



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:01 PM UTC

PDB ID : 6HK3 / pdb_00006hk3
Title : Crystal structure of GSK-3B in complex with pyrazine inhibitor C44
Authors : Piretti, V.; Giabbai, B.; Demitri, N.; Di Martino, R.; Tripathi, S.K.; Gobbo, D.; Decherchi, S.; Storici, P.; Giroto, S.; Cavalli, A.
Deposited on : 2018-09-05
Resolution : 2.35 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

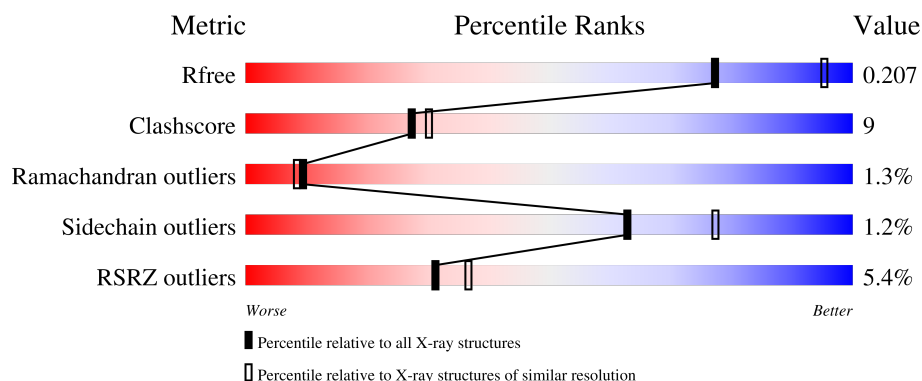
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	350	5% 79% 20% .
1	B	350	5% 85% 13% .
2	N	8	38% 75% 25%

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
4	MLI	A	402	-	-	X	-
5	GOL	A	404	-	X	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5946 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.

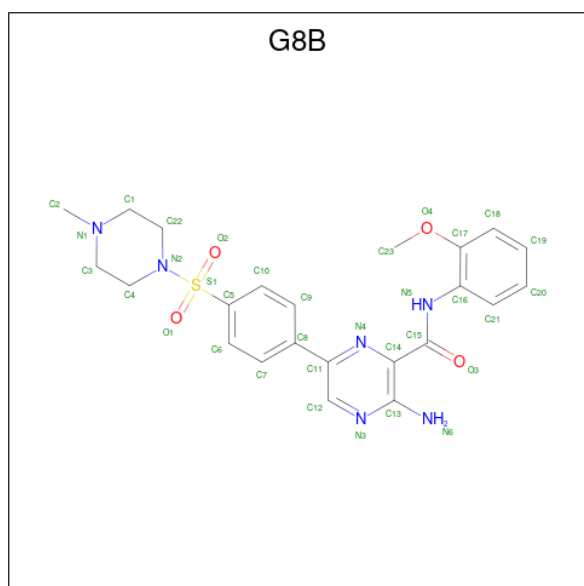
- Molecule 1 is a protein called Glycogen synthase kinase-3 beta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	P	S	0	7	0
			2774	1787	468	506	1	12			
1	B	350	Total	C	N	O	P	S	0	8	0
			2805	1807	478	507	1	12			

- Molecule 2 is a protein called GLY-SER-HIS-GLY-HIS-HIS-HIS-HIS.

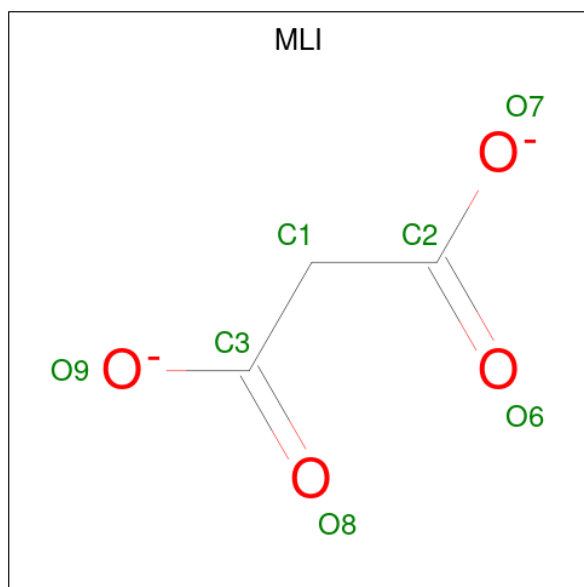
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	N	8	Total	C	N	O	0	0	0
			59	34	16	9			

- Molecule 3 is 3-azanyl- {N}-(2-methoxyphenyl)-6-[4-(4-methylpiperazin-1-yl)sulfonylphenyl]pyrazine-2-carboxamide (CCD ID: G8B) (formula: C₂₃H₂₆N₆O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			34	23	6	4	1		
3	B	1	Total	C	N	O	S	0	0
			34	23	6	4	1		

- Molecule 4 is MALONATE ION (CCD ID: MLI) (formula: $C_3H_2O_4$).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

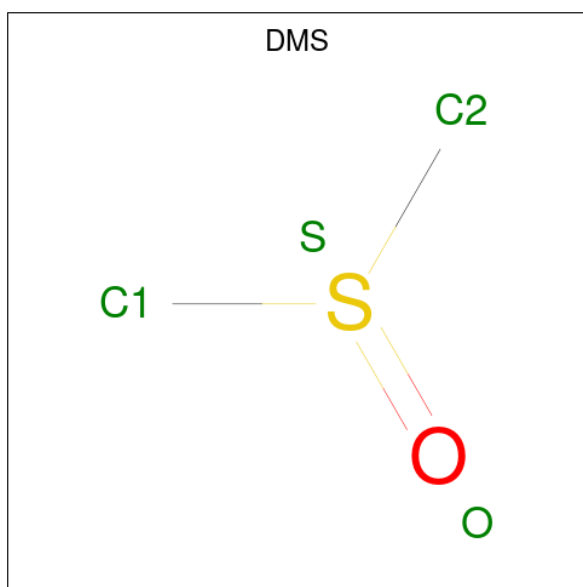


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		
6	B	1	Total	Cl	0	0
			1	1		

- Molecule 7 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



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

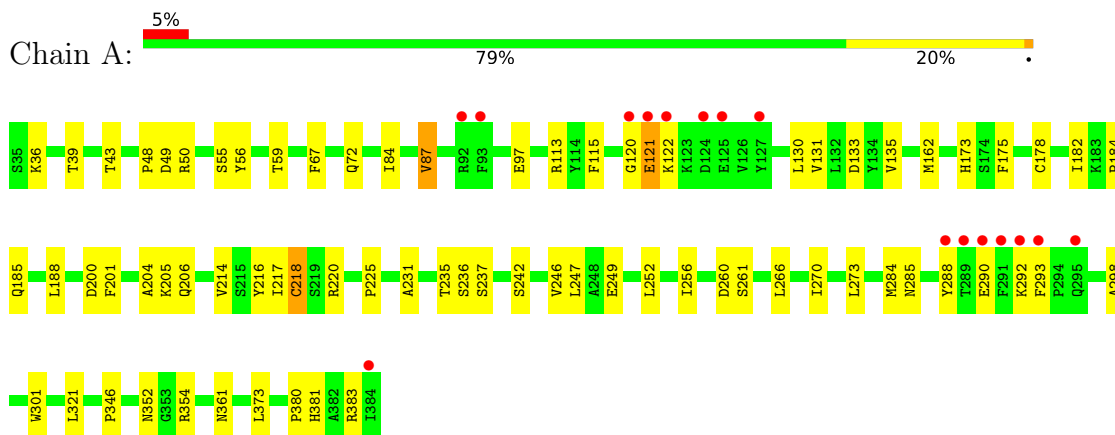
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	84	Total	O	0	3
			87	87		
8	B	102	Total	O	0	1
			103	103		
8	N	2	Total	O	0	0
			2	2		

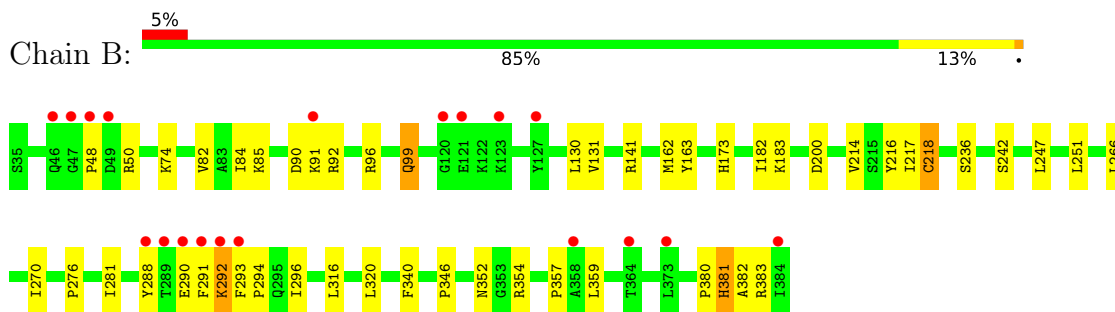
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

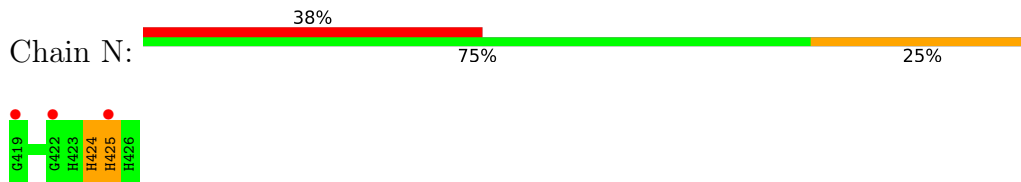
- Molecule 1: Glycogen synthase kinase-3 beta



- Molecule 1: Glycogen synthase kinase-3 beta



- Molecule 2: GLY-SER-HIS-GLY-HIS-HIS-HIS



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	64.32Å 67.12Å 67.24Å 79.84° 76.21° 89.63°	Depositor
Resolution (Å)	42.98 – 2.35 42.98 – 2.35	Depositor EDS
% Data completeness (in resolution range)	97.7 (42.98-2.35) 97.6 (42.98-2.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 2.34Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.204 , 0.234 (Not available) , 0.207	Depositor DCC
R_{free} test set	2321 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.2	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	5946	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MLI, GOL, CL, DMS, G8B, PTR

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	0.39	0/2845	0.59	0/3878
1	B	0.38	0/2880	0.57	1/3921 (0.0%)
2	N	0.41	0/62	0.90	0/82
All	All	0.38	0/5787	0.59	1/7881 (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	B	288	TYR	CB-CA-C	5.55	118.80	109.48

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	2774	0	2779	58	0
1	B	2805	0	2829	47	0
2	N	59	0	40	6	0
3	A	34	0	0	0	0
3	B	34	0	0	2	0
4	A	7	0	2	3	0
4	B	7	0	2	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	18	0	23	2	0
5	B	6	0	8	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	4	0	6	0	0
7	B	4	0	6	0	0
8	A	87	0	0	4	0
8	B	103	0	0	5	0
8	N	2	0	0	0	0
All	All	5946	0	5695	104	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 9.

All (104) 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:292:LYS:HD3	1:B:293:PHE:N	1.28	1.44
1:B:292:LYS:CD	1:B:293:PHE:H	1.58	1.17
1:A:298:ALA:HB1	2:N:425:HIS:NE2	1.60	1.14
1:B:292:LYS:CD	1:B:293:PHE:N	2.20	0.97
1:A:288:TYR:CE2	1:A:290:GLU:HB2	2.06	0.91
1:A:288:TYR:HE2	1:A:290:GLU:HB2	1.38	0.86
1:B:292:LYS:NZ	1:B:293:PHE:O	2.08	0.85
1:B:292:LYS:HD3	1:B:292:LYS:C	2.01	0.79
1:B:162:MET:HE2	1:B:247:LEU:HB2	1.68	0.76
1:B:90:ASP:HB3	1:B:92:ARG:HG2	1.71	0.71
1:A:120:GLY:C	1:A:122:LYS:H	2.00	0.68
1:B:82:VAL:HG11	1:B:131:VAL:HG13	1.77	0.67
1:A:235:THR:HG21	8:A:573:HOH:O	1.94	0.66
1:A:97:GLU:OE2	8:A:540[B]:HOH:O	2.14	0.65
1:B:292:LYS:HD3	1:B:293:PHE:H	0.71	0.63
1:A:217:ILE:HD12	1:A:217:ILE:C	2.24	0.62
1:A:298:ALA:CB	2:N:425:HIS:NE2	2.52	0.62
1:B:141[B]:ARG:NH1	8:B:503:HOH:O	2.32	0.62
1:A:175:PHE:O	1:A:206:GLN:NE2	2.31	0.61
1:A:217:ILE:HD13	1:A:218[B]:CYS:SG	2.41	0.61
1:A:214[B]:VAL:HG12	4:A:402:MLI:C2	2.32	0.60
1:B:292:LYS:HD2	1:B:293:PHE:O	2.01	0.60
1:A:235:THR:HG23	1:A:237:SER:H	1.67	0.59
1:A:260:ASP:OD2	1:B:141[A]:ARG:NH1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ASN:OD1	1:A:354:ARG:HG3	2.03	0.58
1:B:383:ARG:NH2	8:B:504:HOH:O	2.36	0.57
1:B:141[B]:ARG:HD2	3:B:401:G8B:O1	2.06	0.56
1:A:162:MET:HE2	1:A:247:LEU:HB2	1.88	0.56
1:B:292:LYS:CD	1:B:293:PHE:O	2.54	0.55
1:A:121:GLU:O	1:A:122:LYS:HD2	2.07	0.55
1:A:214[A]:VAL:HG22	4:A:402:MLI:C2	2.36	0.55
1:A:120:GLY:O	1:A:122:LYS:HG2	2.08	0.54
1:A:225:PRO:HB2	1:A:284:MET:SD	2.48	0.54
1:A:220:ARG:HD2	1:A:261:SER:C	2.34	0.53
1:A:231:ALA:HB2	1:A:285:ASN:HB2	1.91	0.53
1:B:48:PRO:O	1:B:50:ARG:N	2.38	0.53
1:A:56:TYR:OH	5:A:403:GOL:H31	2.09	0.53
1:B:217:ILE:C	1:B:217:ILE:HD12	2.34	0.52
1:A:113:ARG:HD2	1:A:133:ASP:OD1	2.10	0.52
1:B:90:ASP:CB	1:B:92:ARG:HG2	2.37	0.52
1:B:217:ILE:HD13	1:B:218[B]:CYS:SG	2.49	0.52
1:A:217:ILE:C	1:A:217:ILE:CD1	2.83	0.52
1:B:85:LYS:HD2	3:B:401:G8B:C20	2.40	0.52
1:A:121:GLU:C	1:A:122:LYS:HD2	2.35	0.52
1:A:235:THR:OG1	1:A:236:SER:N	2.42	0.51
1:B:266:LEU:O	1:B:270:ILE:HG13	2.11	0.50
1:B:247:LEU:O	1:B:251:LEU:HG	2.11	0.50
1:A:39:THR:OG1	1:A:55:SER:OG	2.25	0.49
1:A:120:GLY:C	1:A:122:LYS:N	2.70	0.49
1:A:48:PRO:O	1:A:50:ARG:N	2.41	0.49
1:B:96:ARG:O	1:B:99[A]:GLN:HG3	2.13	0.49
1:B:182:ILE:HB	1:B:242:SER:CB	2.42	0.49
1:A:43:THR:HB	1:A:115:PHE:CE1	2.48	0.48
1:A:84:ILE:HA	1:A:130:LEU:O	2.14	0.48
1:A:235:THR:HG22	8:A:501:HOH:O	2.12	0.48
1:A:120:GLY:O	1:A:122:LYS:N	2.44	0.48
1:B:90:ASP:OD1	1:B:92:ARG:N	2.43	0.48
1:A:67:PHE:HB2	1:A:87:VAL:HB	1.96	0.47
1:A:185:GLN:HB3	5:A:404:GOL:H2	1.97	0.47
1:A:135:VAL:HB	1:A:188:LEU:HB3	1.97	0.47
1:A:260:ASP:CG	1:B:141[A]:ARG:HH12	2.23	0.46
1:A:380:PRO:HA	1:A:383:ARG:HE	1.80	0.46
1:B:352:ASN:ND2	1:B:354:ARG:HD3	2.31	0.46
1:B:141[B]:ARG:NH2	8:B:502:HOH:O	2.30	0.46
1:B:84:ILE:HA	1:B:130:LEU:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:LEU:O	1:B:320:LEU:HG	2.16	0.45
1:B:380:PRO:C	1:B:382:ALA:H	2.23	0.45
1:A:162:MET:HG3	1:A:247:LEU:HD13	1.99	0.45
1:B:183:LYS:NZ	8:B:511:HOH:O	2.50	0.45
1:A:36:LYS:HB3	1:A:36:LYS:HE2	1.71	0.45
1:A:59:THR:HA	1:A:72:GLN:O	2.17	0.44
1:A:273[A]:LEU:HD21	1:A:321:LEU:O	2.17	0.44
1:B:291:PHE:HD1	8:B:546:HOH:O	2.00	0.44
1:B:90:ASP:CG	1:B:92:ARG:HG2	2.43	0.44
1:A:184:PRO:HD3	1:A:246:VAL:HG22	2.00	0.44
1:A:205:LYS:NZ	4:A:402:MLI:O8	2.50	0.44
2:N:424:HIS:CD2	2:N:424:HIS:N	2.86	0.44
1:A:361:ASN:OD1	1:A:361:ASN:N	2.51	0.43
1:B:90:ASP:OD1	1:B:91:LYS:N	2.52	0.43
1:A:97:GLU:HG3	1:A:201:PHE:O	2.19	0.42
1:B:173:HIS:CE1	1:B:236:SER:HB2	2.54	0.42
1:B:346:PRO:HB3	1:B:381:HIS:CG	2.55	0.42
1:B:217:ILE:C	1:B:217:ILE:CD1	2.92	0.42
1:A:301:TRP:HE1	2:N:425:HIS:HB3	1.85	0.42
1:B:82:VAL:CG1	1:B:131:VAL:HG13	2.49	0.42
1:B:294:PRO:HG2	1:B:296:ILE:HD11	2.01	0.42
1:B:163:TYR:HB2	1:B:340:PHE:CD1	2.55	0.42
1:B:182:ILE:HB	1:B:242:SER:HB2	2.02	0.42
1:A:173:HIS:CE1	1:A:236:SER:HB3	2.55	0.41
1:A:182:ILE:HB	1:A:242:SER:CB	2.50	0.41
1:A:266:LEU:O	1:A:270:ILE:HG13	2.20	0.41
1:A:301:TRP:NE1	2:N:425:HIS:HB3	2.34	0.41
1:A:178:CYS:O	1:A:204:ALA:HA	2.20	0.41
1:B:294:PRO:O	1:B:296:ILE:HD12	2.20	0.41
1:A:301:TRP:CD1	2:N:425:HIS:HB3	2.56	0.41
1:B:276:PRO:HG2	1:B:281:ILE:HD11	2.02	0.41
1:A:373:LEU:HD23	1:A:373:LEU:HA	1.91	0.40
1:B:214[A]:VAL:HG22	4:B:402:MLI:C2	2.51	0.40
1:A:252:LEU:HD11	1:A:256:ILE:HG13	2.02	0.40
1:B:357:PRO:O	1:B:359:LEU:HG	2.21	0.40
1:A:249:GLU:HB2	8:A:516[A]:HOH:O	2.22	0.40
1:A:346:PRO:HB3	1:A:381:HIS:CD2	2.56	0.40
1:B:74:LYS:HB3	1:B:74:LYS:HE2	1.88	0.40
1:A:182:ILE:HB	1:A:242:SER:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	354/350 (101%)	324 (92%)	23 (6%)	7 (2%)	6	4
1	B	355/350 (101%)	335 (94%)	18 (5%)	2 (1%)	21	24
2	N	6/8 (75%)	4 (67%)	1 (17%)	1 (17%)	0	0
All	All	715/708 (101%)	663 (93%)	42 (6%)	10 (1%)	9	7

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	ASP
1	A	292	LYS
1	B	200	ASP
2	N	425	HIS
1	A	121	GLU
1	A	200	ASP
1	A	218[A]	CYS
1	A	218[B]	CYS
1	B	381	HIS
1	A	293	PHE

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	305/311 (98%)	303 (99%)	2 (1%)	76	86
1	B	310/311 (100%)	304 (98%)	6 (2%)	50	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	5/6 (83%)	4 (80%)	1 (20%)	1	1
All	All	620/628 (99%)	611 (98%)	9 (2%)	63	72

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	VAL
1	A	131	VAL
1	B	99[A]	GLN
1	B	99[B]	GLN
1	B	218[A]	CYS
1	B	218[B]	CYS
1	B	290	GLU
1	B	292	LYS
2	N	424	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	287	ASN
1	B	108	ASN
1	B	206	GLN
1	B	254	GLN
1	B	365	GLN
2	N	424	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	PTR	A	216	1	15,16,17	1.31	1 (6%)	17,22,24	0.44	0
1	PTR	B	216	1	15,16,17	1.24	1 (6%)	17,22,24	0.58	1 (5%)

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
1	PTR	A	216	1	-	0/10/11/13	0/1/1/1
1	PTR	B	216	1	-	0/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	216	PTR	OH-CZ	-4.35	1.30	1.40
1	A	216	PTR	OH-CZ	-4.25	1.31	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	216	PTR	O2P-P-OH	2.07	111.44	105.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	DMS	B	405	-	3,3,3	0.67	0	3,3,3	0.63	0
5	GOL	B	403	-	5,5,5	0.99	0	5,5,5	1.11	0
3	G8B	A	401	-	37,37,37	0.69	1 (2%)	51,53,53	1.69	11 (21%)
4	MLI	A	402	-	6,6,6	1.35	0	7,7,7	0.71	0
4	MLI	B	402	-	6,6,6	1.22	0	7,7,7	1.32	0
7	DMS	A	407	-	3,3,3	0.70	0	3,3,3	0.62	0
3	G8B	B	401	-	37,37,37	0.79	0	51,53,53	1.64	11 (21%)
5	GOL	A	403	-	5,5,5	0.79	0	5,5,5	1.00	0
5	GOL	A	404	-	5,5,5	2.33	2 (40%)	5,5,5	1.36	1 (20%)
5	GOL	A	405	-	5,5,5	1.59	1 (20%)	5,5,5	1.21	1 (20%)

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
5	GOL	B	403	-	-	1/4/4/4	-
3	G8B	A	401	-	-	0/26/36/36	0/4/4/4
4	MLI	A	402	-	-	4/4/4/4	-
4	MLI	B	402	-	-	4/4/4/4	-
3	G8B	B	401	-	-	0/26/36/36	0/4/4/4
5	GOL	A	403	-	-	4/4/4/4	-
5	GOL	A	404	-	-	3/4/4/4	-
5	GOL	A	405	-	-	0/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	404	GOL	O3-C3	3.15	1.55	1.42
5	A	404	GOL	C3-C2	3.13	1.63	1.51
5	A	405	GOL	O2-C2	-2.82	1.35	1.43
3	A	401	G8B	C14-C15	-2.10	1.47	1.50

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	G8B	C5-S1-N2	5.16	113.50	107.28
3	B	401	G8B	C5-S1-N2	4.71	112.96	107.28
3	B	401	G8B	O2-S1-N2	-4.46	102.48	106.69
3	A	401	G8B	C22-N2-C4	4.02	116.74	112.12
3	A	401	G8B	O2-S1-C5	-4.00	103.13	108.10
3	A	401	G8B	O2-S1-O1	3.91	125.68	119.59
3	B	401	G8B	O2-S1-O1	3.48	125.02	119.59
3	B	401	G8B	C22-N2-C4	3.00	115.56	112.12
3	B	401	G8B	C1-C22-N2	2.89	112.03	108.97
3	B	401	G8B	C4-N2-S1	-2.80	111.86	117.06
3	A	401	G8B	C15-C14-N4	-2.66	113.41	116.02
3	A	401	G8B	O2-S1-N2	-2.65	104.19	106.69
3	B	401	G8B	C3-C4-N2	2.64	111.77	108.97
3	B	401	G8B	O1-S1-C5	-2.60	104.87	108.10
3	B	401	G8B	C15-C14-N4	-2.59	113.48	116.02
3	A	401	G8B	C4-N2-S1	-2.46	112.48	117.06
3	A	401	G8B	O1-S1-C5	-2.46	105.05	108.10
3	A	401	G8B	C3-C4-N2	2.41	111.53	108.97
3	B	401	G8B	C14-C15-N5	2.33	116.35	113.99
3	A	401	G8B	C12-C11-C8	2.22	125.06	122.10
5	A	404	GOL	O1-C1-C2	-2.17	100.62	110.38
3	B	401	G8B	O2-S1-C5	-2.16	105.42	108.10
3	A	401	G8B	C14-C13-N6	-2.15	120.44	122.90
5	A	405	GOL	O3-C3-C2	-2.12	100.81	110.38

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	403	GOL	C1-C2-C3-O3
5	A	404	GOL	C1-C2-C3-O3
5	A	403	GOL	O2-C2-C3-O3
5	A	403	GOL	O1-C1-C2-C3
5	A	404	GOL	O2-C2-C3-O3
4	A	402	MLI	C3-C1-C2-O7
5	A	403	GOL	O1-C1-C2-O2
4	A	402	MLI	C3-C1-C2-O6
4	A	402	MLI	C2-C1-C3-O9
5	A	404	GOL	O1-C1-C2-O2
4	A	402	MLI	C2-C1-C3-O8
5	B	403	GOL	O2-C2-C3-O3

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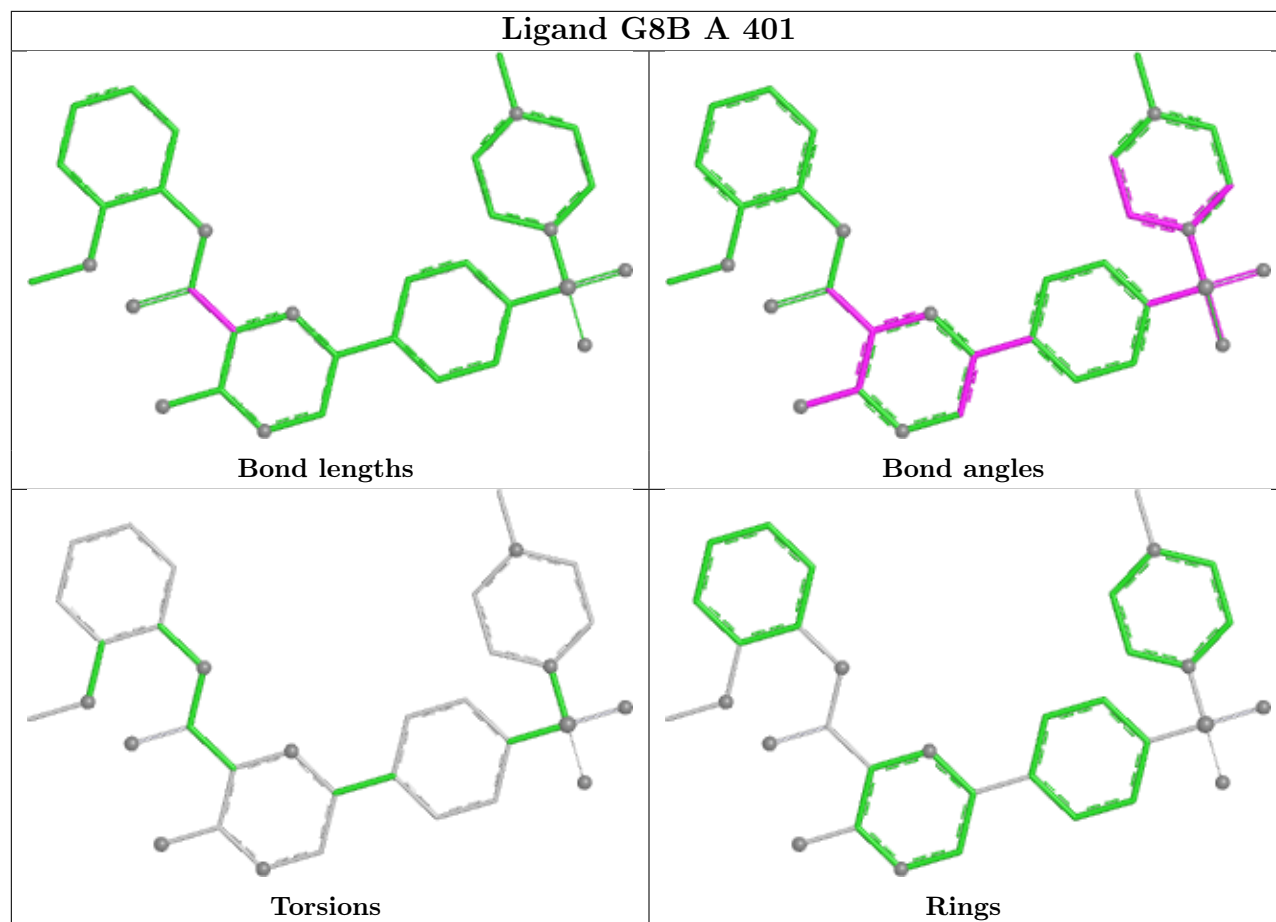
Mol	Chain	Res	Type	Atoms
4	B	402	MLI	C2-C1-C3-O8
4	B	402	MLI	C3-C1-C2-O7
4	B	402	MLI	C2-C1-C3-O9
4	B	402	MLI	C3-C1-C2-O6

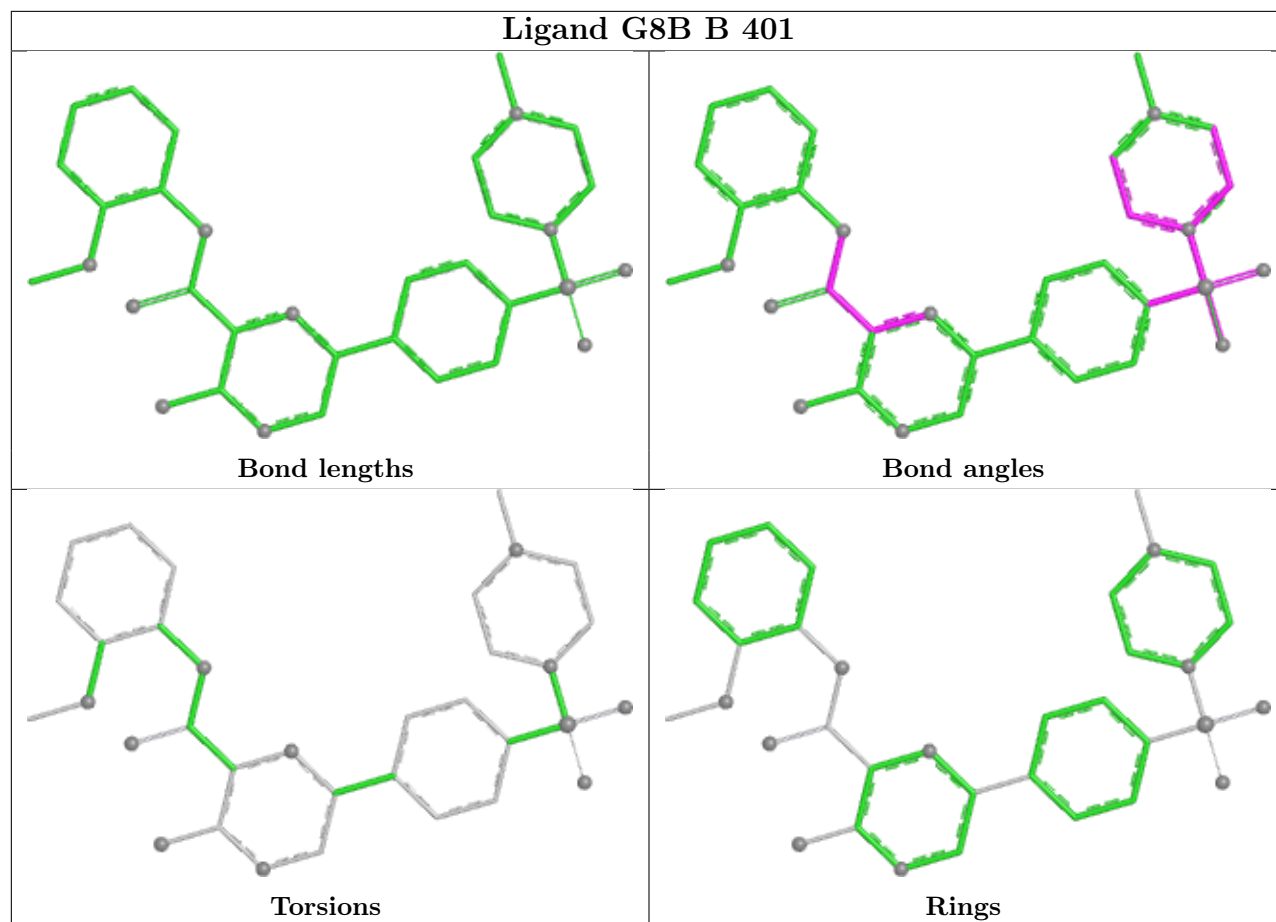
There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	402	MLI	3	0
4	B	402	MLI	1	0
3	B	401	G8B	2	0
5	A	403	GOL	1	0
5	A	404	GOL	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	349/350 (99%)	0.47	16 (4%) 37 43	27, 52, 89, 131	7 (2%)
1	B	349/350 (99%)	0.54	19 (5%) 31 37	26, 54, 93, 130	8 (2%)
2	N	8/8 (100%)	2.27	3 (37%) 1 0	30, 67, 71, 80	0
All	All	706/708 (99%)	0.53	38 (5%) 31 37	26, 52, 91, 131	15 (2%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	419	GLY	6.3
1	A	291	PHE	5.8
1	B	120	GLY	5.4
1	A	121	GLU	5.2
1	B	384	ILE	5.1
1	A	288	TYR	5.0
1	A	120	GLY	4.9
1	B	289	THR	4.9
1	A	384	ILE	4.8
1	B	291	PHE	4.5
1	B	293	PHE	4.5
1	A	295	GLN	3.8
1	B	121	GLU	3.3
1	B	290	GLU	3.3
1	A	92	ARG	3.2
1	A	125	GLU	3.2
1	B	288	TYR	3.1
1	A	290	GLU	3.1
1	B	49	ASP	3.1
1	A	293	PHE	2.8
1	B	364	THR	2.8
1	A	289	THR	2.8
1	A	93	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
2	N	422	GLY	2.6
1	B	48	PRO	2.6
1	A	124	ASP	2.5
1	A	122	LYS	2.3
1	B	46	GLN	2.2
1	B	358	ALA	2.2
1	B	292	LYS	2.2
1	A	127	TYR	2.1
1	B	123	LYS	2.1
1	A	292	LYS	2.1
1	B	47	GLY	2.1
2	N	425	HIS	2.1
1	B	91	LYS	2.0
1	B	127	TYR	2.0
1	B	373	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	PTR	A	216	16/17	0.97	0.07	38,44,51,58	0
1	PTR	B	216	16/17	0.97	0.06	37,42,49,51	0

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	GOL	A	404	6/6	0.77	0.17	20,20,20,20	6

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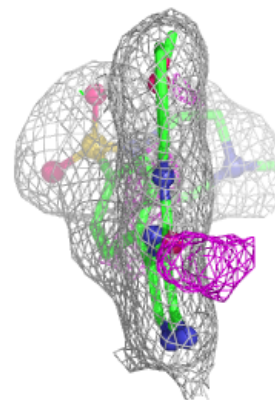
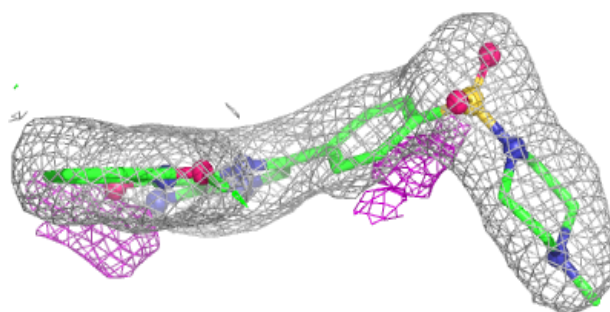
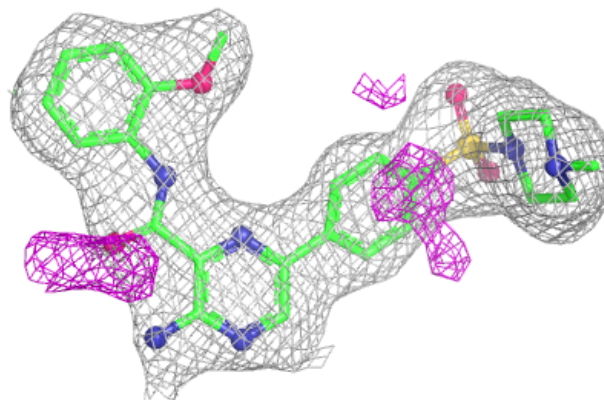
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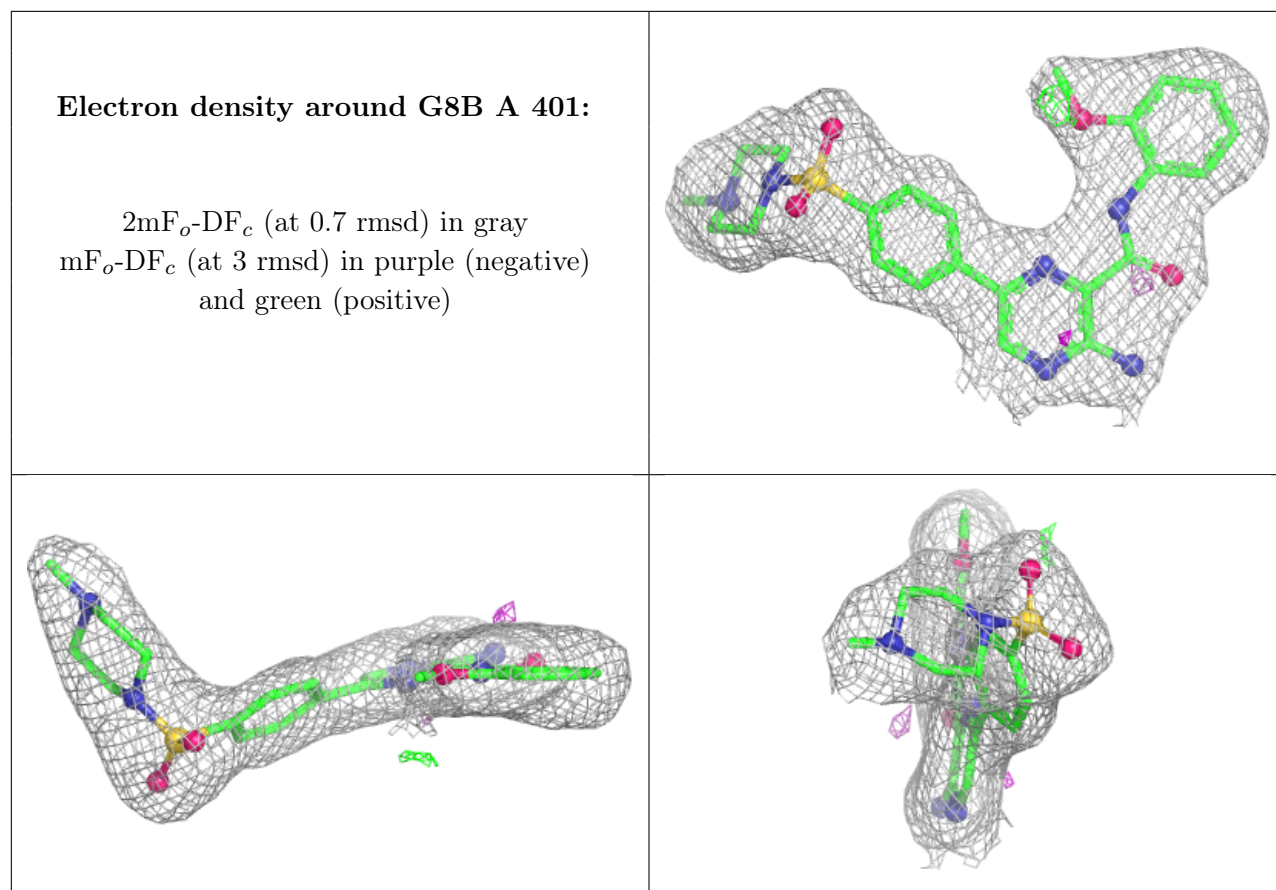
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	A	405	6/6	0.82	0.16	20,20,20,20	6
4	MLI	A	402	7/7	0.91	0.08	44,51,56,59	0
5	GOL	B	403	6/6	0.92	0.12	55,64,69,70	0
7	DMS	A	407	4/4	0.92	0.15	58,64,68,73	0
3	G8B	B	401	34/34	0.93	0.10	37,49,65,73	0
6	CL	B	404	1/1	0.94	0.16	75,75,75,75	0
5	GOL	A	403	6/6	0.95	0.10	54,57,62,66	0
3	G8B	A	401	34/34	0.95	0.09	36,43,58,70	0
4	MLI	B	402	7/7	0.96	0.07	41,49,53,57	0
6	CL	A	406	1/1	0.96	0.11	71,71,71,71	0
7	DMS	B	405	4/4	0.97	0.12	56,67,67,73	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 G8B B 401:

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 ⓘ

There are no such residues in this entry.