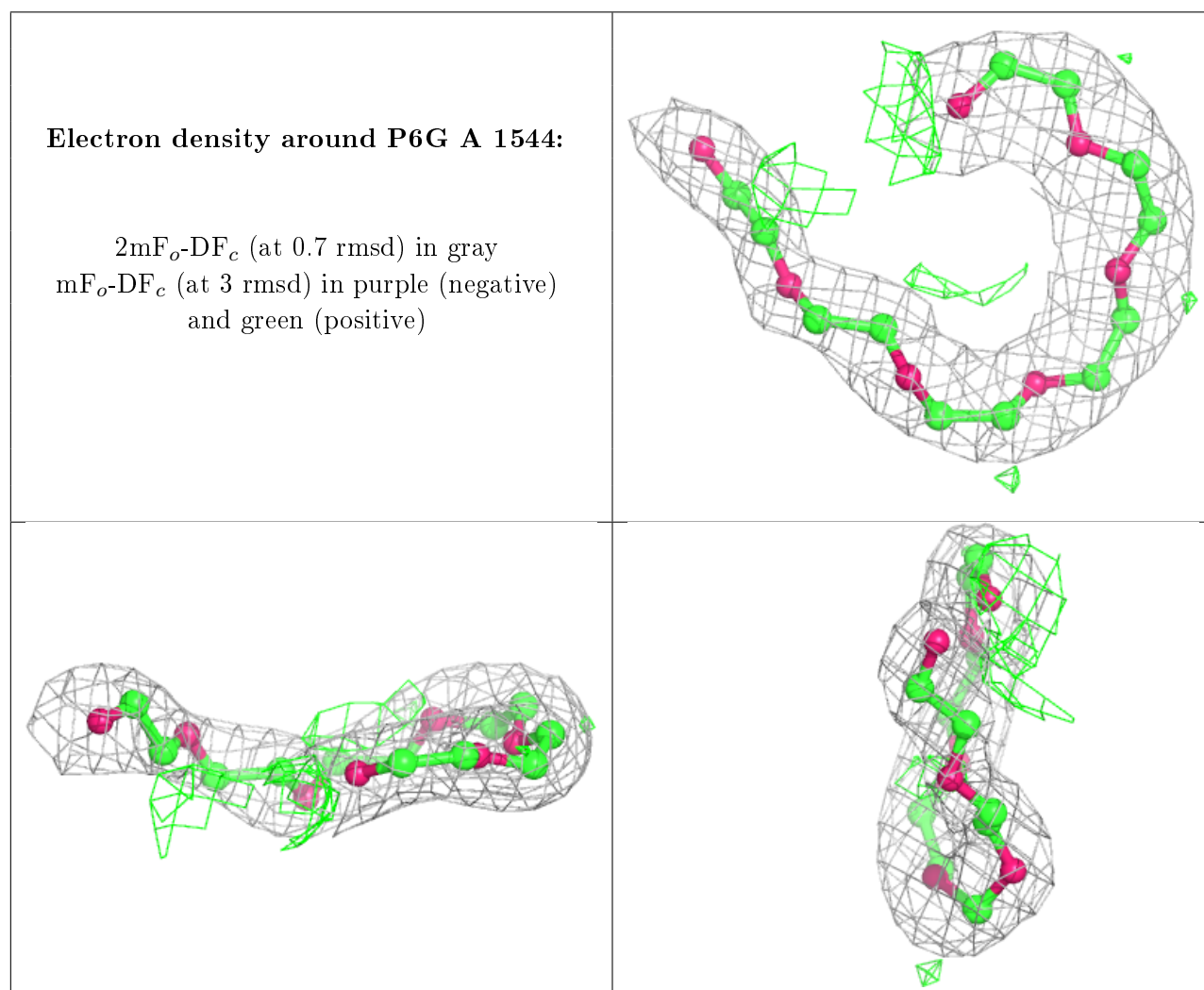
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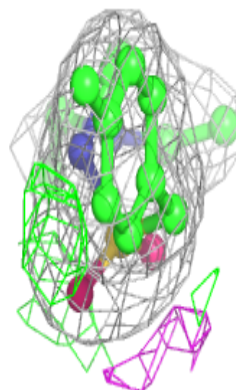
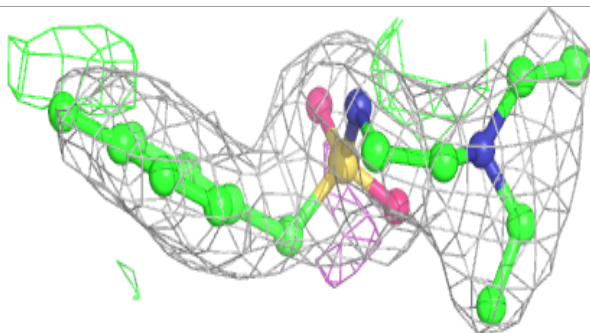
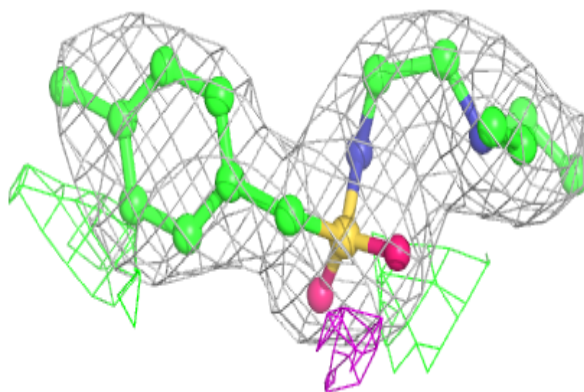
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	A	1546	14/15	0.91	0.38	66,78,91,92	0
3	PEG	A	1543	7/7	0.91	0.14	53,61,72,79	0
3	PEG	B	1551	7/7	0.91	0.15	63,65,72,74	0
6	SO4	B	1549	5/5	0.92	0.16	70,73,76,77	0
6	SO4	A	1553	5/5	0.93	0.17	54,64,66,67	0
4	P6G	A	1544	19/19	0.93	0.26	43,58,81,81	0
2	Q4Q	B	600	19/19	0.96	0.15	41,55,63,64	0
2	Q4Q	A	600	19/19	0.96	0.19	34,45,56,56	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.

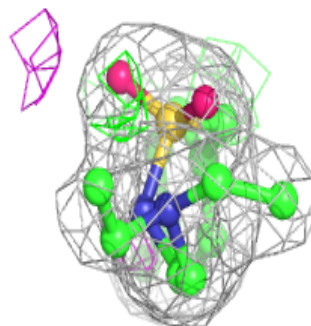
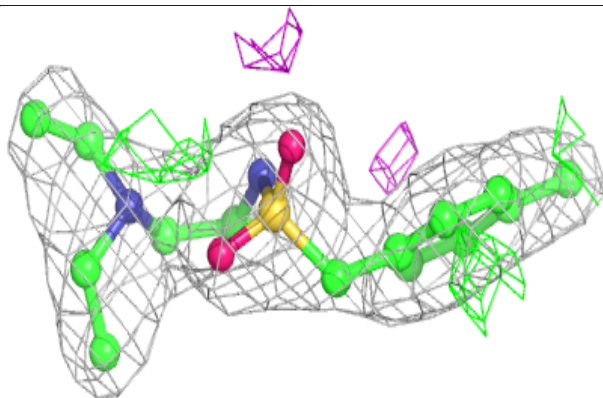
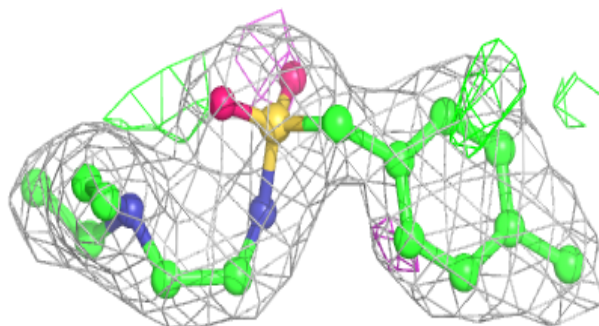


**Electron density around Q4Q B 600:**

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

**Electron density around Q4Q A 600:**

$2mF_o-DF_c$  (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.