



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:50 AM UTC

PDB ID : 5EHZ / pdb_00005ehz
Title : mAChE-syn TZ2PA5 complex from an equimolar mixture of the syn/anti isomers
Authors : Bourne, Y.; Marchot, P.
Deposited on : 2015-10-29
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 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

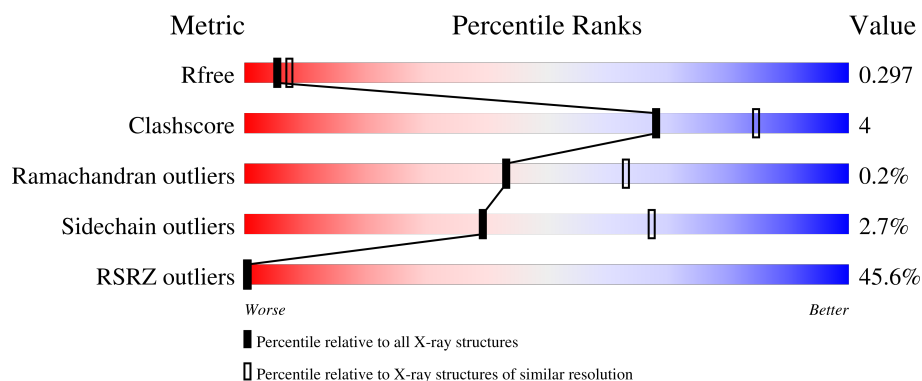
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	543	 40% 87% 11% ..
1	B	543	 50% 88% 9% ..

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8903 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	538	Total	C	N	O	S	0	3	0
			4216	2705	732	765	14			
1	B	534	Total	C	N	O	S	0	3	0
			4182	2685	720	763	14			

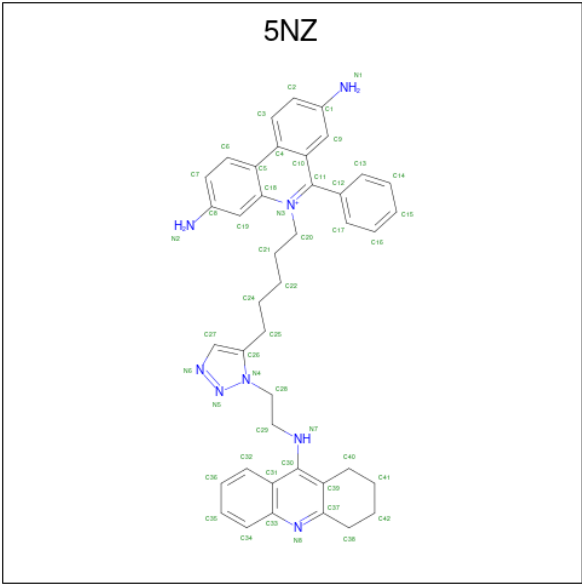
- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

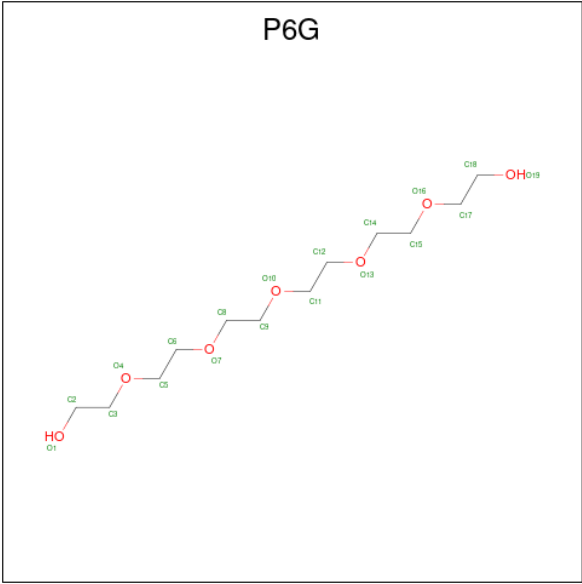
- Molecule 3 is 6-phenyl-5-[5-[3-[2-(1,2,3,4-tetrahydroacridin-9-ylamino)ethyl]-1,2,3-triazol-4-

yl]pentyl]phenanthridin-5-ium-3,8-diamine (CCD ID: 5NZ) (formula: C₄₁H₄₃N₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			49	41	8		
3	B	1	Total	C	N	0	0
			49	41	8		

- Molecule 4 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: C₁₂H₂₆O₇).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	203	Total 203	O 203	0	0
5	B	143	Total 143	O 143	0	0

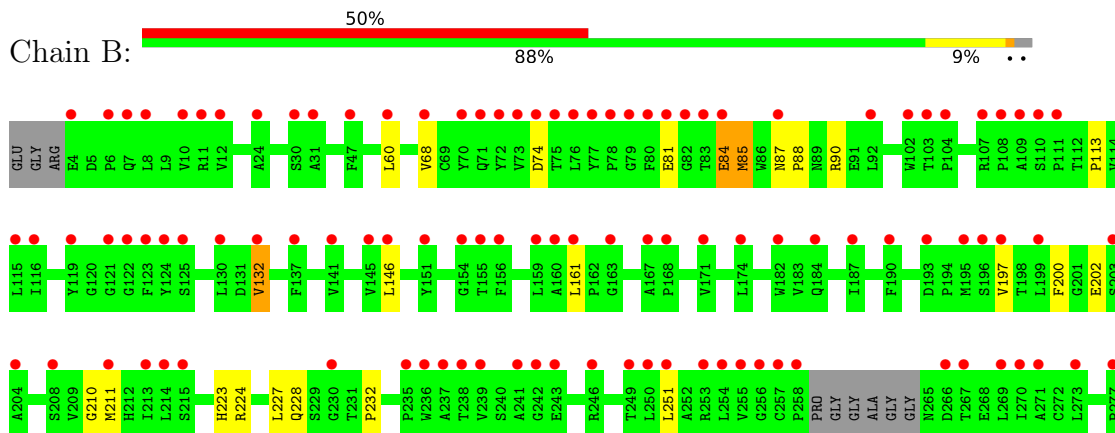
3 Residue-property plots

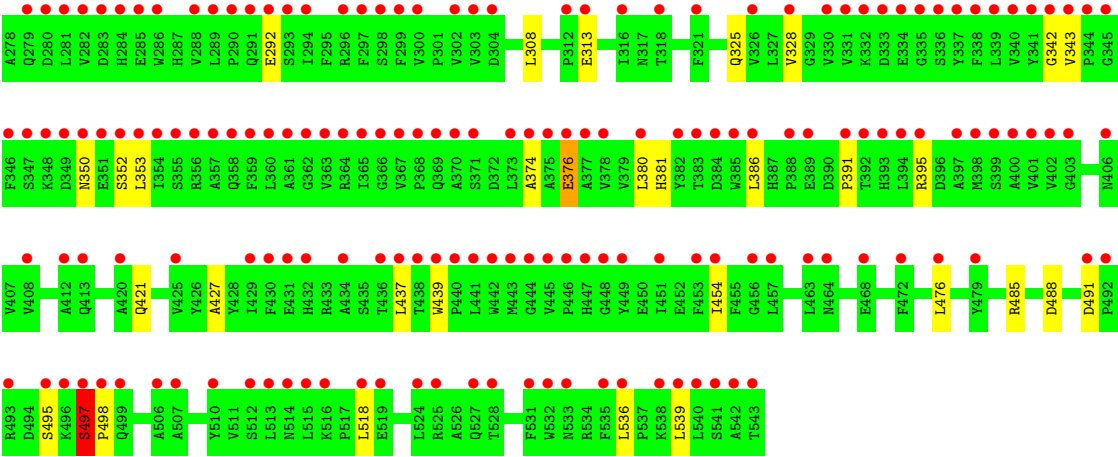
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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, α , β , γ	79.11Å 110.97Å 227.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.00 – 2.50 44.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.00-2.50) 99.4 (44.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.45Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.176 , 0.197 (Not available) , 0.297	Depositor DCC
R_{free} test set	1421 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	51.4	Xtriage
Anisotropy	0.888	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8903	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P6G, 5NZ, NAG

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	0.84	3/4350 (0.1%)	1.25	15/5944 (0.3%)
1	B	0.83	2/4317 (0.0%)	1.24	8/5900 (0.1%)
All	All	0.84	5/8667 (0.1%)	1.24	23/11844 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	443	MET	SD-CE	-8.83	1.57	1.79
1	A	454	ILE	CG1-CD1	-7.76	1.21	1.51
1	B	497	SER	CA-C	7.06	1.61	1.52
1	A	85	MET	SD-CE	-6.80	1.62	1.79
1	B	85	MET	SD-CE	-5.07	1.66	1.79

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	200	PHE	CA-CB-CG	7.66	121.46	113.80
1	B	350	ASN	CA-CB-CG	7.56	120.16	112.60
1	B	343	VAL	N-CA-C	7.17	115.00	107.76
1	B	74	ASP	CA-CB-CG	7.17	119.77	112.60
1	A	350	ASN	CA-CB-CG	7.01	119.61	112.60
1	A	74	ASP	CA-CB-CG	6.90	119.50	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	PHE	CA-CB-CG	6.77	120.57	113.80
1	B	342	GLY	N-CA-C	6.52	122.75	114.66
1	B	292	GLU	N-CA-C	-6.27	100.37	109.59
1	A	292	GLU	N-CA-C	-5.96	100.83	109.59
1	A	342	GLY	N-CA-C	5.87	124.82	115.66
1	A	342	GLY	CA-C-N	-5.66	117.13	123.02
1	A	342	GLY	C-N-CA	-5.66	117.13	123.02
1	A	497	SER	CA-C-N	-5.49	114.05	119.92
1	A	497	SER	C-N-CA	-5.49	114.05	119.92
1	B	491	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	482	ASN	CA-CB-CG	5.27	117.87	112.60
1	A	324	LEU	N-CA-C	5.14	117.78	109.40
1	A	298	SER	N-CA-C	5.13	116.56	111.07
1	A	175	ASP	CA-CB-CG	5.10	117.70	112.60
1	B	488	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	340	VAL	CA-C-N	-5.01	112.77	120.88
1	A	340	VAL	C-N-CA	-5.01	112.77	120.88

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	409	CYS	Mainchain

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	4216	0	4106	30	0
1	B	4182	0	4065	28	0
2	A	28	0	26	0	0
2	B	14	0	13	0	0
3	A	49	0	43	4	0
3	B	49	0	43	2	0
4	B	19	0	26	1	0
5	A	203	0	0	2	0
5	B	143	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8903	0	8322	61	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 (61) 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:B:197:VAL:H	1:B:223:HIS:HD2	1.27	0.83
1:A:197:VAL:H	1:A:223:HIS:HD2	1.28	0.79
1:B:497:SER:HB2	1:B:498:PRO:HA	1.65	0.78
1:B:497:SER:CB	1:B:498:PRO:HA	2.22	0.69
1:B:197:VAL:H	1:B:223:HIS:CD2	2.10	0.68
1:A:197:VAL:H	1:A:223:HIS:CD2	2.10	0.68
1:A:369[B]:GLN:HE22	1:A:405:HIS:CE1	2.15	0.65
1:B:113:PRO:HG2	1:B:485:ARG:HG2	1.82	0.62
1:A:113:PRO:HG2	1:A:485:ARG:HG2	1.84	0.58
1:B:497:SER:HB2	1:B:498:PRO:CA	2.32	0.58
1:B:68:VAL:HG23	1:B:90:ARG:HB2	1.87	0.57
1:A:68:VAL:HG11	1:A:88:PRO:HB3	1.87	0.57
1:B:224:ARG:HG2	1:B:325:GLN:HB2	1.87	0.56
1:B:497:SER:CB	1:B:498:PRO:CA	2.84	0.55
1:A:74:ASP:CG	3:A:603:5NZ:H8	2.32	0.54
1:A:498:PRO:HG2	1:A:518:LEU:HB2	1.90	0.54
1:A:224:ARG:HG2	1:A:325:GLN:HB2	1.89	0.53
1:B:381:HIS:HA	4:B:602:P6G:H51	1.89	0.53
3:A:603:5NZ:H29	5:A:721:HOH:O	2.08	0.53
1:B:68:VAL:HG11	1:B:88:PRO:HB3	1.89	0.53
1:A:337:TYR:O	1:A:340:VAL:HG22	2.09	0.53
1:B:454:ILE:HD13	1:B:476:LEU:HB3	1.90	0.52
1:B:84:GLU:HG3	1:B:87:ASN:HD22	1.74	0.52
3:A:603:5NZ:C29	5:A:721:HOH:O	2.58	0.52
1:A:491:ASP:OD1	1:A:493:ARG:HG3	2.11	0.51
1:B:498:PRO:HG2	1:B:518:LEU:O	2.11	0.50
1:B:81[B]:GLU:H	1:B:81[B]:GLU:CD	2.22	0.48
1:B:328:VAL:O	1:B:427:ALA:HA	2.14	0.48
1:B:439:TRP:CZ2	3:B:603:5NZ:H35	2.49	0.47
1:A:211:MET:HG2	1:A:308:LEU:HD21	1.97	0.47
1:A:340:VAL:HG11	1:A:443:MET:CE	2.45	0.46
1:A:68:VAL:HG23	1:A:90:ARG:HB2	1.97	0.46
1:B:211:MET:HG2	1:B:308:LEU:HD21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ASP:HB3	1:A:8:LEU:HD12	1.97	0.46
1:A:85:MET:HE1	1:A:132:VAL:HG11	1.98	0.45
1:A:370:ALA:HA	1:A:540:LEU:HD11	1.99	0.45
1:B:353:LEU:HB3	1:B:391:PRO:HB2	1.98	0.45
1:B:374:ALA:HA	1:B:539:LEU:HD23	1.99	0.45
1:A:328:VAL:O	1:A:427:ALA:HA	2.16	0.44
1:A:353:LEU:HB3	1:A:391:PRO:HB2	1.98	0.44
1:A:202:GLU:HA	1:A:228:GLN:O	2.17	0.44
1:A:341:TYR:CE1	3:A:603:5NZ:H10	2.53	0.43
1:B:202:GLU:HA	1:B:228:GLN:O	2.18	0.43
1:A:374:ALA:HA	1:A:539:LEU:HD23	2.00	0.43
3:B:603:5NZ:H5	3:B:603:5NZ:H16	1.76	0.43
1:B:85:MET:HE1	1:B:132:VAL:HG11	1.99	0.43
1:B:376:GLU:O	1:B:380:LEU:HG	2.19	0.43
1:A:213:ILE:O	1:A:219[A]:ARG:HD3	2.17	0.43
1:B:536:LEU:HD12	1:B:536:LEU:HA	1.88	0.43
1:A:369[B]:GLN:HE22	1:A:405:HIS:HE1	1.66	0.42
1:A:376:GLU:O	1:A:380:LEU:HG	2.19	0.42
1:B:210:GLY:HA3	1:B:232:PRO:HD3	2.00	0.42
1:A:249:THR:HG23	1:A:259:PRO:HG3	2.02	0.42
1:A:210:GLY:HA3	1:A:232:PRO:HD3	2.01	0.41
1:B:352:SER:O	1:B:395:ARG:HG3	2.21	0.41
1:A:211:MET:HG3	1:A:232:PRO:HB3	2.03	0.40
1:B:211:MET:HG3	1:B:232:PRO:HB3	2.01	0.40
1:A:200:PHE:HB2	1:A:226:VAL:HB	2.02	0.40
1:A:386:LEU:HD23	1:A:386:LEU:HA	1.96	0.40
1:A:103:THR:HG21	1:A:190:PHE:HB3	2.03	0.40
1:B:227:LEU:HB2	1:B:328:VAL:HG12	2.03	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	537/543 (99%)	521 (97%)	15 (3%)	1 (0%)	43	63
1	B	533/543 (98%)	515 (97%)	17 (3%)	1 (0%)	43	63
All	All	1070/1086 (98%)	1036 (97%)	32 (3%)	2 (0%)	43	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	497	SER
1	A	523	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	444/443 (100%)	433 (98%)	11 (2%)	42	69
1	B	442/443 (100%)	429 (97%)	13 (3%)	37	65
All	All	886/886 (100%)	862 (97%)	24 (3%)	39	67

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

Mol	Chain	Res	Type
1	A	7	GLN
1	A	13	ARG
1	A	84	GLU
1	A	146	LEU
1	A	161	LEU
1	A	251	LEU
1	A	386	LEU
1	A	421	GLN
1	A	493	ARG
1	A	495	SER
1	A	540	LEU
1	B	60	LEU
1	B	84	GLU
1	B	132	VAL

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Mol	Chain	Res	Type
1	B	146	LEU
1	B	161	LEU
1	B	251	LEU
1	B	313	GLU
1	B	376	GLU
1	B	386	LEU
1	B	421	GLN
1	B	437	LEU
1	B	495	SER
1	B	497	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	HIS
1	A	287	HIS
1	A	317	ASN
1	A	405	HIS
1	A	413	GLN
1	B	67	ASN
1	B	223	HIS
1	B	317	ASN
1	B	322	GLN
1	B	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 oligosaccharides in this entry.

5.6 Ligand geometry

6 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
4	P6G	B	602	-	18,18,18	0.57	0	17,17,17	0.39	0
2	NAG	A	601	1	14,14,15	0.40	0	17,19,21	0.82	1 (5%)
2	NAG	A	602	1	14,14,15	0.41	0	17,19,21	0.85	1 (5%)
2	NAG	B	601	1	14,14,15	0.41	0	17,19,21	1.49	2 (11%)
3	5NZ	A	603	-	54,56,56	2.19	12 (22%)	70,79,79	1.66	13 (18%)
3	5NZ	B	603	-	54,56,56	2.33	12 (22%)	70,79,79	1.88	13 (18%)

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
4	P6G	B	602	-	-	11/16/16/16	-
2	NAG	A	601	1	-	2/6/23/26	0/1/1/1
2	NAG	A	602	1	-	0/6/23/26	0/1/1/1
2	NAG	B	601	1	-	2/6/23/26	0/1/1/1
3	5NZ	A	603	-	-	6/18/25/25	0/8/8/8
3	5NZ	B	603	-	-	6/18/25/25	0/8/8/8

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	603	5NZ	C30-C39	7.50	1.51	1.39
3	B	603	5NZ	C39-C37	6.64	1.50	1.40
3	A	603	5NZ	C39-C37	6.53	1.50	1.40
3	A	603	5NZ	C30-C39	6.24	1.49	1.39
3	A	603	5NZ	C5-C18	5.25	1.51	1.41
3	B	603	5NZ	C5-C18	5.08	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	603	5NZ	C10-C4	4.90	1.50	1.42
3	B	603	5NZ	N6-N5	4.90	1.40	1.31
3	B	603	5NZ	C31-C33	4.81	1.50	1.42
3	A	603	5NZ	C10-C4	4.78	1.50	1.42
3	A	603	5NZ	N6-N5	4.56	1.39	1.31
3	A	603	5NZ	C31-C33	4.47	1.49	1.42
3	B	603	5NZ	C18-N3	-3.88	1.35	1.40
3	B	603	5NZ	N4-N5	3.70	1.40	1.35
3	A	603	5NZ	C37-N8	3.55	1.36	1.32
3	A	603	5NZ	N4-N5	3.52	1.40	1.35
3	A	603	5NZ	C11-C10	3.49	1.49	1.43
3	B	603	5NZ	C37-N8	3.47	1.36	1.32
3	B	603	5NZ	C11-C10	3.11	1.49	1.43
3	A	603	5NZ	C27-C26	3.11	1.40	1.36
3	B	603	5NZ	C30-C31	2.78	1.48	1.43
3	A	603	5NZ	C30-C31	2.54	1.47	1.43
3	B	603	5NZ	C27-C26	2.31	1.39	1.36
3	A	603	5NZ	C18-N3	-2.22	1.37	1.40

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	603	5NZ	C5-C18-N3	6.51	122.67	118.46
3	B	603	5NZ	C5-C18-N3	6.12	122.42	118.46
3	B	603	5NZ	C37-N8-C33	5.93	124.69	117.67
3	A	603	5NZ	C37-N8-C33	5.05	123.65	117.67
3	B	603	5NZ	C39-C37-N8	-4.92	120.18	123.66
3	B	603	5NZ	C24-C25-C26	-4.83	105.80	113.63
2	B	601	NAG	C1-O5-C5	4.44	118.13	112.19
3	A	603	5NZ	C39-C37-N8	-4.26	120.64	123.66
2	B	601	NAG	O5-C1-C2	-3.93	105.21	111.29
3	B	603	5NZ	C40-C39-C37	-3.37	117.73	120.90
3	B	603	5NZ	C28-N4-C26	3.06	132.02	129.14
2	A	602	NAG	C1-O5-C5	2.83	115.98	112.19
3	B	603	5NZ	C25-C26-C27	-2.76	126.87	131.35
3	B	603	5NZ	C27-C26-N4	2.69	107.32	103.90
3	B	603	5NZ	C31-C30-N7	-2.58	113.82	121.86
3	B	603	5NZ	C13-C12-C11	-2.45	116.86	120.25
3	A	603	5NZ	C28-C29-N7	2.44	117.26	110.29
3	A	603	5NZ	C31-C30-N7	-2.36	114.52	121.86
3	A	603	5NZ	C36-C35-C34	2.35	123.55	120.40
3	A	603	5NZ	C32-C31-C30	-2.32	120.52	124.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	603	5NZ	C32-C31-C33	2.27	120.88	118.36
3	A	603	5NZ	C27-C26-N4	2.26	106.77	103.90
3	A	603	5NZ	C41-C40-C39	-2.22	108.34	112.84
3	B	603	5NZ	C28-C29-N7	2.21	116.60	110.29
2	A	601	NAG	C1-O5-C5	2.17	115.09	112.19
3	B	603	5NZ	C32-C31-C30	-2.11	120.90	124.70
3	B	603	5NZ	C31-C33-N8	-2.10	120.57	122.80
3	A	603	5NZ	C27-N6-N5	-2.06	106.77	108.80
3	A	603	5NZ	C24-C25-C26	-2.00	110.38	113.63
3	A	603	5NZ	C3-C4-C10	2.00	120.19	117.72

There are no chirality outliers.

All (27) torsion outliers are listed below:

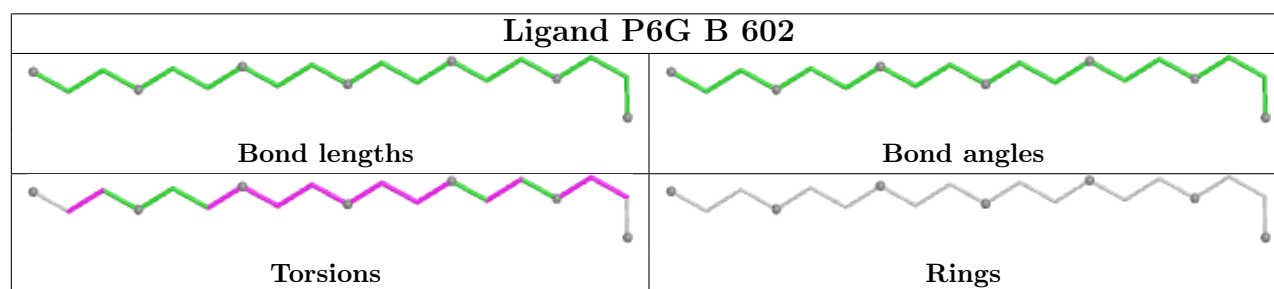
Mol	Chain	Res	Type	Atoms
3	A	603	5NZ	C29-C28-N4-N5
4	B	602	P6G	O4-C5-C6-O7
2	B	601	NAG	O5-C5-C6-O6
4	B	602	P6G	O1-C2-C3-O4
3	A	603	5NZ	N4-C28-C29-N7
3	B	603	5NZ	C22-C24-C25-C26
4	B	602	P6G	O7-C8-C9-O10
4	B	602	P6G	O16-C17-C18-O19
3	A	603	5NZ	C21-C22-C24-C25
3	B	603	5NZ	N4-C28-C29-N7
2	B	601	NAG	C4-C5-C6-O6
3	B	603	5NZ	C29-C28-N4-N5
2	A	601	NAG	C4-C5-C6-O6
3	B	603	5NZ	N3-C20-C21-C22
4	B	602	P6G	C8-C9-O10-C11
4	B	602	P6G	C2-C3-O4-C5
3	A	603	5NZ	C24-C25-C26-N4
4	B	602	P6G	C9-C8-O7-C6
4	B	602	P6G	C11-C12-O13-C14
2	A	601	NAG	O5-C5-C6-O6
4	B	602	P6G	C15-C14-O13-C12
4	B	602	P6G	C12-C11-O10-C9
3	A	603	5NZ	C39-C30-N7-C29
3	A	603	5NZ	C31-C30-N7-C29
3	B	603	5NZ	C31-C30-N7-C29
3	B	603	5NZ	C29-C28-N4-C26
4	B	602	P6G	O10-C11-C12-O13

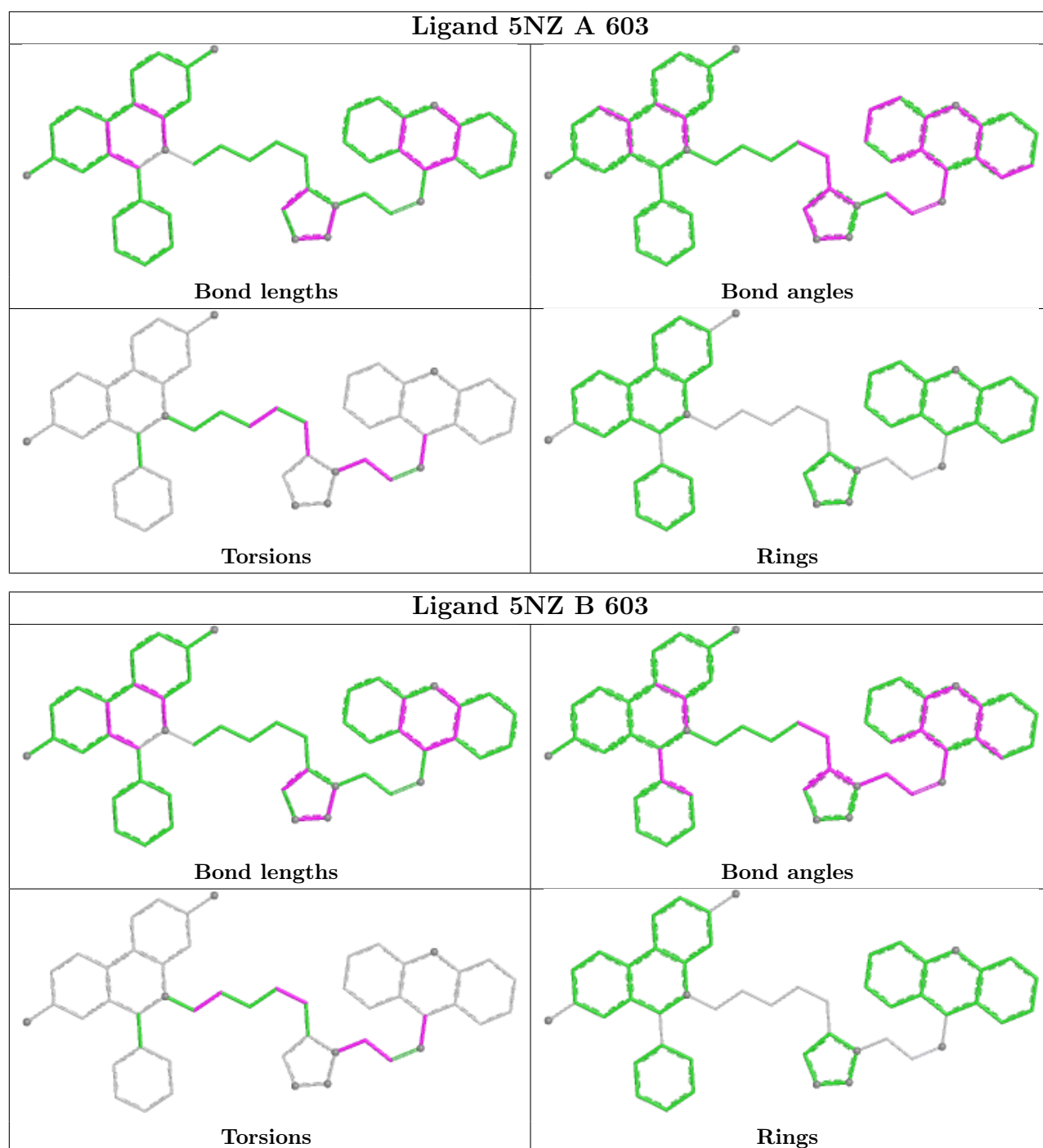
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	602	P6G	1	0
3	A	603	5NZ	4	0
3	B	603	5NZ	2	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	538/543 (99%)	1.84	216 (40%) 0 0	29, 47, 76, 132	3 (0%)
1	B	534/543 (98%)	2.35	273 (51%) 0 0	32, 52, 83, 141	3 (0%)
All	All	1072/1086 (98%)	2.09	489 (45%) 0 0	29, 49, 81, 141	6 (0%)

All (489) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	341	TYR	9.4
1	B	337	TYR	9.4
1	B	341	TYR	9.2
1	B	124	TYR	8.8
1	B	72	TYR	8.3
1	B	344	PRO	8.1
1	B	76	LEU	8.0
1	A	337	TYR	7.6
1	B	497	SER	6.6
1	B	365	ILE	6.5
1	B	77	TYR	6.2
1	B	345	GLY	6.1
1	B	258	PRO	6.1
1	B	342	GLY	6.1
1	A	540	LEU	6.0
1	B	354	ILE	5.9
1	B	75	THR	5.9
1	B	347	SER	5.7
1	B	395	ARG	5.7
1	B	349	ASP	5.6
1	B	394	LEU	5.5
1	A	259	PRO	5.4
1	B	250	LEU	5.4
1	B	492	PRO	5.3

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Mol	Chain	Res	Type	RSRZ
1	B	336	SER	5.2
1	B	430	PHE	5.2
1	B	446	PRO	5.2
1	B	353	LEU	5.2
1	A	543	THR	5.2
1	B	338	PHE	5.1
1	B	343	VAL	5.0
1	B	543	THR	5.0
1	B	439	TRP	5.0
1	B	73	VAL	5.0
1	A	267	THR	4.9
1	A	249	THR	4.9
1	B	340	VAL	4.9
1	B	335	GLY	4.8
1	A	76	LEU	4.8
1	B	360	LEU	4.8
1	B	78	PRO	4.7
1	A	342	GLY	4.7
1	B	447	HIS	4.7
1	A	315	LEU	4.6
1	B	364	ARG	4.6
1	B	540	LEU	4.6
1	B	398	MET	4.5
1	B	493	ARG	4.5
1	B	346	PHE	4.5
1	B	451	ILE	4.5
1	A	241	ALA	4.5
1	B	339	LEU	4.5
1	B	542	ALA	4.4
1	B	382	TYR	4.4
1	B	391	PRO	4.4
1	B	363	VAL	4.4
1	B	532	TRP	4.4
1	B	373	LEU	4.4
1	B	385	TRP	4.3
1	B	74	ASP	4.3
1	A	9	LEU	4.3
1	B	333	ASP	4.3
1	B	442	TRP	4.3
1	A	312	PRO	4.2
1	B	122	GLY	4.2
1	B	249	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	495	SER	4.2
1	B	392	THR	4.2
1	B	401	VAL	4.2
1	A	159	LEU	4.2
1	A	542	ALA	4.1
1	B	368	PRO	4.1
1	B	370	ALA	4.1
1	A	217	PRO	4.1
1	B	498	PRO	4.1
1	A	318	THR	4.0
1	B	533	ASN	4.0
1	B	159	LEU	4.0
1	A	77	TYR	4.0
1	A	307	PHE	4.0
1	B	81[A]	GLU	4.0
1	A	265	ASN	4.0
1	B	298	SER	4.0
1	B	155	THR	4.0
1	B	536	LEU	3.9
1	A	72	TYR	3.9
1	A	397	ALA	3.9
1	B	361	ALA	3.9
1	A	1	GLU	3.9
1	B	496	LYS	3.8
1	A	161	LEU	3.8
1	B	281	LEU	3.8
1	B	288	VAL	3.8
1	B	83	THR	3.8
1	B	400	ALA	3.8
1	B	535	PHE	3.8
1	A	365	ILE	3.8
1	B	71	GLN	3.8
1	A	302	VAL	3.8
1	A	335	GLY	3.8
1	A	394	LEU	3.8
1	A	109	ALA	3.7
1	A	248	ALA	3.7
1	B	300	VAL	3.7
1	B	160	ALA	3.7
1	B	397	ALA	3.7
1	B	362	GLY	3.7
1	B	402	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	352	SER	3.6
1	A	319	GLY	3.6
1	B	539	LEU	3.6
1	B	524	LEU	3.6
1	B	384	ASP	3.6
1	A	4	GLU	3.6
1	A	251	LEU	3.6
1	B	420	ALA	3.6
1	B	359	PHE	3.6
1	B	282	VAL	3.5
1	A	309	SER	3.5
1	A	2	GLY	3.5
1	A	242	GLY	3.5
1	B	79	GLY	3.5
1	B	70	TYR	3.5
1	A	347	SER	3.5
1	A	314	ALA	3.5
1	A	253	ARG	3.5
1	B	279	GLN	3.5
1	B	399	SER	3.5
1	B	156	PHE	3.5
1	B	87	ASN	3.5
1	B	358	GLN	3.5
1	B	441	LEU	3.5
1	B	294	ILE	3.5
1	B	304	ASP	3.4
1	B	239	VAL	3.4
1	A	313[A]	GLU	3.4
1	A	352	SER	3.4
1	B	10	VAL	3.4
1	A	535	PHE	3.3
1	B	151	TYR	3.3
1	B	92	LEU	3.3
1	B	271	ALA	3.3
1	A	323	ASP	3.3
1	B	331	VAL	3.3
1	B	367	VAL	3.3
1	A	137	PHE	3.3
1	A	156	PHE	3.3
1	A	321	PHE	3.3
1	B	123	PHE	3.3
1	A	417	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	296	ARG	3.3
1	A	288	VAL	3.3
1	B	141	VAL	3.3
1	A	419	ALA	3.3
1	B	374	ALA	3.3
1	A	166	GLU	3.3
1	B	313	GLU	3.3
1	B	425	VAL	3.3
1	A	169	GLY	3.3
1	B	286	TRP	3.3
1	A	258	PRO	3.2
1	B	431	GLU	3.2
1	A	82	GLY	3.2
1	A	155	THR	3.2
1	B	434	ALA	3.2
1	A	245	ARG	3.2
1	B	479	TYR	3.2
1	A	472	PHE	3.2
1	B	190	PHE	3.2
1	B	468	GLU	3.2
1	A	374	ALA	3.2
1	A	244	ALA	3.1
1	B	285	GLU	3.1
1	A	214	LEU	3.1
1	B	254	LEU	3.1
1	B	369	GLN	3.1
1	B	30	SER	3.1
1	B	47	PHE	3.1
1	B	531	PHE	3.1
1	A	459	LEU	3.1
1	B	513	LEU	3.1
1	A	511	VAL	3.1
1	A	75	THR	3.1
1	B	103	THR	3.1
1	B	297	PHE	3.1
1	B	321	PHE	3.1
1	A	174	LEU	3.1
1	B	269	LEU	3.1
1	A	141	VAL	3.1
1	A	354	ILE	3.1
1	A	373	LEU	3.1
1	A	401	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	73	VAL	3.0
1	A	171	VAL	3.0
1	B	499	GLN	3.0
1	B	146	LEU	3.0
1	B	348	LYS	3.0
1	A	422	GLY	3.0
1	A	385	TRP	3.0
1	B	378	VAL	3.0
1	B	334	GLU	3.0
1	B	357	ALA	3.0
1	A	465	TYR	3.0
1	A	232	PRO	3.0
1	B	108	PRO	3.0
1	A	418	LEU	3.0
1	B	356	ARG	3.0
1	B	280	ASP	3.0
1	A	517	PRO	3.0
1	B	255	VAL	2.9
1	A	168	PRO	2.9
1	B	355	SER	2.9
1	A	213	ILE	2.9
1	A	303	VAL	2.9
1	B	436	THR	2.9
1	A	78	PRO	2.9
1	B	253	ARG	2.9
1	B	115	LEU	2.9
1	B	302	VAL	2.9
1	B	371	SER	2.9
1	B	429	ILE	2.9
1	B	68	VAL	2.9
1	A	324	LEU	2.9
1	B	413	GLN	2.9
1	A	220	SER	2.8
1	A	410	PRO	2.8
1	B	438	THR	2.8
1	B	109	ALA	2.8
1	B	119	TYR	2.8
1	A	381	HIS	2.8
1	B	145	VAL	2.8
1	A	486	THR	2.8
1	B	366	GLY	2.8
1	A	471	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	414	LEU	2.8
1	A	513	LEU	2.8
1	B	24	ALA	2.8
1	B	241	ALA	2.8
1	B	351	GLU	2.8
1	A	525	ARG	2.8
1	A	25	PRO	2.8
1	A	391	PRO	2.8
1	B	235	PRO	2.8
1	B	383	THR	2.8
1	A	272	CYS	2.8
1	B	292	GLU	2.8
1	B	491	ASP	2.8
1	A	316	ILE	2.7
1	A	170	ASN	2.7
1	B	168	PRO	2.7
1	B	237	ALA	2.7
1	A	79	GLY	2.7
1	B	303	VAL	2.7
1	A	23	LYS	2.7
1	A	271	ALA	2.7
1	A	506	ALA	2.7
1	B	506	ALA	2.7
1	B	389	GLU	2.7
1	A	108	PRO	2.7
1	A	467	THR	2.7
1	A	413	GLN	2.7
1	B	230	GLY	2.7
1	A	290	PRO	2.7
1	B	350	ASN	2.7
1	A	216	LEU	2.7
1	A	443	MET	2.7
1	A	534	ARG	2.7
1	B	60	LEU	2.7
1	B	519	GLU	2.7
1	B	472	PHE	2.6
1	B	443	MET	2.6
1	B	161	LEU	2.6
1	B	457	LEU	2.6
1	B	463	LEU	2.6
1	B	215	SER	2.6
1	A	439	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	440	PRO	2.6
1	A	211	MET	2.6
1	A	380	LEU	2.6
1	A	226	VAL	2.6
1	B	110	SER	2.6
1	A	357	ALA	2.6
1	A	530	ALA	2.6
1	B	242	GLY	2.6
1	B	283	ASP	2.6
1	B	111	PRO	2.6
1	B	454	ILE	2.6
1	B	299	PHE	2.6
1	B	515	LEU	2.6
1	A	402	VAL	2.6
1	B	132	VAL	2.6
1	A	110	SER	2.6
1	A	298	SER	2.6
1	A	223	HIS	2.6
1	A	505	THR	2.6
1	B	412	ALA	2.6
1	B	432	HIS	2.6
1	B	516	LYS	2.6
1	B	236	TRP	2.6
1	A	539	LEU	2.6
1	B	199	LEU	2.6
1	A	445	VAL	2.6
1	B	328	VAL	2.6
1	B	449	TYR	2.6
1	B	388	PRO	2.5
1	A	222	PHE	2.5
1	B	453	PHE	2.5
1	A	233	ASN	2.5
1	A	533	ASN	2.5
1	B	514	ASN	2.5
1	A	144	ALA	2.5
1	B	6	PRO	2.5
1	A	310	ASP	2.5
1	A	199	LEU	2.5
1	A	221	LEU	2.5
1	B	386	LEU	2.5
1	B	437	LEU	2.5
1	B	284	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	434	ALA	2.5
1	A	526	ALA	2.5
1	B	375	ALA	2.5
1	B	238	THR	2.5
1	A	124	TYR	2.5
1	A	503	TYR	2.5
1	A	17	LEU	2.5
1	B	273	LEU	2.5
1	A	328	VAL	2.5
1	B	393	HIS	2.5
1	A	3	ARG	2.5
1	A	165	ARG	2.5
1	A	219[A]	ARG	2.5
1	A	415	ALA	2.5
1	B	293	SER	2.5
1	B	541	SER	2.5
1	A	458	PRO	2.5
1	B	277	PRO	2.5
1	B	163	GLY	2.5
1	A	270	ILE	2.5
1	A	320	ASP	2.5
1	B	193	ASP	2.5
1	A	138	LEU	2.5
1	A	496	LYS	2.5
1	B	12	VAL	2.5
1	B	330	VAL	2.5
1	A	364	ARG	2.5
1	B	203	SER	2.5
1	B	208	SER	2.5
1	B	512	SER	2.5
1	B	121	GLY	2.4
1	A	308	LEU	2.4
1	A	536	LEU	2.4
1	B	130	LEU	2.4
1	B	525	ARG	2.4
1	A	492	PRO	2.4
1	B	104	PRO	2.4
1	A	479	TYR	2.4
1	B	246	ARG	2.4
1	B	195	MET	2.4
1	A	164	SER	2.4
1	A	541	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	376	GLU	2.4
1	B	538	LYS	2.4
1	A	369[A]	GLN	2.4
1	A	515	LEU	2.4
1	B	518	LEU	2.4
1	A	287	HIS	2.4
1	B	464	ASN	2.4
1	B	243	GLU	2.4
1	B	332	LYS	2.4
1	A	135	GLY	2.4
1	A	454	ILE	2.4
1	A	266	ASP	2.4
1	A	70	TYR	2.4
1	A	239	VAL	2.4
1	B	326	VAL	2.4
1	B	445	VAL	2.4
1	A	235	PRO	2.3
1	A	291	GLN	2.3
1	A	524	LEU	2.3
1	B	187	ILE	2.3
1	A	160	ALA	2.3
1	A	377	ALA	2.3
1	B	204	ALA	2.3
1	B	267	THR	2.3
1	A	163	GLY	2.3
1	B	154	GLY	2.3
1	B	256	GLY	2.3
1	B	291	GLN	2.3
1	A	281	LEU	2.3
1	A	457	LEU	2.3
1	B	316	ILE	2.3
1	B	211	MET	2.3
1	A	299	PHE	2.3
1	B	257	CYS	2.3
1	B	406	ASN	2.3
1	A	6	PRO	2.3
1	B	184	GLN	2.3
1	B	456	GLY	2.3
1	A	273	LEU	2.3
1	B	197	VAL	2.3
1	B	403	GLY	2.3
1	A	512	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	266	ASP	2.3
1	A	338	PHE	2.3
1	A	531	PHE	2.3
1	A	153	VAL	2.3
1	A	104	PRO	2.3
1	A	356	ARG	2.3
1	B	11	ARG	2.3
1	A	60	LEU	2.2
1	A	516	LYS	2.2
1	A	538	LYS	2.2
1	B	125	SER	2.2
1	B	4	GLU	2.2
1	A	301	PRO	2.2
1	A	411	VAL	2.2
1	B	171	VAL	2.2
1	B	312	PRO	2.2
1	A	103	THR	2.2
1	A	198	THR	2.2
1	A	218	SER	2.2
1	A	346	PHE	2.2
1	B	137	PHE	2.2
1	A	344	PRO	2.2
1	A	370	ALA	2.2
1	B	528	THR	2.2
1	A	463	LEU	2.2
1	B	8	LEU	2.2
1	B	174	LEU	2.2
1	B	251	LEU	2.2
1	A	252	ALA	2.2
1	A	464	ASN	2.2
1	B	214	LEU	2.2
1	A	389	GLU	2.2
1	A	470	ARG	2.2
1	A	368	PRO	2.2
1	B	290	PRO	2.2
1	B	408	VAL	2.1
1	A	206	ALA	2.1
1	B	448	GLY	2.1
1	A	510	TYR	2.1
1	B	510	TYR	2.1
1	A	485	ARG	2.1
1	A	322	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	325	GLN	2.1
1	A	421	GLN	2.1
1	A	224	ARG	2.1
1	B	84	GLU	2.1
1	A	304	ASP	2.1
1	A	435	SER	2.1
1	A	7	GLN	2.1
1	A	326	VAL	2.1
1	B	7	GLN	2.1
1	A	188	ALA	2.1
1	B	289	LEU	2.1
1	B	444	GLY	2.1
1	A	274	ARG	2.1
1	A	527	GLN	2.1
1	B	167	ALA	2.1
1	A	115	LEU	2.1
1	A	289	LEU	2.1
1	B	182	TRP	2.1
1	B	476	LEU	2.1
1	A	305	GLY	2.1
1	A	504	THR	2.1
1	B	318	THR	2.1
1	A	240	SER	2.1
1	A	501	PRO	2.1
1	A	502	PRO	2.1
1	B	80	PHE	2.0
1	A	54	ARG	2.0
1	A	189	ALA	2.0
1	A	484	ALA	2.0
1	B	31	ALA	2.0
1	B	507	ALA	2.0
1	A	254	LEU	2.0
1	B	380	LEU	2.0
1	A	268	GLU	2.0
1	B	82	GLY	2.0
1	B	102	TRP	2.0
1	B	116	ILE	2.0
1	A	111	PRO	2.0
1	A	498	PRO	2.0
1	B	196	SER	2.0
1	B	527	GLN	2.0
1	B	107	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	377	ALA	2.0
1	B	213	ILE	2.0
1	B	270	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

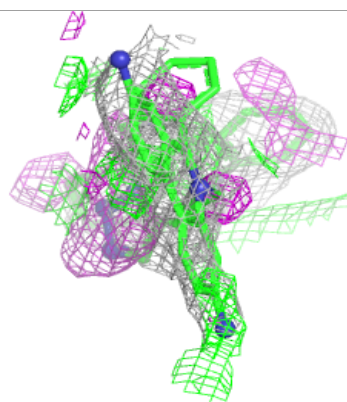
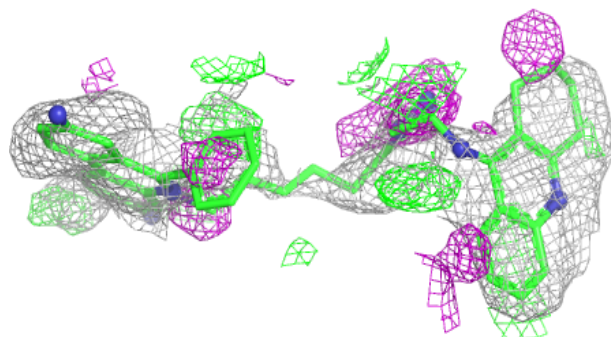
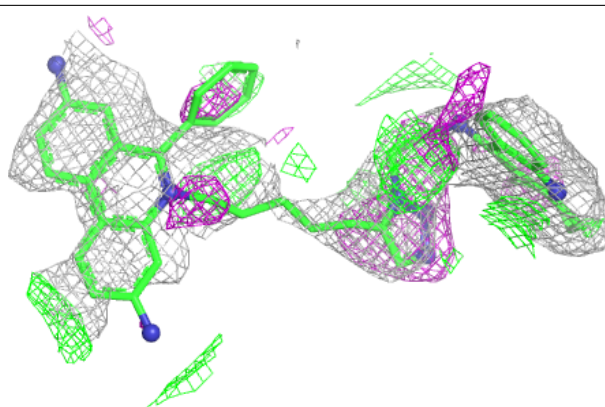
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	B	601	14/15	0.32	0.25	97,102,104,104	0
3	5NZ	B	603	49/49	0.58	0.27	39,53,94,96	0
2	NAG	A	602	14/15	0.64	0.19	105,108,114,115	0
3	5NZ	A	603	49/49	0.71	0.21	30,45,78,79	0
2	NAG	A	601	14/15	0.72	0.17	78,84,88,88	0
4	P6G	B	602	19/19	0.79	0.25	62,69,75,76	0

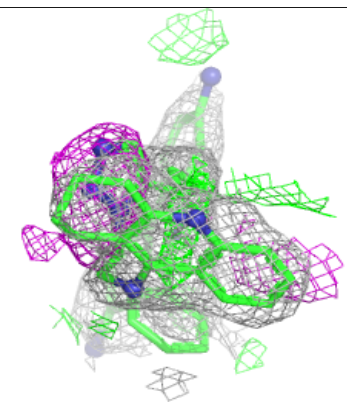
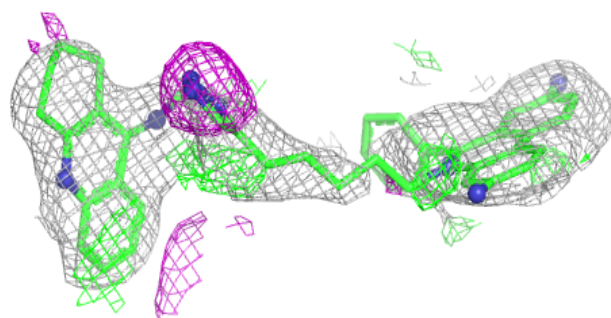
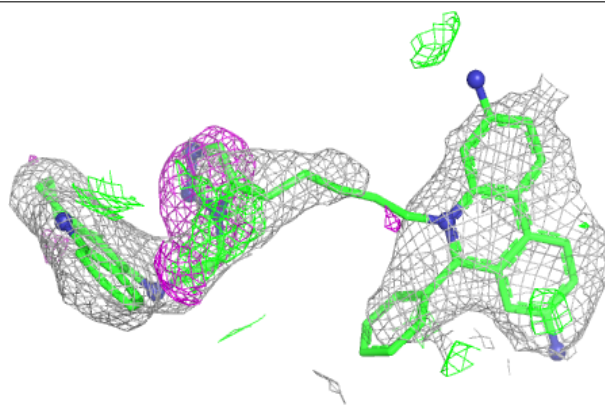
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5NZ B 603:

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

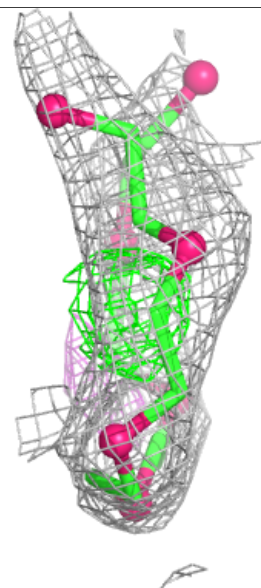
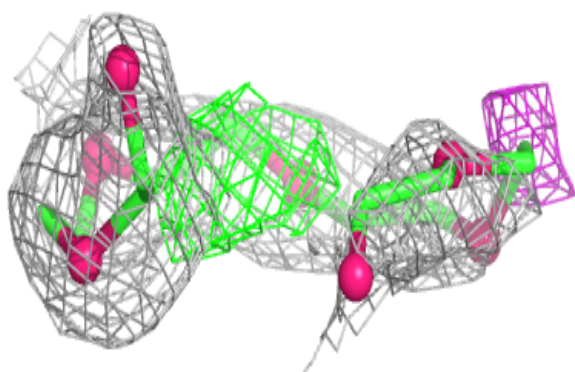
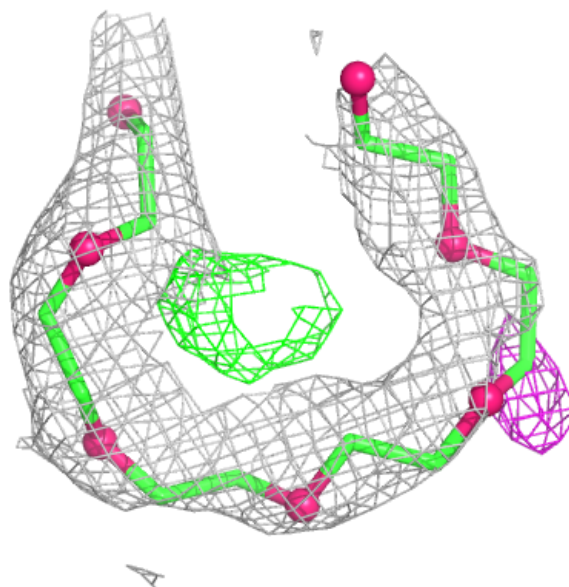
**Electron density around 5NZ A 603:**

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



Electron density around P6G B 602:

$2mF_o-DF_c$ (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.