wwPDB X-ray Structure Validation Summary Report (i)

Feb 3, 2025 – 04:08 PM EST

PDB ID	:	8SCW
Title	:	Crystal structure of IRAK4-HSA complexed with BMS-986147; 6-{5-CYANO-1H-PYRAZOLO[3,4-B]PYRIDIN-1-YL}-N-[(2R)-2-FLUORROXY-3-METHYLBUTYL]-4-[(PROPAN-2-YL)AMINO]PYRIDINE-3-CARBOXAMIDE
Authors	:	Muckelbauer, J.K.; Ghosh, K.
Deposited on	:	2023-04-05
Resolution	:	2.76 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

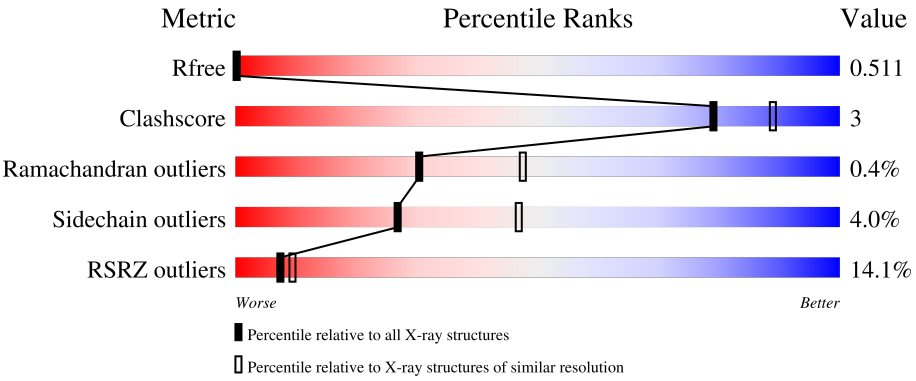
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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}	164625	1606 (2.78-2.74)
Clashscore	180529	1689 (2.78-2.74)
Ramachandran outliers	177936	1665 (2.78-2.74)
Sidechain outliers	177891	1665 (2.78-2.74)
RSRZ outliers	164620	1606 (2.78-2.74)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	305	15% 84% 10% 6%
1	B	305	9% 84% 9% • 6%
1	C	305	11% 84% 9% 7%
1	D	305	17% 84% 9% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8884 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.

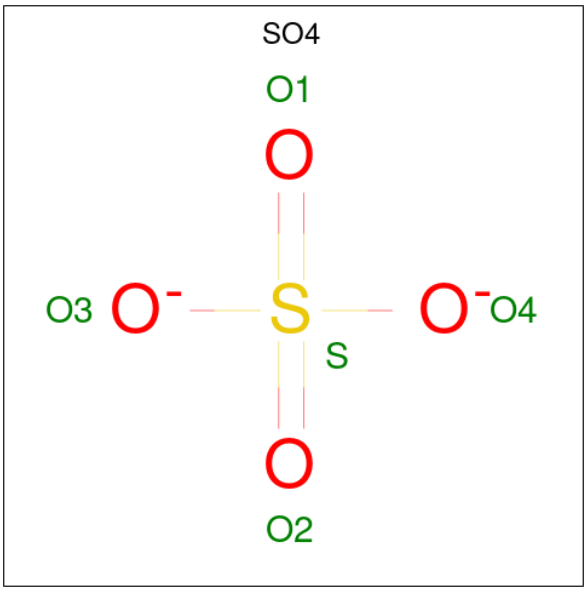
- Molecule 1 is a protein called Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	P	S	0	0	0
			2173	1360	367	429	3	14			
1	B	286	Total	C	N	O	P	S	0	0	0
			2166	1359	367	424	2	14			
1	C	284	Total	C	N	O	P	S	0	0	0
			2157	1352	367	422	2	14			
1	D	284	Total	C	N	O	P	S	0	0	0
			2165	1356	366	426	3	14			

There are 16 discrepancies between the modelled and reference sequences:

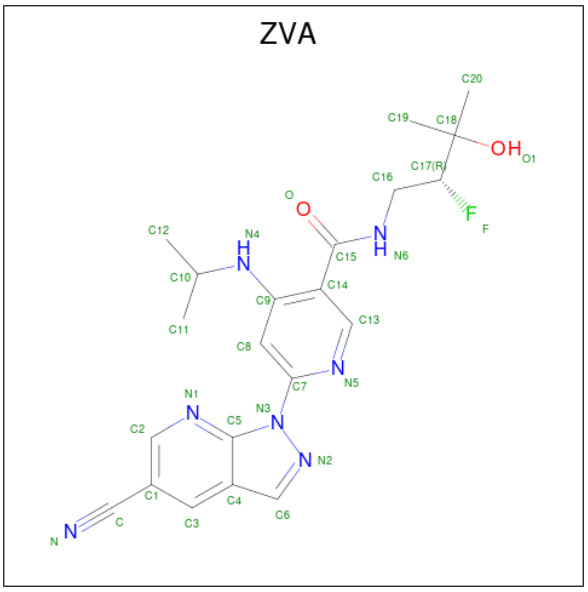
Chain	Residue	Modelled	Actual	Comment	Reference
A	156	GLY	-	expression tag	UNP Q9NWZ3
A	157	ALA	-	expression tag	UNP Q9NWZ3
A	158	MET	-	expression tag	UNP Q9NWZ3
A	159	GLY	-	expression tag	UNP Q9NWZ3
B	156	GLY	-	expression tag	UNP Q9NWZ3
B	157	ALA	-	expression tag	UNP Q9NWZ3
B	158	MET	-	expression tag	UNP Q9NWZ3
B	159	GLY	-	expression tag	UNP Q9NWZ3
C	156	GLY	-	expression tag	UNP Q9NWZ3
C	157	ALA	-	expression tag	UNP Q9NWZ3
C	158	MET	-	expression tag	UNP Q9NWZ3
C	159	GLY	-	expression tag	UNP Q9NWZ3
D	156	GLY	-	expression tag	UNP Q9NWZ3
D	157	ALA	-	expression tag	UNP Q9NWZ3
D	158	MET	-	expression tag	UNP Q9NWZ3
D	159	GLY	-	expression tag	UNP Q9NWZ3

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is (6M)-6-(5-cyano-1H-pyrazolo[3,4-b]pyridin-1-yl)-N-[(2R)-2-fluoro-3-hydroxy-3-methylbutyl]-4-[(propan-2-yl)amino]pyridine-3-carboxamide (three-letter code: ZVA) (formula: $C_{21}H_{24}FN_7O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			31	21	1	7	2		
3	B	1	Total	C	F	N	O	0	0
			31	21	1	7	2		
3	C	1	Total	C	F	N	O	0	0
			31	21	1	7	2		
3	D	1	Total	C	F	N	O	0	0
			31	21	1	7	2		

- Molecule 4 is water.

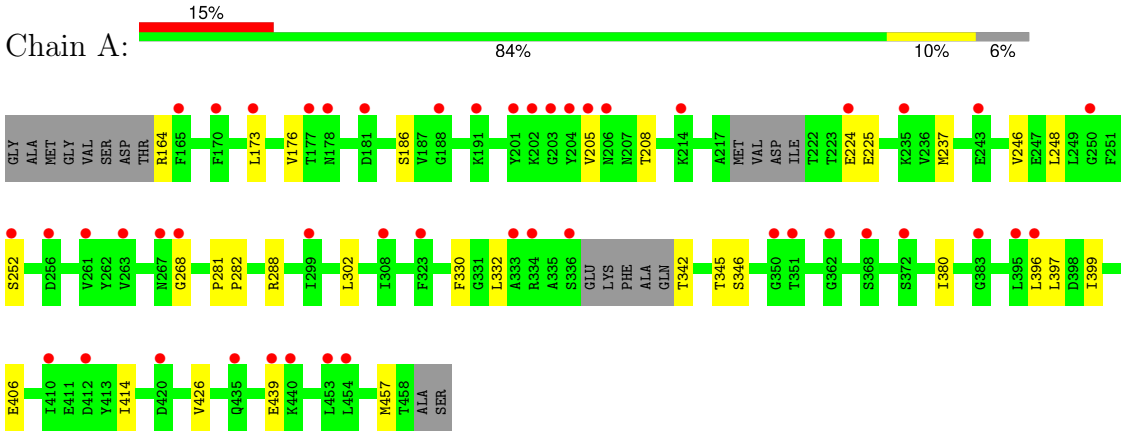
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total	O	0	0
			14	14		
4	B	20	Total	O	0	0
			20	20		
4	C	10	Total	O	0	0
			10	10		
4	D	15	Total	O	0	0
			15	15		

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. 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. 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.

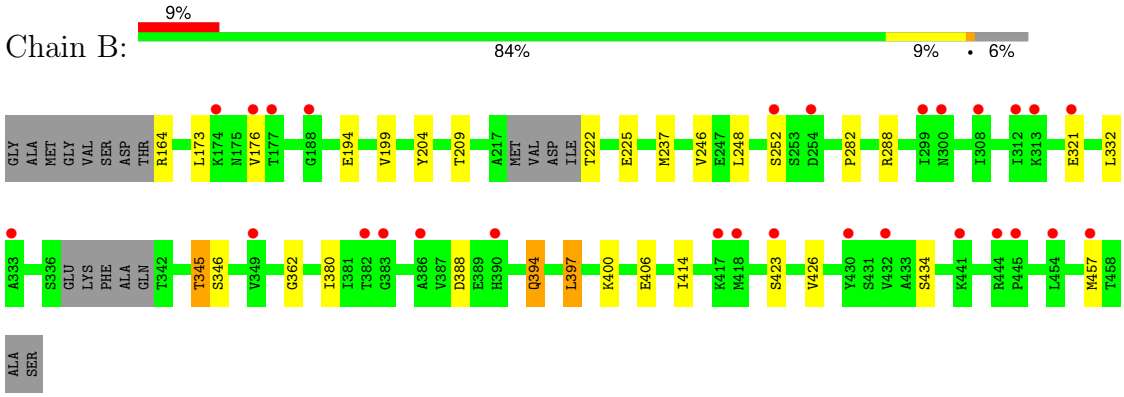
• Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain A:



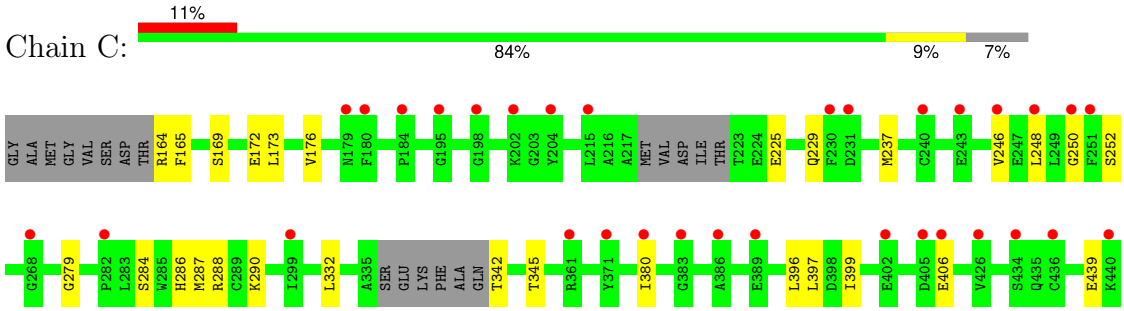
• Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain B:



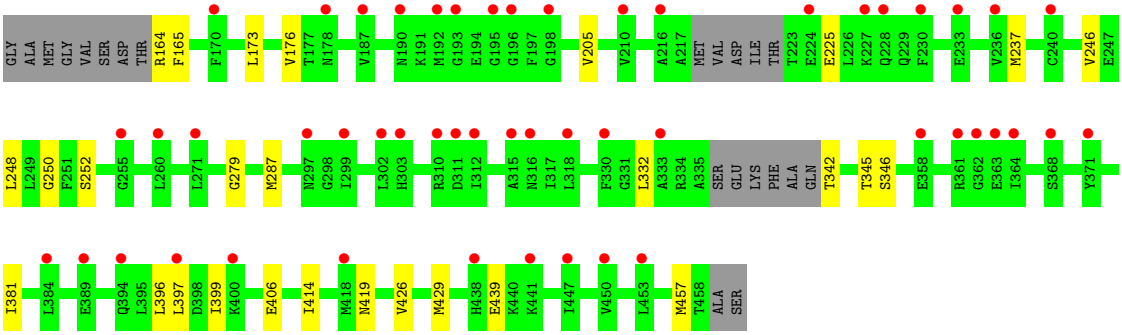
• Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain C:



• Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	135.29Å 140.39Å 85.92Å 90.00° 126.60° 90.00°	Depositor
Resolution (Å)	36.68 – 2.76 36.68 – 2.76	Depositor EDS
% Data completeness (in resolution range)	98.9 (36.68-2.76) 86.5 (36.68-2.76)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.93 (at 2.77Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.195 , 0.238 0.504 , 0.511	Depositor DCC
R_{free} test set	1594 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	44.7	Xtriage
Anisotropy	0.850	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.49 , 544.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.048 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.69	EDS
Total number of atoms	8884	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.5414e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ZVA, SEP, TPO, SO4

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	0.52	0/2176	0.71	0/2948
1	B	0.56	0/2174	0.71	0/2944
1	C	0.54	0/2164	0.69	0/2929
1	D	0.52	0/2168	0.69	0/2935
All	All	0.54	0/8682	0.70	0/11756

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	2173	0	2061	13	0
1	B	2166	0	2065	14	0
1	C	2157	0	2060	11	0
1	D	2165	0	2063	10	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
2	C	15	0	0	0	0
2	D	10	0	0	0	0
3	A	31	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	31	0	0	0	0
3	C	31	0	0	0	0
3	D	31	0	0	0	0
4	A	14	0	0	1	0
4	B	20	0	0	0	0
4	C	10	0	0	0	0
4	D	15	0	0	0	0
All	All	8884	0	8249	44	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 3.

The worst 5 of 44 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:C:284:SER:H	1:C:287:MET:HE3	1.56	0.71
1:B:388:ASP:O	1:B:394:GLN:HG3	1.97	0.64
1:C:165:PHE:HB3	1:C:250:GLY:HA2	1.83	0.60
1:C:237:MET:HG2	1:C:248:LEU:HB2	1.84	0.59
1:A:237:MET:HG2	1:A:248:LEU:HB2	1.85	0.59

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	278/305 (91%)	268 (96%)	9 (3%)	1 (0%)	30	47
1	B	278/305 (91%)	270 (97%)	7 (2%)	1 (0%)	30	47
1	C	276/305 (90%)	266 (96%)	9 (3%)	1 (0%)	30	47
1	D	276/305 (90%)	265 (96%)	10 (4%)	1 (0%)	30	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1108/1220 (91%)	1069 (96%)	35 (3%)	4 (0%)	30 47

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	406	GLU
1	B	406	GLU
1	C	406	GLU
1	D	406	GLU

5.3.2 Protein sidechains (i)

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	224/260 (86%)	215 (96%)	9 (4%)	27 47
1	B	224/260 (86%)	214 (96%)	10 (4%)	23 42
1	C	224/260 (86%)	216 (96%)	8 (4%)	30 51
1	D	224/260 (86%)	215 (96%)	9 (4%)	27 47
All	All	896/1040 (86%)	860 (96%)	36 (4%)	27 47

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	225	GLU
1	D	457	MET
1	D	246	VAL
1	D	332	LEU
1	B	246	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	SEP	C	346	1	3,4,10	0.69	0	2,4,14	1.63	0
1	TPO	D	345	1	8,10,11	1.08	0	10,14,16	1.13	1 (10%)
1	TPO	C	342	1	8,10,11	1.44	1 (12%)	10,14,16	1.36	1 (10%)
1	SEP	D	346	1	8,9,10	0.86	0	7,12,14	2.08	2 (28%)
1	TPO	B	342	1	3,4,11	0.75	0	2,4,16	0.99	0
1	SEP	A	346	1	8,9,10	0.86	0	7,12,14	1.79	1 (14%)
1	TPO	A	345	1	8,10,11	1.13	1 (12%)	10,14,16	1.20	1 (10%)
1	TPO	A	342	1	8,10,11	0.89	0	10,14,16	1.51	1 (10%)
1	TPO	C	345	1	8,10,11	1.08	0	10,14,16	1.05	1 (10%)
1	TPO	D	342	1	8,10,11	1.13	0	10,14,16	1.31	1 (10%)
1	TPO	B	345	1	8,10,11	1.12	0	10,14,16	1.10	1 (10%)
1	SEP	B	346	1	8,9,10	0.70	0	7,12,14	1.93	2 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	C	346	1	-	1/1/2/10	-
1	TPO	D	345	1	-	2/9/11/13	-
1	TPO	C	342	1	-	1/9/11/13	-
1	SEP	D	346	1	-	0/6/8/10	-
1	TPO	B	342	1	-	1/1/2/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	346	1	-	1/6/8/10	-
1	TPO	A	345	1	-	4/9/11/13	-
1	TPO	A	342	1	-	1/9/11/13	-
1	TPO	C	345	1	-	2/9/11/13	-
1	TPO	D	342	1	-	1/9/11/13	-
1	TPO	B	345	1	-	3/9/11/13	-
1	SEP	B	346	1	-	0/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	342	TPO	P-OG1	-2.79	1.54	1.59
1	A	345	TPO	CB-CA	2.07	1.58	1.53

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	346	SEP	OG-CB-CA	4.51	112.54	108.14
1	A	346	SEP	OG-CB-CA	3.93	111.97	108.14
1	B	346	SEP	OG-CB-CA	3.79	111.83	108.14
1	A	342	TPO	P-OG1-CB	-2.81	115.69	123.33
1	C	342	TPO	P-OG1-CB	-2.78	115.78	123.33

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-OG1
1	A	345	TPO	O-C-CA-CB
1	B	342	TPO	O-C-CA-CB
1	B	345	TPO	N-CA-CB-OG1
1	B	345	TPO	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	345	TPO	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	ZVA	B	503	-	30,33,33	1.64	6 (20%)	35,48,48	1.56	6 (17%)
3	ZVA	D	503	-	30,33,33	1.42	5 (16%)	35,48,48	1.44	7 (20%)
2	SO4	A	501	-	4,4,4	0.74	0	6,6,6	0.22	0
2	SO4	C	503	-	4,4,4	0.40	0	6,6,6	0.44	0
2	SO4	D	502	-	4,4,4	0.68	0	6,6,6	0.17	0
2	SO4	B	501	-	4,4,4	0.28	0	6,6,6	0.16	0
2	SO4	C	501	-	4,4,4	0.44	0	6,6,6	0.30	0
3	ZVA	A	502	-	30,33,33	1.52	6 (20%)	35,48,48	1.26	5 (14%)
2	SO4	B	502	-	4,4,4	0.46	0	6,6,6	0.15	0
2	SO4	C	502	-	4,4,4	0.28	0	6,6,6	0.16	0
3	ZVA	C	504	-	30,33,33	1.59	5 (16%)	35,48,48	1.44	6 (17%)
2	SO4	D	501	-	4,4,4	0.34	0	6,6,6	0.07	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	ZVA	B	503	-	-	2/18/25/25	0/3/3/3
3	ZVA	C	504	-	-	2/18/25/25	0/3/3/3
3	ZVA	A	502	-	-	2/18/25/25	0/3/3/3
3	ZVA	D	503	-	-	2/18/25/25	0/3/3/3

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	ZVA	C8-C9	4.33	1.46	1.39
3	C	504	ZVA	C2-C1	4.31	1.45	1.39
3	C	504	ZVA	C8-C9	3.89	1.45	1.39
3	A	502	ZVA	C8-C9	3.86	1.45	1.39
3	D	503	ZVA	C15-N6	3.39	1.41	1.33

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	503	ZVA	C3-C1-C2	4.24	121.84	118.13
3	D	503	ZVA	C3-C1-C2	3.94	121.58	118.13
3	C	504	ZVA	C3-C1-C2	3.81	121.46	118.13
3	B	503	ZVA	C9-N4-C10	3.57	129.75	124.66
3	B	503	ZVA	C14-C9-N4	-3.57	117.93	121.08

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

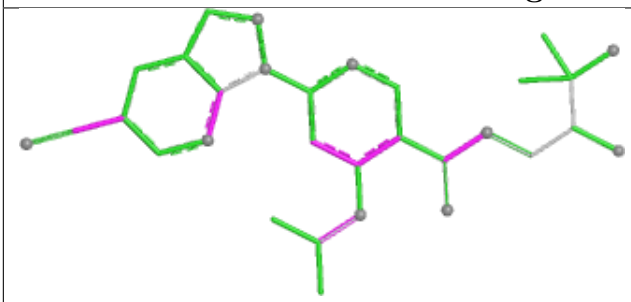
Mol	Chain	Res	Type	Atoms
3	A	502	ZVA	C13-C14-C15-O
3	C	504	ZVA	C13-C14-C15-O
3	D	503	ZVA	C13-C14-C15-O
3	A	502	ZVA	C13-C14-C15-N6
3	C	504	ZVA	C13-C14-C15-N6

There are no ring outliers.

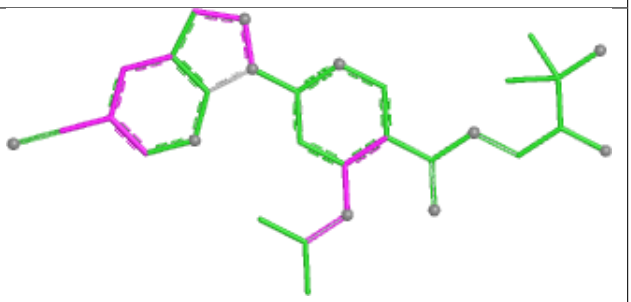
No monomer is involved in short contacts.

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 then 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.

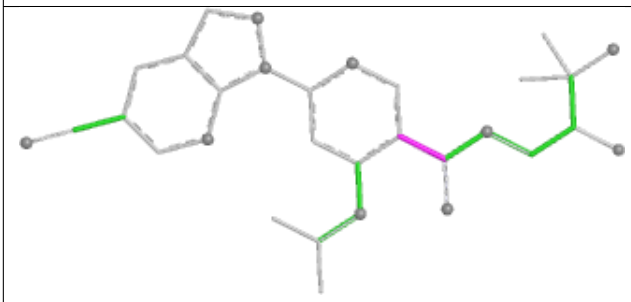
Ligand ZVA B 503



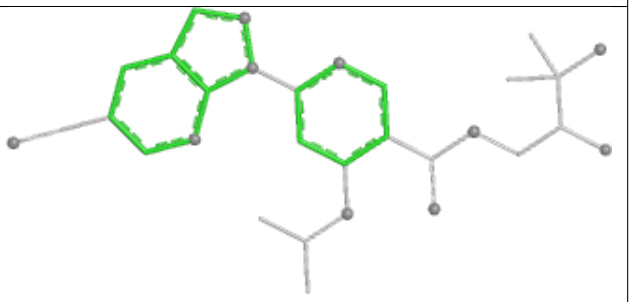
Bond lengths



Bond angles

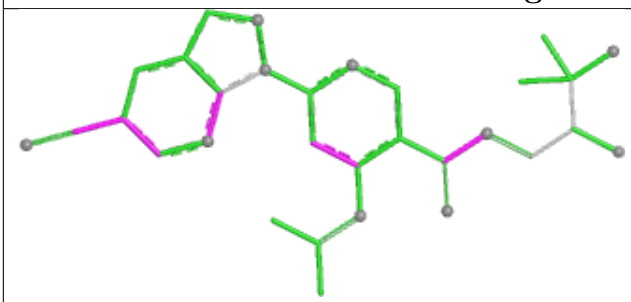


Torsions

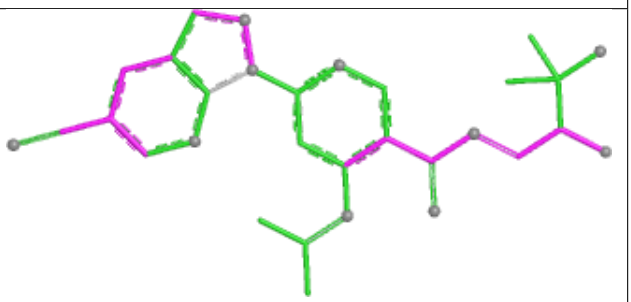


Rings

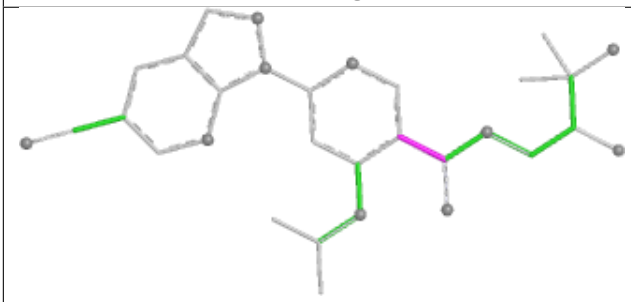
Ligand ZVA D 503



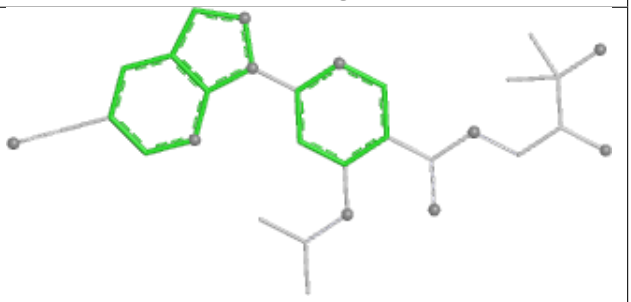
Bond lengths



Bond angles

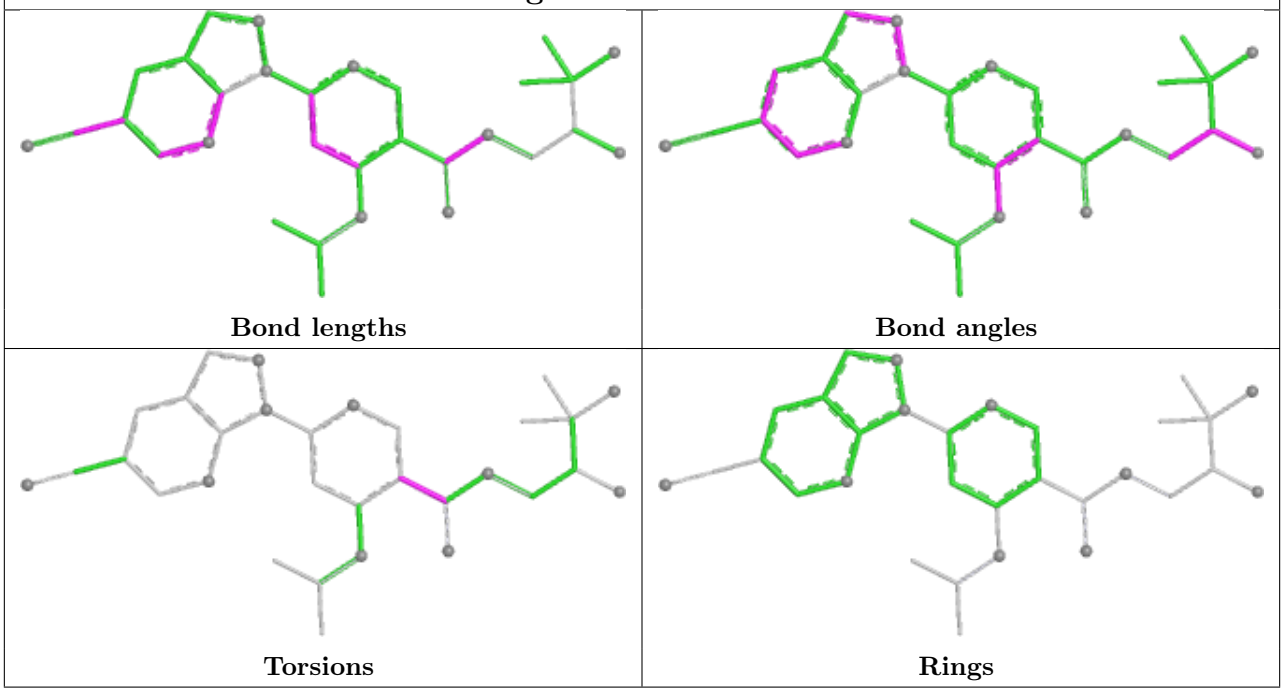


Torsions

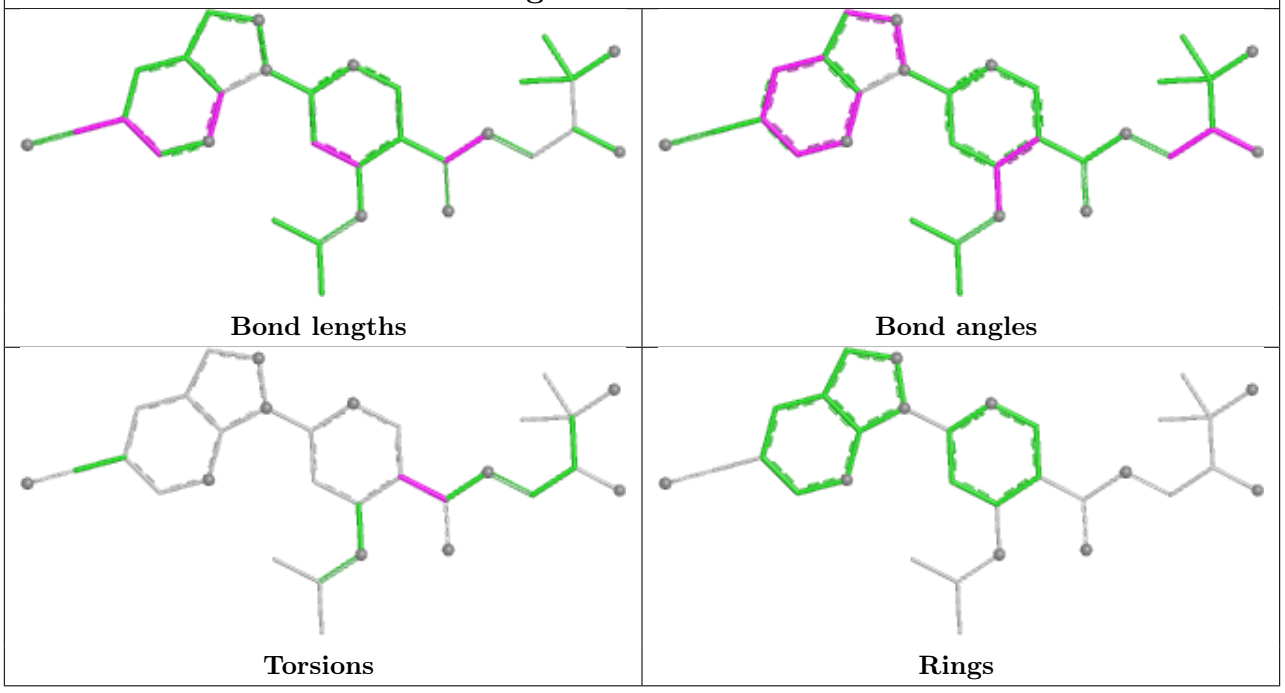


Rings

Ligand ZVA A 502



Ligand ZVA C 504



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

Warning: The R factor obtained from EDS is 0.3844, which does not match the depositor's R factor of 0.195. Please interpret the results in this section carefully.

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, 95^{th} 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	283/305 (92%)	0.95	47 (16%) 5 6	29, 54, 85, 123	0
1	B	283/305 (92%)	0.64	28 (9%) 14 17	29, 54, 83, 113	0
1	C	281/305 (92%)	0.96	33 (11%) 10 13	30, 56, 100, 116	0
1	D	281/305 (92%)	1.08	51 (18%) 4 5	33, 59, 94, 115	0
All	All	1128/1220 (92%)	0.91	159 (14%) 7 9	29, 55, 92, 123	0

The worst 5 of 159 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	434	SER	13.5
1	C	426	VAL	7.4
1	D	193	GLY	7.1
1	C	231	ASP	6.3
1	D	255	GLY	6.0

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

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	SEP	C	346	5/11	0.91	0.14	96,96,99,99	0
1	TPO	D	342	11/12	0.91	0.14	80,83,88,88	0
1	TPO	D	345	11/12	0.94	0.13	72,73,76,78	0
1	TPO	C	342	11/12	0.96	0.14	116,118,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	TPO	A	342	11/12	0.96	0.15	119,122,127,127	0
1	SEP	A	346	10/11	0.96	0.11	112,115,120,120	0
1	TPO	B	342	5/12	0.96	0.18	89,90,93,94	0
1	SEP	D	346	10/11	0.96	0.09	77,84,94,95	0
1	TPO	B	345	11/12	0.97	0.15	93,100,102,103	0
1	TPO	A	345	11/12	0.97	0.14	109,111,112,113	0
1	SEP	B	346	10/11	0.98	0.19	98,102,110,110	0
1	TPO	C	345	11/12	0.98	0.17	98,100,101,101	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

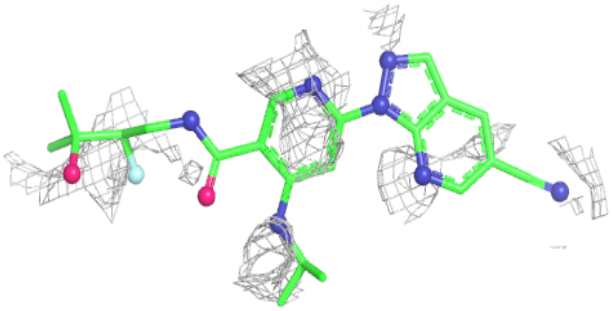
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

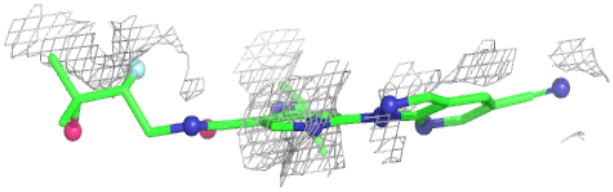
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	D	502	5/5	0.94	0.25	74,77,79,81	0
3	ZVA	A	502	31/31	0.94	0.13	26,33,40,50	0
3	ZVA	D	503	31/31	0.95	0.11	22,37,43,47	0
2	SO4	C	502	5/5	0.96	0.10	142,147,147,148	0
3	ZVA	B	503	31/31	0.96	0.10	27,35,41,42	0
2	SO4	B	502	5/5	0.96	0.15	120,124,125,125	0
2	SO4	C	501	5/5	0.97	0.12	84,89,89,90	0
2	SO4	B	501	5/5	0.97	0.12	108,113,113,113	0
2	SO4	C	503	5/5	0.97	0.08	66,69,71,72	0
3	ZVA	C	504	31/31	0.97	0.12	34,40,50,51	0
2	SO4	D	501	5/5	0.97	0.13	159,163,164,164	0
2	SO4	A	501	5/5	0.98	0.12	85,89,90,91	0

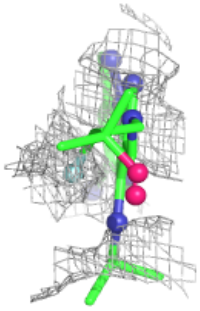
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ZVA A 502:

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

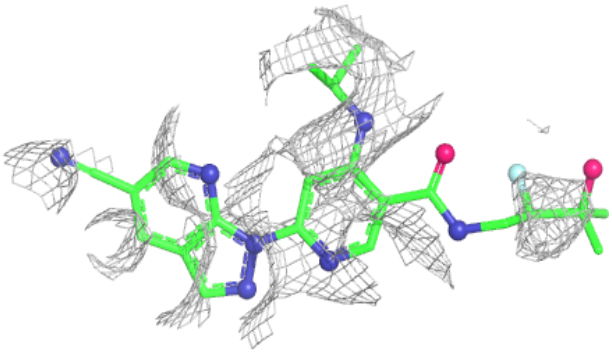


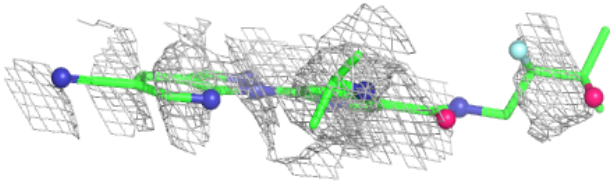


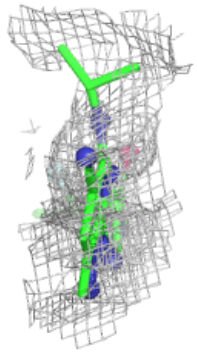


Electron density around ZVA D 503:

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

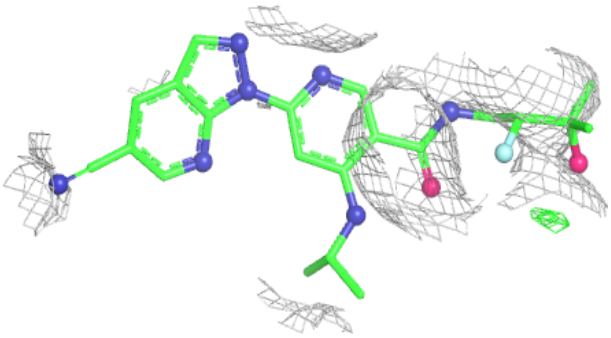


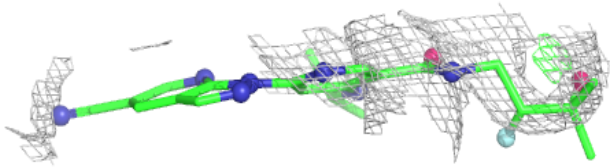


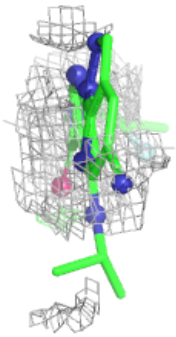


Electron density around ZVA B 503:

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

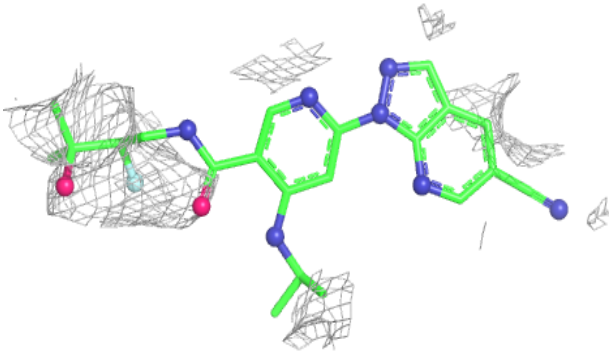


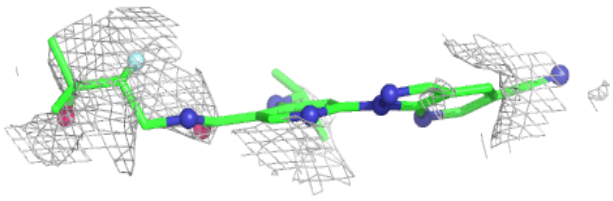


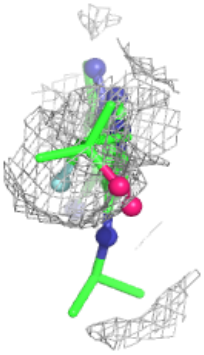


Electron density around ZVA C 504:

$2mF_o$-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.