



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:11 PM UTC

PDB ID : 4B82 / pdb_00004b82
Title : Mus musculus Acetylcholinesterase in complex with N-(2-Diethylamino- ethyl)-2-fluoranyl-benzenesulfonamide
Authors : Andersson, C.D.; Forsgren, N.; Akfur, C.; Allgardsson, A.; Berg, L.; Qian, W.; Ekstrom, F.; Linusson, A.
Deposited on : 2012-08-24
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

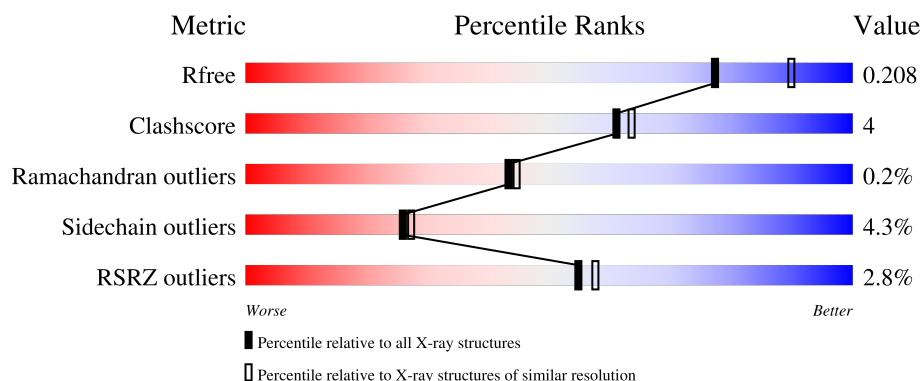
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	548	2% 87% 10% ..
1	B	548	3% 87% 9% ..

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	B3Z	A	1543[A]	-	X	-	-
2	B3Z	A	1543[B]	-	X	-	-
2	B3Z	B	1544	-	X	-	-
3	PEG	A	1547	-	-	X	-
5	NAG	A	1548	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9484 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.

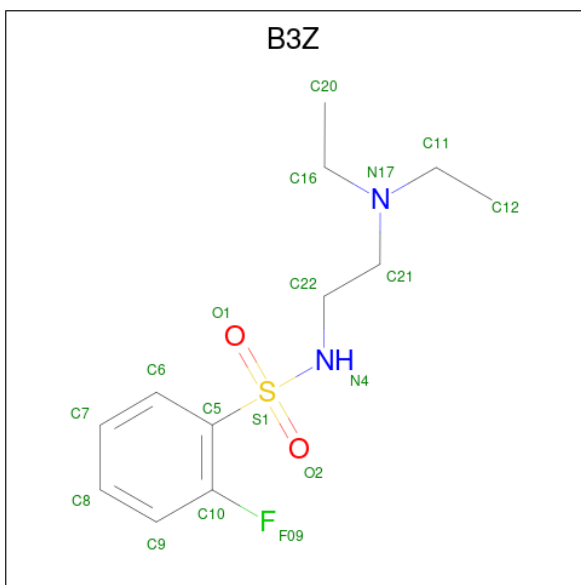
- Molecule 1 is a protein called ACETYLCHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	4	0
			4207	2697	733	763	14			
1	B	533	Total	C	N	O	S	0	1	0
			4167	2675	720	758	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 N-[2-(diethylamino)ethyl]-2-fluoranyl-benzenesulfonamide (CCD ID: B3Z) (formula: C₁₂H₁₉FN₂O₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	1
			36	24	2	4	4	2		
2	B	1	Total	C	F	N	O	S	0	0
			18	12	1	2	2	1		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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		

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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

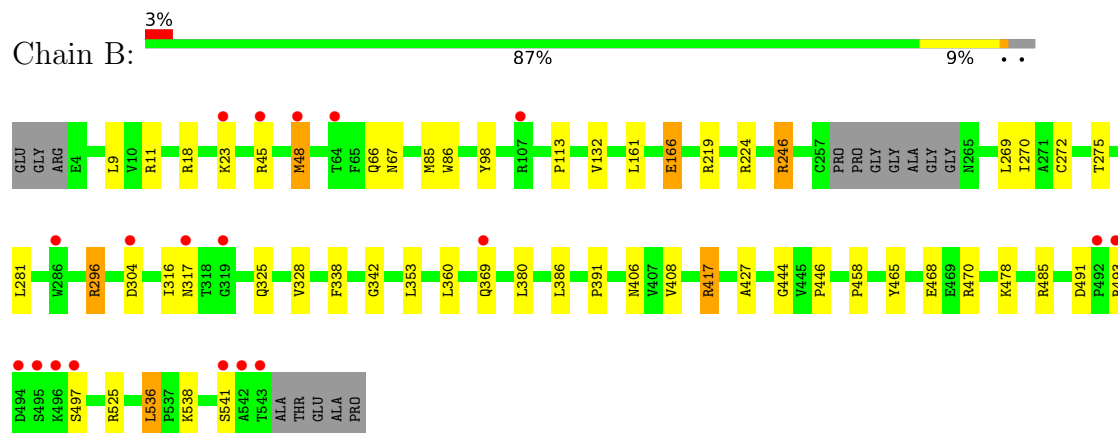


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	537	Total	O	0	0
			537	537		
6	B	397	Total	O	0	0
			397	397		

● 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	80.46Å 111.86Å 226.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.81 – 2.10 28.81 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (28.81-2.10) 99.8 (28.81-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.27 (at 2.10Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, R_{free}	0.191 , 0.215 0.185 , 0.208	Depositor DCC
R_{free} test set	2419 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 64.4	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	0.95	EDS
Total number of atoms	9484	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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: SO4, B3Z, NAG, 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	0.33	0/4339	0.74	1/5927 (0.0%)
1	B	0.33	0/4290	0.74	0/5863
All	All	0.33	0/8629	0.74	1/11790 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	305	GLY	N-CA-C	-5.25	108.08	115.32

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	4207	0	4100	35	0
1	B	4167	0	4053	30	0
2	A	36	0	38	4	0
2	B	18	0	19	4	0
3	A	35	0	50	6	0
3	B	35	0	50	3	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	28	0	26	0	0
5	B	14	0	13	0	0
6	A	537	0	0	6	0
6	B	397	0	0	4	0
All	All	9484	0	8349	71	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (71) 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:186:ASN:HD21	3:A:1547:PEG:H11	1.32	0.94
1:B:296:ARG:NH2	1:B:406:ASN:OD1	2.24	0.71
1:A:182:TRP:HA	3:A:1547:PEG:H21	1.74	0.69
1:A:246:ARG:NH2	6:A:2313:HOH:O	2.27	0.68
1:B:246:ARG:NH2	6:B:2225:HOH:O	2.27	0.66
1:A:45:ARG:NH1	1:A:51:GLU:OE1	2.27	0.66
1:A:304[A]:ASP:OD2	6:A:2246:HOH:O	2.14	0.66
1:B:380:LEU:HD12	3:B:1548:PEG:H32	1.80	0.62
1:B:219:ARG:NH2	6:B:2197:HOH:O	2.33	0.62
1:B:353:LEU:HB3	1:B:391:PRO:HB2	1.80	0.61
1:A:9:LEU:HG	1:A:18[B]:ARG:HH12	1.65	0.61
1:B:113:PRO:HG2	1:B:485:ARG:HG2	1.81	0.61
1:A:219:ARG:HE	3:A:1544:PEG:H31	1.68	0.59
1:A:219:ARG:HG2	3:A:1544:PEG:H21	1.85	0.58
3:A:1547:PEG:O1	6:A:2030:HOH:O	2.17	0.58
1:B:166:GLU:HG2	1:B:270:ILE:HD12	1.85	0.57
3:A:1547:PEG:O1	6:A:2079:HOH:O	2.11	0.56
1:B:408:VAL:HG11	1:B:525:ARG:HG3	1.87	0.56
1:A:316:ILE:HG13	1:A:417:ARG:HG2	1.88	0.56
1:B:67:ASN:ND2	6:B:2070:HOH:O	2.34	0.56
1:A:424:ARG:NH1	6:A:2460:HOH:O	2.34	0.55
1:A:304[A]:ASP:OD1	1:A:304[A]:ASP:N	2.36	0.55
1:A:433:ARG:NH2	1:A:440:PRO:O	2.40	0.55
1:B:219:ARG:HG2	3:B:1545:PEG:H21	1.88	0.54
1:A:207:ALA:O	1:A:211:MET:HG2	2.07	0.54
1:A:161:LEU:HD11	1:A:269:LEU:HD22	1.89	0.54
1:A:86:TRP:CD2	2:A:1543[B]:B3Z:H212	2.44	0.53
1:B:18:ARG:NH2	6:B:2012:HOH:O	2.28	0.53
1:A:86:TRP:CD2	2:A:1543[A]:B3Z:H212	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:ASP:OD1	1:B:304:ASP:N	2.42	0.51
1:B:85:MET:HA	3:B:1547:PEG:H12	1.91	0.51
1:A:245:ARG:O	1:A:249:THR:HG23	2.12	0.50
1:A:113:PRO:HG2	1:A:485:ARG:HG2	1.93	0.50
1:A:458:PRO:HA	1:A:465:TYR:CD1	2.47	0.50
1:B:161:LEU:HD12	1:B:270:ILE:HD11	1.94	0.50
1:B:86:TRP:CD2	2:B:1544:B3Z:H212	2.47	0.49
1:B:328:VAL:O	1:B:427:ALA:HA	2.14	0.48
1:A:224:ARG:HG2	1:A:325:GLN:HB2	1.94	0.48
1:B:316:ILE:HG13	1:B:417:ARG:HG2	1.95	0.48
1:A:433:ARG:CZ	1:A:437:LEU:HD23	2.44	0.48
1:B:338:PHE:CE2	2:B:1544:B3Z:H6	2.49	0.47
2:B:1544:B3Z:F09	2:B:1544:B3Z:N4	2.36	0.47
1:B:161:LEU:HD11	1:B:269:LEU:HD22	1.97	0.46
1:A:404:ASP:HA	1:A:408:VAL:HB	1.98	0.45
2:A:1543[A]:B3Z:F09	2:A:1543[A]:B3Z:N4	2.38	0.45
1:B:45:ARG:HA	1:B:48:MET:HG3	1.99	0.45
1:B:224:ARG:HG2	1:B:325:GLN:HB2	1.98	0.45
1:A:265:ASN:ND2	6:A:2324:HOH:O	2.50	0.44
1:A:23:LYS:HA	1:A:23:LYS:HD2	1.71	0.44
1:A:408:VAL:HG11	1:A:525:ARG:HG3	2.00	0.43
1:A:211:MET:HE3	1:A:301:PRO:HG2	2.00	0.43
1:B:45:ARG:HA	1:B:45:ARG:HD3	1.86	0.43
1:B:48:MET:HE3	1:B:166:GLU:HA	2.01	0.43
1:B:458:PRO:HA	1:B:465:TYR:CD1	2.54	0.43
1:A:166:GLU:HB2	1:A:270:ILE:HD13	2.01	0.43
1:A:374:ALA:HA	1:A:539:LEU:HD23	2.01	0.42
1:B:66:GLN:HG3	1:B:98:TYR:CD1	2.54	0.42
1:B:444:GLY:O	1:B:446:PRO:HD3	2.20	0.42
1:B:272:CYS:O	1:B:275:THR:OG1	2.37	0.42
1:A:386:LEU:HD23	1:A:386:LEU:HA	1.88	0.42
1:A:353:LEU:HB3	1:A:391:PRO:HB2	2.02	0.42
2:B:1544:B3Z:H203	2:B:1544:B3Z:H211	1.74	0.41
1:A:390:ASP:HA	1:A:391:PRO:HD3	1.80	0.41
1:B:491:ASP:C	1:B:493:ARG:H	2.28	0.41
1:B:166:GLU:HG2	1:B:270:ILE:CD1	2.51	0.41
1:A:216:LEU:HA	1:A:219:ARG:HD2	2.03	0.41
1:A:66:GLN:HG3	1:A:98:TYR:CD2	2.56	0.40
2:A:1543[A]:B3Z:H203	2:A:1543[A]:B3Z:H211	1.74	0.40
1:A:539:LEU:HD12	1:A:539:LEU:HA	1.92	0.40
1:B:536:LEU:HD22	1:B:536:LEU:HA	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304[A]:ASP:OD2	1:A:306:ASP: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	535/548 (98%)	524 (98%)	10 (2%)	1 (0%)	43	44
1	B	530/548 (97%)	513 (97%)	16 (3%)	1 (0%)	43	44
All	All	1065/1096 (97%)	1037 (97%)	26 (2%)	2 (0%)	43	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	342	GLY
1	A	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	443/446 (99%)	426 (96%)	17 (4%)	29	32
1	B	439/446 (98%)	417 (95%)	22 (5%)	22	22
All	All	882/892 (99%)	843 (96%)	39 (4%)	26	26

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	13	ARG
1	A	23	LYS
1	A	48	MET
1	A	81	GLU
1	A	132	VAL
1	A	200	PHE
1	A	246	ARG
1	A	332	LYS
1	A	369	GLN
1	A	376	GLU
1	A	417	ARG
1	A	418	LEU
1	A	424	ARG
1	A	470	ARG
1	A	536	LEU
1	A	540	LEU
1	B	9	LEU
1	B	11	ARG
1	B	23	LYS
1	B	48	MET
1	B	132	VAL
1	B	166	GLU
1	B	246	ARG
1	B	281	LEU
1	B	296	ARG
1	B	317	ASN
1	B	360	LEU
1	B	369[A]	GLN
1	B	369[B]	GLN
1	B	386	LEU
1	B	417	ARG
1	B	468	GLU
1	B	470	ARG
1	B	478	LYS
1	B	497	SER
1	B	536	LEU
1	B	538	LYS
1	B	541	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	508	GLN
1	A	509	GLN
1	B	317	ASN
1	B	474	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

18 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	1544	-	6,6,6	0.65	0	5,5,5	1.22	0
3	PEG	B	1550	-	6,6,6	0.66	0	5,5,5	1.38	0
4	SO4	B	1546	-	4,4,4	0.23	0	6,6,6	0.09	0
3	PEG	A	1551	-	6,6,6	0.64	0	5,5,5	1.31	0
2	B3Z	A	1543[B]	-	18,18,18	2.19	7 (38%)	24,24,24	3.21	9 (37%)
3	PEG	B	1545	-	6,6,6	0.65	0	5,5,5	1.24	0
3	PEG	B	1551	-	6,6,6	0.65	0	5,5,5	1.43	0
3	PEG	A	1549	-	6,6,6	0.66	0	5,5,5	1.24	0
5	NAG	A	1548	1	14,14,15	1.37	1 (7%)	17,19,21	1.53	2 (11%)
5	NAG	A	1546	1	14,14,15	1.37	1 (7%)	17,19,21	1.34	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PEG	A	1547	-	6,6,6	0.68	0	5,5,5	1.23	0
3	PEG	A	1550	-	6,6,6	0.64	0	5,5,5	1.40	0
3	PEG	B	1547	-	6,6,6	0.63	0	5,5,5	1.47	0
3	PEG	B	1548	-	6,6,6	0.65	0	5,5,5	1.32	0
4	SO4	A	1545	-	4,4,4	0.23	0	6,6,6	0.09	0
2	B3Z	B	1544	-	18,18,18	2.09	7 (38%)	24,24,24	3.16	9 (37%)
2	B3Z	A	1543[A]	-	18,18,18	2.12	7 (38%)	24,24,24	3.09	9 (37%)
5	NAG	B	1549	1	14,14,15	1.42	1 (7%)	17,19,21	1.34	2 (11%)

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	1544	-	-	2/4/4/4	-
3	PEG	B	1550	-	-	2/4/4/4	-
3	PEG	A	1551	-	-	2/4/4/4	-
2	B3Z	A	1543[B]	-	-	8/17/17/17	0/1/1/1
3	PEG	B	1545	-	-	2/4/4/4	-
3	PEG	B	1551	-	-	2/4/4/4	-
3	PEG	A	1549	-	-	2/4/4/4	-
5	NAG	A	1548	1	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	A	1546	1	-	0/6/23/26	0/1/1/1
3	PEG	A	1547	-	-	3/4/4/4	-
3	PEG	A	1550	-	-	3/4/4/4	-
3	PEG	B	1547	-	-	1/4/4/4	-
3	PEG	B	1548	-	-	3/4/4/4	-
2	B3Z	B	1544	-	-	9/17/17/17	0/1/1/1
2	B3Z	A	1543[A]	-	-	9/17/17/17	0/1/1/1
5	NAG	B	1549	1	-	4/6/23/26	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1544	B3Z	S1-N4	5.07	1.69	1.61
2	A	1543[A]	B3Z	S1-N4	5.03	1.69	1.61
2	A	1543[B]	B3Z	S1-N4	4.94	1.69	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1549	NAG	C7-N2	4.13	1.47	1.34
5	A	1548	NAG	C7-N2	4.04	1.47	1.34
5	A	1546	NAG	C7-N2	3.99	1.47	1.34
2	A	1543[B]	B3Z	C10-C5	3.76	1.41	1.39
2	A	1543[B]	B3Z	C5-S1	-3.33	1.72	1.77
2	A	1543[A]	B3Z	C5-S1	-3.27	1.73	1.77
2	B	1544	B3Z	C5-S1	-3.22	1.73	1.77
2	B	1544	B3Z	C10-C5	3.16	1.41	1.39
2	A	1543[A]	B3Z	C10-C5	3.14	1.41	1.39
2	A	1543[A]	B3Z	C6-C5	2.88	1.42	1.39
2	A	1543[B]	B3Z	C6-C5	2.82	1.42	1.39
2	B	1544	B3Z	C6-C5	2.73	1.42	1.39
2	A	1543[B]	B3Z	C21-N17	2.66	1.53	1.47
2	A	1543[B]	B3Z	O1-S1	-2.59	1.40	1.43
2	A	1543[A]	B3Z	O1-S1	-2.59	1.40	1.43
2	A	1543[A]	B3Z	C21-N17	2.58	1.53	1.47
2	A	1543[B]	B3Z	F09-C10	-2.56	1.28	1.35
2	B	1544	B3Z	C21-N17	2.53	1.53	1.47
2	B	1544	B3Z	F09-C10	-2.51	1.28	1.35
2	A	1543[A]	B3Z	F09-C10	-2.47	1.28	1.35
2	B	1544	B3Z	O1-S1	-2.26	1.40	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1543[B]	B3Z	C10-C5-S1	9.66	127.39	121.21
2	B	1544	B3Z	C6-C5-C10	-8.68	112.86	118.53
2	A	1543[B]	B3Z	C6-C5-C10	-8.58	112.93	118.53
2	A	1543[A]	B3Z	C6-C5-C10	-8.21	113.17	118.53
2	A	1543[A]	B3Z	C6-C5-S1	6.41	126.73	117.51
2	B	1544	B3Z	C6-C5-S1	6.25	126.50	117.51
2	B	1544	B3Z	C9-C10-C5	5.93	125.10	122.22
2	A	1543[A]	B3Z	C9-C10-C5	5.69	124.98	122.22
2	A	1543[A]	B3Z	C5-S1-N4	-4.98	101.08	107.86
2	B	1544	B3Z	C5-S1-N4	-4.91	101.18	107.86
2	B	1544	B3Z	C21-C22-N4	4.82	119.33	110.35
2	A	1543[B]	B3Z	C21-C22-N4	4.71	119.11	110.35
5	A	1548	NAG	C1-O5-C5	4.48	118.19	112.19
2	A	1543[A]	B3Z	C21-C22-N4	4.48	118.69	110.35
5	A	1546	NAG	C1-O5-C5	3.94	117.46	112.19
5	B	1549	NAG	C1-O5-C5	3.87	117.38	112.19
2	A	1543[A]	B3Z	O1-S1-C5	3.32	113.17	107.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1544	B3Z	O1-S1-N4	3.23	112.06	107.03
2	A	1543[B]	B3Z	C9-C10-C5	3.17	123.76	122.22
2	A	1543[A]	B3Z	O1-S1-N4	3.00	111.70	107.03
2	B	1544	B3Z	O1-S1-C5	2.99	112.61	107.68
2	A	1543[B]	B3Z	C7-C6-C5	2.92	123.98	118.76
2	A	1543[B]	B3Z	O1-S1-C5	2.89	112.45	107.68
5	B	1549	NAG	C8-C7-N2	2.75	120.67	116.12
2	A	1543[B]	B3Z	C5-S1-N4	-2.72	104.16	107.86
2	A	1543[B]	B3Z	O1-S1-N4	2.67	111.19	107.03
5	A	1548	NAG	C8-C7-N2	2.40	120.10	116.12
5	A	1546	NAG	C8-C7-N2	2.29	119.91	116.12
2	B	1544	B3Z	C7-C6-C5	2.26	122.80	118.76
2	A	1543[A]	B3Z	O2-S1-N4	-2.22	103.57	107.03
2	B	1544	B3Z	O2-S1-N4	-2.21	103.59	107.03
2	A	1543[A]	B3Z	C7-C6-C5	2.09	122.50	118.76
2	A	1543[B]	B3Z	O2-S1-N4	-2.09	103.78	107.03

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1548	NAG	C1

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1543[A]	B3Z	C22-N4-S1-C5
2	A	1543[A]	B3Z	C10-C5-S1-O1
2	A	1543[A]	B3Z	C10-C5-S1-O2
2	A	1543[A]	B3Z	N17-C21-C22-N4
2	A	1543[B]	B3Z	C22-N4-S1-C5
2	A	1543[B]	B3Z	C10-C5-S1-O2
2	A	1543[B]	B3Z	N17-C21-C22-N4
2	B	1544	B3Z	C10-C5-S1-O1
2	B	1544	B3Z	C10-C5-S1-O2
2	B	1544	B3Z	N17-C21-C22-N4
2	A	1543[A]	B3Z	C22-N4-S1-O2
2	A	1543[B]	B3Z	C22-N4-S1-O2
2	B	1544	B3Z	C6-C5-S1-N4
2	B	1544	B3Z	C22-N4-S1-O2
5	B	1549	NAG	O5-C5-C6-O6
5	A	1548	NAG	O5-C5-C6-O6
5	A	1548	NAG	C4-C5-C6-O6

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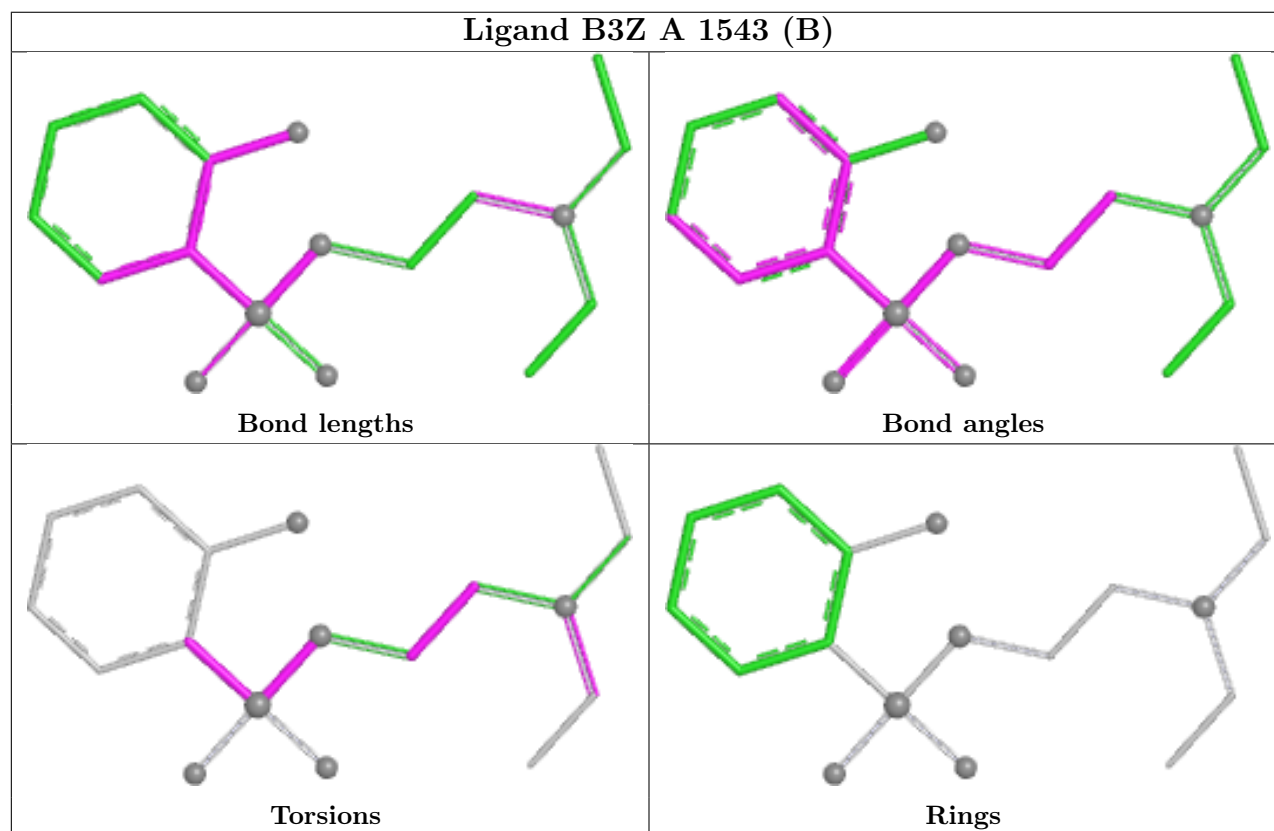
Mol	Chain	Res	Type	Atoms
5	B	1549	NAG	C4-C5-C6-O6
2	B	1544	B3Z	C22-N4-S1-C5
5	B	1549	NAG	C8-C7-N2-C2
5	B	1549	NAG	O7-C7-N2-C2
2	A	1543[A]	B3Z	C10-C5-S1-N4
2	B	1544	B3Z	C10-C5-S1-N4
3	A	1544	PEG	O2-C3-C4-O4
3	A	1547	PEG	O1-C1-C2-O2
3	A	1549	PEG	O2-C3-C4-O4
3	B	1550	PEG	O1-C1-C2-O2
2	A	1543[A]	B3Z	C6-C5-S1-N4
3	A	1547	PEG	O2-C3-C4-O4
3	B	1551	PEG	O2-C3-C4-O4
3	B	1545	PEG	O1-C1-C2-O2
2	A	1543[B]	B3Z	C10-C5-S1-N4
2	A	1543[B]	B3Z	C6-C5-S1-N4
3	A	1544	PEG	O1-C1-C2-O2
3	A	1550	PEG	O1-C1-C2-O2
3	B	1548	PEG	O2-C3-C4-O4
2	A	1543[B]	B3Z	C6-C5-S1-O2
2	B	1544	B3Z	C6-C5-S1-O2
3	A	1551	PEG	O2-C3-C4-O4
3	B	1547	PEG	O2-C3-C4-O4
2	A	1543[A]	B3Z	C6-C5-S1-O2
3	B	1551	PEG	C4-C3-O2-C2
2	B	1544	B3Z	C6-C5-S1-O1
3	B	1550	PEG	O2-C3-C4-O4
3	A	1550	PEG	C1-C2-O2-C3
3	A	1551	PEG	C4-C3-O2-C2
3	B	1548	PEG	O1-C1-C2-O2
3	A	1549	PEG	C1-C2-O2-C3
3	B	1548	PEG	C1-C2-O2-C3
3	B	1545	PEG	O2-C3-C4-O4
3	A	1547	PEG	C1-C2-O2-C3
2	A	1543[A]	B3Z	C6-C5-S1-O1
3	A	1550	PEG	C4-C3-O2-C2
2	A	1543[B]	B3Z	C12-C11-N17-C21

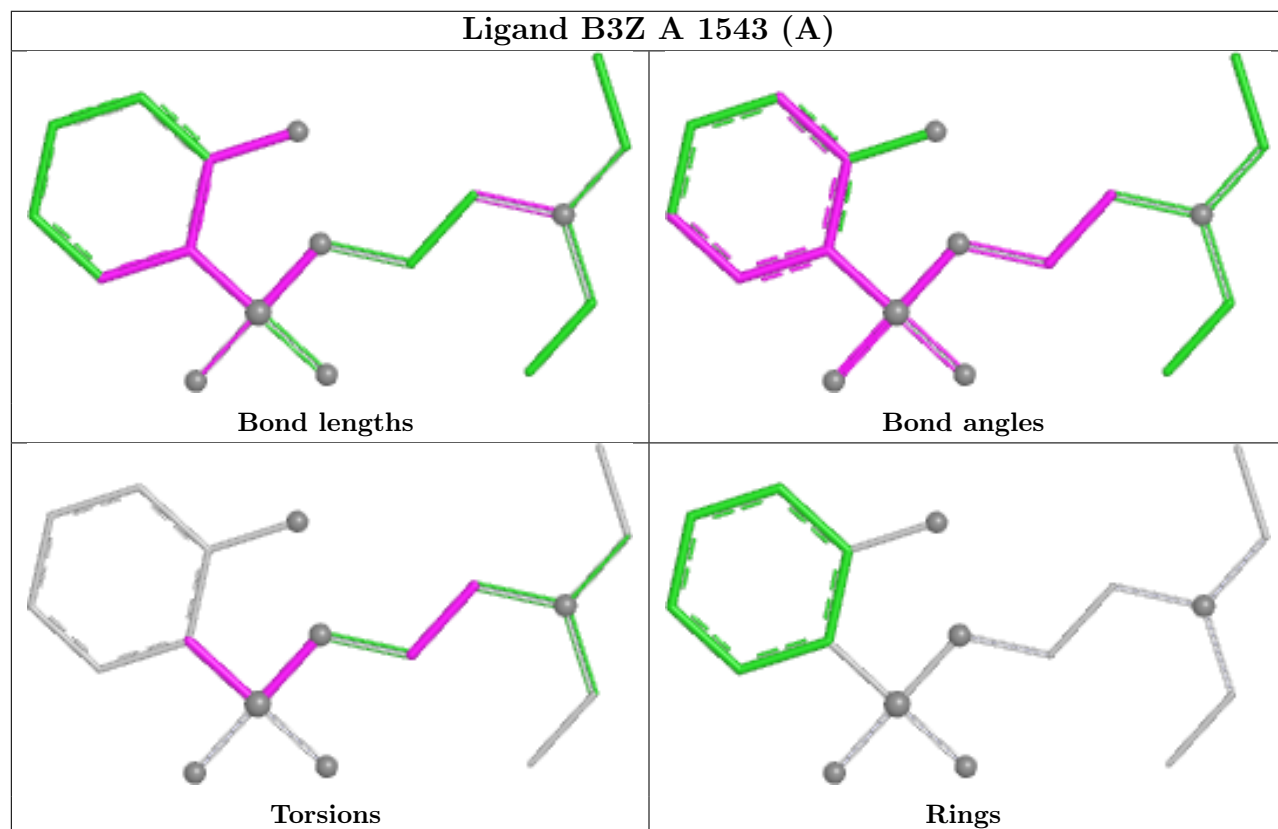
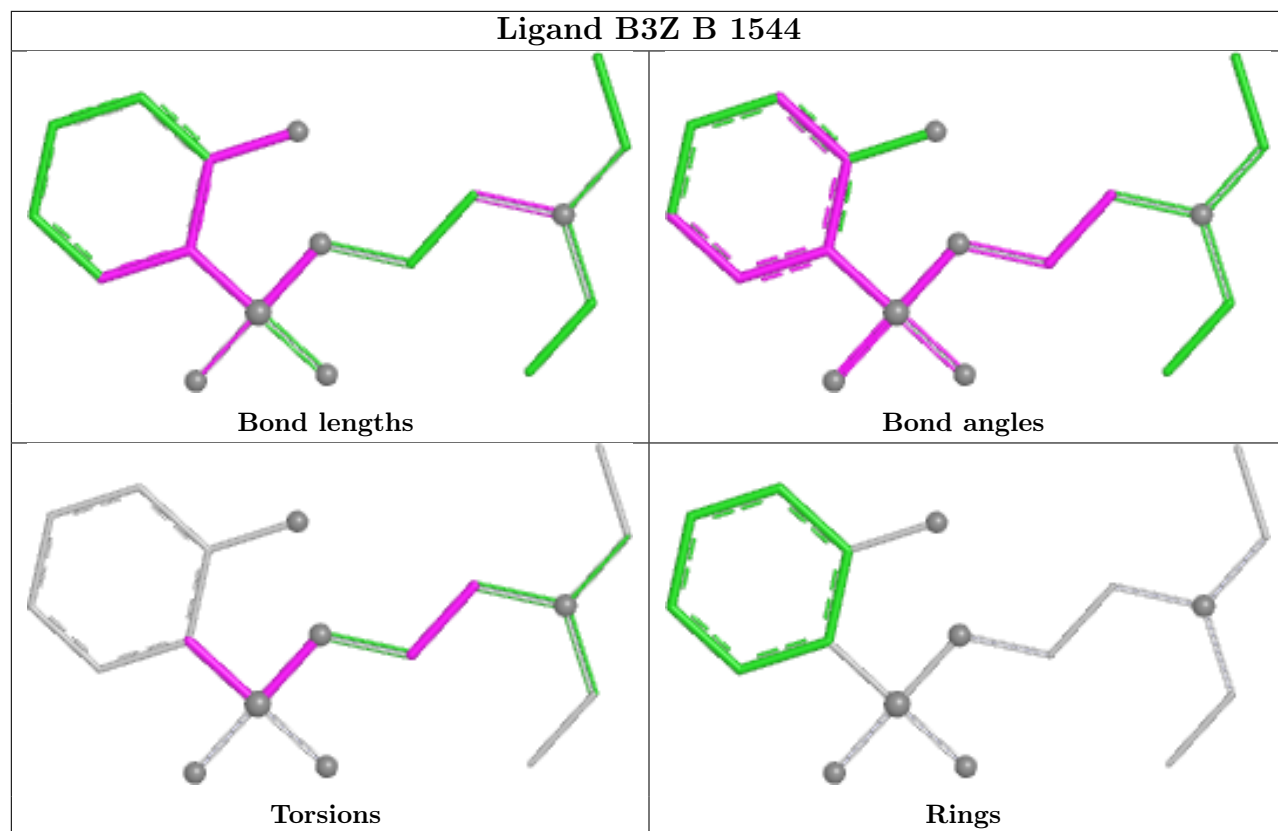
There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1544	PEG	2	0
2	A	1543[B]	B3Z	1	0
3	B	1545	PEG	1	0
3	A	1547	PEG	4	0
3	B	1547	PEG	1	0
3	B	1548	PEG	1	0
2	B	1544	B3Z	4	0
2	A	1543[A]	B3Z	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	535/548 (97%)	-0.11	11 (2%) 63 66	21, 34, 58, 116	4 (0%)
1	B	533/548 (97%)	0.02	19 (3%) 46 48	22, 38, 63, 116	1 (0%)
All	All	1068/1096 (97%)	-0.04	30 (2%) 55 57	21, 36, 60, 116	5 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	496	LYS	7.5
1	B	497	SER	6.3
1	B	495	SER	5.9
1	B	494	ASP	4.4
1	B	542	ALA	3.7
1	A	494	ASP	3.6
1	A	9	LEU	3.6
1	B	492	PRO	3.6
1	B	543	THR	3.4
1	B	541	SER	3.0
1	A	493	ARG	2.9
1	B	493	ARG	2.9
1	A	542	ALA	2.8
1	A	495	SER	2.7
1	B	304	ASP	2.7
1	A	541	SER	2.5
1	B	317	ASN	2.5
1	A	319	GLY	2.5
1	B	64	THR	2.5
1	A	23	LYS	2.2
1	A	485	ARG	2.2
1	B	48	MET	2.2
1	B	286	TRP	2.1
1	A	540	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	45	ARG	2.1
1	A	323	ASP	2.0
1	B	369[A]	GLN	2.0
1	B	107	ARG	2.0
1	B	23	LYS	2.0
1	B	319	GLY	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
5	NAG	B	1549	14/15	0.56	0.19	68,81,89,92	0
5	NAG	A	1548	14/15	0.63	0.16	82,89,92,93	0
5	NAG	A	1546	14/15	0.69	0.17	63,74,80,81	0
3	PEG	B	1548	7/7	0.72	0.33	64,69,72,72	0
3	PEG	B	1545	7/7	0.77	0.24	46,49,54,55	0
3	PEG	A	1544	7/7	0.79	0.24	46,51,55,56	0
3	PEG	B	1547	7/7	0.80	0.26	71,71,74,77	0
3	PEG	B	1551	7/7	0.81	0.22	82,83,85,85	0
3	PEG	A	1547	7/7	0.82	0.18	43,52,61,64	0
3	PEG	B	1550	7/7	0.84	0.17	63,65,68,71	0
3	PEG	A	1551	7/7	0.85	0.15	69,70,73,74	0
3	PEG	A	1550	7/7	0.86	0.18	64,66,70,72	0
3	PEG	A	1549	7/7	0.86	0.19	73,74,79,81	0
4	SO4	B	1546	5/5	0.89	0.11	70,72,73,75	0
2	B3Z	A	1543[A]	18/18	0.90	0.15	36,42,46,49	18
2	B3Z	A	1543[B]	18/18	0.90	0.15	36,42,46,48	18
4	SO4	A	1545	5/5	0.91	0.12	63,66,66,68	0

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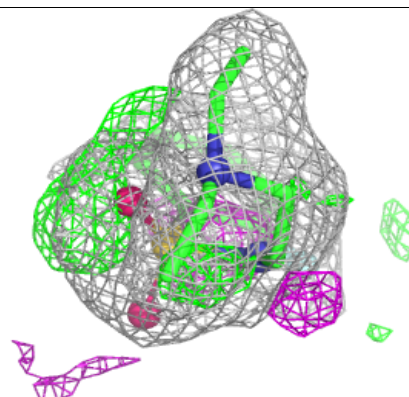
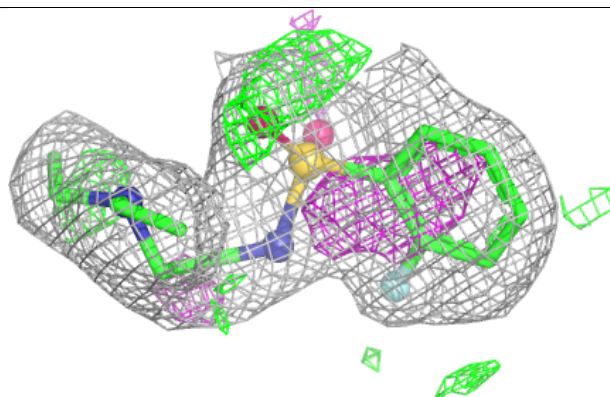
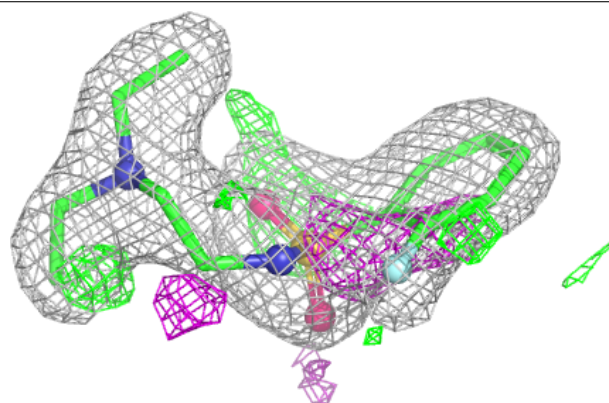
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	B3Z	B	1544	18/18	0.92	0.14	39,46,57,61	0

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.

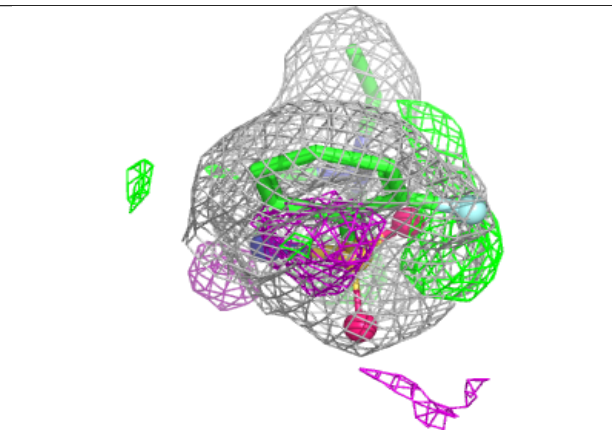
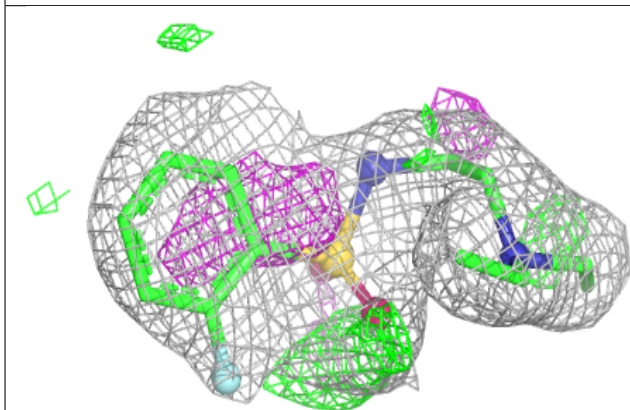
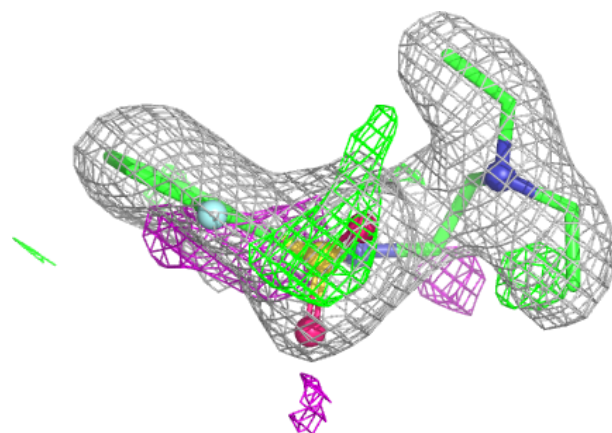
Electron density around B3Z A 1543 (A):

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

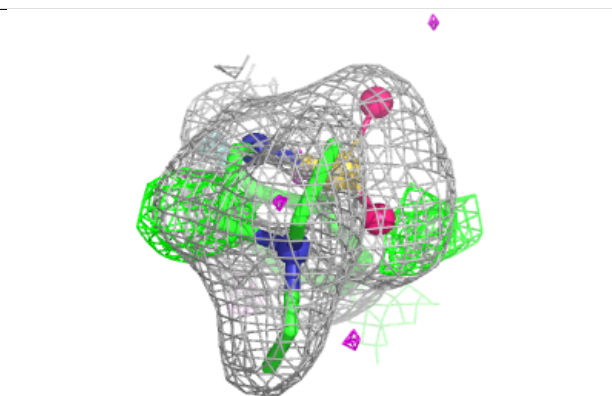
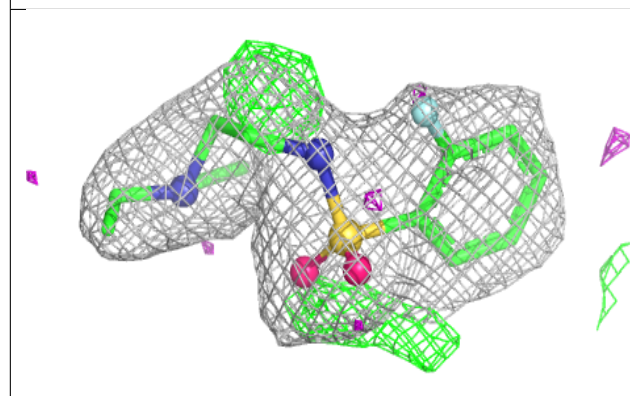
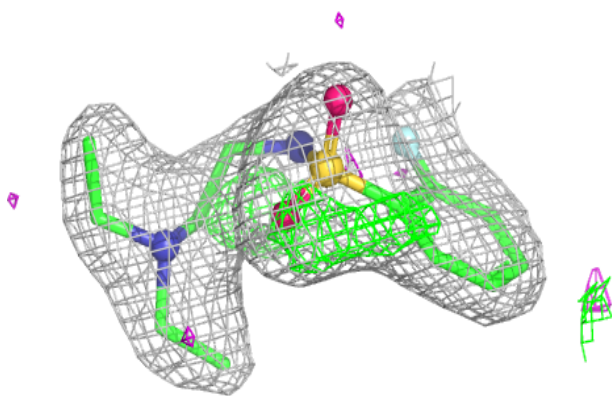


Electron density around B3Z A 1543 (B):

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

**Electron density around B3Z B 1544:**

$2mF_o-DF_c$ (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.