



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 09:58 AM EDT

PDB ID : 7XYH / pdb_00007xyh
Title : Crystal structure of CK2a2 complexed with AG1112
Authors : Ikeda, A.; Kinoshita, T.; Tsuyuguchi, M.
Deposited on : 2022-06-01
Resolution : 2.04 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

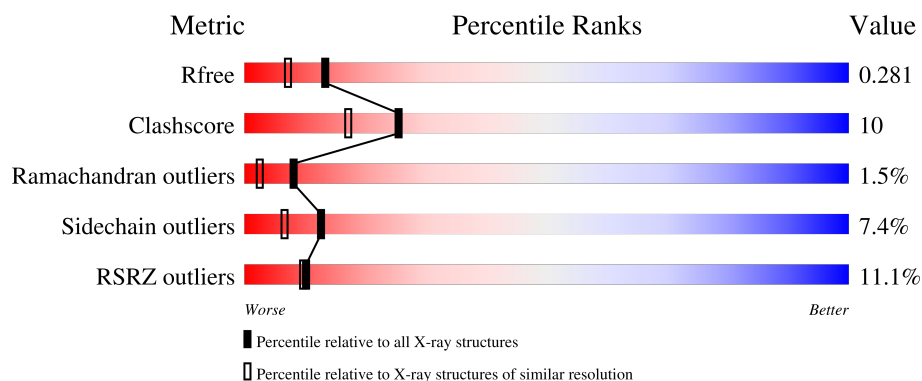
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	339	
1	B	339	

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	8BH	A	401	-	X	-	-
2	8BH	B	401	-	X	-	-
3	EDO	A	406	-	X	-	-
3	EDO	B	403	-	-	X	-
3	EDO	B	405	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5752 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.

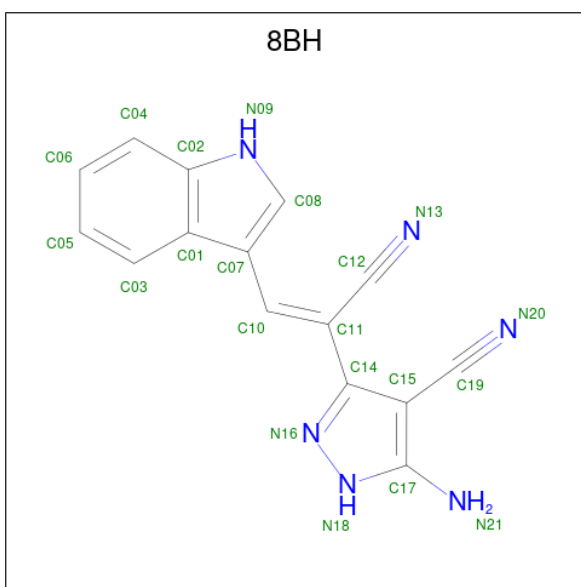
- Molecule 1 is a protein called Casein kinase II subunit alpha'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	0	0
			2749	1770	480	489	10			
1	B	325	Total	C	N	O	S	0	0	0
			2749	1770	480	489	10			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P19784
A	-3	PRO	-	expression tag	UNP P19784
A	-2	LEU	-	expression tag	UNP P19784
A	-1	GLY	-	expression tag	UNP P19784
A	0	SER	-	expression tag	UNP P19784
B	-4	GLY	-	expression tag	UNP P19784
B	-3	PRO	-	expression tag	UNP P19784
B	-2	LEU	-	expression tag	UNP P19784
B	-1	GLY	-	expression tag	UNP P19784
B	0	SER	-	expression tag	UNP P19784

- Molecule 2 is 5-azanyl-3-[({Z})-1-cyano-2-(1 {H}-indol-3-yl)ethenyl]-1 {H}-pyrazole-4-carbonitrile (CCD ID: 8BH) (formula: C₁₅H₁₀N₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			21	15	6		
2	B	1	Total	C	N	0	0
			21	15	6		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

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

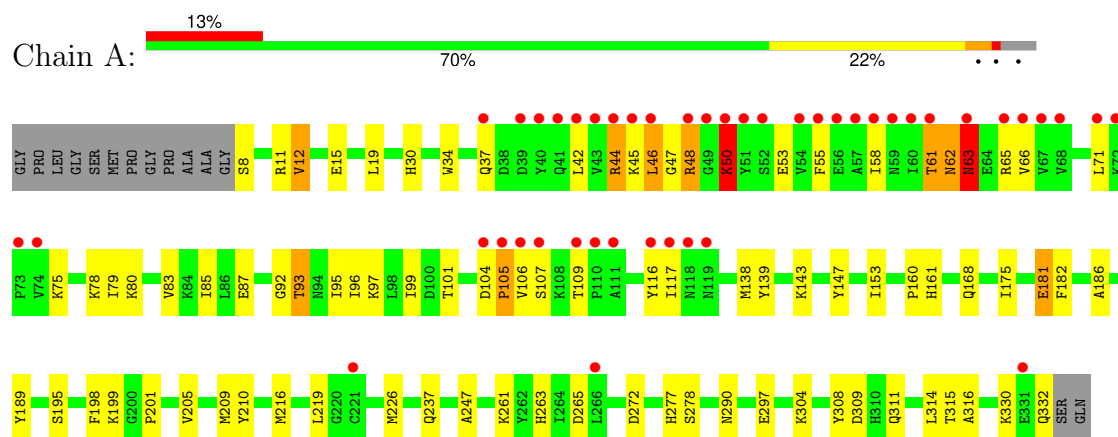
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	85	Total O 85 85	0	0
4	B	79	Total O 79 79	0	0

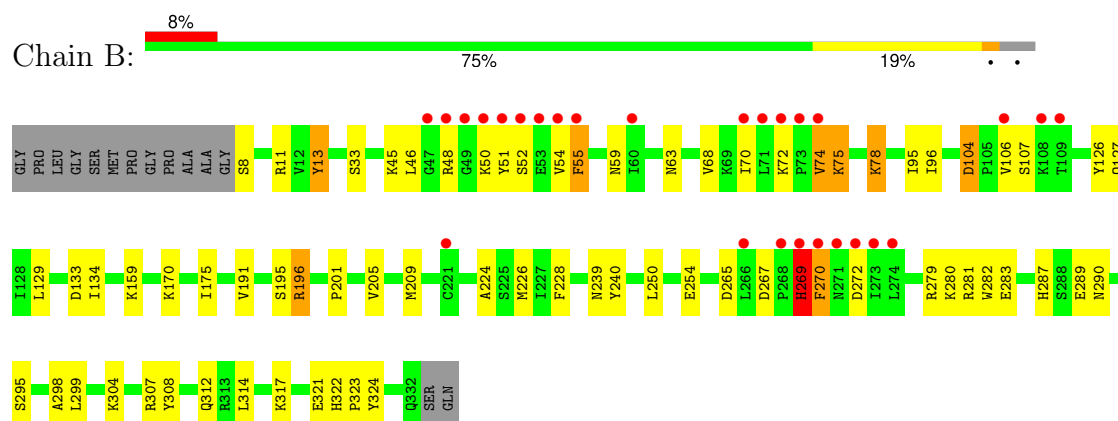
3 Residue-property plots [i](#)

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: Casein kinase II subunit alpha'



• Molecule 1: Casein kinase II subunit alpha'



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	46.55Å 62.54Å 74.06Å 81.42° 75.37° 72.00°	Depositor
Resolution (Å)	35.72 – 2.04 35.72 – 2.04	Depositor EDS
% Data completeness (in resolution range)	97.0 (35.72-2.04) 97.2 (35.72-2.04)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.231 , 0.282 0.232 , 0.281	Depositor DCC
R_{free} test set	2384 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5752	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.74% 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: EDO, 8BH

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	0.69	0/2820	0.81	0/3807
1	B	0.63	0/2820	0.75	0/3807
All	All	0.66	0/5640	0.78	0/7614

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	2749	0	2725	58	0
1	B	2749	0	2725	51	0
2	A	21	0	0	4	0
2	B	21	0	0	1	0
3	A	28	0	42	3	0
3	B	20	0	30	12	0
4	A	85	0	0	6	0
4	B	79	0	0	5	0
All	All	5752	0	5522	107	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 10.

All (107) 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:44:ARG:NE	1:A:44:ARG:HA	1.74	0.99
1:B:104:ASP:OD2	1:B:107:SER:OG	1.94	0.85
1:A:44:ARG:HA	1:A:44:ARG:HE	1.41	0.83
1:A:19:LEU:O	4:A:501:HOH:O	1.99	0.81
1:B:201:PRO:O	1:B:205:VAL:HG22	1.83	0.78
2:A:401:8BH:C10	2:A:401:8BH:C19	2.58	0.77
1:B:13:TYR:N	3:B:403:EDO:H12	2.04	0.72
1:B:45:LYS:O	1:B:46:LEU:HD23	1.90	0.72
1:B:13:TYR:H	3:B:403:EDO:H12	1.56	0.69
1:B:191:VAL:HG22	4:B:503:HOH:O	1.93	0.68
1:B:279:ARG:HE	3:B:405:EDO:C1	2.08	0.66
1:A:263:HIS:ND1	1:B:74:VAL:HG21	2.10	0.66
1:A:277:HIS:HA	3:A:406:EDO:C1	2.27	0.65
1:B:196:ARG:NH2	4:B:501:HOH:O	2.29	0.62
1:A:11:ARG:HD3	1:A:311:GLN:O	1.99	0.62
1:A:30:HIS:O	1:A:80:LYS:NZ	2.31	0.61
1:B:239:ASN:OD1	3:B:406:EDO:O1	2.18	0.61
1:A:62:ASN:O	1:A:63:ASN:HB2	1.98	0.61
1:A:46:LEU:O	2:A:401:8BH:C02	2.49	0.60
1:A:247:ALA:HA	1:A:308:TYR:OH	2.03	0.59
1:A:277:HIS:HA	3:A:406:EDO:H12	1.84	0.59
1:B:298:ALA:HB2	1:B:324:TYR:CE1	2.38	0.59
1:A:45:LYS:C	1:A:47:GLY:H	2.10	0.59
1:B:282:TRP:CE2	3:B:405:EDO:O2	2.56	0.58
1:B:279:ARG:HE	3:B:405:EDO:H12	1.68	0.57
1:A:45:LYS:O	1:A:47:GLY:N	2.37	0.56
1:A:139:TYR:CE2	1:A:143:LYS:HE3	2.41	0.55
1:A:186:ALA:O	1:A:209:MET:HE2	2.08	0.54
1:A:12:VAL:HG22	1:A:315:THR:HG21	1.90	0.54
1:A:116:TYR:O	1:A:117:ILE:HD13	2.07	0.54
1:A:138:MET:HE3	1:A:226:MET:HE1	1.89	0.54
1:A:46:LEU:O	2:A:401:8BH:N09	2.42	0.53
2:B:401:8BH:C12	2:B:401:8BH:C08	2.87	0.53
1:B:240:TYR:HA	1:B:270:PHE:HZ	1.75	0.51
1:B:240:TYR:HA	1:B:270:PHE:CZ	2.46	0.51
1:A:85:ILE:HG23	1:A:153:ILE:HD13	1.92	0.51
1:B:59:ASN:O	1:B:63:ASN:N	2.43	0.51
1:A:216:MET:HE2	1:A:316:ALA:HA	1.93	0.51
1:B:51:TYR:CZ	1:B:78:LYS:HE2	2.46	0.50
1:A:42:LEU:HD13	1:A:55:PHE:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:THR:O	1:A:61:THR:HG23	2.12	0.49
1:A:50:LYS:HZ3	1:B:265:ASP:HB3	1.76	0.49
1:A:261:LYS:NZ	4:A:505:HOH:O	2.44	0.49
1:B:287:HIS:CE1	1:B:289:GLU:HB2	2.48	0.49
3:B:403:EDO:H22	4:B:554:HOH:O	2.12	0.49
1:B:134:ILE:HG23	1:B:226:MET:HE2	1.93	0.49
1:A:263:HIS:CG	1:B:74:VAL:HG21	2.47	0.49
1:A:181:GLU:OE2	1:A:182:PHE:N	2.45	0.48
1:B:304:LYS:HB3	1:B:314:LEU:HG	1.96	0.48
1:B:106:VAL:HG12	1:B:106:VAL:O	2.13	0.48
1:B:126:TYR:HA	1:B:129:LEU:HD12	1.95	0.48
1:A:237:GLN:HG2	4:A:536:HOH:O	2.13	0.48
1:B:307:ARG:HD3	4:B:565:HOH:O	2.14	0.47
1:A:92:GLY:HA3	1:A:147:TYR:CE2	2.48	0.47
1:B:13:TYR:H	3:B:403:EDO:C1	2.27	0.47
1:A:71:LEU:HD13	1:A:79:ILE:HG12	1.95	0.47
1:A:216:MET:CE	1:A:316:ALA:HA	2.45	0.47
1:A:44:ARG:HD3	1:A:45:LYS:N	2.29	0.47
1:A:96:ILE:HB	1:A:175:ILE:HG22	1.96	0.47
1:B:8:SER:O	1:B:209:MET:CE	2.63	0.47
1:A:290:ASN:OD1	1:A:290:ASN:C	2.57	0.47
1:A:34:TRP:CZ3	1:A:101:THR:HB	2.50	0.46
1:A:201:PRO:O	1:A:205:VAL:HG22	2.15	0.46
1:B:267:ASP:OD1	1:B:269:HIS:HB2	2.16	0.46
1:A:195:SER:O	1:A:199:LYS:HG3	2.16	0.46
1:A:37:GLN:O	1:A:37:GLN:HG2	2.15	0.46
1:B:254:GLU:HA	1:B:254:GLU:OE1	2.16	0.46
1:A:277:HIS:HA	3:A:406:EDO:H11	1.97	0.46
1:A:83:VAL:HG13	4:A:548:HOH:O	2.15	0.45
1:B:322:HIS:CG	1:B:323:PRO:HD2	2.52	0.45
1:B:317:LYS:O	1:B:321:GLU:HG3	2.16	0.45
1:B:51:TYR:OH	1:B:75:LYS:HG3	2.18	0.44
1:B:196:ARG:NH1	4:B:508:HOH:O	2.49	0.44
1:A:175:ILE:CD1	2:A:401:8BH:C12	2.96	0.44
1:B:281:ARG:C	1:B:283:GLU:N	2.73	0.44
1:A:161:HIS:ND1	4:A:502:HOH:O	2.21	0.43
1:A:48:ARG:HA	1:A:53:GLU:HA	2.00	0.43
1:A:139:TYR:CD2	1:A:143:LYS:HE3	2.54	0.43
1:B:133:ASP:OD1	3:B:404:EDO:O2	2.18	0.43
1:B:224:ALA:O	1:B:228:PHE:HB2	2.19	0.43
1:A:12:VAL:CG2	1:A:315:THR:HG21	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ASP:OD2	1:B:51:TYR:OH	2.32	0.43
1:B:270:PHE:C	1:B:272:ASP:H	2.27	0.42
1:B:280:LYS:O	3:B:405:EDO:H22	2.19	0.42
1:A:83:VAL:CG1	4:A:548:HOH:O	2.67	0.42
1:A:160:PRO:HD3	1:A:198:PHE:CZ	2.54	0.42
1:B:54:VAL:O	1:B:68:VAL:O	2.38	0.42
1:B:170:LYS:HD2	3:B:404:EDO:H21	2.01	0.42
1:A:216:MET:HE2	1:A:316:ALA:N	2.35	0.42
1:A:65:ARG:C	1:A:66:VAL:HG13	2.45	0.42
1:A:304:LYS:HB3	1:A:314:LEU:HG	2.01	0.41
1:B:290:ASN:OD1	1:B:290:ASN:C	2.62	0.41
1:B:54:VAL:O	1:B:55:PHE:HB2	2.20	0.41
1:B:270:PHE:C	1:B:272:ASP:N	2.75	0.41
1:A:46:LEU:H	1:A:46:LEU:HG	1.62	0.41
1:A:97:LYS:HE2	1:A:99:ILE:CG1	2.50	0.41
1:B:283:GLU:N	1:B:283:GLU:OE2	2.54	0.41
1:A:189:TYR:HB2	1:A:210:TYR:CE2	2.55	0.41
1:B:96:ILE:HB	1:B:175:ILE:HG22	2.02	0.41
1:A:97:LYS:HE2	1:A:99:ILE:HG13	2.03	0.41
1:A:104:ASP:OD1	1:A:104:ASP:C	2.63	0.41
1:B:250:LEU:HB3	1:B:308:TYR:CE2	2.55	0.41
1:A:104:ASP:O	1:A:105:PRO:C	2.64	0.41
1:A:263:HIS:HB3	1:B:74:VAL:CG1	2.51	0.40
1:B:195:SER:O	1:B:196:ARG:C	2.63	0.40
1:B:279:ARG:HE	3:B:405:EDO:H11	1.84	0.40
1:B:282:TRP:HB3	1:B:299:LEU:HD22	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	323/339 (95%)	293 (91%)	24 (7%)	6 (2%)	6	2
1	B	323/339 (95%)	300 (93%)	19 (6%)	4 (1%)	10	4
All	All	646/678 (95%)	593 (92%)	43 (7%)	10 (2%)	8	2

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	50	LYS
1	B	13	TYR
1	A	309	ASP
1	B	55	PHE
1	B	269	HIS
1	A	62	ASN
1	A	93	THR
1	B	196	ARG
1	A	105	PRO

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	298/306 (97%)	272 (91%)	26 (9%)	9	4
1	B	298/306 (97%)	280 (94%)	18 (6%)	17	10
All	All	596/612 (97%)	552 (93%)	44 (7%)	13	6

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	12	VAL
1	A	15	GLU
1	A	44	ARG
1	A	46	LEU
1	A	48	ARG

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Mol	Chain	Res	Type
1	A	50	LYS
1	A	58	ILE
1	A	61	THR
1	A	63	ASN
1	A	75	LYS
1	A	78	LYS
1	A	87	GLU
1	A	93	THR
1	A	95	ILE
1	A	106	VAL
1	A	107	SER
1	A	109	THR
1	A	168	GLN
1	A	181	GLU
1	A	219	LEU
1	A	272	ASP
1	A	278	SER
1	A	297	GLU
1	A	330	LYS
1	A	332	GLN
1	B	11	ARG
1	B	33	SER
1	B	48	ARG
1	B	50	LYS
1	B	52	SER
1	B	70	ILE
1	B	72	LYS
1	B	74	VAL
1	B	75	LYS
1	B	78	LYS
1	B	95	ILE
1	B	104	ASP
1	B	127	GLN
1	B	159	LYS
1	B	269	HIS
1	B	270	PHE
1	B	295	SER
1	B	312	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	ASN
1	A	119	ASN
1	A	124	GLN
1	A	167	HIS
1	A	237	GLN
1	A	276	GLN
1	B	30	HIS
1	B	37	GLN
1	B	168	GLN
1	B	269	HIS
1	B	287	HIS

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 ⓘ

14 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	EDO	A	402	-	3,3,3	0.94	0	2,2,2	0.93	0
3	EDO	B	402	-	3,3,3	0.56	0	2,2,2	1.11	0
2	8BH	A	401	-	23,23,23	4.20	18 (78%)	23,32,32	5.96	17 (73%)
3	EDO	A	408	-	3,3,3	0.54	0	2,2,2	1.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	A	407	-	3,3,3	1.23	0	2,2,2	0.55	0
3	EDO	B	406	-	3,3,3	0.92	0	2,2,2	1.50	0
3	EDO	B	405	-	3,3,3	0.70	0	2,2,2	1.16	0
3	EDO	B	404	-	3,3,3	1.07	0	2,2,2	0.52	0
3	EDO	A	404	-	3,3,3	1.00	0	2,2,2	0.94	0
3	EDO	A	406	-	3,3,3	1.30	1 (33%)	2,2,2	2.40	1 (50%)
3	EDO	B	403	-	3,3,3	0.88	0	2,2,2	1.03	0
2	8BH	B	401	-	23,23,23	3.85	14 (60%)	23,32,32	5.04	14 (60%)
3	EDO	A	403	-	3,3,3	0.79	0	2,2,2	1.03	0
3	EDO	A	405	-	3,3,3	0.78	0	2,2,2	1.31	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	402	-	-	1/1/1/1	-
3	EDO	B	402	-	-	1/1/1/1	-
2	8BH	A	401	-	-	5/9/12/12	0/3/3/3
3	EDO	A	408	-	-	1/1/1/1	-
3	EDO	A	407	-	-	1/1/1/1	-
3	EDO	B	406	-	-	1/1/1/1	-
3	EDO	B	405	-	-	1/1/1/1	-
3	EDO	B	404	-	-	0/1/1/1	-
3	EDO	A	404	-	-	1/1/1/1	-
3	EDO	A	406	-	-	1/1/1/1	-
3	EDO	B	403	-	-	1/1/1/1	-
2	8BH	B	401	-	-	1/9/12/12	0/3/3/3
3	EDO	A	403	-	-	0/1/1/1	-
3	EDO	A	405	-	-	1/1/1/1	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	8BH	C11-C14	7.83	1.57	1.42
2	A	401	8BH	C12-C11	7.73	1.57	1.43
2	B	401	8BH	C01-C07	7.59	1.55	1.45
2	A	401	8BH	C12-N13	7.22	1.27	1.14
2	A	401	8BH	C17-N21	6.87	1.48	1.34
2	A	401	8BH	C11-C14	6.59	1.54	1.42
2	B	401	8BH	C08-N09	-6.44	1.26	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	8BH	C02-N09	-6.28	1.27	1.37
2	A	401	8BH	C17-N18	6.27	1.39	1.34
2	A	401	8BH	C01-C07	5.74	1.52	1.45
2	B	401	8BH	C10-C07	5.29	1.58	1.43
2	B	401	8BH	C12-C11	4.86	1.52	1.43
2	B	401	8BH	C19-C15	4.72	1.53	1.43
2	A	401	8BH	C08-N09	-4.37	1.30	1.37
2	B	401	8BH	C17-N21	4.37	1.43	1.34
2	A	401	8BH	C19-C15	4.32	1.52	1.43
2	A	401	8BH	C14-N16	4.13	1.39	1.34
2	B	401	8BH	C19-N20	3.63	1.21	1.14
2	A	401	8BH	N18-N16	3.47	1.43	1.36
2	A	401	8BH	C08-C07	3.00	1.43	1.38
2	A	401	8BH	C19-N20	2.81	1.19	1.14
2	A	401	8BH	C03-C01	2.76	1.44	1.39
2	A	401	8BH	C05-C03	2.75	1.43	1.38
2	A	401	8BH	C15-C17	-2.56	1.35	1.41
2	A	401	8BH	C06-C04	2.47	1.43	1.38
2	B	401	8BH	C12-N13	2.44	1.19	1.14
2	B	401	8BH	N18-N16	2.36	1.41	1.36
2	A	401	8BH	C01-C02	2.30	1.44	1.41
3	A	406	EDO	O2-C2	2.10	1.52	1.42
2	A	401	8BH	C10-C11	2.08	1.40	1.35
2	B	401	8BH	C05-C03	2.05	1.42	1.38
2	B	401	8BH	C03-C01	2.02	1.43	1.39
2	B	401	8BH	C06-C05	2.02	1.42	1.38

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	8BH	C07-C08-N09	-17.27	101.38	110.20
2	B	401	8BH	C02-N09-C08	16.46	123.72	109.08
2	A	401	8BH	C02-N09-C08	14.03	121.56	109.08
2	A	401	8BH	C11-C14-N16	9.15	139.05	119.81
2	B	401	8BH	C01-C02-N09	-7.97	100.88	107.52
2	B	401	8BH	C01-C07-C08	-7.64	101.93	106.12
2	A	401	8BH	C01-C07-C08	7.39	110.18	106.12
2	B	401	8BH	C07-C08-N09	-6.41	106.93	110.20
2	A	401	8BH	C02-C01-C07	-6.21	102.32	106.53
2	A	401	8BH	N21-C17-N18	6.11	132.81	123.68
2	B	401	8BH	C17-N18-N16	-5.33	106.80	112.65
2	A	401	8BH	C08-C07-C10	-5.13	119.16	129.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	8BH	C03-C01-C02	-4.98	113.68	118.84
2	B	401	8BH	C04-C02-C01	4.87	126.89	122.19
2	B	401	8BH	C01-C07-C10	4.85	133.06	124.54
2	B	401	8BH	C03-C01-C07	3.82	139.79	133.99
2	A	401	8BH	C01-C02-N09	-3.56	104.56	107.52
2	A	401	8BH	C01-C07-C10	3.48	130.65	124.54
2	B	401	8BH	C14-N16-N18	3.06	110.10	104.90
2	A	401	8BH	C05-C06-C04	3.04	123.98	120.24
2	A	401	8BH	C03-C01-C07	2.90	138.40	133.99
3	A	406	EDO	O2-C2-C1	-2.83	90.81	112.39
2	A	401	8BH	C10-C11-C12	-2.71	117.71	122.76
2	A	401	8BH	C11-C12-N13	-2.60	172.94	177.68
2	A	401	8BH	C19-C15-C14	-2.57	122.24	128.75
2	B	401	8BH	C05-C06-C04	-2.53	117.12	120.24
2	B	401	8BH	C10-C11-C12	-2.47	118.17	122.76
2	B	401	8BH	C06-C05-C03	2.46	123.28	120.24
2	A	401	8BH	C17-N18-N16	-2.29	110.13	112.65
2	B	401	8BH	C08-C07-C10	-2.28	124.95	129.59
2	A	401	8BH	C06-C05-C03	-2.05	117.71	120.24
2	A	401	8BH	C15-C19-N20	-2.01	172.81	177.39

There are no chirality outliers.

All (16) torsion outliers are listed below:

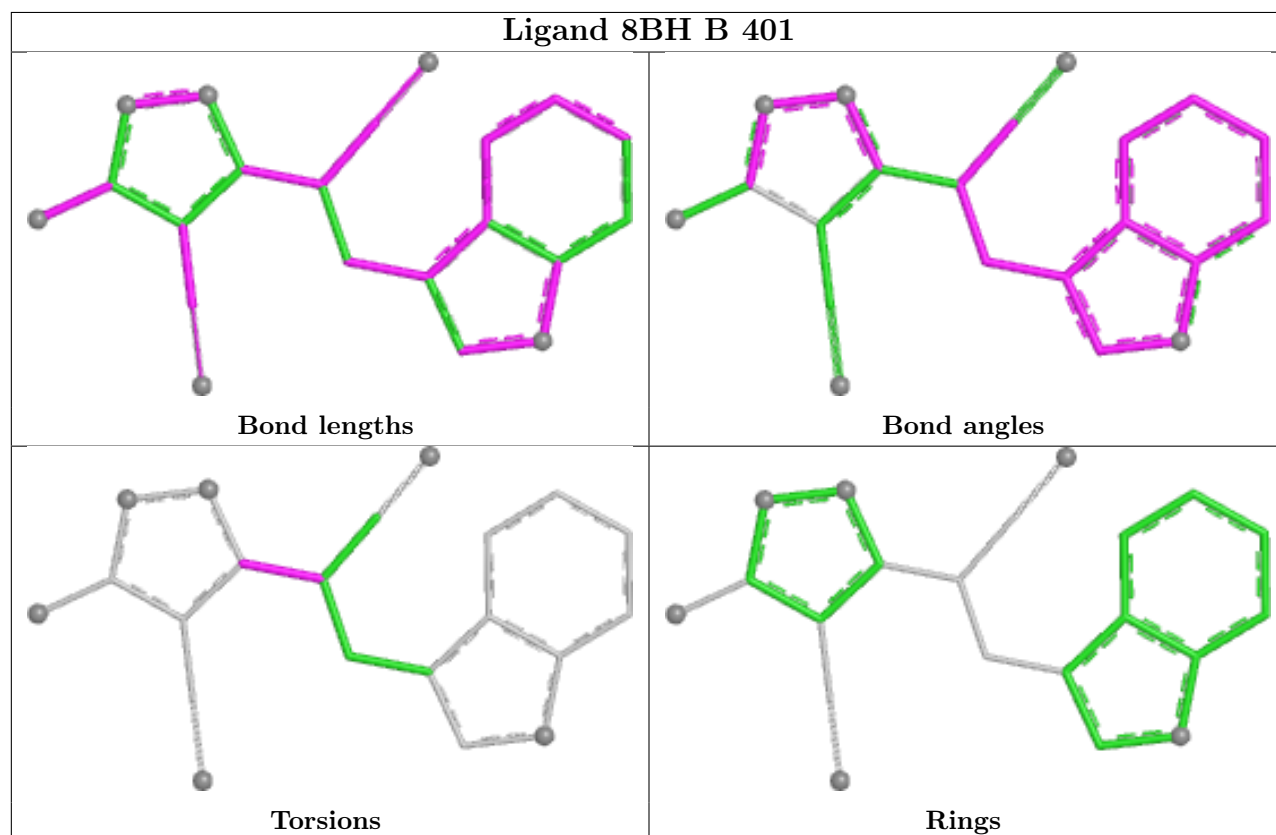
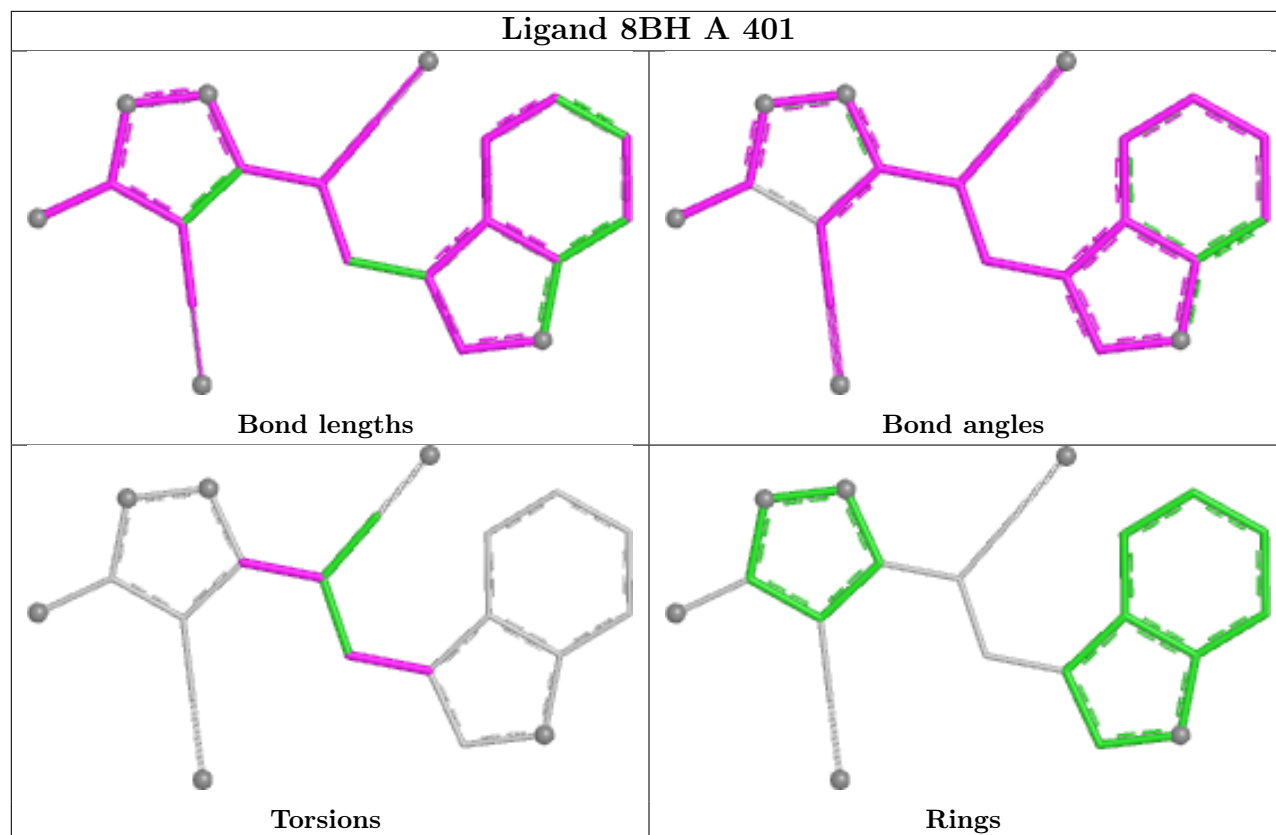
Mol	Chain	Res	Type	Atoms
2	A	401	8BH	C08-C07-C10-C11
2	A	401	8BH	C10-C11-C14-N16
2	A	401	8BH	C12-C11-C14-C15
2	B	401	8BH	C10-C11-C14-C15
3	B	403	EDO	O1-C1-C2-O2
3	A	404	EDO	O1-C1-C2-O2
3	A	406	EDO	O1-C1-C2-O2
3	B	405	EDO	O1-C1-C2-O2
2	A	401	8BH	C01-C07-C10-C11
2	A	401	8BH	C10-C11-C14-C15
3	A	405	EDO	O1-C1-C2-O2
3	A	407	EDO	O1-C1-C2-O2
3	A	408	EDO	O1-C1-C2-O2
3	B	402	EDO	O1-C1-C2-O2
3	A	402	EDO	O1-C1-C2-O2
3	B	406	EDO	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	8BH	4	0
3	B	406	EDO	1	0
3	B	405	EDO	5	0
3	B	404	EDO	2	0
3	A	406	EDO	3	0
3	B	403	EDO	4	0
2	B	401	8BH	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	325/339 (95%)	0.71	45 (13%) 6 6	23, 38, 100, 212	0
1	B	325/339 (95%)	0.55	27 (8%) 17 17	24, 39, 93, 174	0
All	All	650/678 (95%)	0.63	72 (11%) 10 10	23, 39, 95, 212	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	106	VAL	7.1
1	B	51	TYR	7.0
1	A	58	ILE	6.5
1	B	73	PRO	5.7
1	A	105	PRO	5.6
1	A	43	VAL	5.2
1	A	44	ARG	5.1
1	B	52	SER	4.9
1	A	66	VAL	4.9
1	B	54	VAL	4.8
1	A	117	ILE	4.4
1	A	60	ILE	4.4
1	A	40	TYR	4.4
1	A	42	LEU	4.4
1	A	74	VAL	4.3
1	A	51	TYR	4.3
1	A	104	ASP	4.2
1	B	72	LYS	4.0
1	B	74	VAL	4.0
1	A	73	PRO	4.0
1	B	50	LYS	4.0
1	A	116	TYR	3.9
1	A	52	SER	3.9
1	A	57	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	65	ARG	3.6
1	B	266	LEU	3.5
1	A	54	VAL	3.5
1	A	221	CYS	3.5
1	A	71	LEU	3.4
1	A	50	LYS	3.3
1	A	56	GLU	3.3
1	B	71	LEU	3.2
1	A	107	SER	3.1
1	A	59	ASN	3.0
1	B	47	GLY	2.9
1	B	273	ILE	2.9
1	A	63	ASN	2.9
1	B	60	ILE	2.9
1	A	331	GLU	2.8
1	A	68	VAL	2.8
1	B	221	CYS	2.8
1	A	46	LEU	2.8
1	A	67	VAL	2.7
1	B	55	PHE	2.7
1	B	269	HIS	2.7
1	A	49	GLY	2.7
1	B	53	GLU	2.6
1	A	266	LEU	2.6
1	B	268	PRO	2.6
1	A	111	ALA	2.6
1	B	106	VAL	2.6
1	A	41	GLN	2.6
1	A	55	PHE	2.5
1	A	118	ASN	2.5
1	B	49	GLY	2.5
1	B	271	ASN	2.5
1	B	109	THR	2.4
1	B	270	PHE	2.4
1	A	45	LYS	2.4
1	A	37	GLN	2.3
1	B	70	ILE	2.3
1	A	109	THR	2.3
1	A	48	ARG	2.3
1	A	119	ASN	2.3
1	B	48	ARG	2.2
1	A	39	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	272	ASP	2.2
1	A	72	LYS	2.2
1	B	108	LYS	2.1
1	A	110	PRO	2.1
1	B	274	LEU	2.0
1	A	61	THR	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.

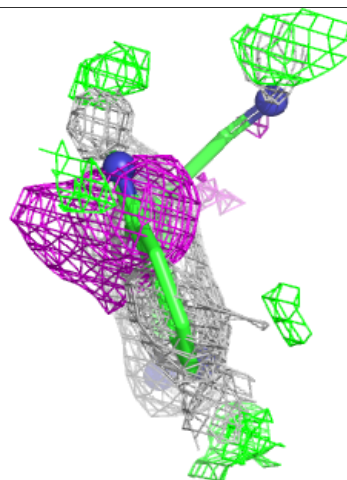
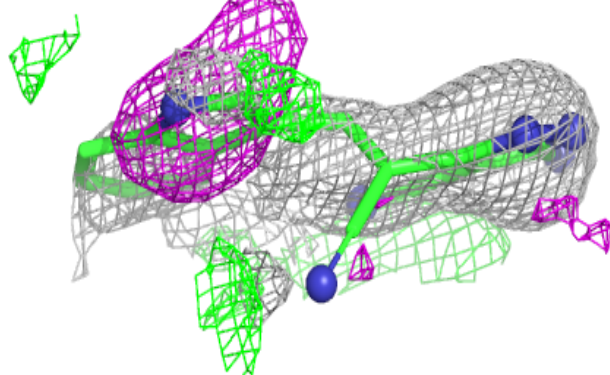
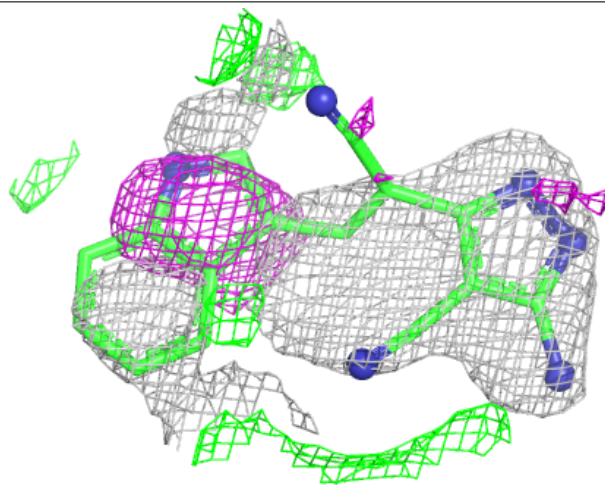
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	8BH	A	401	21/21	0.53	0.19	46,59,65,66	0
3	EDO	B	403	4/4	0.67	0.17	37,39,39,43	0
3	EDO	A	403	4/4	0.69	0.19	34,36,39,42	0
3	EDO	B	406	4/4	0.73	0.16	44,46,47,48	0
3	EDO	A	408	4/4	0.74	0.18	49,49,52,55	0
3	EDO	A	402	4/4	0.75	0.16	34,34,36,44	0
3	EDO	A	407	4/4	0.76	0.12	40,41,44,46	0
2	8BH	B	401	21/21	0.79	0.19	35,48,58,58	21
3	EDO	B	404	4/4	0.85	0.10	42,42,44,46	0
3	EDO	B	402	4/4	0.86	0.10	38,40,41,42	0
3	EDO	A	406	4/4	0.86	0.12	38,39,41,42	0
3	EDO	A	404	4/4	0.89	0.11	29,31,32,39	0
3	EDO	B	405	4/4	0.90	0.15	35,36,41,42	0
3	EDO	A	405	4/4	0.90	0.15	33,34,35,44	0

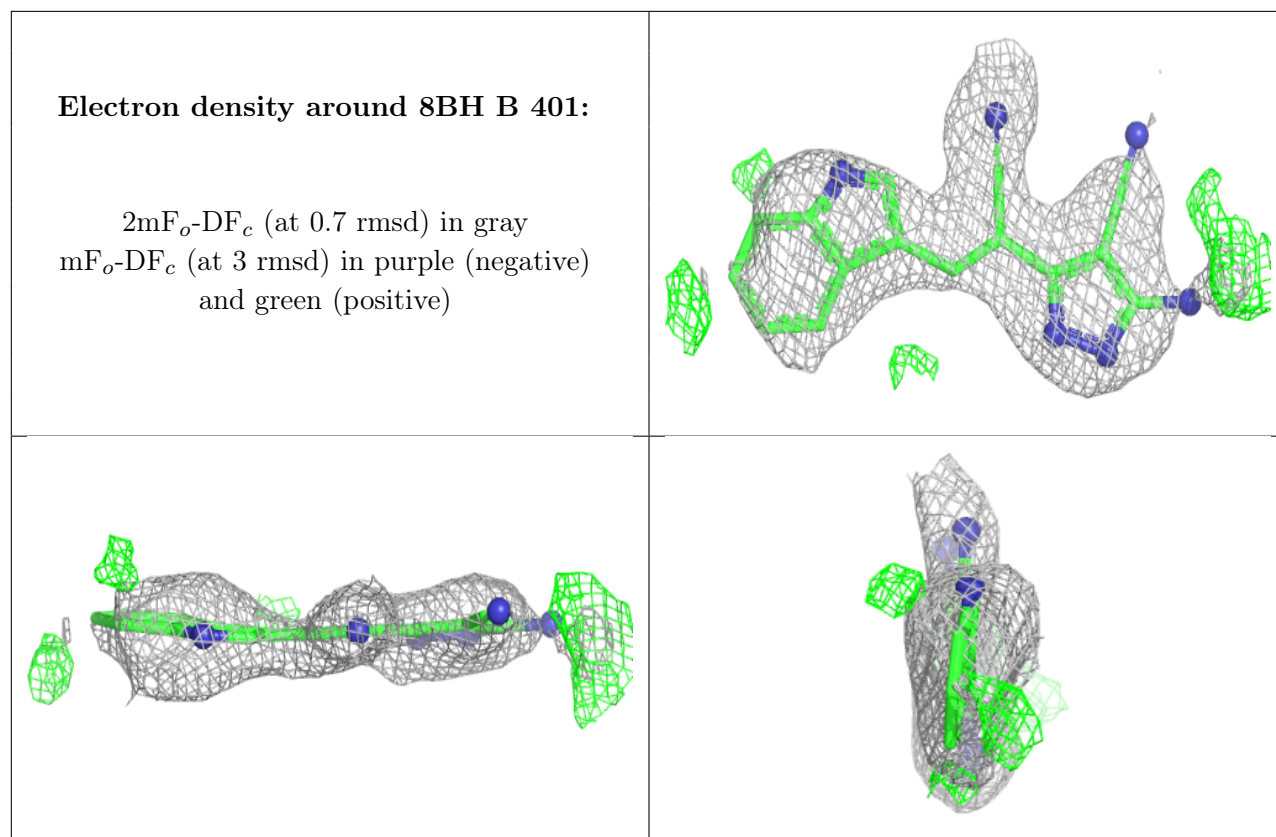
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

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 8BH A 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 [i](#)

There are no such residues in this entry.