



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2021 – 10:04 AM EST

PDB ID : 6UX9
Title : Crystal Structure Analysis of PIP4K2A
Authors : Seo, H.-S.; Dhe-Paganon, S.
Deposited on : 2019-11-07
Resolution : 1.71 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 : 2.24
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) : 2.24

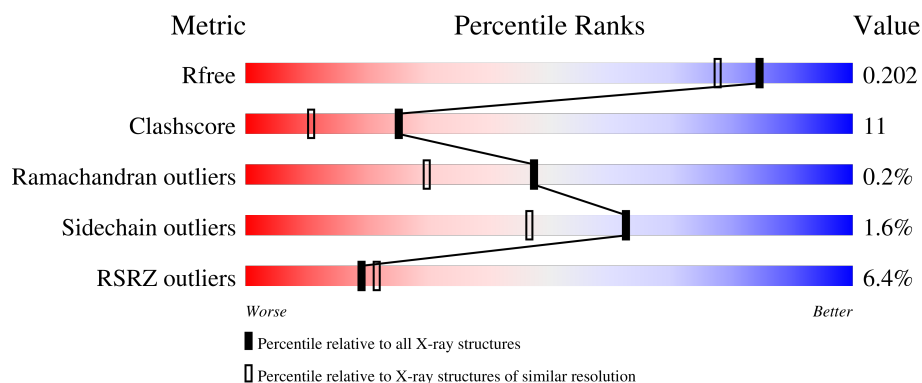
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.71 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	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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	370	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>11%</div> <div>•</div> <div>15%</div> </div> </div>
1	B	370	<div> <div>6%</div> <div> <div></div> <div>67%</div> <div>16%</div> <div>•</div> <div>16%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5639 atoms, of which 28 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 Phosphatidylinositol 5-phosphate 4-kinase type-2 alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	4	0
			2630	1692	442	483	13			
1	B	312	Total	C	N	O	S	0	1	0
			2573	1656	434	470	13			

There are 94 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	initiating methionine	UNP P48426
A	13	HIS	-	expression tag	UNP P48426
A	14	HIS	-	expression tag	UNP P48426
A	15	HIS	-	expression tag	UNP P48426
A	16	HIS	-	expression tag	UNP P48426
A	17	HIS	-	expression tag	UNP P48426
A	18	HIS	-	expression tag	UNP P48426
A	19	SER	-	expression tag	UNP P48426
A	20	SER	-	expression tag	UNP P48426
A	21	GLY	-	expression tag	UNP P48426
A	22	VAL	-	expression tag	UNP P48426
A	23	ASP	-	expression tag	UNP P48426
A	24	LEU	-	expression tag	UNP P48426
A	25	GLY	-	expression tag	UNP P48426
A	26	THR	-	expression tag	UNP P48426
A	27	GLU	-	expression tag	UNP P48426
A	28	ASN	-	expression tag	UNP P48426
A	29	LEU	-	expression tag	UNP P48426
A	30	TYR	-	expression tag	UNP P48426
A	31	PHE	-	expression tag	UNP P48426
A	32	GLN	-	expression tag	UNP P48426
A	33	SER	-	expression tag	UNP P48426
A	34	MET	-	expression tag	UNP P48426
A	?	-	GLY	deletion	UNP P48426
A	?	-	GLU	deletion	UNP P48426

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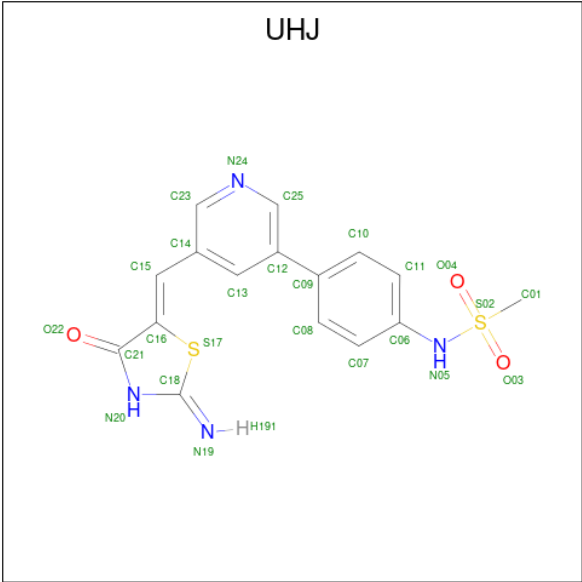
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP P48426
A	?	-	GLU	deletion	UNP P48426
A	?	-	GLY	deletion	UNP P48426
A	?	-	GLU	deletion	UNP P48426
A	?	-	SER	deletion	UNP P48426
A	?	-	ASP	deletion	UNP P48426
A	?	-	GLY	deletion	UNP P48426
A	?	-	THR	deletion	UNP P48426
A	?	-	HIS	deletion	UNP P48426
A	?	-	PRO	deletion	UNP P48426
A	?	-	VAL	deletion	UNP P48426
A	?	-	GLY	deletion	UNP P48426
A	?	-	THR	deletion	UNP P48426
A	?	-	PRO	deletion	UNP P48426
A	?	-	PRO	deletion	UNP P48426
A	?	-	ASP	deletion	UNP P48426
A	?	-	SER	deletion	UNP P48426
A	?	-	PRO	deletion	UNP P48426
A	?	-	GLY	deletion	UNP P48426
A	?	-	ASN	deletion	UNP P48426
A	?	-	THR	deletion	UNP P48426
A	?	-	LEU	deletion	UNP P48426
B	12	MET	-	initiating methionine	UNP P48426
B	13	HIS	-	expression tag	UNP P48426
B	14	HIS	-	expression tag	UNP P48426
B	15	HIS	-	expression tag	UNP P48426
B	16	HIS	-	expression tag	UNP P48426
B	17	HIS	-	expression tag	UNP P48426
B	18	HIS	-	expression tag	UNP P48426
B	19	SER	-	expression tag	UNP P48426
B	20	SER	-	expression tag	UNP P48426
B	21	GLY	-	expression tag	UNP P48426
B	22	VAL	-	expression tag	UNP P48426
B	23	ASP	-	expression tag	UNP P48426
B	24	LEU	-	expression tag	UNP P48426
B	25	GLY	-	expression tag	UNP P48426
B	26	THR	-	expression tag	UNP P48426
B	27	GLU	-	expression tag	UNP P48426
B	28	ASN	-	expression tag	UNP P48426
B	29	LEU	-	expression tag	UNP P48426
B	30	TYR	-	expression tag	UNP P48426
B	31	PHE	-	expression tag	UNP P48426

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Chain	Residue	Modelled	Actual	Comment	Reference
B	32	GLN	-	expression tag	UNP P48426
B	33	SER	-	expression tag	UNP P48426
B	34	MET	-	expression tag	UNP P48426
B	?	-	GLY	deletion	UNP P48426
B	?	-	GLU	deletion	UNP P48426
B	?	-	GLU	deletion	UNP P48426
B	?	-	GLU	deletion	UNP P48426
B	?	-	GLY	deletion	UNP P48426
B	?	-	GLU	deletion	UNP P48426
B	?	-	SER	deletion	UNP P48426
B	?	-	ASP	deletion	UNP P48426
B	?	-	GLY	deletion	UNP P48426
B	?	-	THR	deletion	UNP P48426
B	?	-	HIS	deletion	UNP P48426
B	?	-	PRO	deletion	UNP P48426
B	?	-	VAL	deletion	UNP P48426
B	?	-	GLY	deletion	UNP P48426
B	?	-	THR	deletion	UNP P48426
B	?	-	PRO	deletion	UNP P48426
B	?	-	PRO	deletion	UNP P48426
B	?	-	ASP	deletion	UNP P48426
B	?	-	SER	deletion	UNP P48426
B	?	-	PRO	deletion	UNP P48426
B	?	-	GLY	deletion	UNP P48426
B	?	-	ASN	deletion	UNP P48426
B	?	-	THR	deletion	UNP P48426
B	?	-	LEU	deletion	UNP P48426

- Molecule 2 is N-[4-(5-{(Z)-[(2E)-2-imino-4-oxo-1,3-thiazolidin-5-ylidene]methyl}pyridin-3-yl)phenyl]methanesulfonamide (three-letter code: UHJ) (formula: C₁₆H₁₄N₄O₃S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	0
			39	16	14	4	3	2		
2	B	1	Total	C	H	N	O	S	0	0
			39	16	14	4	3	2		

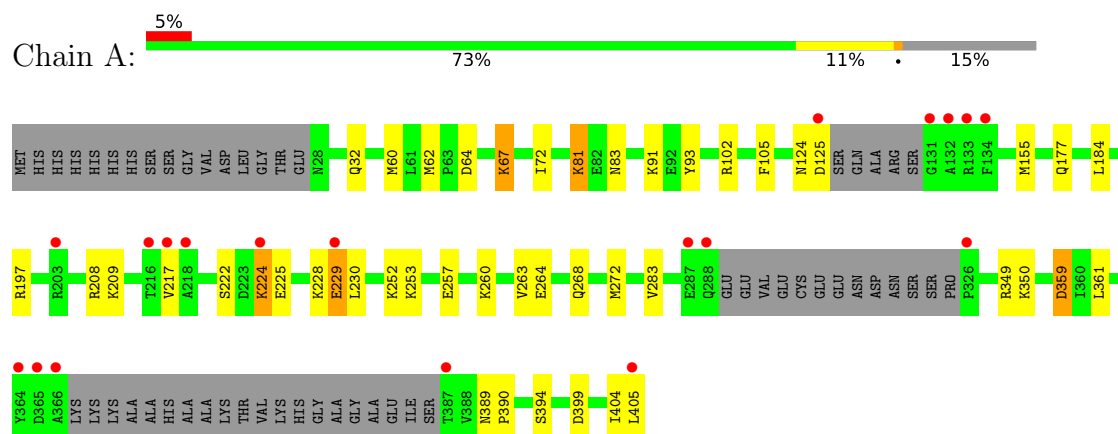
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	209	Total	O	0	0
			209	209		
3	B	149	Total	O	0	0
			149	149		

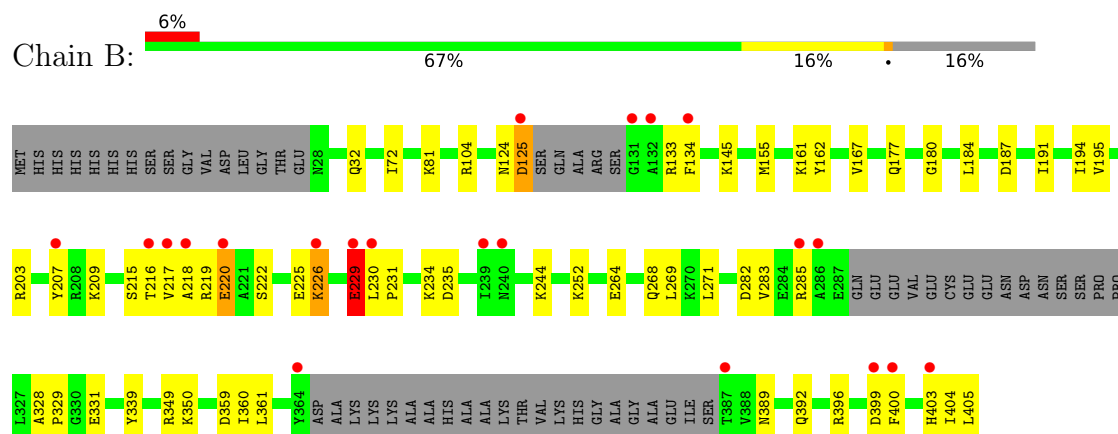
3 Residue-property plots [i](#)

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: Phosphatidylinositol 5-phosphate 4-kinase type-2 alpha



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.23Å 88.58Å 105.78Å 90.00° 92.91° 90.00°	Depositor
Resolution (Å)	45.37 – 1.71 45.37 – 1.71	Depositor EDS
% Data completeness (in resolution range)	97.7 (45.37-1.71) 97.8 (45.37-1.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 1.71Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.177 , 0.204 0.175 , 0.202	Depositor DCC
R_{free} test set	4205 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.742	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5639	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 8.61% 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: UHJ

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	0.80	1/2700 (0.0%)	1.10	5/3641 (0.1%)
1	B	0.73	2/2635 (0.1%)	0.82	4/3553 (0.1%)
All	All	0.76	3/5335 (0.1%)	0.97	9/7194 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	229	GLU	CD-OE2	11.26	1.38	1.25
1	B	162	TYR	CD1-CE1	5.09	1.47	1.39
1	A	105	PHE	CE2-CZ	5.08	1.47	1.37

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	ARG	NE-CZ-NH1	33.99	137.30	120.30
1	A	102	ARG	NE-CZ-NH2	-29.83	105.39	120.30
1	A	102	ARG	CD-NE-CZ	12.67	141.34	123.60
1	B	226	LYS	CD-CE-NZ	-11.92	84.29	111.70
1	A	102	ARG	CG-CD-NE	-8.04	94.92	111.80
1	B	220	GLU	CG-CD-OE2	-5.84	106.63	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	331	GLU	N-CA-CB	-5.61	100.50	110.60
1	A	359	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	B	226	LYS	CG-CD-CE	5.15	127.36	111.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	229	GLU	Peptide
1	B	229	GLU	Peptide

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	2630	0	2596	50	0
1	B	2573	0	2543	64	0
2	A	25	14	0	0	0
2	B	25	14	0	0	0
3	A	209	0	0	5	1
3	B	149	0	0	3	0
All	All	5611	28	5139	111	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 (111) 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:215:SER:OG	1:B:217:VAL:O	1.77	1.03
1:B:229:GLU:O	1:B:229:GLU:HG3	1.64	0.96
1:B:218:ALA:HB1	1:B:220:GLU:OE1	1.66	0.93
1:A:229:GLU:HG3	1:A:229:GLU:O	1.72	0.86
1:B:222:SER:O	1:B:226:LYS:HB2	1.77	0.85
1:B:215:SER:O	1:B:216:THR:HG22	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:GLN:OE1	3:B:4101:HOH:O	1.95	0.83
1:B:209:LYS:CE	1:B:230:LEU:HD12	2.09	0.82
1:B:209:LYS:HE2	1:B:230:LEU:HD12	1.66	0.77
1:B:209:LYS:HE2	1:B:230:LEU:CD1	2.16	0.76
1:B:217:VAL:HG12	1:B:218:ALA:H	1.54	0.73
1:B:399:ASP:O	1:B:403:HIS:CG	2.41	0.73
1:A:60:MET:HG3	1:A:62:MET:HE1	1.71	0.70
1:A:222:SER:OG	1:A:224:LYS:HE2	1.92	0.69
1:B:400:PHE:O	1:B:403:HIS:HB2	1.92	0.69
1:A:155:MET:CE	1:A:361:LEU:HD21	2.23	0.69
1:A:209:LYS:HE2	1:A:230:LEU:HG	1.74	0.69
1:B:216:THR:HG21	1:B:396:ARG:NH1	2.09	0.67
1:A:272:MET:HE1	1:A:390:PRO:N	2.10	0.66
1:A:60:MET:CG	1:A:62:MET:HE1	2.25	0.66
1:A:155:MET:HE2	1:A:361:LEU:HD21	1.77	0.65
1:A:264:GLU:O	1:A:268:GLN:HG3	1.95	0.65
1:A:81:LYS:NZ	3:A:4101:HOH:O	1.93	0.65
1:A:217:VAL:N	3:A:4106:HOH:O	2.30	0.64
1:A:124:ASN:O	1:A:125:ASP:HB2	1.96	0.64
1:B:184:LEU:HD12	1:B:191:ILE:HD11	1.79	0.64
1:A:208:ARG:NE	3:A:4103:HOH:O	2.25	0.62
1:B:209:LYS:CE	1:B:230:LEU:CD1	2.75	0.62
1:B:180:GLY:O	1:B:194:ILE:HD12	2.00	0.61
1:A:272:MET:HE1	1:A:389:ASN:C	2.21	0.61
1:B:389:ASN:H	1:B:392:GLN:HE21	1.48	0.61
1:B:124:ASN:OD1	1:B:125:ASP:N	2.34	0.60
1:A:399:ASP:OD1	3:A:4102:HOH:O	2.16	0.60
1:B:133:ARG:NH2	1:B:133:ARG:HG3	2.17	0.60
1:B:229:GLU:O	1:B:229:GLU:CG	2.41	0.60
1:A:60:MET:SD	1:A:62:MET:HE1	2.41	0.59
1:B:133:ARG:HG3	1:B:133:ARG:HH21	1.66	0.59
1:B:219:ARG:O	1:B:220:GLU:HG3	2.03	0.59
1:A:404:ILE:O	1:A:405:LEU:HB2	2.04	0.57
1:B:389:ASN:OD1	1:B:392:GLN:HG3	2.04	0.57
1:A:263:VAL:CG1	1:A:394:SER:HB2	2.35	0.57
1:B:216:THR:HB	1:B:396:ARG:HD2	1.88	0.54
1:A:253:LYS:O	1:A:257[B]:GLU:HG2	2.07	0.54
1:A:177:GLN:OE1	1:A:197:ARG:NH2	2.40	0.54
1:A:272:MET:CE	1:A:390:PRO:N	2.71	0.53
1:B:145:LYS:NZ	1:B:359:ASP:OD1	2.38	0.53
1:A:60:MET:CG	1:A:62:MET:CE	2.87	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:SER:C	1:B:217:VAL:H	2.11	0.52
1:A:67:LYS:HE2	3:A:4259:HOH:O	2.09	0.52
1:B:209:LYS:NZ	1:B:230:LEU:HD12	2.25	0.51
1:A:72:ILE:CG2	1:B:72:ILE:HD11	2.40	0.51
1:B:264:GLU:O	1:B:268:GLN:HG3	2.12	0.50
1:A:222:SER:HG	1:A:224:LYS:HB2	1.76	0.50
1:B:209:LYS:CD	1:B:230:LEU:CD1	2.89	0.50
1:B:219:ARG:NH2	1:B:234:LYS:HD3	2.26	0.50
1:B:155:MET:CE	1:B:361:LEU:HD11	2.41	0.49
1:B:225:GLU:O	1:B:231:PRO:HB3	2.13	0.48
1:B:134:PHE:CE2	1:B:145:LYS:HG3	2.48	0.48
1:B:328:ALA:HB1	1:B:329:PRO:HD2	1.95	0.48
1:B:161:LYS:HD2	1:B:269:LEU:HD21	1.96	0.48
1:B:349:ARG:HB2	1:B:349:ARG:HH11	1.79	0.48
1:A:252:LYS:HZ3	1:A:405:LEU:HB3	1.79	0.48
1:B:282:ASP:OD1	1:B:285:ARG:HG3	2.14	0.47
1:A:60:MET:HG3	1:A:62:MET:CE	2.41	0.47
1:A:60:MET:SD	1:A:62:MET:CE	3.01	0.47
1:A:252:LYS:NZ	1:A:405:LEU:HD23	2.29	0.47
1:B:399:ASP:O	1:B:403:HIS:HB2	2.14	0.47
1:B:104:ARG:CZ	1:B:167:VAL:HG22	2.44	0.47
1:A:225:GLU:O	1:A:228:LYS:HG3	2.15	0.47
1:A:252:LYS:HZ3	1:A:405:LEU:CB	2.27	0.47
1:B:216:THR:HG21	1:B:396:ARG:HH11	1.77	0.47
1:B:230:LEU:C	1:B:230:LEU:HD13	2.36	0.46
1:A:224:LYS:HE2	1:A:224:LYS:HB2	1.67	0.46
1:A:252:LYS:NZ	1:A:405:LEU:HB3	2.31	0.46
1:B:155:MET:HE2	1:B:361:LEU:HD21	1.98	0.46
1:A:32:GLN:HG3	1:A:83:ASN:HA	1.99	0.45
1:B:219:ARG:HB3	1:B:234:LYS:HD2	1.98	0.45
1:B:399:ASP:O	1:B:403:HIS:CB	2.65	0.45
1:B:81:LYS:HG3	3:B:4118:HOH:O	2.17	0.45
1:B:177:GLN:HG3	1:B:339:TYR:OH	2.16	0.45
1:A:283:VAL:HB	1:A:350:LYS:HB3	1.97	0.45
1:A:155:MET:HE1	1:A:361:LEU:HD21	1.97	0.44
1:A:272:MET:CE	1:A:390:PRO:CA	2.95	0.44
1:B:271:LEU:HD13	1:B:360:ILE:O	2.17	0.44
1:B:404:ILE:O	1:B:405:LEU:HB2	2.18	0.44
1:A:260:LYS:O	1:A:264:GLU:HG3	2.18	0.44
1:B:219:ARG:C	1:B:220:GLU:HG3	2.37	0.44
1:B:216:THR:CG2	1:B:396:ARG:NH1	2.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:VAL:HG21	1:B:350:LYS:HG2	2.00	0.43
1:B:217:VAL:HG12	1:B:218:ALA:N	2.30	0.43
1:A:64:ASP:OD1	1:A:67:LYS:HE3	2.18	0.43
1:A:222:SER:OG	1:A:224:LYS:CE	2.65	0.43
1:B:230:LEU:HD22	1:B:230:LEU:HA	1.91	0.43
1:B:203:ARG:HE	1:B:203:ARG:HB3	1.48	0.43
1:B:400:PHE:C	1:B:403:HIS:HB2	2.38	0.43
1:A:272:MET:CE	1:A:390:PRO:HA	2.47	0.43
1:A:272:MET:HB3	1:A:272:MET:HE3	1.65	0.43
1:A:184:LEU:HD12	1:A:184:LEU:N	2.34	0.42
1:A:272:MET:HE3	1:A:390:PRO:HG3	2.01	0.42
1:B:283:VAL:HB	1:B:350:LYS:HB3	2.00	0.42
1:A:263:VAL:HG12	1:A:394:SER:HB2	2.01	0.42
1:B:399:ASP:O	1:B:403:HIS:ND1	2.53	0.42
1:B:252:LYS:HD2	1:B:405:LEU:HG	2.02	0.42
1:B:194:ILE:HG13	1:B:195:VAL:N	2.34	0.42
1:A:272:MET:HE1	1:A:390:PRO:CD	2.50	0.41
1:B:209:LYS:HD3	1:B:230:LEU:HD11	2.02	0.41
1:B:282:ASP:OD1	3:B:4102:HOH:O	2.22	0.41
1:A:72:ILE:HG21	1:B:72:ILE:HD11	2.02	0.41
1:A:72:ILE:HG23	1:B:72:ILE:HD11	2.03	0.40
1:A:91:LYS:HE2	1:A:93:TYR:CE1	2.56	0.40
1:A:155:MET:HE2	1:A:361:LEU:CD2	2.49	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)
3:A:4221:HOH:O	3:A:4259:HOH:O[2_655]	2.05	0.15

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	312/370 (84%)	305 (98%)	7 (2%)	0	100	100
1	B	305/370 (82%)	296 (97%)	8 (3%)	1 (0%)	41	24
All	All	617/740 (83%)	601 (97%)	15 (2%)	1 (0%)	47	30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	187	ASP

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	294/335 (88%)	289 (98%)	5 (2%)	60	44
1	B	287/335 (86%)	283 (99%)	4 (1%)	67	52
All	All	581/670 (87%)	572 (98%)	9 (2%)	62	49

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

Mol	Chain	Res	Type
1	A	67	LYS
1	A	81	LYS
1	A	224	LYS
1	A	349	ARG
1	A	359	ASP
1	B	125	ASP
1	B	207	TYR
1	B	235	ASP
1	B	244	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	392	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides 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	UHJ	B	4000	-	27,27,27	3.56	12 (44%)	35,39,39	3.33	16 (45%)
2	UHJ	A	4000	-	27,27,27	3.26	8 (29%)	35,39,39	3.79	20 (57%)

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	UHJ	B	4000	-	-	4/13/25/25	0/3/3/3
2	UHJ	A	4000	-	-	2/13/25/25	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4000	UHJ	C21-N20	12.60	1.64	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4000	UHJ	C21-N20	11.80	1.62	1.38
2	A	4000	UHJ	C18-N20	7.49	1.53	1.36
2	B	4000	UHJ	C18-N20	7.26	1.53	1.36
2	B	4000	UHJ	C21-C16	5.41	1.57	1.48
2	A	4000	UHJ	C21-C16	5.14	1.56	1.48
2	B	4000	UHJ	S02-N05	4.79	1.69	1.63
2	A	4000	UHJ	C18-S17	-4.67	1.68	1.74
2	B	4000	UHJ	C18-S17	-3.95	1.69	1.74
2	B	4000	UHJ	C16-S17	-3.38	1.66	1.73
2	A	4000	UHJ	C14-C15	3.06	1.52	1.46
2	B	4000	UHJ	C15-C16	-2.99	1.31	1.34
2	B	4000	UHJ	C14-C15	2.75	1.52	1.46
2	A	4000	UHJ	C16-S17	-2.63	1.68	1.73
2	A	4000	UHJ	C01-S02	2.30	1.80	1.75
2	B	4000	UHJ	C01-S02	2.25	1.80	1.75
2	B	4000	UHJ	O22-C21	-2.21	1.19	1.23
2	A	4000	UHJ	O22-C21	-2.21	1.19	1.23
2	B	4000	UHJ	O03-S02	2.07	1.47	1.43
2	B	4000	UHJ	C12-C09	2.00	1.54	1.49

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4000	UHJ	O04-S02-O03	-14.52	97.97	118.85
2	B	4000	UHJ	O04-S02-O03	-11.13	102.84	118.85
2	A	4000	UHJ	C18-S17-C16	9.40	102.68	89.50
2	B	4000	UHJ	C18-S17-C16	9.35	102.61	89.50
2	A	4000	UHJ	C14-C15-C16	-6.21	122.44	130.94
2	B	4000	UHJ	C14-C15-C16	-5.97	122.77	130.94
2	A	4000	UHJ	O04-S02-N05	4.94	117.17	107.10
2	B	4000	UHJ	C16-C21-N20	-4.42	106.54	110.22
2	B	4000	UHJ	O04-S02-N05	4.24	115.75	107.10
2	A	4000	UHJ	C07-C06-N05	-3.71	112.06	120.09
2	A	4000	UHJ	C10-C11-C06	-3.63	116.10	120.30
2	A	4000	UHJ	C16-C21-N20	-3.50	107.31	110.22
2	B	4000	UHJ	C08-C09-C12	-3.40	115.46	121.36
2	B	4000	UHJ	C13-C14-C23	3.39	120.82	117.10
2	B	4000	UHJ	C14-C13-C12	-3.31	117.21	121.08
2	A	4000	UHJ	C08-C09-C12	-3.08	116.02	121.36
2	A	4000	UHJ	C25-N24-C23	3.06	121.65	117.48
2	A	4000	UHJ	C11-C06-C07	2.99	123.12	119.03
2	A	4000	UHJ	C01-S02-N05	2.97	110.02	106.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4000	UHJ	C25-N24-C23	2.83	121.35	117.48
2	A	4000	UHJ	O04-S02-C01	2.83	112.81	108.28
2	B	4000	UHJ	C07-C06-N05	-2.71	114.22	120.09
2	B	4000	UHJ	C15-C16-C21	-2.66	118.36	120.47
2	B	4000	UHJ	O03-S02-N05	2.62	112.45	107.10
2	A	4000	UHJ	C13-C14-C23	2.46	119.80	117.10
2	A	4000	UHJ	C10-C09-C08	2.45	122.48	117.59
2	A	4000	UHJ	C07-C08-C09	-2.39	117.69	121.13
2	B	4000	UHJ	C11-C06-N05	2.38	125.24	120.09
2	A	4000	UHJ	O22-C21-C16	2.25	128.84	126.01
2	B	4000	UHJ	C13-C12-C25	2.21	119.30	117.11
2	B	4000	UHJ	C10-C11-C06	-2.19	117.77	120.30
2	A	4000	UHJ	C11-C06-N05	2.18	124.81	120.09
2	B	4000	UHJ	O04-S02-C01	2.18	111.78	108.28
2	A	4000	UHJ	C25-C12-C09	-2.17	117.91	121.69
2	A	4000	UHJ	C14-C23-N24	-2.15	119.67	123.91
2	A	4000	UHJ	O03-S02-N05	2.12	111.42	107.10

There are no chirality outliers.

All (6) torsion outliers are listed below:

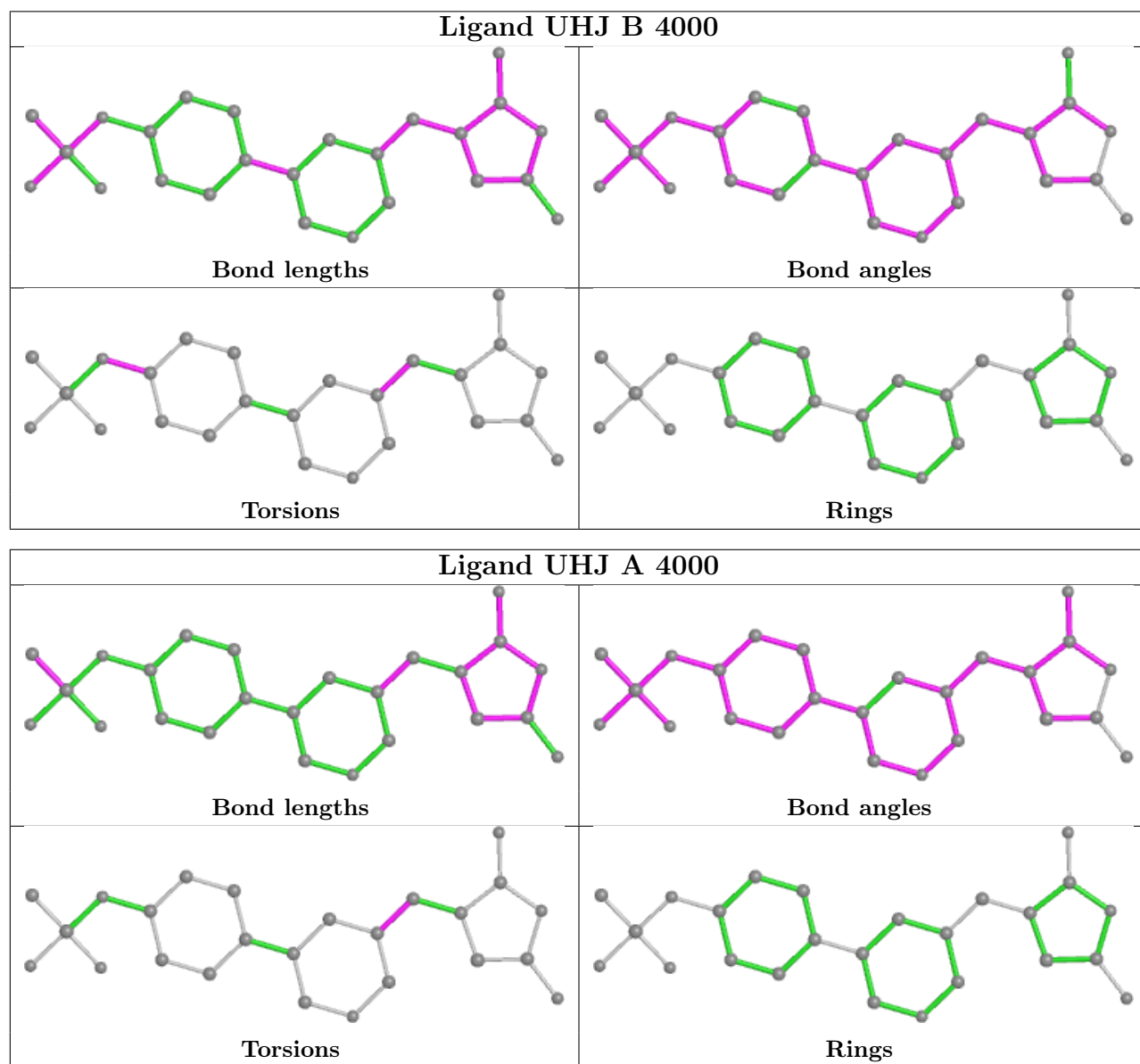
Mol	Chain	Res	Type	Atoms
2	A	4000	UHJ	C23-C14-C15-C16
2	A	4000	UHJ	C13-C14-C15-C16
2	B	4000	UHJ	C23-C14-C15-C16
2	B	4000	UHJ	C13-C14-C15-C16
2	B	4000	UHJ	C07-C06-N05-S02
2	B	4000	UHJ	C11-C06-N05-S02

There are no ring outliers.

No monomer is involved in short contacts.

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	316/370 (85%)	0.26	19 (6%) 21 24	28, 42, 89, 139	0
1	B	312/370 (84%)	0.30	21 (6%) 17 20	31, 51, 99, 124	0
All	All	628/740 (84%)	0.28	40 (6%) 19 21	28, 46, 96, 139	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	366	ALA	10.8
1	A	216	THR	7.8
1	A	132	ALA	7.6
1	B	216	THR	6.3
1	A	364	TYR	5.9
1	A	218	ALA	5.5
1	B	132	ALA	5.5
1	A	387	THR	4.8
1	B	403	HIS	4.6
1	A	217	VAL	4.5
1	B	286	ALA	4.5
1	B	229	GLU	4.4
1	B	239	ILE	4.1
1	B	217	VAL	3.9
1	A	405	LEU	3.9
1	A	288	GLN	3.8
1	B	134	PHE	3.7
1	B	218	ALA	3.6
1	A	326	PRO	3.4
1	A	365	ASP	3.4
1	A	131	GLY	3.3
1	B	387	THR	3.2
1	A	125	ASP	2.9
1	B	285	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	134	PHE	2.8
1	A	287	GLU	2.7
1	A	224	LYS	2.7
1	B	230	LEU	2.6
1	B	207	TYR	2.5
1	B	226	LYS	2.5
1	B	364	TYR	2.4
1	B	400	PHE	2.4
1	A	229	GLU	2.4
1	B	220	GLU	2.3
1	A	133	ARG	2.2
1	B	131	GLY	2.2
1	B	240	ASN	2.1
1	B	125	ASP	2.1
1	B	399	ASP	2.1
1	A	203	ARG	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 monosaccharides in this entry.

6.4 Ligands [i](#)

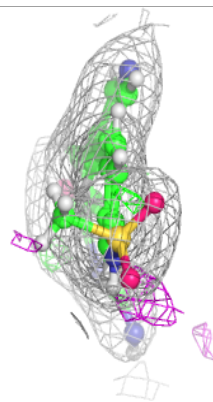
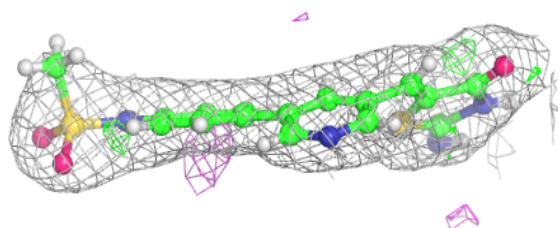
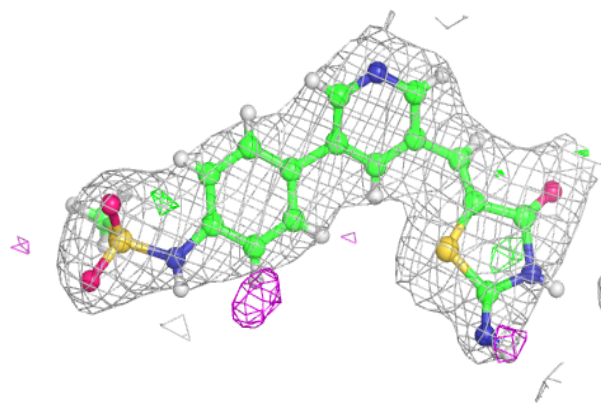
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	UHJ	B	4000	25/25	0.96	0.08	37,50,62,74	0
2	UHJ	A	4000	25/25	0.98	0.09	34,45,55,58	0

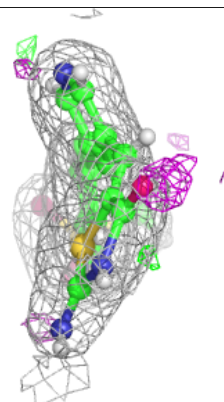
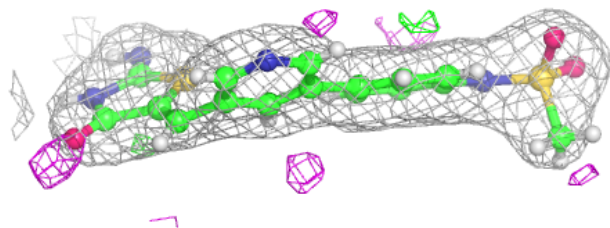
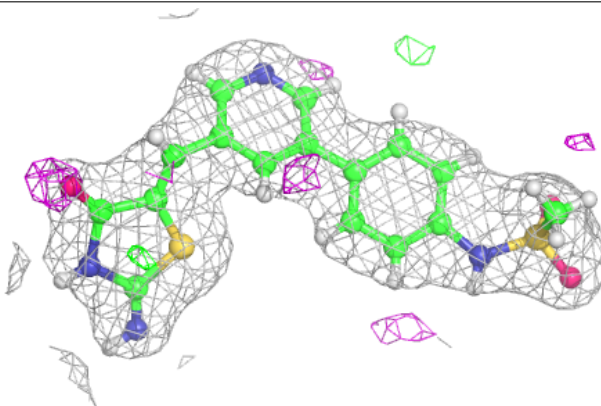
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UHJ B 4000:

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

**Electron density around UHJ A 4000:**

$2mF_o-DF_c$ (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.