



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:44 pm BST

PDB ID : 1Q3D
Title : GSK-3 Beta complexed with Staurosporine
Authors : Bertrand, J.A.; Thieffine, S.; Vulpetti, A.; Cristiani, C.; Valsasina, B.; Knapp, S.; Kalisz, H.M.; Flocco, M.
Deposited on : 2003-07-29
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

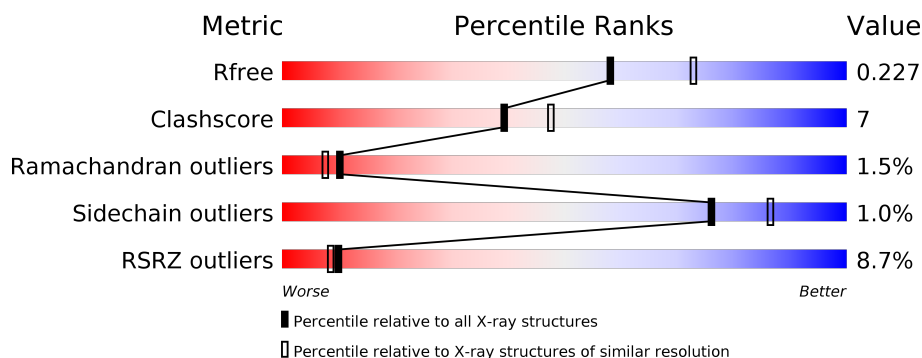
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	424	<div> <div>8%</div> <div>69%</div> <div>10%</div> <div>20%</div> </div>
1	B	424	<div> <div>6%</div> <div>70%</div> <div>8%</div> <div>20%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5644 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.

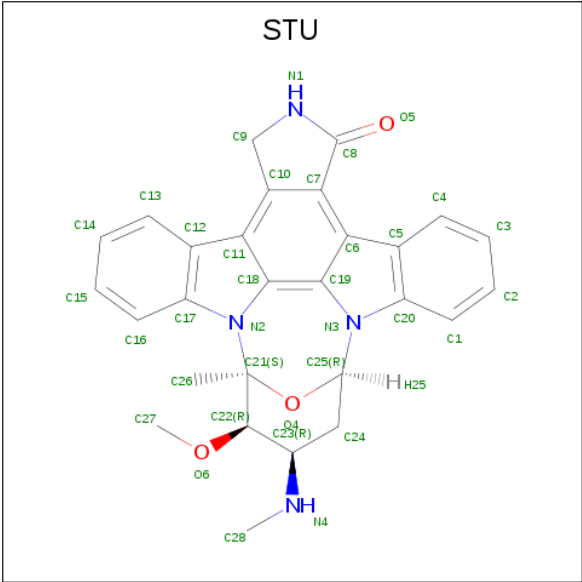
- Molecule 1 is a protein called GLYCOGEN SYNTHASE KINASE-3 BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2709	1744	467	487	11			
1	B	339	Total	C	N	O	S	0	0	0
			2709	1742	466	490	11			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	CLONING ARTIFACT	UNP P49841
A	-2	PRO	-	CLONING ARTIFACT	UNP P49841
A	-1	LEU	-	CLONING ARTIFACT	UNP P49841
A	0	GLY	-	CLONING ARTIFACT	UNP P49841
A	1	SER	-	CLONING ARTIFACT	UNP P49841
B	-3	GLY	-	CLONING ARTIFACT	UNP P49841
B	-2	PRO	-	CLONING ARTIFACT	UNP P49841
B	-1	LEU	-	CLONING ARTIFACT	UNP P49841
B	0	GLY	-	CLONING ARTIFACT	UNP P49841
B	1	SER	-	CLONING ARTIFACT	UNP P49841

- Molecule 2 is STAUROSPORINE (three-letter code: STU) (formula: C₂₈H₂₆N₄O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			35	28	4	3		
2	B	1	Total	C	N	O	0	0
			35	28	4	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	71	Total	O	0	0
			71	71		
3	B	85	Total	O	0	0
			85	85		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.73Å 87.05Å 177.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.12 – 2.20 20.11 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.4 (20.12-2.20) 95.6 (20.11-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.19Å)	Xtriage
Refinement program	CNX 2000	Depositor
R, R_{free}	0.230 , 0.252 0.224 , 0.227	Depositor DCC
R_{free} test set	3235 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.625	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5644	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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: STU

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	0.49	0/2776	0.68	0/3777
1	B	0.52	0/2776	0.68	0/3777
All	All	0.51	0/5552	0.68	0/7554

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

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	2709	0	2744	40	0
1	B	2709	0	2735	42	0
2	A	35	0	26	0	0
2	B	35	0	26	1	0
3	A	71	0	0	1	0
3	B	85	0	0	1	0
All	All	5644	0	5531	81	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 7.

All (81) 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:285:ASN:HB3	1:A:286:PRO:HD3	1.25	1.09
1:A:285:ASN:HB3	1:A:286:PRO:CD	1.96	0.94
1:B:383:ARG:NE	1:B:383:ARG:HA	1.93	0.84
1:B:383:ARG:HA	1:B:383:ARG:HE	1.49	0.78
1:B:65:GLY:O	1:B:67:PHE:N	2.20	0.75
1:B:90:ASP:HB3	1:B:93:PHE:CD1	2.23	0.74
1:B:308:ARG:HG2	1:B:308:ARG:HH11	1.54	0.73
1:A:370:ASN:HD22	1:A:372:PRO:HD2	1.55	0.71
1:B:370:ASN:HD22	1:B:372:PRO:HD2	1.56	0.70
1:A:285:ASN:CB	1:A:286:PRO:HD3	2.13	0.69
1:B:285:ASN:OD1	1:B:286:PRO:HD2	1.94	0.67
1:A:384:ILE:HG22	1:A:385:GLN:N	2.11	0.66
1:A:229:PHE:O	1:A:286:PRO:HB2	1.96	0.65
1:B:293:PHE:N	1:B:294:PRO:HD3	2.10	0.65
1:B:308:ARG:HG2	1:B:308:ARG:NH1	2.14	0.62
1:A:370:ASN:ND2	1:A:372:PRO:HD2	2.17	0.59
1:A:65:GLY:O	1:A:67:PHE:N	2.35	0.59
1:B:67:PHE:O	1:B:87:VAL:HG23	2.02	0.59
1:A:220:ARG:O	1:A:221:TYR:HB2	2.03	0.58
1:A:276:PRO:HG3	1:A:323:TYR:CZ	2.38	0.58
1:B:93:PHE:CD1	1:B:93:PHE:N	2.71	0.58
1:B:285:ASN:CG	1:B:286:PRO:HD2	2.24	0.58
1:B:379:PRO:HG2	1:B:382:ALA:HB2	1.86	0.58
1:A:285:ASN:CB	1:A:286:PRO:CD	2.76	0.56
1:B:370:ASN:ND2	1:B:372:PRO:HD2	2.20	0.56
1:A:208:VAL:HB	1:A:211:GLU:OE1	2.04	0.56
1:A:220:ARG:HH11	1:B:220:ARG:HD3	1.71	0.56
1:B:208:VAL:HB	1:B:211:GLU:OE1	2.06	0.56
1:B:90:ASP:O	1:B:91:LYS:HB2	2.04	0.56
1:A:185:GLN:HG3	3:A:501:HOH:O	2.07	0.55
1:B:220:ARG:HH11	1:B:220:ARG:HG2	1.71	0.55
1:A:149:ALA:O	1:A:151:GLN:HG3	2.07	0.55
1:A:220:ARG:HD2	1:B:220:ARG:HD3	1.89	0.54
1:A:220:ARG:NH2	1:A:221:TYR:OH	2.40	0.54
1:A:299:HIS:HE1	1:A:303:LYS:HB3	1.74	0.52
1:B:196:LEU:HD23	1:B:196:LEU:C	2.30	0.52
1:A:381:HIS:HA	1:A:384:ILE:HD12	1.91	0.51
1:A:220:ARG:O	1:A:221:TYR:CB	2.58	0.51
1:A:384:ILE:CG2	1:A:385:GLN:N	2.74	0.51
1:B:276:PRO:HG3	1:B:323:TYR:CZ	2.45	0.51
1:A:196:LEU:HD23	1:A:196:LEU:C	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LYS:HE2	1:A:72:GLN:NE2	2.26	0.50
1:B:42:ALA:HB1	1:B:114:TYR:HB3	1.95	0.49
1:B:296:ILE:HG22	1:B:297:LYS:N	2.28	0.49
1:B:220:ARG:O	1:B:221:TYR:HB2	2.14	0.48
1:A:50:ARG:HG2	1:A:50:ARG:NH1	2.29	0.48
1:B:38:THR:O	1:B:55:SER:HA	2.15	0.47
1:A:299:HIS:CE1	1:A:303:LYS:HB3	2.50	0.46
1:B:185:GLN:HG3	3:B:522:HOH:O	2.14	0.46
1:A:67:PHE:HD1	1:A:67:PHE:H	1.64	0.46
1:A:50:ARG:HH11	1:A:50:ARG:HG2	1.80	0.46
1:A:115:PHE:HA	1:A:129:ASN:O	2.15	0.45
1:B:98:LEU:O	1:B:102:ARG:HG3	2.16	0.45
1:B:220:ARG:HH11	1:B:220:ARG:CG	2.29	0.45
1:A:278:ARG:HA	1:A:281:ILE:HD12	1.99	0.45
1:B:308:ARG:HH11	1:B:308:ARG:H	1.65	0.45
1:B:293:PHE:N	1:B:294:PRO:CD	2.79	0.44
1:B:152:THR:OG1	1:B:306:ARG:NH1	2.50	0.44
1:B:308:ARG:N	1:B:308:ARG:HD3	2.32	0.44
1:A:319:ARG:HH11	1:A:319:ARG:HG3	1.82	0.44
1:A:57:THR:O	1:A:58:ASP:HB2	2.17	0.44
1:B:220:ARG:O	1:B:221:TYR:CB	2.65	0.43
1:A:370:ASN:C	1:A:370:ASN:HD22	2.20	0.43
1:B:196:LEU:HD23	1:B:197:LYS:N	2.33	0.43
1:B:370:ASN:HD22	1:B:370:ASN:C	2.21	0.42
1:A:275:THR:OG1	1:A:295:GLN:HA	2.19	0.42
1:A:67:PHE:N	1:A:67:PHE:CD1	2.88	0.42
1:A:217:ILE:O	1:A:218:CYS:CB	2.68	0.42
1:B:91:LYS:C	1:B:93:PHE:H	2.22	0.42
1:B:90:ASP:CB	1:B:93:PHE:CD1	3.01	0.42
1:A:310:PRO:HA	1:A:311:PRO:HD3	1.95	0.41
1:A:332:LEU:HD12	1:A:332:LEU:HA	1.93	0.41
1:B:307:PRO:HB2	1:B:308:ARG:NH1	2.35	0.41
1:B:285:ASN:CG	1:B:286:PRO:CD	2.89	0.41
1:A:280:GLN:HA	1:A:283:GLU:OE1	2.20	0.41
1:A:162:MET:HG3	1:A:247:LEU:HD13	2.02	0.41
2:B:452:STU:H261	2:B:452:STU:H16	2.02	0.41
1:A:252:LEU:HG	1:A:305:PHE:CE1	2.56	0.41
1:B:92:ARG:C	1:B:93:PHE:CD1	2.94	0.41
1:B:296:ILE:CG2	1:B:297:LYS:N	2.84	0.40
1:B:319:ARG:HH11	1:B:319:ARG:HG3	1.87	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	333/424 (78%)	316 (95%)	12 (4%)	5 (2%)	10	8
1	B	333/424 (78%)	313 (94%)	15 (4%)	5 (2%)	10	8
All	All	666/848 (78%)	629 (94%)	27 (4%)	10 (2%)	10	8

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	SER
1	A	149	ALA
1	A	285	ASN
1	B	66	SER
1	B	91	LYS
1	B	221	TYR
1	A	65	GLY
1	A	221	TYR
1	B	36	LYS
1	B	47	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	302/366 (82%)	300 (99%)	2 (1%)	84	91
1	B	302/366 (82%)	298 (99%)	4 (1%)	69	81
All	All	604/732 (82%)	598 (99%)	6 (1%)	76	86

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	370	ASN
1	B	93	PHE
1	B	308	ARG
1	B	370	ASN
1	B	383	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	99	GLN
1	A	108	ASN
1	A	254	GLN
1	A	365	GLN
1	A	370	ASN
1	B	72	GLN
1	B	108	ASN
1	B	145	HIS
1	B	254	GLN
1	B	365	GLN
1	B	370	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 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
2	STU	B	452	-	30,42,42	2.32	14 (46%)	31,68,68	1.90	8 (25%)
2	STU	A	451	-	30,42,42	2.09	13 (43%)	31,68,68	1.83	7 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	STU	B	452	-	-	1/4/42/42	-
2	STU	A	451	-	-	1/4/42/42	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	452	STU	C22-C23	5.51	1.58	1.52
2	A	451	STU	C22-C23	5.42	1.58	1.52
2	B	452	STU	C9-N1	-3.77	1.42	1.45
2	B	452	STU	C13-C12	3.47	1.48	1.41
2	B	452	STU	C3-C4	3.28	1.44	1.36
2	A	451	STU	C26-C21	2.96	1.55	1.51
2	B	452	STU	C14-C13	2.95	1.43	1.36
2	A	451	STU	C9-N1	-2.90	1.42	1.45
2	B	452	STU	C15-C16	2.90	1.43	1.36
2	B	452	STU	C16-C17	2.67	1.46	1.41
2	A	451	STU	C14-C15	2.59	1.44	1.38
2	B	452	STU	C1-C20	2.57	1.46	1.41
2	A	451	STU	C2-C1	2.54	1.42	1.36
2	B	452	STU	C14-C15	2.52	1.44	1.38
2	A	451	STU	C1-C20	2.49	1.46	1.41
2	B	452	STU	C4-C5	2.43	1.45	1.41
2	A	451	STU	C3-C4	2.43	1.42	1.36
2	A	451	STU	C13-C12	2.40	1.45	1.41
2	B	452	STU	C2-C1	2.29	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	452	STU	C26-C21	2.24	1.54	1.51
2	A	451	STU	C15-C16	2.23	1.41	1.36
2	A	451	STU	C16-C17	2.23	1.45	1.41
2	A	451	STU	C24-C25	2.21	1.55	1.51
2	A	451	STU	O6-C22	2.21	1.46	1.42
2	B	452	STU	C28-N4	2.19	1.52	1.46
2	A	451	STU	C4-C5	2.07	1.45	1.41
2	B	452	STU	C24-C25	2.06	1.55	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	451	STU	C1-C20-N3	-5.17	126.06	132.25
2	B	452	STU	C1-C20-N3	-5.12	126.12	132.25
2	B	452	STU	C3-C4-C5	-3.76	114.53	120.86
2	A	451	STU	C2-C1-C20	-3.61	112.53	119.44
2	B	452	STU	C2-C1-C20	-3.55	112.64	119.44
2	A	451	STU	C3-C4-C5	-3.34	115.25	120.86
2	B	452	STU	C1-C20-C5	3.00	125.06	120.73
2	A	451	STU	C1-C20-C5	2.81	124.79	120.73
2	B	452	STU	C24-C23-N4	2.57	117.88	112.17
2	B	452	STU	C3-C2-C1	2.56	124.02	120.44
2	B	452	STU	O5-C8-C7	-2.53	126.32	129.32
2	B	452	STU	C26-C21-C22	-2.42	107.92	112.64
2	A	451	STU	C3-C2-C1	2.41	123.81	120.44
2	A	451	STU	O4-C25-C24	2.40	115.78	112.31
2	A	451	STU	O5-C8-C7	-2.08	126.85	129.32

There are no chirality outliers.

All (2) torsion outliers are listed below:

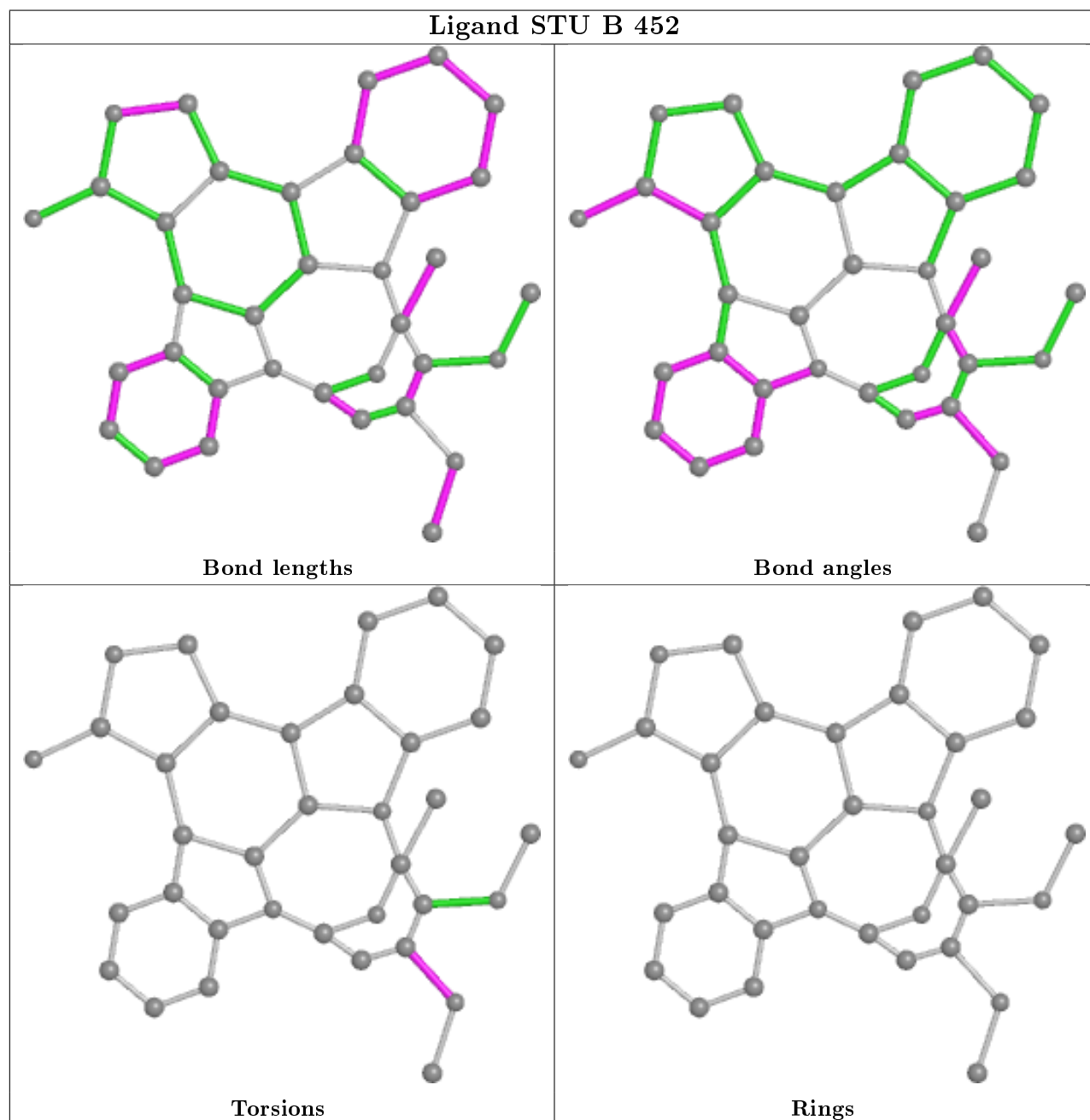
Mol	Chain	Res	Type	Atoms
2	B	452	STU	C24-C23-N4-C28
2	A	451	STU	C24-C23-N4-C28

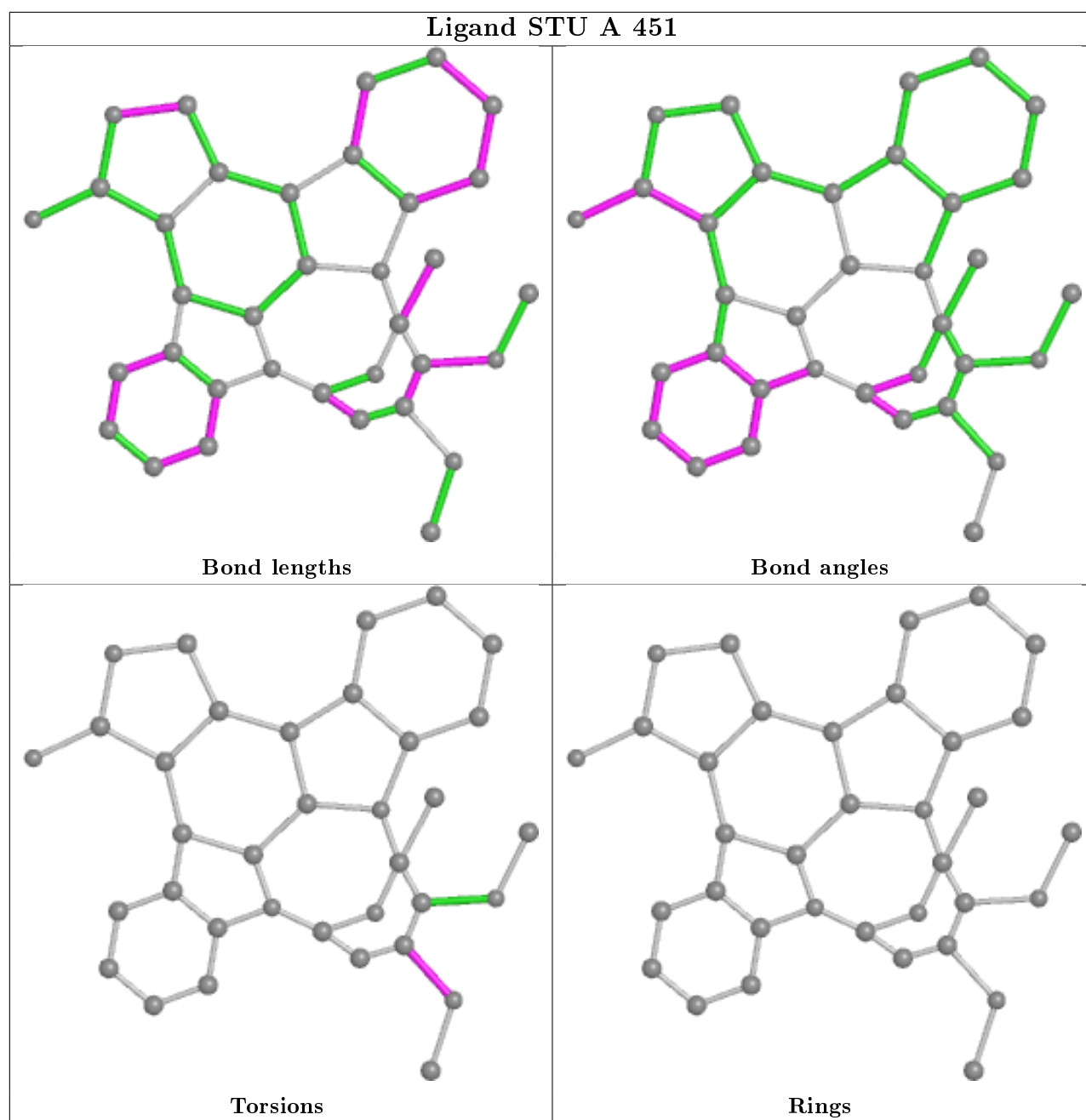
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	452	STU	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 [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	339/424 (79%)	0.29	32 (9%) 8 7	31, 51, 86, 116	0
1	B	339/424 (79%)	0.09	27 (7%) 12 11	30, 45, 82, 118	0
All	All	678/848 (79%)	0.19	59 (8%) 10 8	30, 48, 84, 118	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	293	PHE	9.3
1	A	93	PHE	6.5
1	A	293	PHE	5.4
1	A	92	ARG	4.8
1	B	278	ARG	4.6
1	B	93	PHE	4.5
1	A	119	SER	4.2
1	A	66	SER	4.0
1	A	94	LYS	4.0
1	A	35	SER	4.0
1	A	91	LYS	3.9
1	A	278	ARG	3.9
1	A	385	GLN	3.8
1	B	92	ARG	3.8
1	B	35	SER	3.6
1	A	282	ARG	3.4
1	B	124	ASP	3.4
1	B	67	PHE	3.3
1	B	308	ARG	3.2
1	A	132	LEU	3.1
1	A	297	LYS	3.0
1	B	282	ARG	3.0
1	A	150	LYS	2.9
1	A	131	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	84	ILE	2.9
1	B	279	GLU	2.8
1	A	83	ALA	2.8
1	A	67	PHE	2.8
1	B	132	LEU	2.7
1	B	66	SER	2.7
1	A	48	PRO	2.7
1	B	298	ALA	2.7
1	B	36	LYS	2.6
1	A	130	LEU	2.6
1	A	286	PRO	2.5
1	A	300	PRO	2.4
1	A	209	ARG	2.4
1	A	303	LYS	2.4
1	A	295	GLN	2.4
1	B	209	ARG	2.3
1	B	84	ILE	2.3
1	A	90	ASP	2.3
1	A	299	HIS	2.3
1	B	294	PRO	2.3
1	B	77	ASP	2.3
1	A	307	PRO	2.2
1	B	119	SER	2.2
1	B	286	PRO	2.2
1	A	36	LYS	2.2
1	B	295	GLN	2.2
1	B	150	LYS	2.1
1	B	90	ASP	2.1
1	B	91	LYS	2.1
1	B	297	LYS	2.1
1	A	126	VAL	2.1
1	A	298	ALA	2.0
1	B	64	ASN	2.0
1	B	130	LEU	2.0
1	A	65	GLY	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

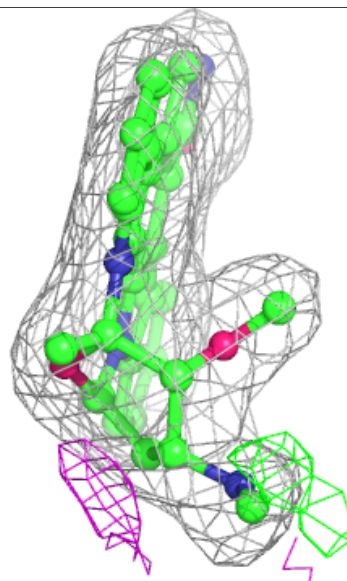
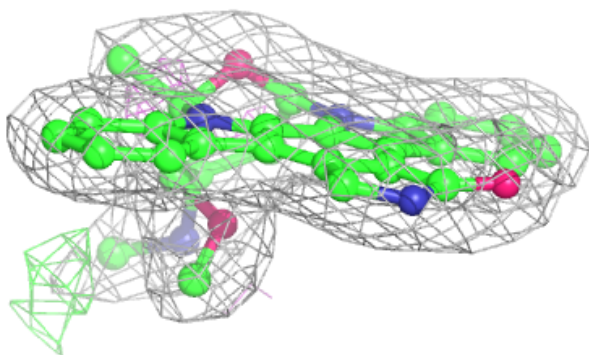
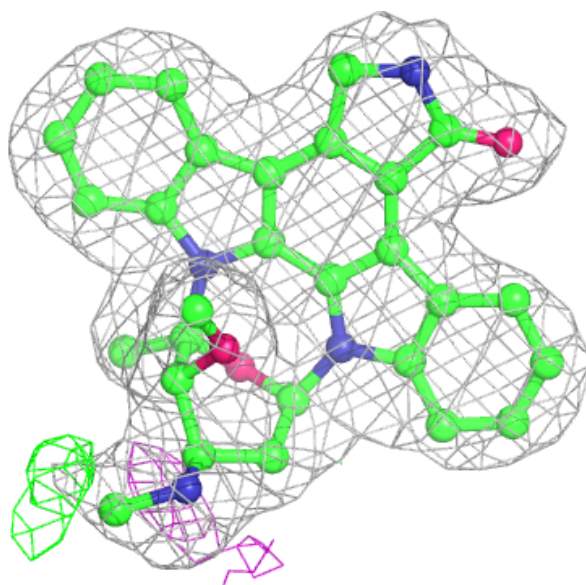
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	STU	A	451	35/35	0.96	0.12	28,34,39,41	0
2	STU	B	452	35/35	0.97	0.10	29,32,35,41	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.

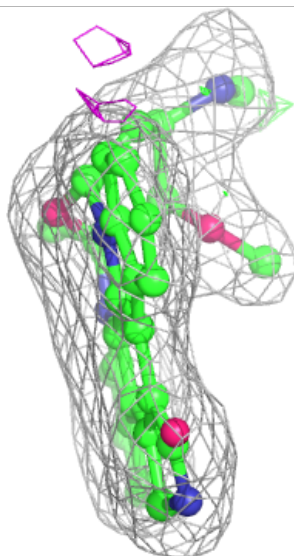
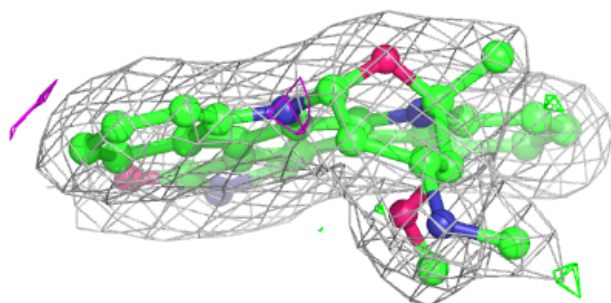
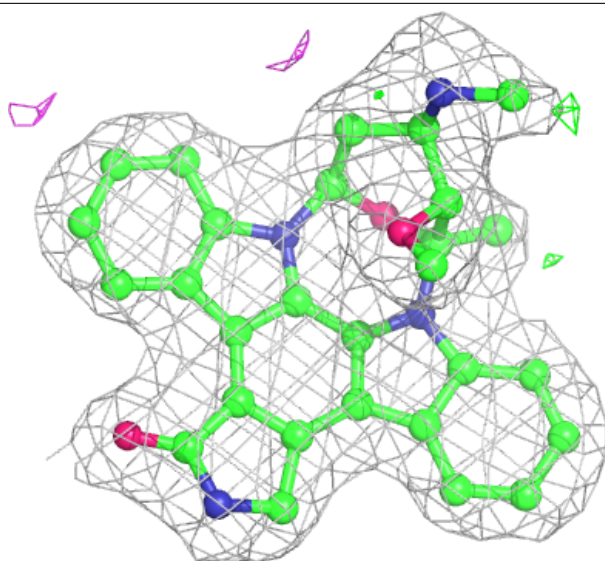
Electron density around STU A 451:

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



Electron density around STU B 452:

$2mF_o-DF_c$ (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.