



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:39 PM UTC

PDB ID : 5UKF / pdb_00005ukf
Title : Crystal Structure of the Human Vaccinia-related Kinase 1 Bound to an Oxindole Inhibitor
Authors : Counago, R.M.; Wells, C.; Zuercher, W.; Willson, T.M.; Bountra, C.; Edwards, A.M.; Arruda, P.; Gileadi, O.; Structural Genomics Consortium (SGC)
Deposited on : 2017-01-22
Resolution : 2.40 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

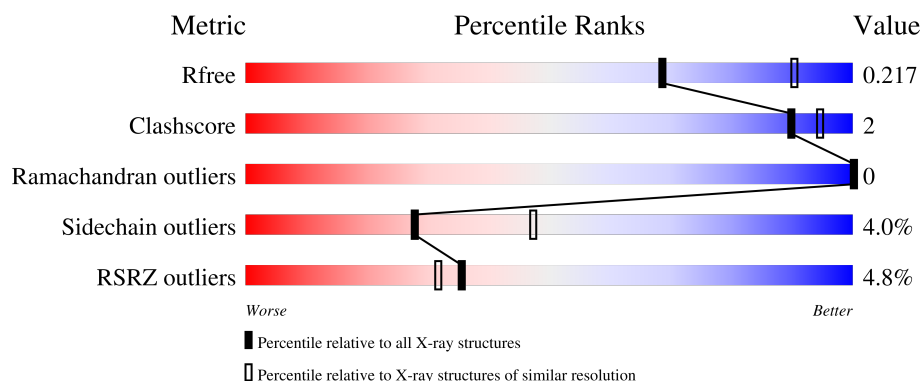
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	363	5% 83% 5% 11%
1	B	363	4% 66% 7% 27%
1	C	363	2% 81% 7% 13%
1	D	363	5% 68% 6% 26%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9854 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 Serine/threonine-protein kinase VRK1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2473	1586	420	455	12			
1	B	265	Total	C	N	O	S	0	0	0
			2073	1331	352	381	9			
1	C	317	Total	C	N	O	S	0	0	0
			2478	1589	418	459	12			
1	D	268	Total	C	N	O	S	0	0	0
			2130	1369	365	387	9			

There are 48 discrepancies between the modelled and reference sequences:

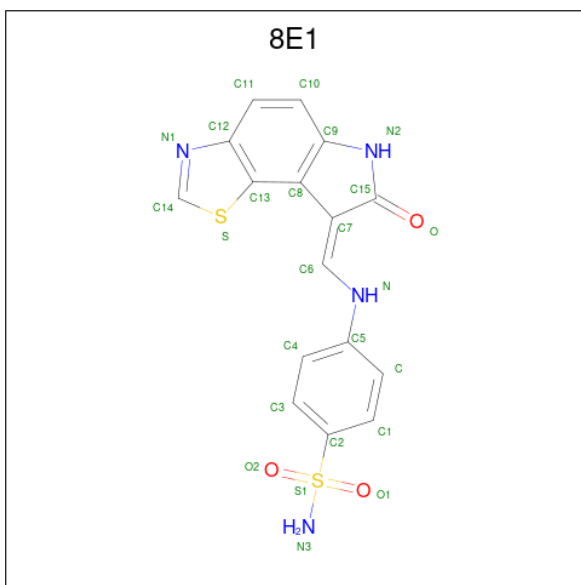
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MET	-	initiating methionine	UNP Q99986
A	34	ALA	LYS	engineered mutation	UNP Q99986
A	35	ALA	LYS	engineered mutation	UNP Q99986
A	36	ALA	GLU	engineered mutation	UNP Q99986
A	212	ALA	GLU	engineered mutation	UNP Q99986
A	214	ALA	LYS	engineered mutation	UNP Q99986
A	215	ALA	GLU	engineered mutation	UNP Q99986
A	292	ALA	GLU	engineered mutation	UNP Q99986
A	293	ALA	LYS	engineered mutation	UNP Q99986
A	295	ALA	LYS	engineered mutation	UNP Q99986
A	359	ALA	LYS	engineered mutation	UNP Q99986
A	360	ALA	LYS	engineered mutation	UNP Q99986
B	2	MET	-	initiating methionine	UNP Q99986
B	34	ALA	LYS	engineered mutation	UNP Q99986
B	35	ALA	LYS	engineered mutation	UNP Q99986
B	36	ALA	GLU	engineered mutation	UNP Q99986
B	212	ALA	GLU	engineered mutation	UNP Q99986
B	214	ALA	LYS	engineered mutation	UNP Q99986
B	215	ALA	GLU	engineered mutation	UNP Q99986
B	292	ALA	GLU	engineered mutation	UNP Q99986
B	293	ALA	LYS	engineered mutation	UNP Q99986

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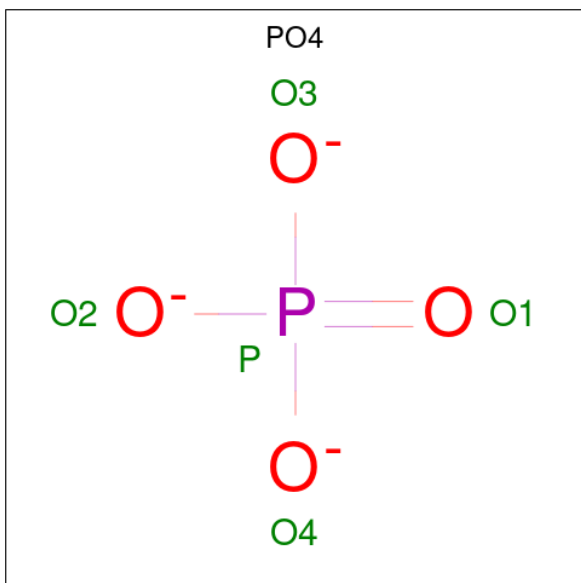
Chain	Residue	Modelled	Actual	Comment	Reference
B	295	ALA	LYS	engineered mutation	UNP Q99986
B	359	ALA	LYS	engineered mutation	UNP Q99986
B	360	ALA	LYS	engineered mutation	UNP Q99986
C	2	MET	-	initiating methionine	UNP Q99986
C	34	ALA	LYS	engineered mutation	UNP Q99986
C	35	ALA	LYS	engineered mutation	UNP Q99986
C	36	ALA	GLU	engineered mutation	UNP Q99986
C	212	ALA	GLU	engineered mutation	UNP Q99986
C	214	ALA	LYS	engineered mutation	UNP Q99986
C	215	ALA	GLU	engineered mutation	UNP Q99986
C	292	ALA	GLU	engineered mutation	UNP Q99986
C	293	ALA	LYS	engineered mutation	UNP Q99986
C	295	ALA	LYS	engineered mutation	UNP Q99986
C	359	ALA	LYS	engineered mutation	UNP Q99986
C	360	ALA	LYS	engineered mutation	UNP Q99986
D	2	MET	-	initiating methionine	UNP Q99986
D	34	ALA	LYS	engineered mutation	UNP Q99986
D	35	ALA	LYS	engineered mutation	UNP Q99986
D	36	ALA	GLU	engineered mutation	UNP Q99986
D	212	ALA	GLU	engineered mutation	UNP Q99986
D	214	ALA	LYS	engineered mutation	UNP Q99986
D	215	ALA	GLU	engineered mutation	UNP Q99986
D	292	ALA	GLU	engineered mutation	UNP Q99986
D	293	ALA	LYS	engineered mutation	UNP Q99986
D	295	ALA	LYS	engineered mutation	UNP Q99986
D	359	ALA	LYS	engineered mutation	UNP Q99986
D	360	ALA	LYS	engineered mutation	UNP Q99986

- Molecule 2 is 4-{{[(Z)-(7-oxo-6,7-dihydro-8H-[1,3]thiazolo[5,4-e]indol-8-ylidene)methyl]amino}benzene-1-sulfonamide (CCD ID: 8E1) (formula: C₁₆H₁₂N₄O₃S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			25	16	4	3	2		
2	B	1	Total	C	N	O	S	0	0
			25	16	4	3	2		
2	C	1	Total	C	N	O	S	0	0
			25	16	4	3	2		
2	D	1	Total	C	N	O	S	0	0
			25	16	4	3	2		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

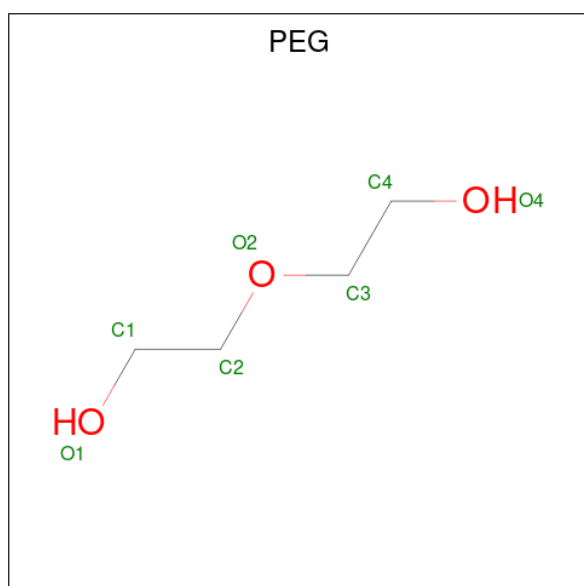


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	B	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0
4	D	4	Total Cl 4 4	0	0

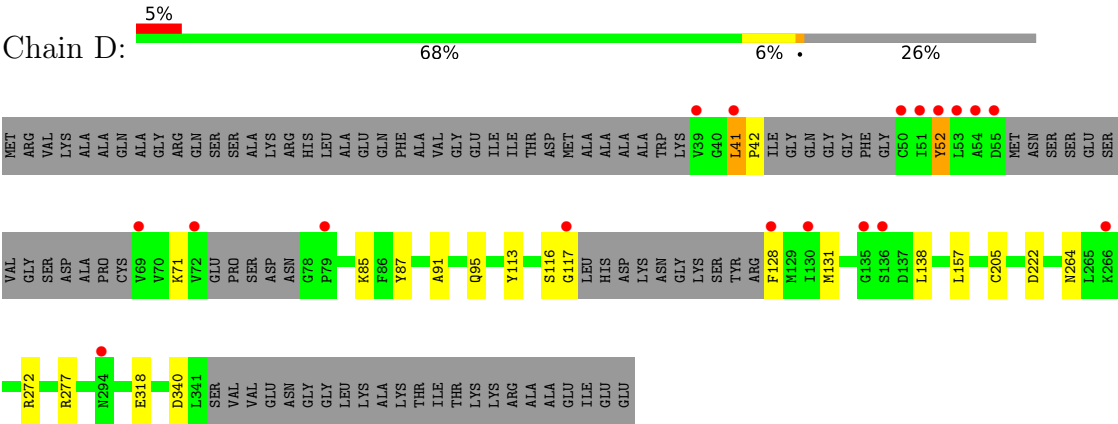
- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	132	Total	O	0	0
			132	132		
6	B	122	Total	O	0	0
			122	122		
6	C	141	Total	O	0	0
			141	141		
6	D	156	Total	O	0	0
			156	156		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.14Å 96.05Å 192.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.19 – 2.40 24.19 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.19-2.40) 99.9 (24.19-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.39Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.177 , 0.214 0.187 , 0.217	Depositor DCC
R_{free} test set	3417 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.576	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 69.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9854	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, 8E1, CL, PO4

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	0.82	0/2534	1.19	4/3444 (0.1%)
1	B	0.75	0/2120	1.09	3/2875 (0.1%)
1	C	0.76	0/2538	1.10	0/3446
1	D	0.82	0/2179	1.26	7/2946 (0.2%)
All	All	0.79	0/9371	1.17	14/12711 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	225	ILE	N-CA-C	6.77	117.52	110.62
1	B	91	ALA	N-CA-C	5.85	120.01	112.41
1	D	264	ASN	N-CA-C	5.48	119.50	112.26
1	A	292	ALA	N-CA-C	5.45	119.09	111.74
1	D	272	ARG	CA-C-N	5.44	127.57	120.28
1	D	272	ARG	C-N-CA	5.44	127.57	120.28
1	D	95	GLN	CA-C-N	5.26	127.19	120.56
1	D	95	GLN	C-N-CA	5.26	127.19	120.56
1	A	265	LEU	N-CA-C	5.25	117.75	111.71
1	B	172	GLU	N-CA-C	5.20	118.92	112.58
1	A	316	LEU	CA-C-N	5.19	127.18	120.44
1	A	316	LEU	C-N-CA	5.19	127.18	120.44
1	D	157	LEU	CA-C-N	5.04	127.03	120.28
1	D	157	LEU	C-N-CA	5.04	127.03	120.28

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	2473	0	2352	7	0
1	B	2073	0	1972	12	0
1	C	2478	0	2383	9	0
1	D	2130	0	2059	5	0
2	A	25	0	0	0	0
2	B	25	0	0	0	0
2	C	25	0	0	0	0
2	D	25	0	0	0	0
3	A	5	0	0	0	0
3	B	20	0	0	0	0
3	C	10	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	4	0	0	0	0
5	D	7	0	10	0	0
6	A	132	0	0	0	0
6	B	122	0	0	0	0
6	C	141	0	0	0	0
6	D	156	0	0	0	0
All	All	9854	0	8776	33	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 2.

All (33) 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:248:GLY:HA2	1:B:251:MET:HE2	1.79	0.63
1:B:109:GLY:HA3	1:B:164:ILE:HD11	1.84	0.60
1:B:84:LEU:HB2	1:B:129:MET:HE2	1.86	0.57
1:C:185:LEU:HD11	1:C:341:LEU:HD12	1.89	0.55
1:C:169:HIS:CG	1:C:240:ARG:HG2	2.47	0.50
1:C:204:TYR:CE2	1:C:205:CYS:HB2	2.47	0.49
1:B:138:LEU:CD2	1:B:157:LEU:HD21	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:ILE:HG21	1:B:247:LEU:HD13	1.95	0.48
1:B:204:TYR:CE2	1:B:205:CYS:HB2	2.49	0.48
1:D:41:LEU:H	1:D:41:LEU:HD12	1.79	0.47
1:B:155:LEU:HD21	1:B:298:GLU:HG3	1.97	0.47
1:A:138:LEU:HD23	1:A:138:LEU:HA	1.67	0.46
1:C:174:VAL:HG13	1:C:204:TYR:CD1	2.50	0.46
1:B:138:LEU:HD21	1:B:157:LEU:HD21	1.96	0.46
1:A:117:GLY:O	1:A:127:ARG:HD3	2.16	0.45
1:A:131:MET:HE3	1:A:131:MET:HB3	1.69	0.45
1:B:109:GLY:HA3	1:B:164:ILE:CD1	2.46	0.45
1:C:85:LYS:HA	1:C:85:LYS:HD2	1.54	0.45
1:D:117:GLY:HA3	1:D:128:PHE:CE2	2.51	0.45
1:C:185:LEU:HD11	1:C:341:LEU:CD1	2.47	0.45
1:D:87:TYR:HA	1:D:91:ALA:HB3	1.99	0.44
1:A:85:LYS:HA	1:A:85:LYS:HD2	1.65	0.44
1:B:227:PHE:O	1:B:246:ILE:HG12	2.18	0.44
1:B:128:PHE:C	1:B:128:PHE:CD1	2.96	0.44
1:D:87:TYR:CE2	1:D:131:MET:HE1	2.53	0.43
1:A:77:ASN:ND2	1:A:79:PRO:HD2	2.33	0.43
1:C:189:ASN:HA	1:C:190:PRO:HD2	1.93	0.43
1:B:169:HIS:CG	1:B:240:ARG:HG2	2.53	0.43
1:C:52:TYR:HB2	1:C:70:VAL:HG13	2.01	0.42
1:A:78:GLY:N	1:A:79:PRO:CD	2.83	0.42
1:C:155:LEU:HD21	1:C:298:GLU:HG3	2.02	0.42
1:A:205:CYS:O	1:A:205:CYS:SG	2.78	0.41
1:D:42:PRO:HA	1:D:52:TYR:HA	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	320/363 (88%)	315 (98%)	5 (2%)	0	100	100
1	B	257/363 (71%)	253 (98%)	4 (2%)	0	100	100
1	C	313/363 (86%)	307 (98%)	6 (2%)	0	100	100
1	D	258/363 (71%)	253 (98%)	5 (2%)	0	100	100
All	All	1148/1452 (79%)	1128 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	244/303 (80%)	235 (96%)	9 (4%)	30	51
1	B	206/303 (68%)	200 (97%)	6 (3%)	37	60
1	C	253/303 (84%)	243 (96%)	10 (4%)	28	47
1	D	215/303 (71%)	203 (94%)	12 (6%)	19	33
All	All	918/1212 (76%)	881 (96%)	37 (4%)	28	47

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	SER
1	A	76	ASP
1	A	80	LEU
1	A	125	SER
1	A	138	LEU
1	A	140	LYS
1	A	184	LEU
1	A	185	LEU
1	A	274	SER
1	B	118	LEU
1	B	132	ASP
1	B	145	ASN
1	B	157	LEU

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Mol	Chain	Res	Type
1	B	218	LYS
1	B	225	ILE
1	C	38	LYS
1	C	51	ILE
1	C	72	VAL
1	C	80	LEU
1	C	84	LEU
1	C	112	LYS
1	C	133	ARG
1	C	138	LEU
1	C	228	THR
1	C	236	VAL
1	D	41	LEU
1	D	52	TYR
1	D	71	LYS
1	D	85	LYS
1	D	113	TYR
1	D	116	SER
1	D	138	LEU
1	D	205	CYS
1	D	222	ASP
1	D	277	ARG
1	D	318	GLU
1	D	340	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	281	ASN
1	B	145	ASN
1	B	326	GLN
1	D	281	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 7 are monoatomic - leaving 12 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
3	PO4	B	404	-	4,4,4	2.57	3 (75%)	6,6,6	0.60	0
3	PO4	B	402	-	4,4,4	2.62	3 (75%)	6,6,6	0.48	0
3	PO4	B	403	-	4,4,4	2.57	2 (50%)	6,6,6	0.52	0
2	8E1	A	401	-	28,28,28	0.77	2 (7%)	37,42,42	1.04	3 (8%)
5	PEG	D	401	-	6,6,6	0.33	0	5,5,5	0.51	0
3	PO4	A	402	-	4,4,4	2.57	2 (50%)	6,6,6	0.61	0
3	PO4	C	402	-	4,4,4	2.51	1 (25%)	6,6,6	0.63	0
2	8E1	B	401	-	28,28,28	0.70	1 (3%)	37,42,42	0.59	1 (2%)
2	8E1	D	402	-	28,28,28	0.73	1 (3%)	37,42,42	0.77	2 (5%)
3	PO4	B	405	-	4,4,4	1.23	0	6,6,6	0.48	0
3	PO4	C	403	-	4,4,4	2.57	2 (50%)	6,6,6	0.52	0
2	8E1	C	401	-	28,28,28	0.74	1 (3%)	37,42,42	0.94	2 (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
2	8E1	A	401	-	-	3/11/23/23	0/4/4/4
5	PEG	D	401	-	-	0/4/4/4	-
2	8E1	B	401	-	-	6/11/23/23	0/4/4/4
2	8E1	D	402	-	-	3/11/23/23	0/4/4/4
2	8E1	C	401	-	-	5/11/23/23	0/4/4/4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	PO4	P-O1	4.30	1.60	1.50
3	B	403	PO4	P-O1	4.26	1.60	1.50
3	A	402	PO4	P-O1	4.26	1.60	1.50
3	C	403	PO4	P-O1	4.25	1.60	1.50
3	B	404	PO4	P-O1	4.24	1.60	1.50
3	C	402	PO4	P-O1	4.17	1.60	1.50
2	C	401	8E1	C11-C10	2.52	1.42	1.38
2	B	401	8E1	C11-C10	2.51	1.42	1.38
2	A	401	8E1	C11-C10	2.44	1.42	1.38
2	D	402	8E1	C11-C10	2.42	1.42	1.38
2	A	401	8E1	C7-C15	-2.09	1.47	1.50
3	B	402	PO4	P-O2	2.07	1.60	1.54
3	A	402	PO4	P-O2	2.05	1.60	1.54
3	C	403	PO4	P-O3	2.05	1.60	1.54
3	B	404	PO4	P-O3	2.04	1.60	1.54
3	B	402	PO4	P-O4	2.01	1.60	1.54
3	B	403	PO4	P-O4	2.01	1.60	1.54
3	B	404	PO4	P-O4	2.00	1.60	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	8E1	C7-C6-N	-4.78	115.27	123.90
2	C	401	8E1	C7-C6-N	-4.33	116.08	123.90
2	D	402	8E1	C7-C6-N	-2.38	119.60	123.90
2	D	402	8E1	C11-C12-N1	-2.28	125.42	129.62
2	A	401	8E1	C6-C7-C15	-2.22	121.52	124.74
2	B	401	8E1	C11-C12-N1	-2.11	125.73	129.62
2	A	401	8E1	C11-C12-N1	-2.11	125.73	129.62
2	C	401	8E1	C11-C12-N1	-2.05	125.85	129.62

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	402	8E1	N-C6-C7-C8
2	D	402	8E1	N-C6-C7-C15
2	C	401	8E1	C7-C6-N-C5
2	C	401	8E1	C1-C2-S1-N3
2	C	401	8E1	C3-C2-S1-N3
2	B	401	8E1	C1-C2-S1-N3

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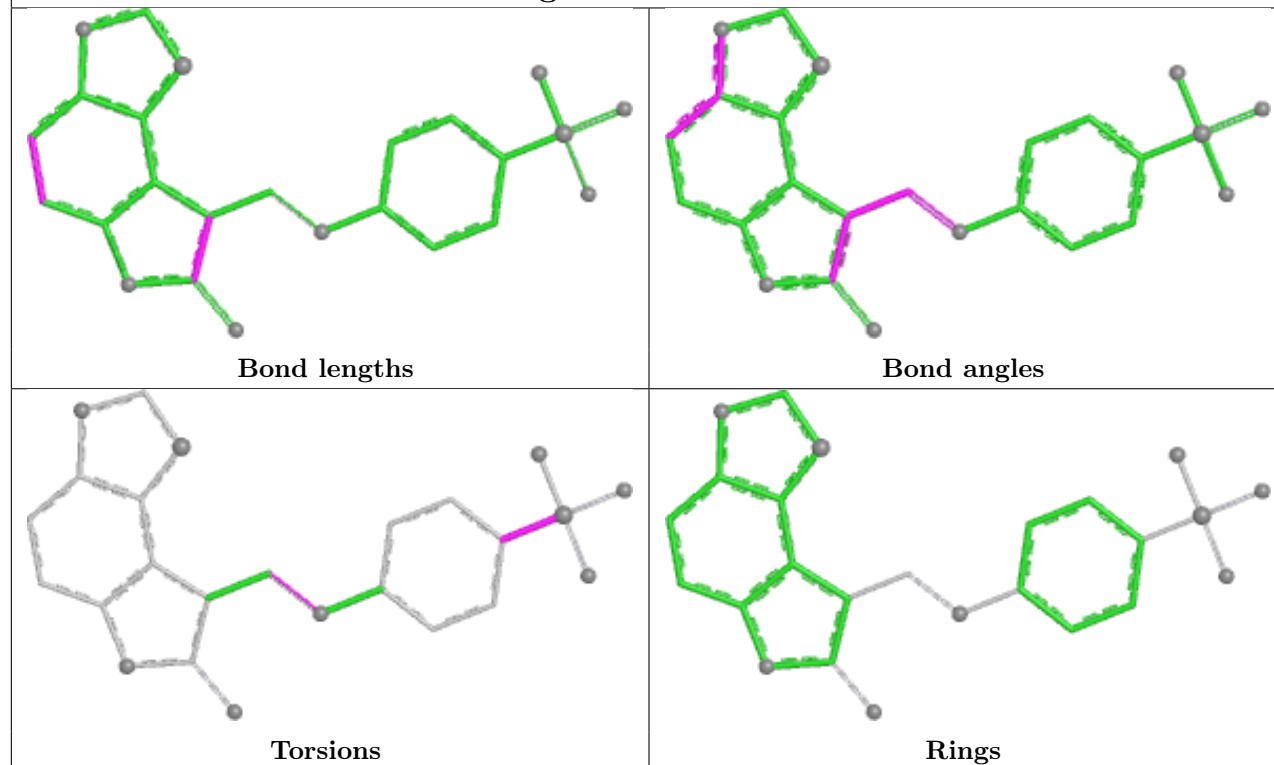
Mol	Chain	Res	Type	Atoms
2	B	401	8E1	C3-C2-S1-N3
2	C	401	8E1	C1-C2-S1-O1
2	D	402	8E1	C7-C6-N-C5
2	C	401	8E1	C3-C2-S1-O1
2	A	401	8E1	C7-C6-N-C5
2	B	401	8E1	C7-C6-N-C5
2	B	401	8E1	C3-C2-S1-O2
2	B	401	8E1	C1-C2-S1-O2
2	A	401	8E1	C1-C2-S1-O1
2	A	401	8E1	C3-C2-S1-O1
2	B	401	8E1	C1-C2-S1-O1

There are no ring outliers.

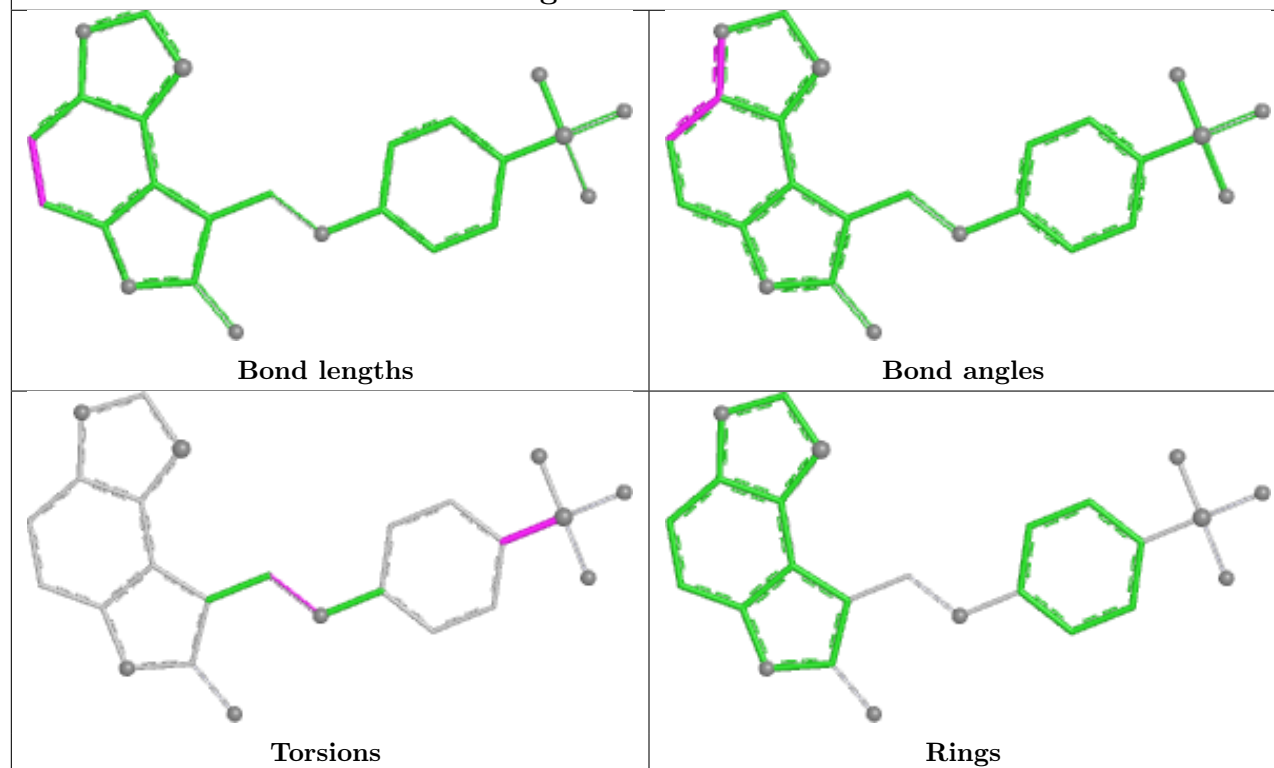
No monomer is involved in short contacts.

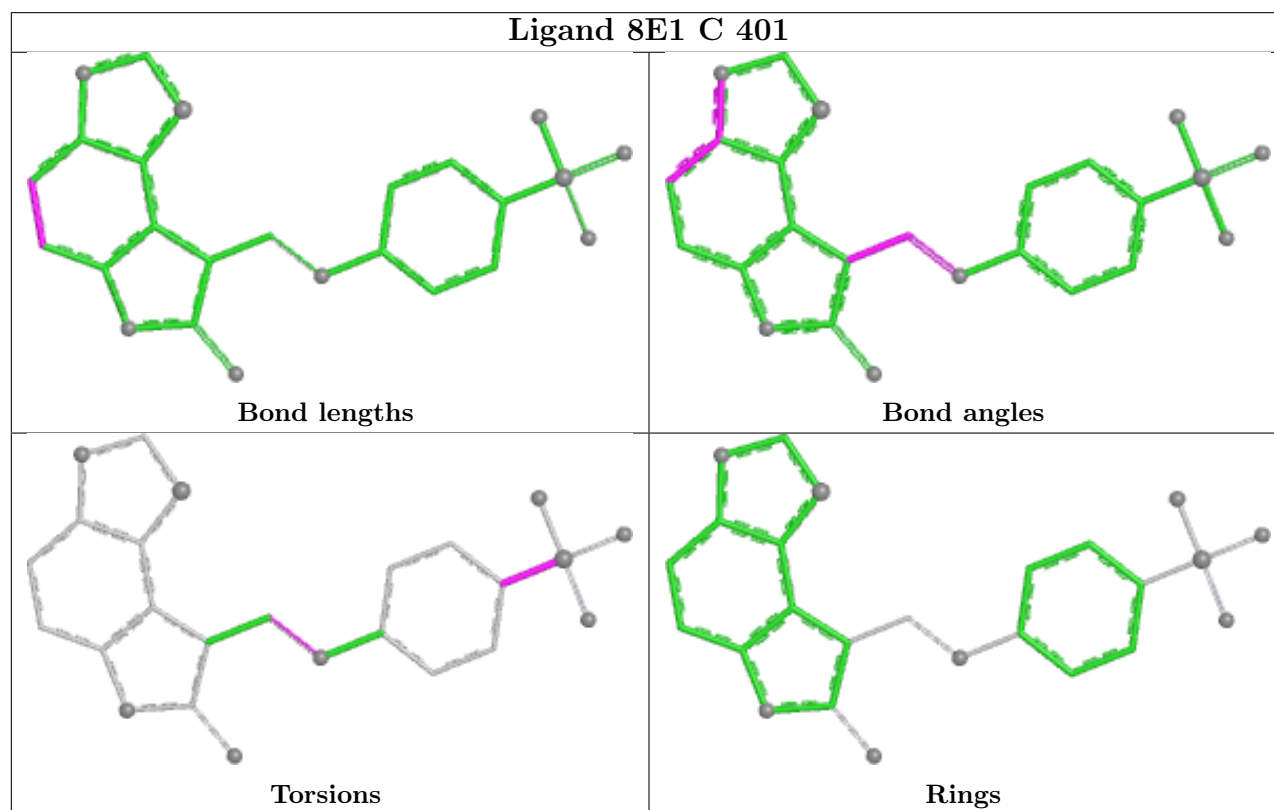
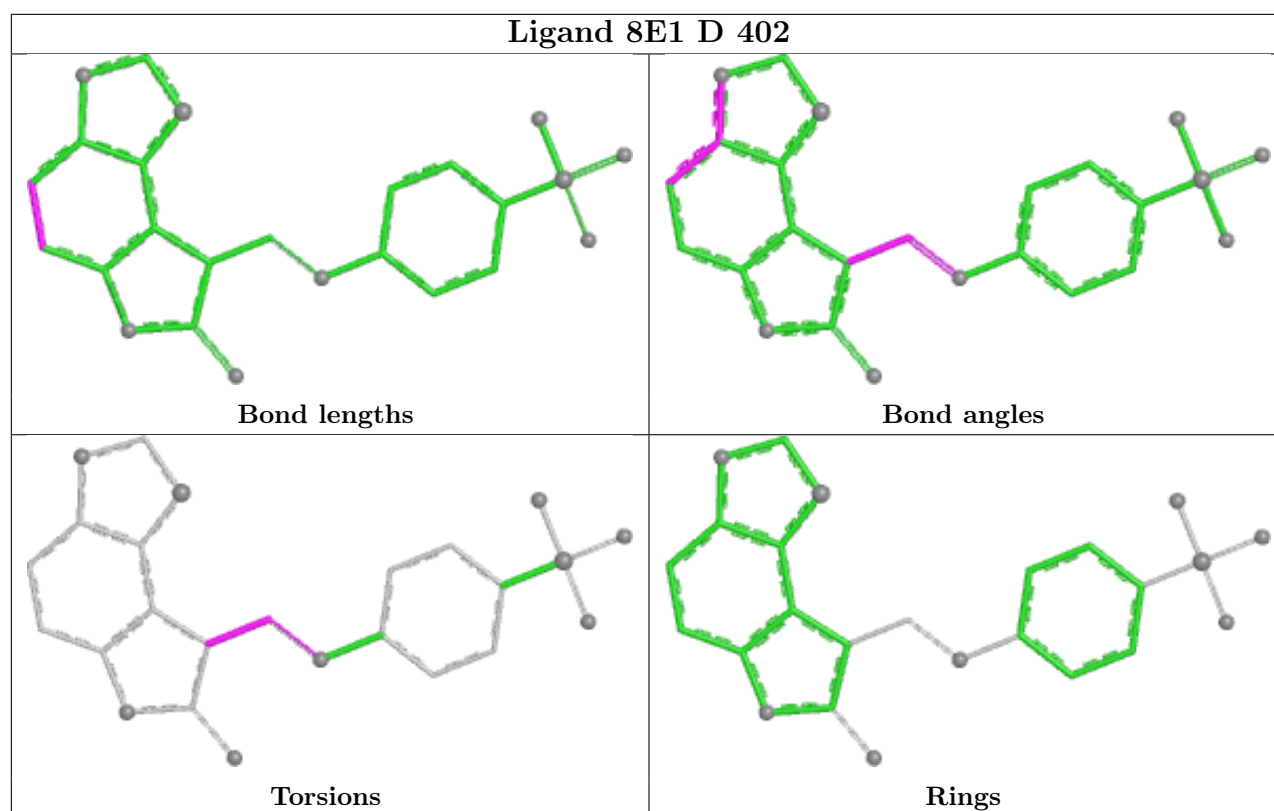
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand 8E1 A 401



Ligand 8E1 B 401





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	322/363 (88%)	0.02	17 (5%) 32 28	37, 57, 90, 119	0
1	B	265/363 (73%)	0.04	13 (4%) 35 31	36, 58, 109, 153	0
1	C	317/363 (87%)	0.02	8 (2%) 58 54	35, 58, 100, 119	0
1	D	268/363 (73%)	-0.04	18 (6%) 24 20	33, 50, 84, 138	0
All	All	1172/1452 (80%)	0.01	56 (4%) 35 32	33, 56, 99, 153	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	20	ALA	5.8
1	B	131	MET	4.8
1	D	39	VAL	4.7
1	D	41	LEU	4.5
1	D	72	VAL	4.3
1	D	117	GLY	4.2
1	A	292	ALA	4.1
1	A	341	LEU	4.1
1	C	43	ILE	3.9
1	D	69	VAL	3.9
1	D	55	ASP	3.7
1	A	25	VAL	3.5
1	B	69	VAL	3.4
1	B	54	ALA	3.4
1	B	114	TRP	3.3
1	A	21	GLU	3.3
1	A	294	ASN	3.2
1	B	73	GLU	3.2
1	D	54	ALA	3.1
1	D	51	ILE	3.1
1	A	291	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	53	LEU	3.0
1	B	135	GLY	2.8
1	A	220	CYS	2.7
1	C	64	SER	2.7
1	A	218	LYS	2.7
1	C	65	ASP	2.7
1	B	118	LEU	2.6
1	D	135	GLY	2.5
1	A	77	ASN	2.5
1	B	200	LEU	2.4
1	C	48	PHE	2.4
1	D	79	PRO	2.4
1	B	340	ASP	2.4
1	B	127	ARG	2.4
1	D	50	CYS	2.4
1	C	76	ASP	2.3
1	A	74	PRO	2.3
1	B	132	ASP	2.3
1	D	52	TYR	2.3
1	A	43	ILE	2.2
1	D	128	PHE	2.2
1	A	293	ALA	2.2
1	A	80	LEU	2.2
1	C	220	CYS	2.2
1	A	215	ALA	2.1
1	C	123	GLY	2.1
1	D	266	LYS	2.1
1	A	64	SER	2.1
1	D	136	SER	2.1
1	D	294	ASN	2.0
1	B	130	ILE	2.0
1	C	218	LYS	2.0
1	D	130	ILE	2.0
1	A	222	ASP	2.0
1	B	187	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

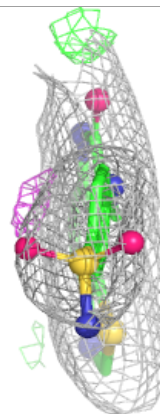
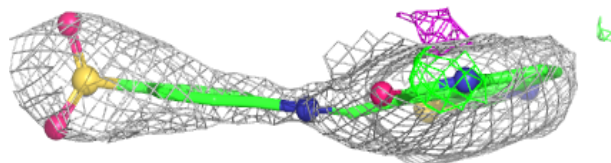
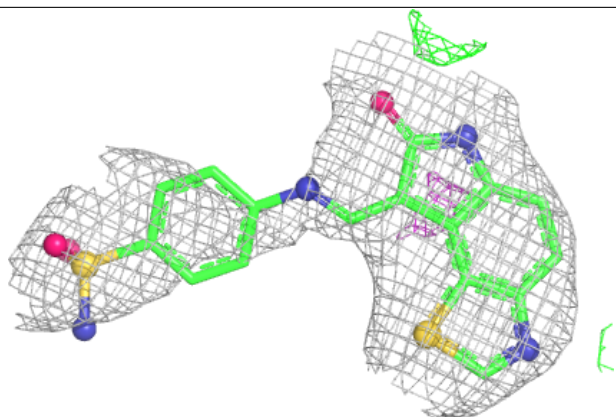
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	PO4	C	403	5/5	0.70	0.17	133,135,135,136	0
3	PO4	B	404	5/5	0.81	0.09	103,104,106,106	0
2	8E1	B	401	25/25	0.82	0.14	87,93,126,127	0
3	PO4	B	405	5/5	0.82	0.09	103,104,107,107	0
2	8E1	C	401	25/25	0.82	0.14	85,90,122,123	0
5	PEG	D	401	7/7	0.82	0.16	61,71,73,74	0
3	PO4	B	402	5/5	0.83	0.10	98,98,100,100	0
2	8E1	D	402	25/25	0.86	0.14	58,69,114,115	0
3	PO4	B	403	5/5	0.87	0.12	134,135,135,136	0
4	CL	C	404	1/1	0.88	0.20	102,102,102,102	0
3	PO4	A	402	5/5	0.88	0.12	92,96,97,99	0
4	CL	D	403	1/1	0.90	0.27	81,81,81,81	0
3	PO4	C	402	5/5	0.93	0.09	69,70,72,78	0
2	8E1	A	401	25/25	0.93	0.09	50,54,93,95	0
4	CL	A	403	1/1	0.93	0.14	89,89,89,89	0
4	CL	B	406	1/1	0.94	0.23	86,86,86,86	0
4	CL	D	406	1/1	0.95	0.23	82,82,82,82	0
4	CL	D	405	1/1	0.95	0.21	86,86,86,86	0
4	CL	D	404	1/1	0.98	0.24	72,72,72,72	0

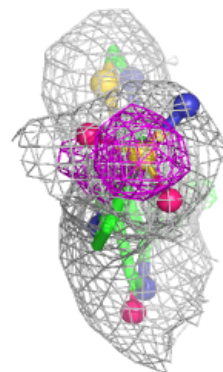
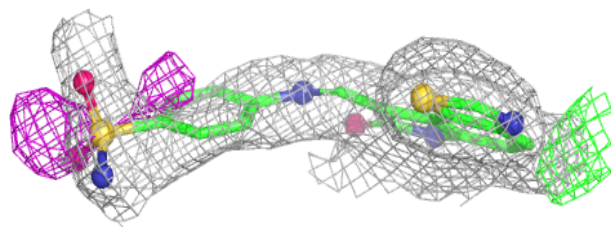
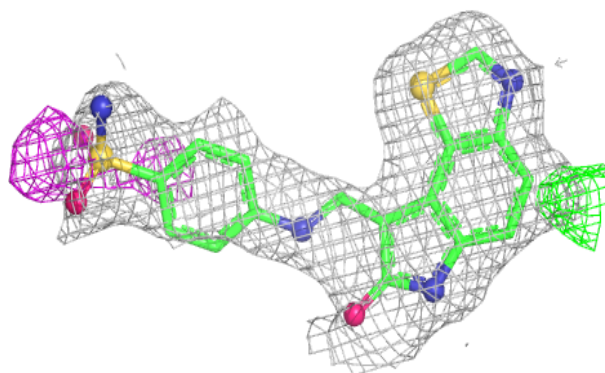
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8E1 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)

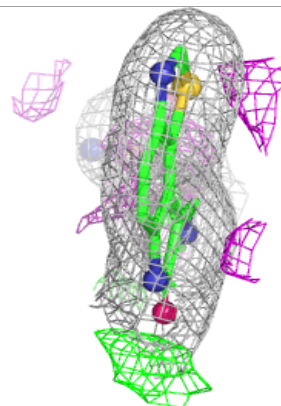
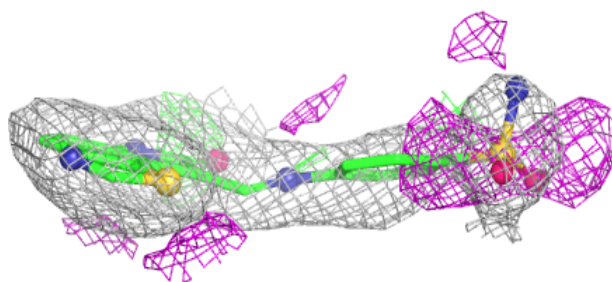
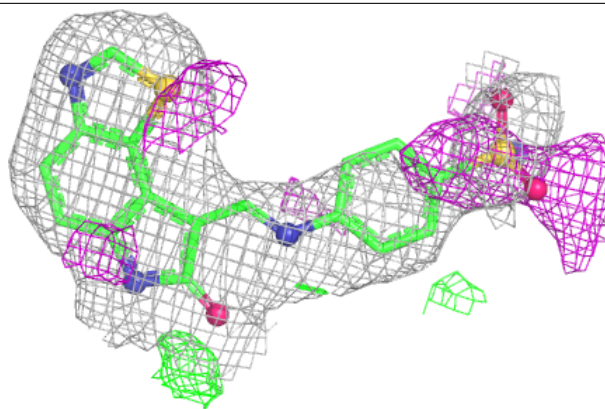
**Electron density around 8E1 C 401:**

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

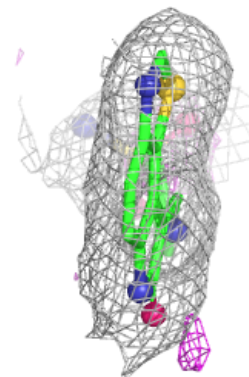
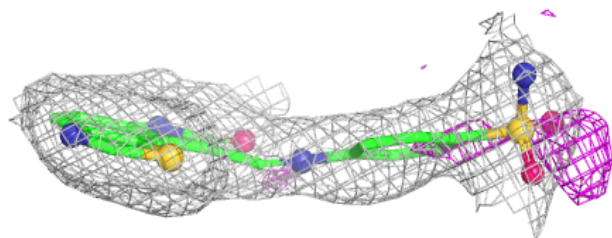
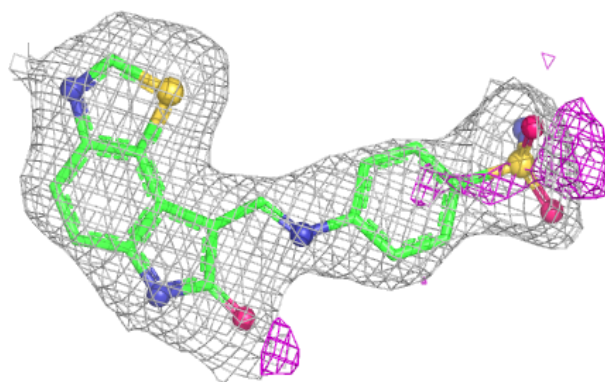


Electron density around 8E1 D 402:

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

**Electron density around 8E1 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.