



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:26 PM UTC

PDB ID : 7X4U / pdb_00007x4u
Title : Crystal structure of ERK2 with an allosteric inhibitor 2
Authors : Yoshida, M.; Kinoshita, T.
Deposited on : 2022-03-03
Resolution : 1.98 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

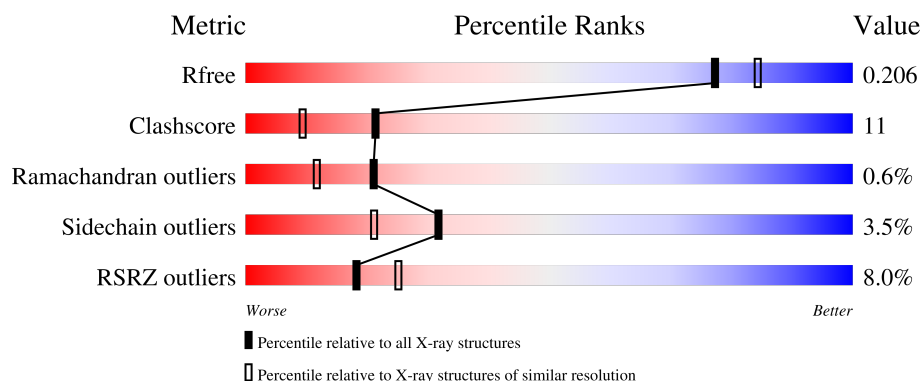
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	368	8% 75% 18% • 5%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3290 atoms, of which 96 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.

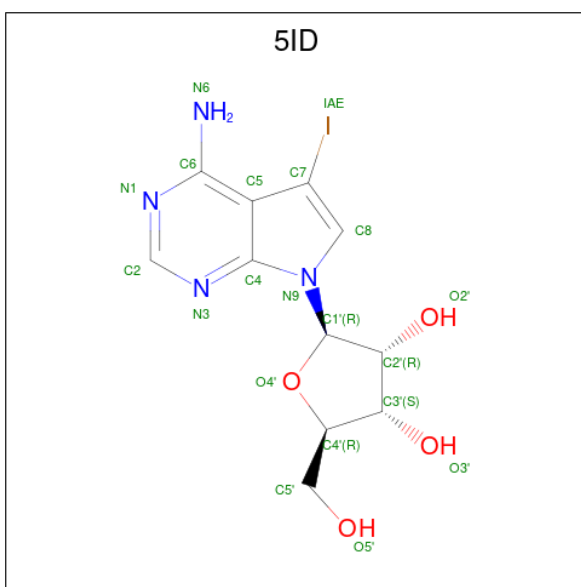
- Molecule 1 is a protein called Mitogen-activated protein kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	350	2887	1852	496	524	15	0	4	0

There are 8 discrepancies between the modelled and reference sequences:

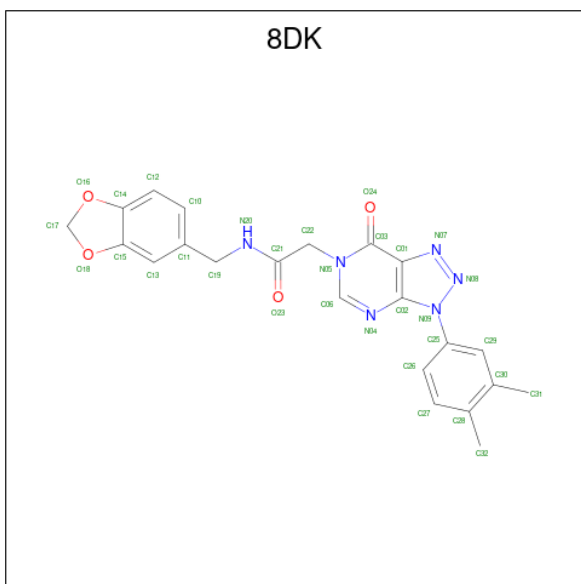
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP P28482
A	-6	ASP	-	expression tag	UNP P28482
A	-5	LEU	-	expression tag	UNP P28482
A	-4	GLY	-	expression tag	UNP P28482
A	-3	SER	-	expression tag	UNP P28482
A	-2	ASP	-	expression tag	UNP P28482
A	-1	GLU	-	expression tag	UNP P28482
A	0	LEU	-	expression tag	UNP P28482

- Molecule 2 is (2R,3R,4S,5R)-2-(4-AMINO-5-iodo-7H-pyrrolo[2,3-d]pyrimidin-7-yl)-5-(hydroxymethyl)tetrahydrofuran-3,4-diol (CCD ID: 5ID) (formula: C₁₁H₁₃IN₄O₄).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	I	N	O	0	0
			33	11	13	1	4	4		

- Molecule 3 is N-(1,3-benzodioxol-5-ylmethyl)-2-[3-(3,4-dimethylphenyl)-7-oxidanylidene-[1,2,3]triazolo[4,5-d]pyrimidin-6-yl]ethanamide (CCD ID: 8DK) (formula: $C_{22}H_{20}N_6O_4$).



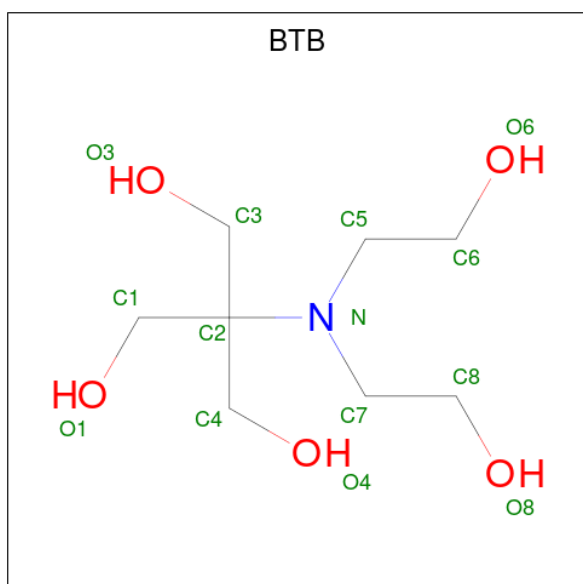
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	1
			104	44	40	12	8		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



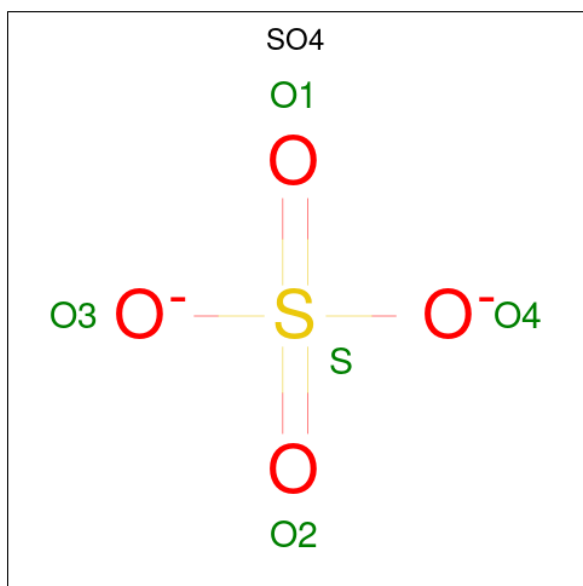
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: BTB) (formula: $C_8H_{19}NO_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			33	8	19	1	5		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

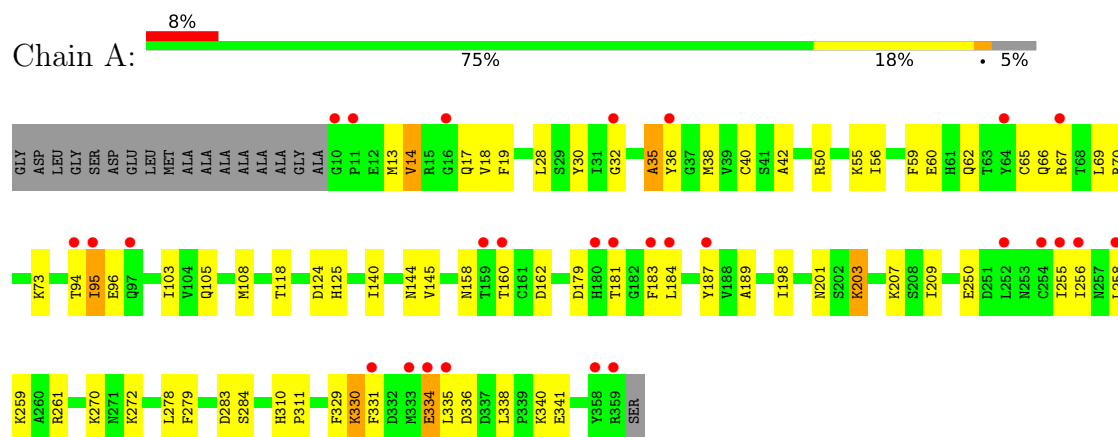
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	186	Total	O	0	0
			186	186		

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: Mitogen-activated protein kinase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	91.74Å 91.74Å 100.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.87 – 1.98 45.87 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.87-1.98) 100.0 (45.87-1.98)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.197 , 0.235 0.200 , 0.206	Depositor DCC
R_{free} test set	1727 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3290	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% 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: 8DK, 5ID, BTB, SO4, GOL

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	0.35	0/2961	0.47	0/4013

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 [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	2887	0	2877	63	0
2	A	20	13	12	3	0
3	A	64	40	0	3	0
4	A	18	24	24	2	0
5	A	14	19	18	1	0
6	A	5	0	0	0	0
7	A	186	0	0	5	1
All	All	3194	96	2931	65	1

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 11.

All (65) 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)
2:A:401:5ID:O4'	2:A:401:5ID:C1'	1.64	1.21
1:A:181:THR:HB	1:A:203:LYS:HD2	1.41	1.02
1:A:13:MET:HB3	1:A:18:VAL:HA	1.58	0.83
1:A:56:ILE:HD12	1:A:103:ILE:HD12	1.65	0.77
1:A:158:ASN:OD1	1:A:160:THR:HG22	1.85	0.76
1:A:270:LYS:HE2	7:A:513:HOH:O	1.86	0.75
1:A:124:ASP:HB3	3:A:402[B]:8DK:O23	1.97	0.65
1:A:62:GLN:NE2	1:A:338:LEU:O	2.28	0.64
1:A:179:ASP:O	1:A:203:LYS:HG2	1.98	0.63
1:A:56:ILE:HD12	1:A:103:ILE:CD1	2.27	0.63
1:A:198:ILE:HD11	1:A:209:ILE:HD11	1.82	0.61
1:A:278:LEU:HD23	1:A:279:PHE:CE2	2.35	0.61
1:A:30:TYR:CZ	1:A:32:GLY:HA2	2.36	0.61
1:A:66:GLN:OE1	1:A:336:ASP:HA	2.03	0.59
1:A:160:THR:HG23	1:A:162:ASP:OD1	2.02	0.58
1:A:187:TYR:HE2	1:A:189:ALA:HB3	1.69	0.58
1:A:187:TYR:CE2	1:A:189:ALA:HB3	2.38	0.58
1:A:73:LYS:HD3	1:A:331:PHE:HE1	1.69	0.57
1:A:96:GLU:OE1	1:A:96:GLU:N	2.32	0.57
1:A:272:LYS:HE2	7:A:575:HOH:O	2.05	0.57
1:A:66:GLN:O	1:A:70:ARG:HG2	2.05	0.56
1:A:105:GLN:OE1	2:A:401:5ID:IAE	2.94	0.56
1:A:183:PHE:HD2	1:A:259:LYS:HD3	1.71	0.56
1:A:94:THR:O	1:A:95:ILE:HB	2.04	0.56
1:A:69:LEU:HD23	1:A:335:LEU:HD13	1.87	0.55
1:A:183:PHE:O	1:A:184:LEU:HB2	2.06	0.55
1:A:283:ASP:HA	4:A:403:GOL:H11	1.88	0.54
1:A:201:ASN:ND2	1:A:255:ILE:HG23	2.23	0.54
1:A:14:VAL:HG13	1:A:38:MET:HE1	1.90	0.53
1:A:96:GLU:H	1:A:96:GLU:CD	2.17	0.53
1:A:108:MET:O	2:A:401:5ID:H2	2.08	0.53
1:A:94:THR:O	1:A:95:ILE:CB	2.58	0.52
1:A:13:MET:HB2	1:A:17:GLN:O	2.10	0.51
1:A:329:PHE:O	1:A:330:LYS:NZ	2.43	0.51
1:A:334:GLU:OE1	1:A:334:GLU:HA	2.12	0.50
1:A:95:ILE:HG23	1:A:96:GLU:N	2.27	0.49
1:A:334:GLU:C	1:A:335:LEU:HD23	2.38	0.49
1:A:201:ASN:HD22	1:A:255:ILE:HG23	1.79	0.48
1:A:28:LEU:HD22	1:A:42:ALA:HB2	1.94	0.48
1:A:272:LYS:NZ	7:A:508:HOH:O	2.46	0.48
1:A:340:LYS:NZ	1:A:341:GLU:OE2	2.38	0.48
1:A:198:ILE:HD11	1:A:209:ILE:CD1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:404:BTB:H31	5:A:404:BTB:H52	1.73	0.47
1:A:56:ILE:CD1	1:A:103:ILE:HD12	2.41	0.47
1:A:198:ILE:CD1	1:A:209:ILE:HD11	2.45	0.46
1:A:18:VAL:O	1:A:55:LYS:NZ	2.47	0.45
1:A:95:ILE:HG23	1:A:96:GLU:H	1.82	0.45
1:A:60:GLU:HA	1:A:60:GLU:OE1	2.16	0.45
1:A:140:ILE:HG22	1:A:145:VAL:O	2.17	0.44
1:A:124:ASP:HB3	3:A:402[A]:8DK:O23	2.18	0.44
1:A:329:PHE:O	1:A:330:LYS:HD2	2.18	0.43
1:A:35:ALA:O	1:A:36:TYR:C	2.61	0.43
1:A:125[A]:HIS:NE2	3:A:402[A]:8DK:C01	2.82	0.43
1:A:14:VAL:HG11	1:A:40:CYS:SG	2.58	0.43
1:A:42:ALA:O	1:A:50:ARG:HA	2.19	0.42
1:A:73:LYS:HD3	1:A:331:PHE:CE1	2.53	0.42
1:A:207:LYS:NZ	7:A:505:HOH:O	2.38	0.42
1:A:329:PHE:O	1:A:330:LYS:CE	2.68	0.42
1:A:118:THR:HA	4:A:405:GOL:H11	2.02	0.42
1:A:256:ILE:HD13	1:A:256:ILE:HA	1.89	0.41
1:A:30:TYR:OH	1:A:32:GLY:HA2	2.21	0.41
1:A:272:LYS:HE2	7:A:629:HOH:O	2.21	0.41
1:A:203:LYS:HG2	1:A:203:LYS:H	1.49	0.41
1:A:59:PHE:HA	1:A:65:CYS:SG	2.60	0.40
1:A:310:HIS:CG	1:A:311:PRO:HD2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:639:HOH:O	7:A:641:HOH:O[4_555]	1.98	0.22

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	352/368 (96%)	324 (92%)	26 (7%)	2 (1%)	21	12

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	ILE
1	A	35	ALA

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	319/324 (98%)	306 (96%)	13 (4%)	27	16

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	19	PHE
1	A	67[A]	ARG
1	A	67[B]	ARG
1	A	144	ASN
1	A	203	LYS
1	A	250	GLU
1	A	258	LEU
1	A	261	ARG
1	A	284[A]	SER
1	A	284[B]	SER
1	A	330	LYS
1	A	334	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN

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Mol	Chain	Res	Type
1	A	120	HIS
1	A	123	ASN
1	A	224	ASN
1	A	249	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
5	BTB	A	404	-	13,13,13	4.67	5 (38%)	7,16,16	1.32	0
6	SO4	A	407	-	4,4,4	0.27	0	6,6,6	0.13	0
2	5ID	A	401	-	21,22,22	3.47	9 (42%)	28,33,33	2.46	8 (28%)
3	8DK	A	402[A]	-	36,36,36	3.63	10 (27%)	51,52,52	3.10	17 (33%)
4	GOL	A	405	-	5,5,5	0.61	0	5,5,5	1.00	0
4	GOL	A	406	-	5,5,5	0.73	0	5,5,5	0.93	0
4	GOL	A	403	-	5,5,5	0.48	0	5,5,5	0.92	0
3	8DK	A	402[B]	-	36,36,36	3.78	11 (30%)	51,52,52	3.04	18 (35%)

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	BTB	A	404	-	-	5/21/21/21	-
2	5ID	A	401	-	-	2/6/22/22	0/3/3/3
3	8DK	A	402[A]	-	-	4/13/19/19	0/5/5/5
4	GOL	A	405	-	-	2/4/4/4	-
4	GOL	A	406	-	-	3/4/4/4	-
4	GOL	A	403	-	-	4/4/4/4	-
3	8DK	A	402[B]	-	-	4/13/19/19	0/5/5/5

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402[B]	8DK	C22-N05	16.25	1.67	1.46
3	A	402[A]	8DK	C22-N05	15.14	1.65	1.46
5	A	404	BTB	C4-C2	13.77	1.69	1.53
2	A	401	5ID	O4'-C1'	9.90	1.64	1.42
5	A	404	BTB	C1-C2	7.99	1.62	1.53
2	A	401	5ID	O4'-C4'	-7.18	1.29	1.45
3	A	402[B]	8DK	C25-N09	6.62	1.55	1.43
2	A	401	5ID	C2'-C1'	-6.53	1.33	1.53
3	A	402[B]	8DK	O24-C03	6.37	1.36	1.23
3	A	402[A]	8DK	C25-N09	6.35	1.54	1.43
3	A	402[A]	8DK	O24-C03	6.22	1.35	1.23
3	A	402[A]	8DK	C01-N07	6.04	1.44	1.36
3	A	402[B]	8DK	C02-N09	5.91	1.45	1.36
3	A	402[B]	8DK	C01-N07	5.86	1.44	1.36
3	A	402[A]	8DK	C02-N09	5.51	1.44	1.36
3	A	402[A]	8DK	N09-N08	4.89	1.43	1.36
3	A	402[B]	8DK	N09-N08	4.53	1.43	1.36
3	A	402[A]	8DK	C06-N05	4.47	1.42	1.36
2	A	401	5ID	C6-N6	4.39	1.45	1.34
3	A	402[B]	8DK	C06-N05	4.18	1.42	1.36
3	A	402[B]	8DK	C21-N20	4.02	1.42	1.33
3	A	402[A]	8DK	C21-N20	3.99	1.42	1.33
3	A	402[A]	8DK	C01-C02	3.47	1.48	1.38
5	A	404	BTB	O4-C4	-3.24	1.32	1.42
2	A	401	5ID	O2'-C2'	3.21	1.50	1.43
3	A	402[B]	8DK	C01-C02	3.18	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	404	BTB	C3-C2	2.75	1.56	1.53
2	A	401	5ID	O3'-C3'	-2.53	1.36	1.43
2	A	401	5ID	C8-C7	2.52	1.40	1.36
5	A	404	BTB	C7-N	-2.47	1.44	1.48
3	A	402[B]	8DK	C06-N04	2.34	1.34	1.30
2	A	401	5ID	C5-C4	-2.16	1.38	1.40
2	A	401	5ID	C8-N9	-2.15	1.34	1.38
3	A	402[A]	8DK	C06-N04	2.10	1.34	1.30
3	A	402[B]	8DK	C02-N04	2.01	1.39	1.35

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402[B]	8DK	C06-N05-C03	-11.92	114.55	123.06
3	A	402[A]	8DK	C06-N05-C03	-11.40	114.93	123.06
3	A	402[A]	8DK	C22-N05-C03	10.88	125.38	117.38
3	A	402[B]	8DK	C22-N05-C03	7.90	123.19	117.38
2	A	401	5ID	C5-C4-N3	-7.61	118.90	126.97
3	A	402[A]	8DK	N09-N08-N07	7.49	114.34	107.08
3	A	402[B]	8DK	N09-N08-N07	7.43	114.27	107.08
3	A	402[B]	8DK	N09-C02-N04	6.45	134.86	125.85
3	A	402[A]	8DK	N09-C02-N04	6.17	134.46	125.85
3	A	402[B]	8DK	C01-C02-N04	-5.83	118.69	127.27
3	A	402[A]	8DK	C01-C02-N04	-5.63	118.98	127.27
2	A	401	5ID	N3-C2-N1	-4.77	121.37	128.58
3	A	402[B]	8DK	O24-C03-N05	-4.09	115.10	120.53
3	A	402[A]	8DK	O24-C03-N05	-4.08	115.10	120.53
3	A	402[B]	8DK	C02-N09-N08	-3.90	104.23	109.06
3	A	402[A]	8DK	C02-N09-N08	-3.83	104.32	109.06
3	A	402[B]	8DK	C21-C22-N05	3.83	116.06	111.16
2	A	401	5ID	C2-N3-C4	3.78	121.06	111.83
2	A	401	5ID	C4-N9-C8	3.73	109.62	108.08
2	A	401	5ID	C6-C5-C4	3.64	118.47	115.74
2	A	401	5ID	N3-C4-N9	3.24	132.67	127.17
3	A	402[B]	8DK	O23-C21-N20	-2.91	117.33	123.03
2	A	401	5ID	C5-C6-N6	-2.82	119.68	123.40
3	A	402[B]	8DK	C22-N05-C06	2.73	122.24	119.55
3	A	402[A]	8DK	N05-C06-N04	2.73	129.11	126.45
3	A	402[A]	8DK	O23-C21-N20	-2.71	117.71	123.03
3	A	402[A]	8DK	C02-C01-N07	-2.57	106.09	109.27
3	A	402[B]	8DK	C02-C01-N07	-2.53	106.14	109.27
3	A	402[A]	8DK	C15-C13-C11	-2.52	116.30	120.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402[B]	8DK	C19-N20-C21	-2.50	118.37	122.42
2	A	401	5ID	O4'-C4'-C3'	-2.47	100.24	105.15
3	A	402[B]	8DK	C15-C13-C11	-2.45	116.41	120.04
3	A	402[B]	8DK	C03-C01-N07	2.45	133.62	130.14
3	A	402[A]	8DK	C03-C01-N07	2.43	133.60	130.14
3	A	402[B]	8DK	C06-N04-C02	2.42	117.28	112.53
3	A	402[A]	8DK	C21-C22-N05	2.39	114.22	111.16
3	A	402[A]	8DK	C10-C11-C13	2.30	121.71	118.55
3	A	402[B]	8DK	C10-C11-C13	2.29	121.70	118.55
3	A	402[B]	8DK	N05-C06-N04	2.15	128.55	126.45
3	A	402[A]	8DK	C25-N09-N08	2.12	123.38	119.76
3	A	402[A]	8DK	C19-N20-C21	-2.10	119.02	122.42
3	A	402[B]	8DK	C01-C03-N05	2.09	120.68	115.10
3	A	402[A]	8DK	C06-N04-C02	2.08	116.60	112.53

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403	GOL	O1-C1-C2-C3
4	A	403	GOL	C1-C2-C3-O3
4	A	405	GOL	O1-C1-C2-C3
5	A	404	BTB	O1-C1-C2-C4
5	A	404	BTB	O1-C1-C2-N
2	A	401	5ID	O4'-C4'-C5'-O5'
4	A	403	GOL	O2-C2-C3-O3
5	A	404	BTB	N-C5-C6-O6
4	A	406	GOL	O1-C1-C2-C3
4	A	406	GOL	C1-C2-C3-O3
4	A	403	GOL	O1-C1-C2-O2
4	A	405	GOL	O1-C1-C2-O2
3	A	402[B]	8DK	O23-C21-C22-N05
2	A	401	5ID	C3'-C4'-C5'-O5'
5	A	404	BTB	N-C7-C8-O8
3	A	402[A]	8DK	O23-C21-C22-N05
3	A	402[B]	8DK	N20-C21-C22-N05
3	A	402[A]	8DK	N20-C21-C22-N05
3	A	402[A]	8DK	C26-C25-N09-N08
3	A	402[A]	8DK	C29-C25-N09-N08
3	A	402[B]	8DK	C21-C22-N05-C06
4	A	406	GOL	O1-C1-C2-O2
3	A	402[B]	8DK	C21-C22-N05-C03

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Mol	Chain	Res	Type	Atoms
5	A	404	BTB	N-C2-C4-O4

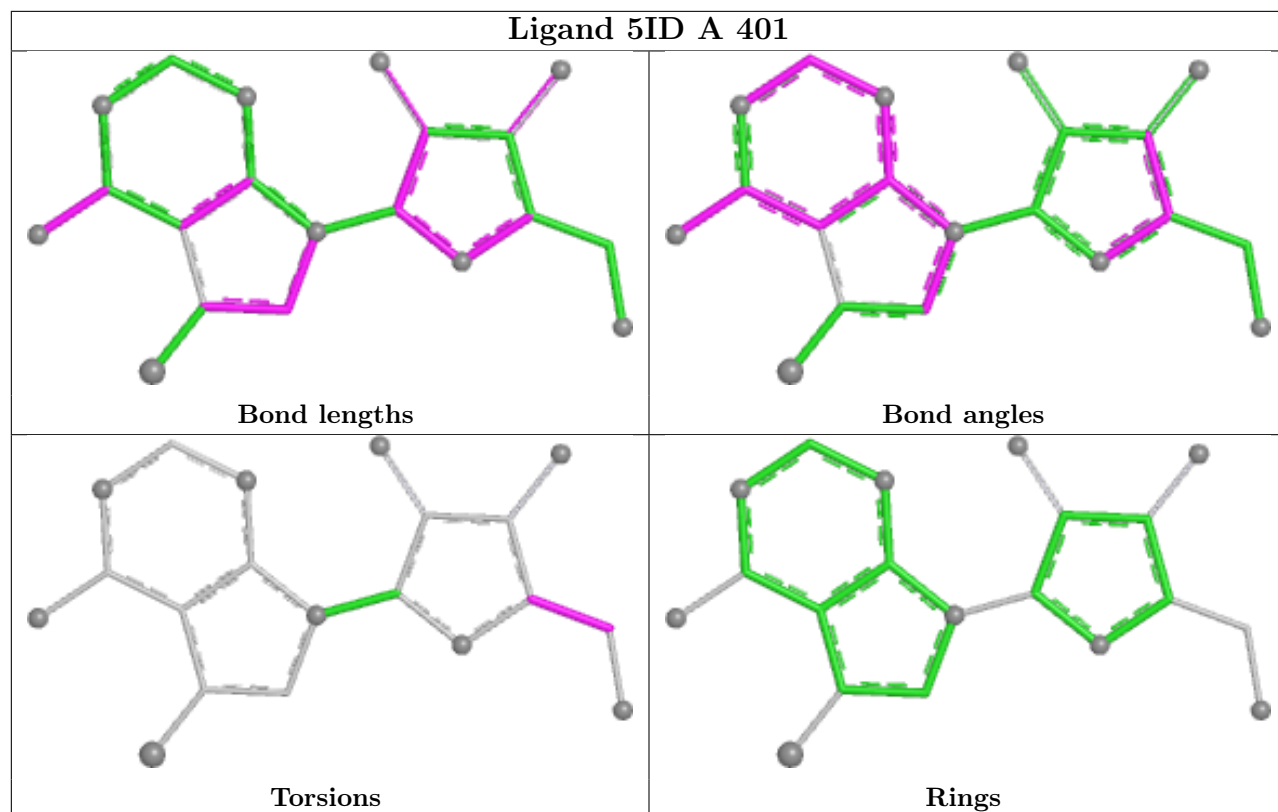
There are no ring outliers.

6 monomers are involved in 9 short contacts:

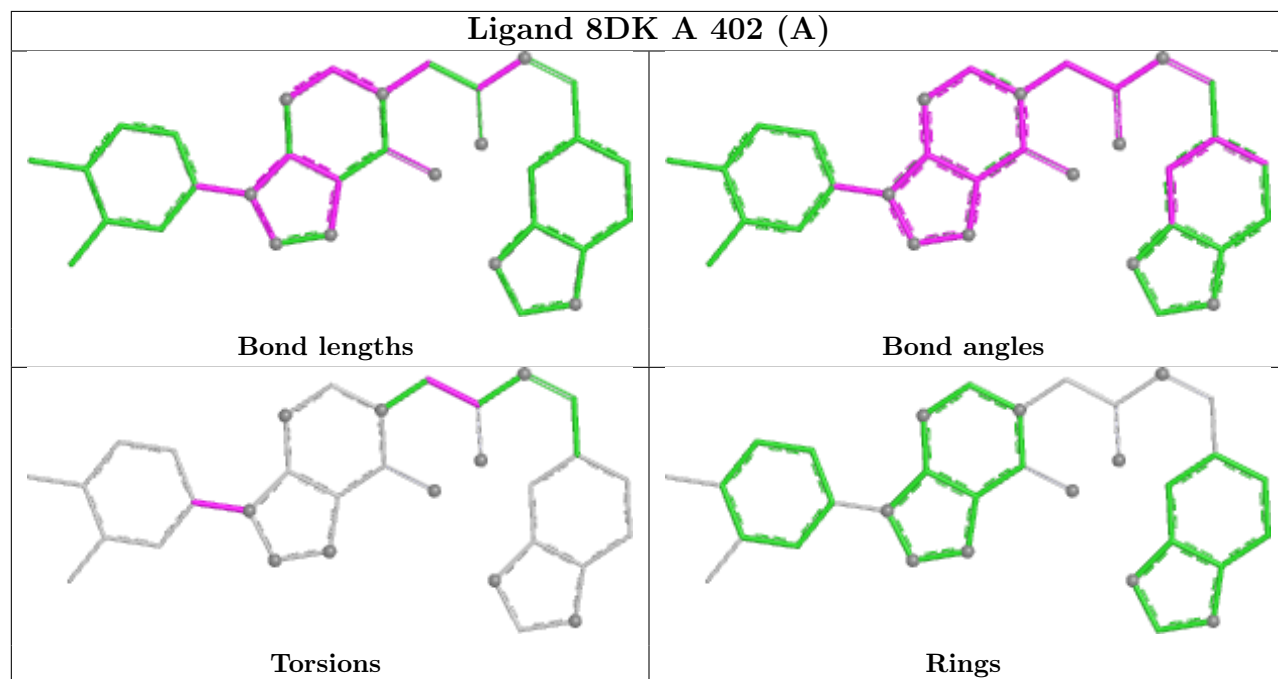
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	404	BTB	1	0
2	A	401	5ID	3	0
3	A	402[A]	8DK	2	0
4	A	405	GOL	1	0
4	A	403	GOL	1	0
3	A	402[B]	8DK	1	0

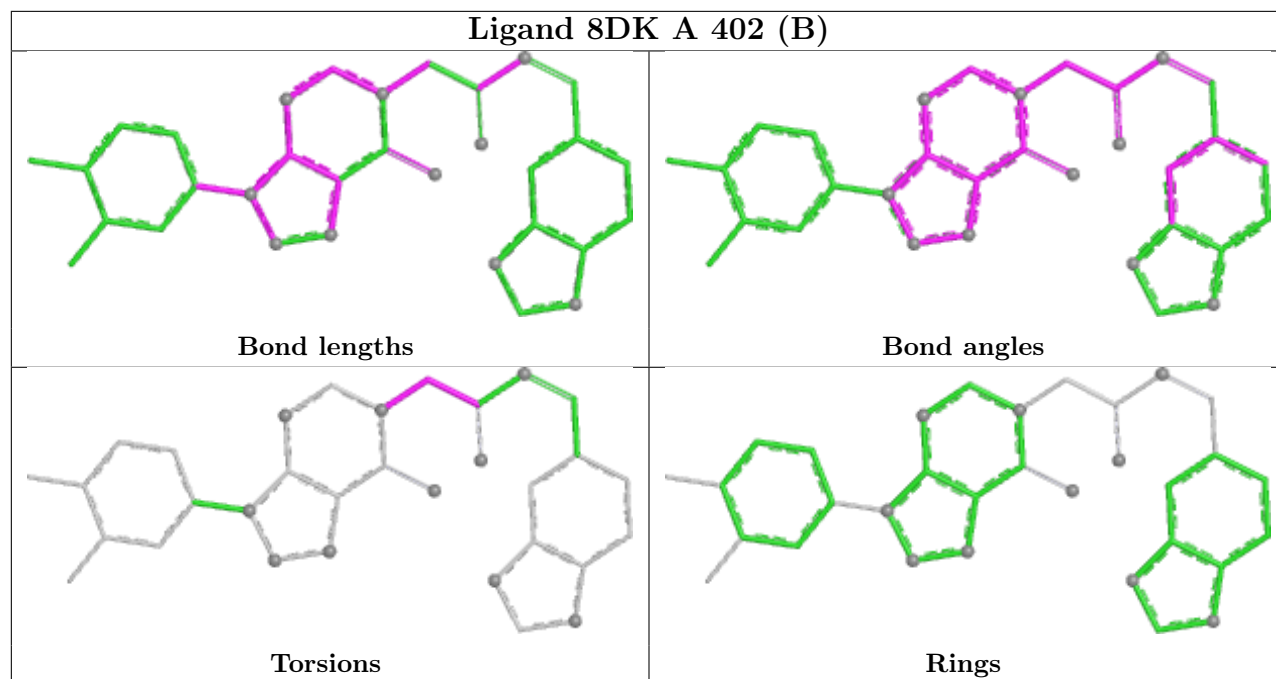
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand 5ID A 401



Ligand 8DK A 402 (A)





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	350/368 (95%)	0.42	28 (8%)	18 25	24, 44, 78, 105	4 (1%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	36	TYR	4.9
1	A	256	ILE	3.7
1	A	183	PHE	3.5
1	A	16	GLY	3.4
1	A	358	TYR	3.3
1	A	10	GLY	3.2
1	A	359	ARG	3.0
1	A	184	LEU	2.8
1	A	254	CYS	2.8
1	A	64	TYR	2.7
1	A	258	LEU	2.7
1	A	95	ILE	2.7
1	A	160	THR	2.6
1	A	180	HIS	2.5
1	A	331	PHE	2.5
1	A	335	LEU	2.5
1	A	255	ILE	2.4
1	A	159	THR	2.4
1	A	333	MET	2.4
1	A	97	GLN	2.3
1	A	67[A]	ARG	2.3
1	A	181	THR	2.3
1	A	94	THR	2.2
1	A	334	GLU	2.1
1	A	252	LEU	2.1
1	A	187	TYR	2.0
1	A	11	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	32	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

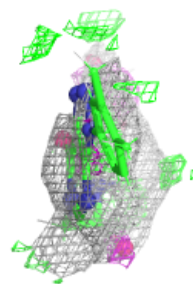
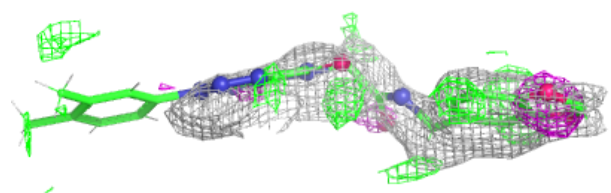
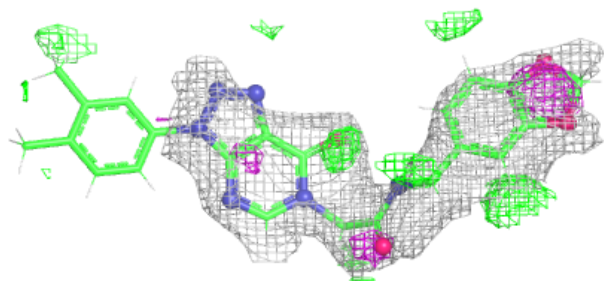
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	8DK	A	402[A]	32/32	0.59	0.24	65,72,87,92	52
3	8DK	A	402[B]	32/32	0.59	0.24	56,72,87,91	52
4	GOL	A	406	6/6	0.61	0.19	54,73,84,88	0
4	GOL	A	405	6/6	0.75	0.12	68,82,90,91	0
6	SO4	A	407	5/5	0.76	0.12	77,77,88,106	0
5	BTB	A	404	14/14	0.77	0.14	47,63,75,80	0
4	GOL	A	403	6/6	0.79	0.10	55,70,83,84	0
2	5ID	A	401	20/20	0.93	0.12	32,64,85,92	0

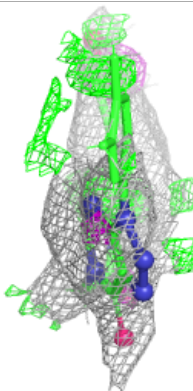
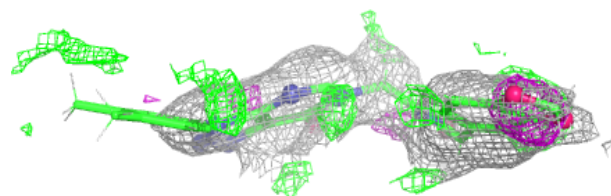
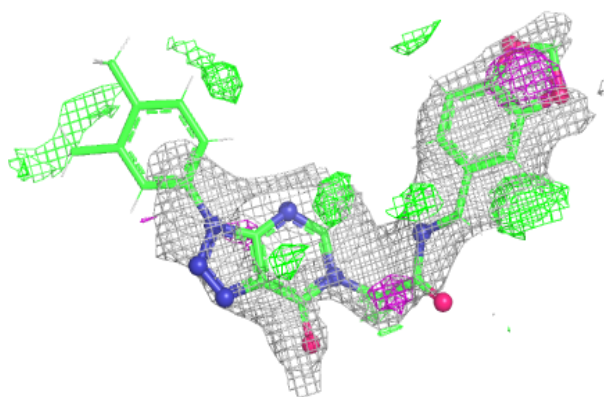
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8DK A 402 (A):

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

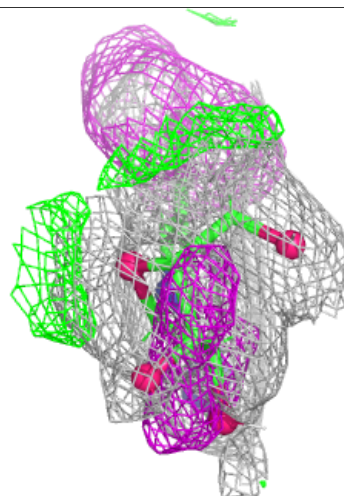
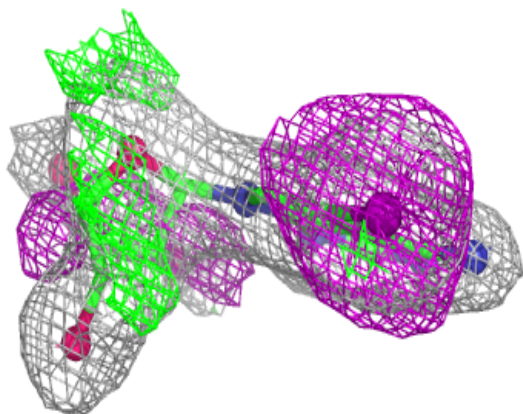
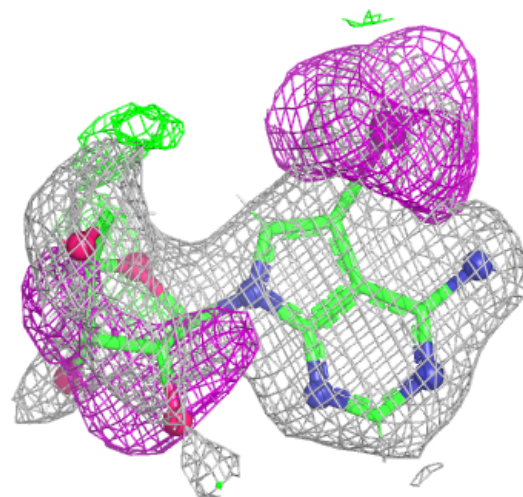
**Electron density around 8DK A 402 (B):**

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



Electron density around 5ID 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.