



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 05:57 pm BST

PDB ID : 4JFW
Title : Crystal structure of a bacterial fucosidase with iminosugar inhibitor (2S,3S,4R,5S)-2-[N-(propylferrocene)]aminoethyl-5-methylpyrrolidine-3,4-diol
Authors : Wright, D.W.; Davies, G.J.
Deposited on : 2013-02-28
Resolution : 2.10 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	:	2.11
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)	:	2.11

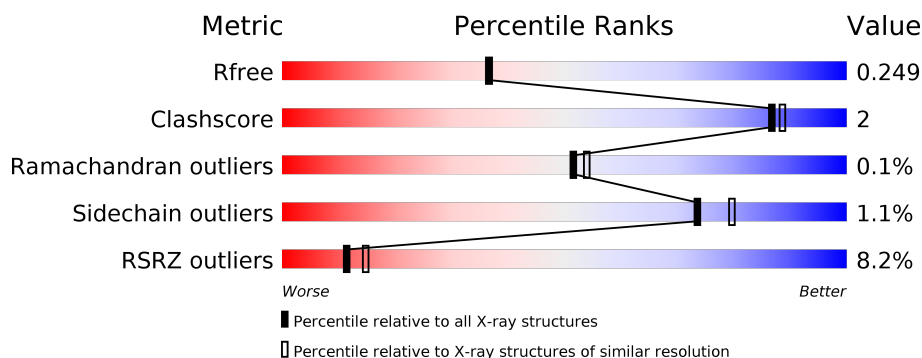
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 on 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	450	<div> <div>6%</div> <div>92%</div> <div>5%</div> </div>
1	B	450	<div> <div>7%</div> <div>92%</div> <div>6%</div> </div>
1	C	450	<div> <div>8%</div> <div>92%</div> <div>6%</div> </div>
1	D	450	<div> <div>11%</div> <div>92%</div> <div>5%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	B	503	-	-	X	-

2 Entry composition [i](#)

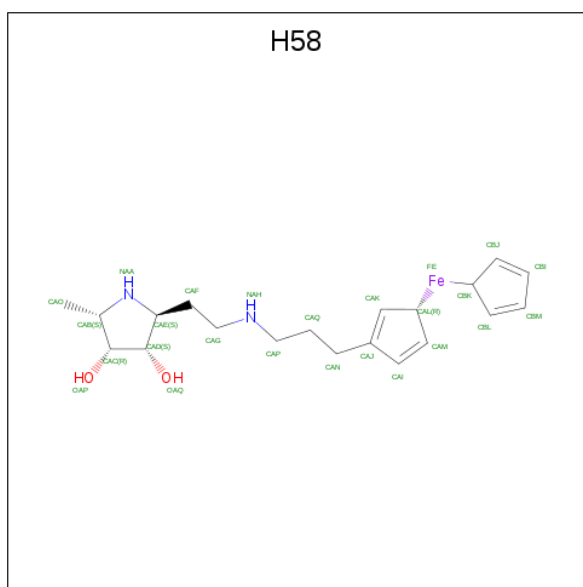
There are 5 unique types of molecules in this entry. The entry contains 14229 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 alpha-L-fucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	0	0
			3491	2248	584	643	16			
1	B	439	Total	C	N	O	S	0	0	0
			3461	2227	578	640	16			
1	C	439	Total	C	N	O	S	0	0	0
			3460	2224	577	643	16			
1	D	438	Total	C	N	O	S	0	0	0
			3447	2215	576	640	16			

- Molecule 2 is (3alpha)-[3-({2-[(2S,3S,4R,5S)-3,4-dihydroxy-5-methylpyrrolidin-2-yl]ethyl}amino)propyl]ferrocene (three-letter code: H58) (formula: C₂₀H₃₀FeN₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N O	0	0
			25	20	1	2 2		
2	B	1	Total	C	Fe	N O	0	0
			25	20	1	2 2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	Fe	N	O	0	0
			25	20	1	2	2		
2	D	1	Total	C	Fe	N	O	0	0
			25	20	1	2	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is IMIDAZOLE (three-letter code: IMD) (formula: C₃H₅N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			5	3	2		
4	B	1	Total	C	N	0	0
			5	3	2		
4	C	1	Total	C	N	0	0
			5	3	2		
4	D	1	Total	C	N	0	0
			5	3	2		

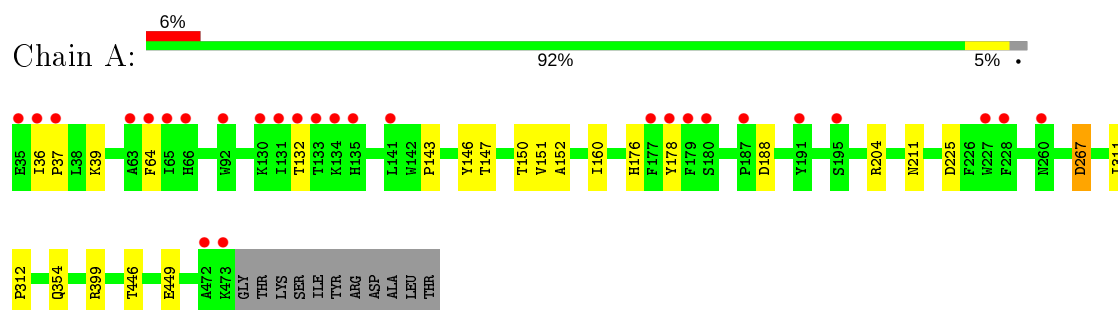
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	74	Total	O	0	0
			74	74		
5	B	58	Total	O	0	0
			58	58		
5	C	38	Total	O	0	0
			38	38		
5	D	45	Total	O	0	0
			45	45		

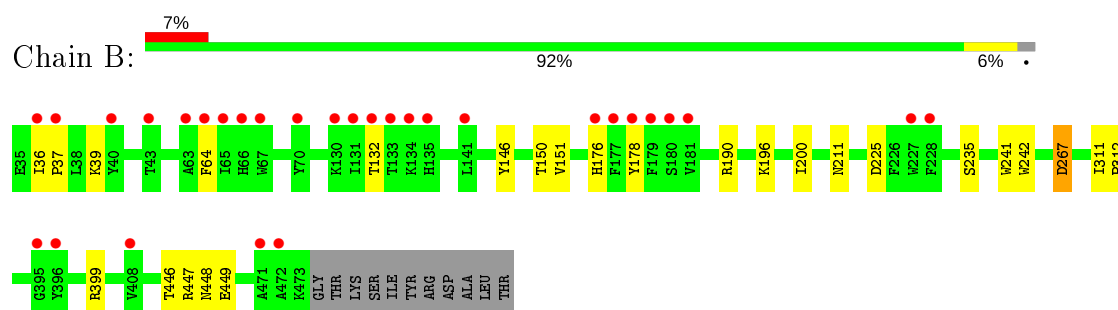
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

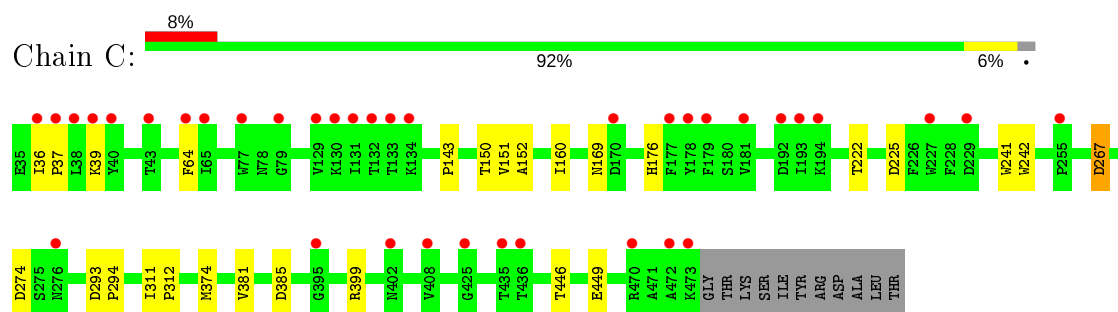
- Molecule 1: alpha-L-fucosidase



- Molecule 1: alpha-L-fucosidase

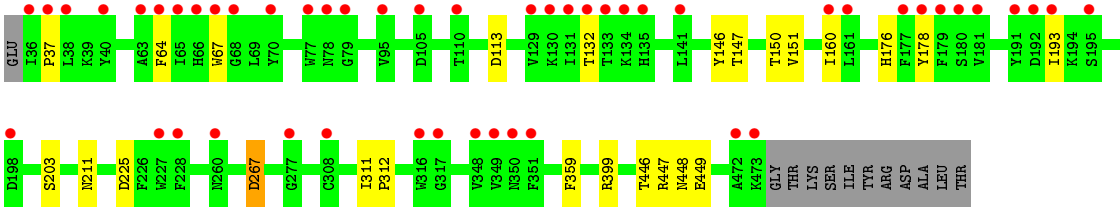


- Molecule 1: alpha-L-fucosidase



- Molecule 1: alpha-L-fucosidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.51 Å 189.98 Å 97.54 Å 90.00° 94.09° 90.00°	Depositor
Resolution (Å)	97.27 – 2.10 29.77 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (97.27-2.10) 99.9 (29.77-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.10 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.207 , 0.244 0.213 , 0.249	Depositor DCC
R_{free} test set	5986 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14229	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: H58, IMD, 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	0.68	0/3598	0.73	1/4901 (0.0%)
1	B	0.66	0/3568	0.73	1/4869 (0.0%)
1	C	0.68	0/3567	0.73	2/4869 (0.0%)
1	D	0.67	0/3554	0.73	2/4850 (0.0%)
All	All	0.67	0/14287	0.73	6/19489 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	399	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	B	399	ARG	NE-CZ-NH1	6.87	123.74	120.30
1	C	399	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	D	399	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	D	113	ASP	CB-CG-OD1	5.54	123.29	118.30
1	C	385	ASP	CB-CG-OD1	5.36	123.12	118.30

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	3491	0	3257	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3461	0	3192	12	0
1	C	3460	0	3171	17	0
1	D	3447	0	3157	10	0
2	A	25	0	28	0	0
2	B	25	0	28	2	0
2	C	25	0	28	0	0
2	D	25	0	28	1	0
3	A	5	0	0	0	0
3	B	10	0	0	2	0
3	C	10	0	0	0	0
3	D	10	0	0	1	0
4	A	5	0	5	0	0
4	B	5	0	5	0	0
4	C	5	0	5	0	0
4	D	5	0	5	1	0
5	A	74	0	0	1	0
5	B	58	0	0	0	0
5	C	38	0	0	0	0
5	D	45	0	0	0	0
All	All	14229	0	12909	57	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 (57) 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:150:THR:HG22	1:C:152:ALA:H	1.34	0.89
1:A:150:THR:HG22	1:A:152:ALA:H	1.42	0.81
1:A:446:THR:HG22	1:A:449:GLU:HB3	1.76	0.67
1:B:446:THR:HG22	1:B:449:GLU:HB3	1.76	0.67
1:D:446:THR:HG22	1:D:449:GLU:HB3	1.77	0.66
1:C:446:THR:HG22	1:C:449:GLU:HB3	1.79	0.64
1:A:143:PRO:HA	1:A:150:THR:CG2	2.29	0.63
1:C:150:THR:HG22	1:C:152:ALA:N	2.13	0.60
1:C:143:PRO:HA	1:C:150:THR:CG2	2.33	0.59
1:C:176:HIS:CG	1:C:225:ASP:HB3	2.41	0.56
1:D:176:HIS:CG	1:D:225:ASP:HB3	2.42	0.55
1:A:176:HIS:CG	1:A:225:ASP:HB3	2.43	0.54
2:D:501:H58:NAH	3:D:503:SO4:O2	2.40	0.54
1:A:143:PRO:HA	1:A:150:THR:HG21	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:HIS:CG	1:B:225:ASP:HB3	2.45	0.52
1:A:143:PRO:HA	1:A:150:THR:HG23	1.93	0.51
1:C:311:ILE:HB	1:C:312:PRO:HD3	1.93	0.50
1:D:193:ILE:O	1:D:193:ILE:HG23	2.11	0.50
1:C:143:PRO:HA	1:C:150:THR:HG23	1.95	0.49
1:A:188:ASP:OD2	1:A:204:ARG:NE	2.39	0.49
1:A:311:ILE:HB	1:A:312:PRO:HD3	1.96	0.48
1:C:143:PRO:HA	1:C:150:THR:HG21	1.96	0.47
1:A:267:ASP:N	1:A:267:ASP:OD1	2.47	0.47
1:D:267:ASP:OD1	1:D:267:ASP:N	2.46	0.47
1:B:36:ILE:HG23	1:B:37:PRO:HD2	1.96	0.46
1:B:267:ASP:OD1	1:B:267:ASP:N	2.48	0.46
1:C:36:ILE:HG23	1:C:37:PRO:HD2	1.97	0.46
1:D:311:ILE:HB	1:D:312:PRO:HD3	1.97	0.46
2:B:501:H58:H20	3:B:503:SO4:O4	2.17	0.45
1:B:311:ILE:HB	1:B:312:PRO:HD3	1.98	0.45
1:A:354:GLN:NE2	5:A:647:HOH:O	2.49	0.44
1:D:132:THR:HA	1:D:178:TYR:HB3	2.01	0.43
1:A:151:VAL:HG21	1:A:160:ILE:HG12	2.01	0.43
1:C:151:VAL:HG21	1:C:160:ILE:HG12	2.00	0.43
1:D:146:TYR:CZ	1:D:211:ASN:HB3	2.54	0.43
1:A:36:ILE:HG23	1:A:37:PRO:HD2	1.99	0.43
1:D:359:PHE:CZ	4:D:504:IMD:H4	2.54	0.43
1:A:39:LYS:N	1:A:267:ASP:OD2	2.44	0.42
1:D:151:VAL:HG21	1:D:160:ILE:HG12	2.00	0.42
1:B:196:LYS:O	1:B:200:ILE:HG12	2.19	0.42
1:B:241:TRP:CD2	1:B:242:TRP:N	2.88	0.42
1:D:447:ARG:O	1:D:448:ASN:HB2	2.20	0.42
1:B:447:ARG:O	1:B:448:ASN:HB2	2.21	0.41
1:B:132:THR:HA	1:B:178:TYR:HB3	2.02	0.41
1:C:241:TRP:CD2	1:C:242:TRP:N	2.88	0.41
1:C:39:LYS:N	1:C:267:ASP:OD2	2.49	0.41
1:C:293:ASP:HA	1:C:294:PRO:HD3	1.95	0.41
2:B:501:H58:NAH	3:B:503:SO4:O4	2.54	0.41
1:C:267:ASP:OD1	1:C:267:ASP:N	2.48	0.41
1:B:190:ARG:O	1:B:235:SER:CB	2.69	0.41
1:B:39:LYS:N	1:B:267:ASP:OD2	2.44	0.40
1:A:146:TYR:CZ	1:A:211:ASN:HB3	2.55	0.40
1:C:374:MET:HE1	1:C:381:VAL:HG11	2.03	0.40
1:C:169:ASN:ND2	1:C:222:THR:OG1	2.52	0.40
1:A:132:THR:HA	1:A:178:TYR:HB3	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:TYR:CZ	1:B:211:ASN:HB3	2.56	0.40
1:C:274:ASP:C	1:C:274:ASP:OD1	2.60	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	437/450 (97%)	421 (96%)	16 (4%)	0	100	100
1	B	437/450 (97%)	422 (97%)	15 (3%)	0	100	100
1	C	437/450 (97%)	423 (97%)	14 (3%)	0	100	100
1	D	436/450 (97%)	419 (96%)	16 (4%)	1 (0%)	47	49
All	All	1747/1800 (97%)	1685 (96%)	61 (4%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	37	PRO

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	346/383 (90%)	343 (99%)	3 (1%)	78	84

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	340/383 (89%)	336 (99%)	4 (1%)	71	77
1	C	338/383 (88%)	336 (99%)	2 (1%)	86	90
1	D	337/383 (88%)	331 (98%)	6 (2%)	59	65
All	All	1361/1532 (89%)	1346 (99%)	15 (1%)	73	79

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	PHE
1	A	147	THR
1	A	267	ASP
1	B	64	PHE
1	B	150	THR
1	B	151	VAL
1	B	267	ASP
1	C	64	PHE
1	C	267	ASP
1	D	64	PHE
1	D	67	TRP
1	D	147	THR
1	D	150	THR
1	D	203	SER
1	D	267	ASP

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

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 carbohydrates in this entry.

5.6 Ligand geometry

15 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	SO4	B	502	-	4,4,4	0.41	0	6,6,6	0.27	0
2	H58	C	501	-	21,27,27	1.41	2 (9%)	16,36,36	0.97	0
4	IMD	D	504	-	3,5,5	0.46	0	4,5,5	0.47	0
2	H58	A	501	-	21,27,27	1.53	2 (9%)	16,36,36	1.42	2 (12%)
2	H58	B	501	-	21,27,27	1.61	3 (14%)	16,36,36	1.18	2 (12%)
2	H58	D	501	-	21,27,27	1.48	2 (9%)	16,36,36	1.59	3 (18%)
3	SO4	C	502	-	4,4,4	0.38	0	6,6,6	0.31	0
3	SO4	A	502	-	4,4,4	0.53	0	6,6,6	0.49	0
4	IMD	A	503	-	3,5,5	0.42	0	4,5,5	0.62	0
4	IMD	C	504	-	3,5,5	0.28	0	4,5,5	0.84	0
3	SO4	B	503	-	4,4,4	0.52	0	6,6,6	0.53	0
3	SO4	C	503	-	4,4,4	0.37	0	6,6,6	0.47	0
4	IMD	B	504	-	3,5,5	0.49	0	4,5,5	0.27	0
3	SO4	D	503	-	4,4,4	0.30	0	6,6,6	0.22	0
3	SO4	D	502	-	4,4,4	0.43	0	6,6,6	0.65	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
4	IMD	D	504	-	-	-	0/1/1/1
2	H58	C	501	-	-	5/9/45/45	0/3/3/3
2	H58	A	501	-	-	2/9/45/45	0/3/3/3
2	H58	B	501	-	-	4/9/45/45	0/3/3/3
2	H58	D	501	-	-	5/9/45/45	0/3/3/3
4	IMD	A	503	-	-	-	0/1/1/1
4	IMD	C	504	-	-	-	0/1/1/1
4	IMD	B	504	-	-	-	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	H58	CAK-CAJ	4.83	1.43	1.34
2	D	501	H58	CAK-CAJ	4.54	1.42	1.34
2	B	501	H58	CAK-CAJ	4.53	1.42	1.34
2	C	501	H58	CAK-CAJ	4.42	1.42	1.34
2	A	501	H58	CAI-CAM	4.21	1.41	1.33
2	B	501	H58	CAI-CAM	4.11	1.41	1.33
2	D	501	H58	CAI-CAM	4.10	1.41	1.33
2	C	501	H58	CAI-CAM	3.95	1.41	1.33
2	B	501	H58	CAC-CAB	-3.53	1.48	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	H58	CAO-CAB-NAA	4.07	116.45	111.70
2	A	501	H58	CAQ-CAN-CAJ	3.64	120.78	114.25
2	A	501	H58	CAC-CAD-CAE	2.69	106.81	102.55
2	B	501	H58	CAO-CAB-NAA	2.56	114.70	111.70
2	D	501	H58	CAQ-CAN-CAJ	2.56	118.84	114.25
2	B	501	H58	CAC-CAD-CAE	2.33	106.23	102.55
2	D	501	H58	CAP-CAQ-CAN	2.22	119.42	112.84

There are no chirality outliers.

All (16) torsion outliers are listed below:

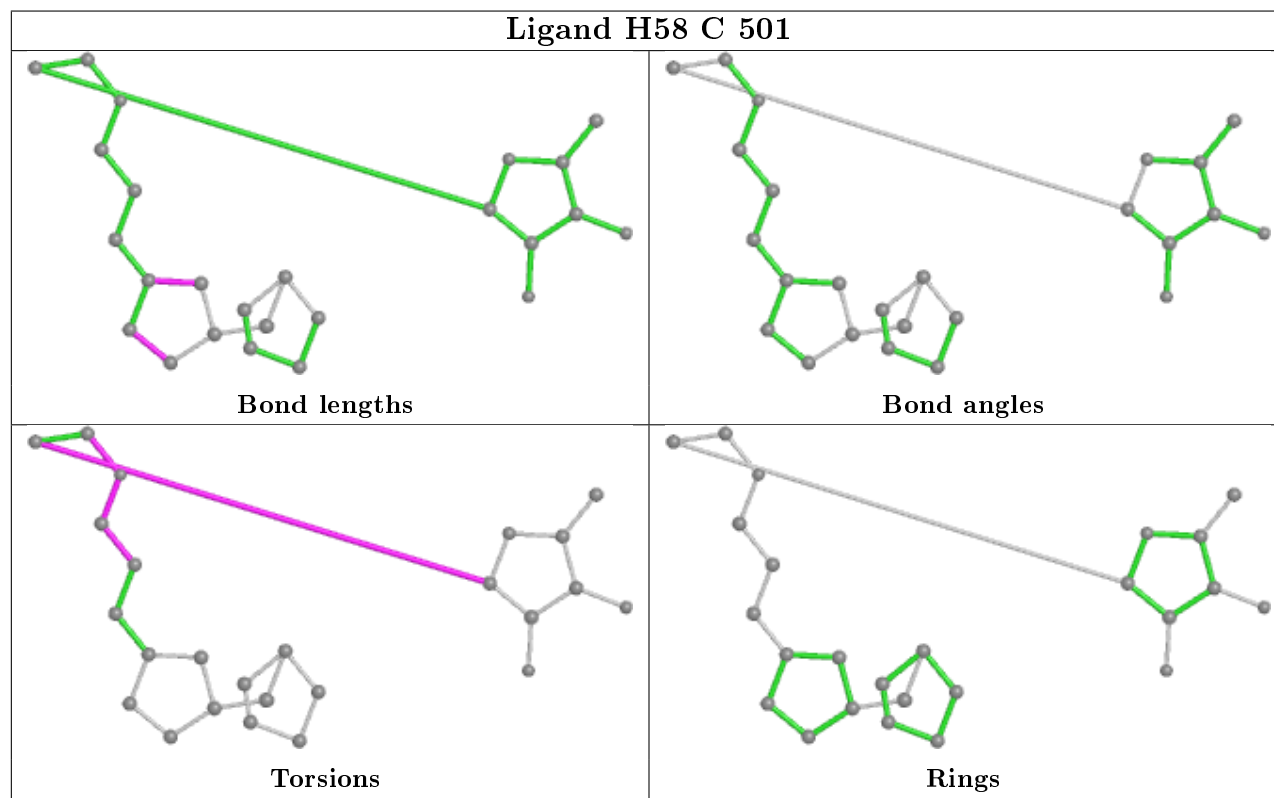
Mol	Chain	Res	Type	Atoms
2	C	501	H58	NAA-CAE-CAF-CAG
2	C	501	H58	CAD-CAE-CAF-CAG
2	B	501	H58	NAA-CAE-CAF-CAG
2	B	501	H58	CAD-CAE-CAF-CAG
2	D	501	H58	NAA-CAE-CAF-CAG
2	D	501	H58	CAK-CAJ-CAN-CAQ
2	D	501	H58	CAI-CAJ-CAN-CAQ
2	C	501	H58	NAH-CAP-CAQ-CAN
2	C	501	H58	CAQ-CAP-NAH-CAG
2	D	501	H58	CAQ-CAP-NAH-CAG
2	B	501	H58	CAQ-CAP-NAH-CAG
2	A	501	H58	CAI-CAJ-CAN-CAQ
2	C	501	H58	CAF-CAG-NAH-CAP
2	A	501	H58	NAA-CAE-CAF-CAG
2	D	501	H58	NAH-CAP-CAQ-CAN
2	B	501	H58	CAF-CAG-NAH-CAP

There are no ring outliers.

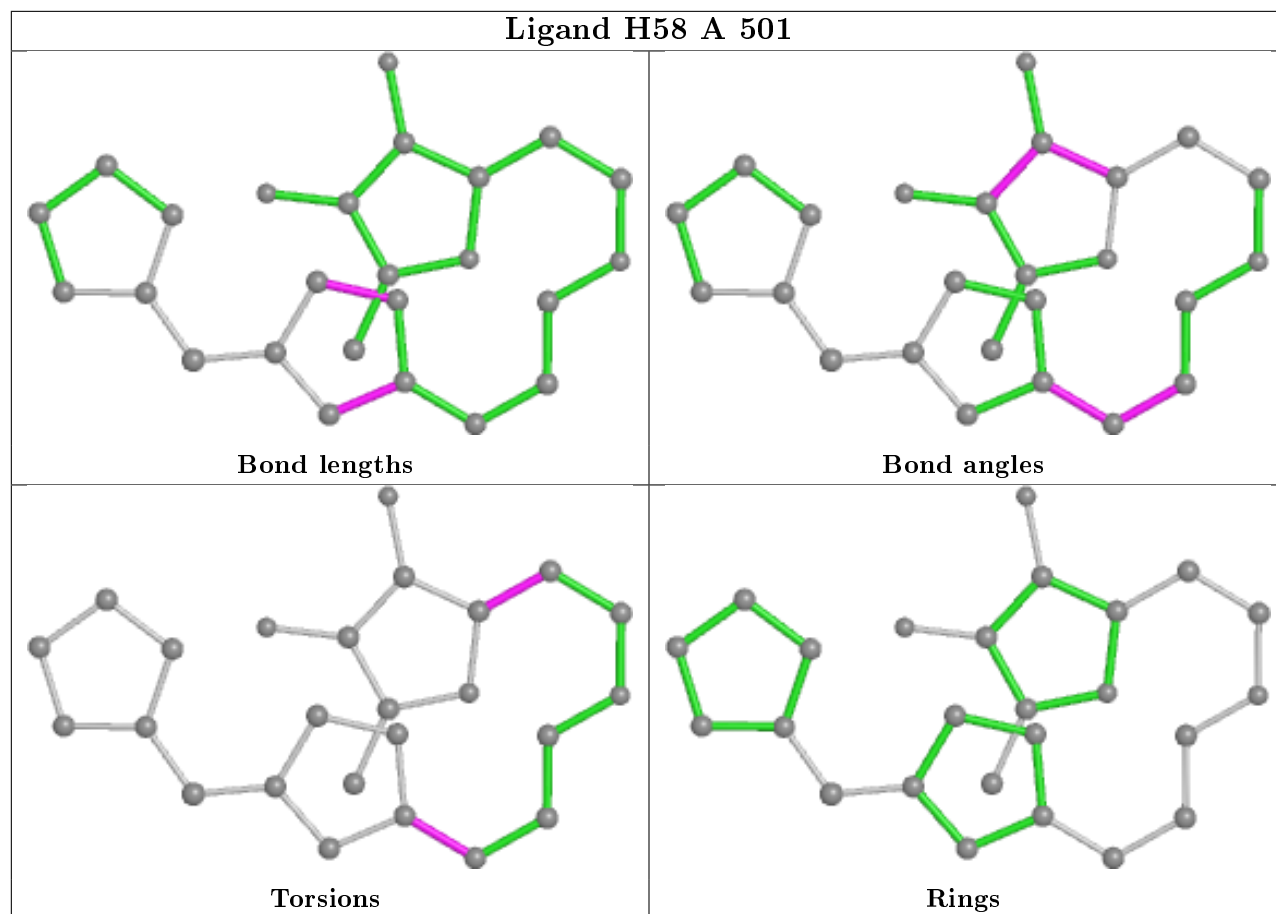
5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	504	IMD	1	0
2	B	501	H58	2	0
2	D	501	H58	1	0
3	B	503	SO4	2	0
3	D	503	SO4	1	0

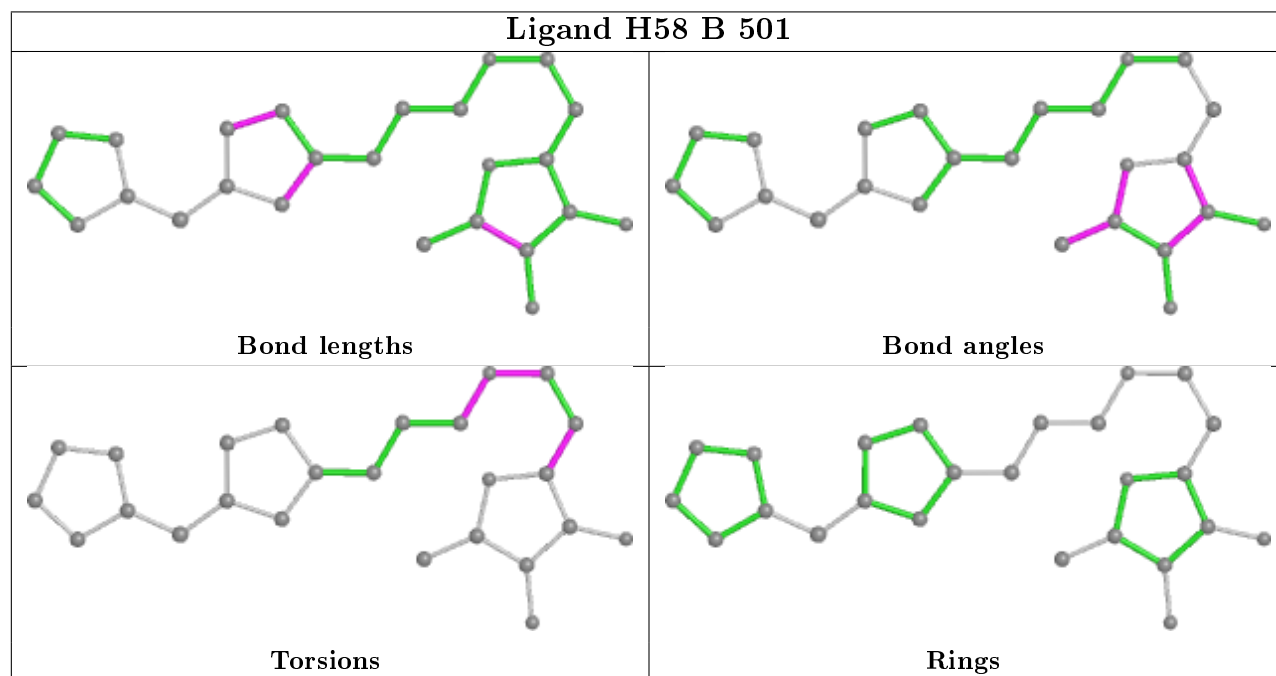
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

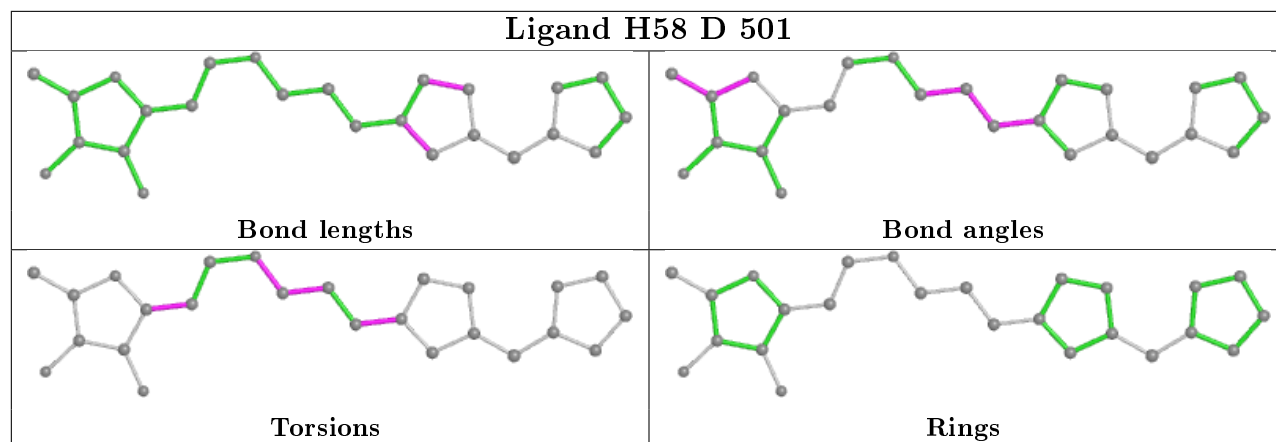


Ligand H58 A 501



Ligand H58 B 501





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	439/450 (97%)	0.20	27 (6%)	20 25	30, 49, 68, 93	2 (0%)
1	B	439/450 (97%)	0.29	30 (6%)	17 21	33, 51, 75, 99	0
1	C	439/450 (97%)	0.41	37 (8%)	11 14	32, 53, 80, 100	1 (0%)
1	D	438/450 (97%)	0.57	50 (11%)	5 6	36, 56, 82, 107	1 (0%)
All	All	1755/1800 (97%)	0.37	144 (8%)	11 15	30, 52, 78, 107	4 (0%)

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	178	TYR	7.5
1	C	472	ALA	6.7
1	B	178	TYR	6.7
1	D	132	THR	6.5
1	D	65	ILE	5.6
1	B	132	THR	5.5
1	A	178	TYR	5.4
1	A	36	ILE	5.2
1	D	133	THR	5.1
1	A	472	ALA	4.9
1	A	37	PRO	4.9
1	D	37	PRO	4.8
1	B	179	PHE	4.6
1	C	178	TYR	4.6
1	D	193	ILE	4.5
1	D	64	PHE	4.4
1	B	131	ILE	4.4
1	D	179	PHE	4.4
1	C	132	THR	4.4
1	B	65	ILE	4.2
1	A	132	THR	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	131	ILE	4.1
1	D	227	TRP	4.0
1	A	131	ILE	4.0
1	B	472	ALA	4.0
1	B	227	TRP	4.0
1	C	193	ILE	4.0
1	D	66	HIS	3.9
1	D	141	LEU	3.8
1	C	131	ILE	3.8
1	D	135	HIS	3.7
1	B	64	PHE	3.7
1	D	134	LYS	3.7
1	C	227	TRP	3.7
1	A	64	PHE	3.7
1	B	133	THR	3.7
1	C	64	PHE	3.7
1	B	471	ALA	3.6
1	D	79	GLY	3.6
1	C	37	PRO	3.6
1	B	134	LYS	3.5
1	D	130	LYS	3.5
1	A	65	ILE	3.5
1	B	36	ILE	3.4
1	D	195	SER	3.4
1	D	177	PHE	3.4
1	D	228	PHE	3.4
1	B	135	HIS	3.3
1	B	141	LEU	3.3
1	D	67	TRP	3.3
1	B	228	PHE	3.3
1	C	65	ILE	3.3
1	A	179	PHE	3.3
1	D	473	LYS	3.2
1	A	227	TRP	3.2
1	B	130	LYS	3.2
1	D	472	ALA	3.2
1	D	180	SER	3.2
1	B	180	SER	3.1
1	C	170	ASP	3.1
1	C	38	LEU	3.1
1	D	63	ALA	3.1
1	D	110	THR	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	228	PHE	3.1
1	D	40	TYR	3.1
1	C	79	GLY	3.0
1	C	40	TYR	2.9
1	B	40	TYR	2.9
1	B	66	HIS	2.9
1	C	473	LYS	2.9
1	D	348	VAL	2.9
1	C	402	ASN	2.9
1	C	36	ILE	2.8
1	C	276	ASN	2.8
1	C	133	THR	2.8
1	C	435	THR	2.8
1	C	179	PHE	2.7
1	D	36	ILE	2.7
1	A	133	THR	2.7
1	D	277	GLY	2.7
1	A	180	SER	2.7
1	B	395	GLY	2.7
1	D	68	GLY	2.7
1	D	129	VAL	2.7
1	D	308	CYS	2.7
1	D	351	PHE	2.6
1	D	349	VAL	2.6
1	B	177	PHE	2.6
1	C	255	PRO	2.6
1	D	181	VAL	2.6
1	B	181	VAL	2.6
1	D	78	ASN	2.6
1	C	39	LYS	2.5
1	D	317	GLY	2.5
1	D	95	VAL	2.5
1	D	70	TYR	2.5
1	D	191	TYR	2.5
1	A	130	LYS	2.5
1	B	176	HIS	2.5
1	B	67	TRP	2.5
1	C	470	ARG	2.5
1	B	396	TYR	2.5
1	C	425	GLY	2.5
1	B	43	THR	2.4
1	C	408	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	66	HIS	2.4
1	C	129	VAL	2.4
1	C	43	THR	2.4
1	A	35	GLU	2.4
1	C	134	LYS	2.4
1	D	192	ASP	2.4
1	D	316	TRP	2.4
1	A	135	HIS	2.4
1	B	408	VAL	2.3
1	A	63	ALA	2.3
1	C	229	ASP	2.3
1	D	260	ASN	2.3
1	A	177	PHE	2.3
1	A	92	TRP	2.3
1	C	192	ASP	2.3
1	B	63	ALA	2.2
1	C	395	GLY	2.2
1	D	77	TRP	2.2
1	C	194	LYS	2.2
1	A	473	LYS	2.2
1	A	191	TYR	2.2
1	B	70	TYR	2.2
1	D	350	ASN	2.2
1	A	187	PRO	2.2
1	A	141	LEU	2.1
1	C	177	PHE	2.1
1	D	198	ASP	2.1
1	B	37	PRO	2.1
1	A	195	SER	2.1
1	C	130	LYS	2.1
1	D	160	ILE	2.1
1	C	77	TRP	2.1
1	C	436	THR	2.1
1	D	105	ASP	2.1
1	D	161	LEU	2.1
1	C	181	VAL	2.1
1	A	260	ASN	2.0
1	D	38	LEU	2.0
1	A	134	LYS	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

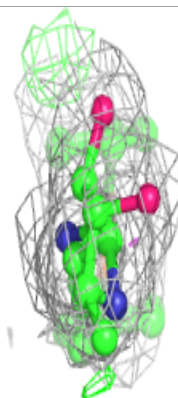
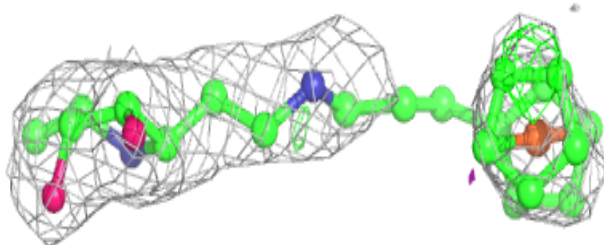
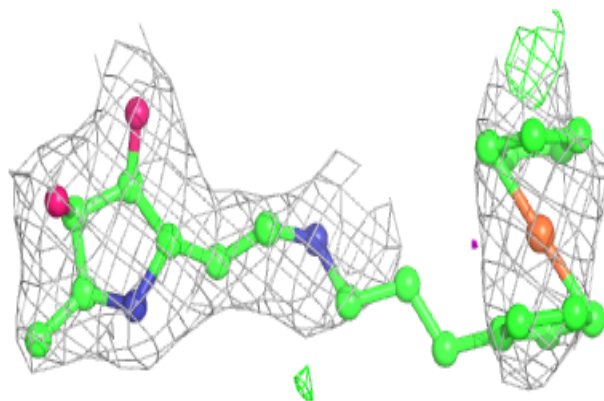
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	H58	B	501	25/25	0.65	0.31	42,98,170,187	0
2	H58	A	501	25/25	0.69	0.26	37,91,157,172	0
2	H58	D	501	25/25	0.70	0.31	43,96,152,163	0
2	H58	C	501	25/25	0.86	0.21	35,85,116,119	0
3	SO4	A	502	5/5	0.91	0.21	66,78,81,87	5
3	SO4	C	503	5/5	0.91	0.29	77,80,87,88	5
4	IMD	C	504	5/5	0.92	0.26	62,66,70,73	5
4	IMD	A	503	5/5	0.93	0.23	71,75,77,81	0
3	SO4	D	502	5/5	0.93	0.19	74,76,83,85	5
4	IMD	B	504	5/5	0.94	0.19	51,55,58,58	5
3	SO4	D	503	5/5	0.94	0.16	72,77,77,79	5
3	SO4	B	503	5/5	0.94	0.26	65,70,77,79	5
4	IMD	D	504	5/5	0.95	0.21	63,63,68,73	0
3	SO4	B	502	5/5	0.95	0.15	72,73,79,80	5
3	SO4	C	502	5/5	0.97	0.13	60,70,72,73	0

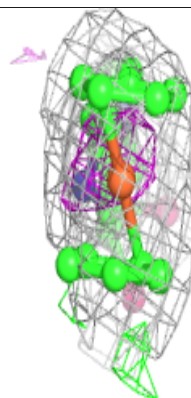
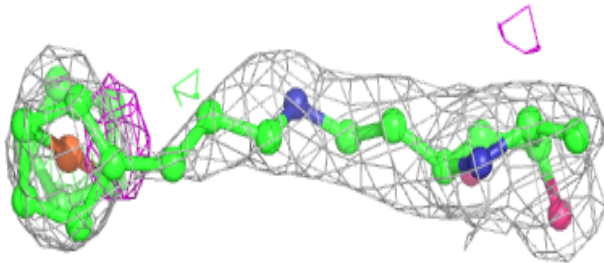
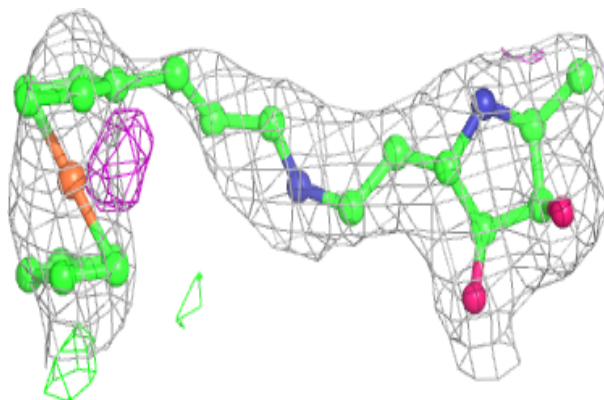
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around H58 B 501:

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

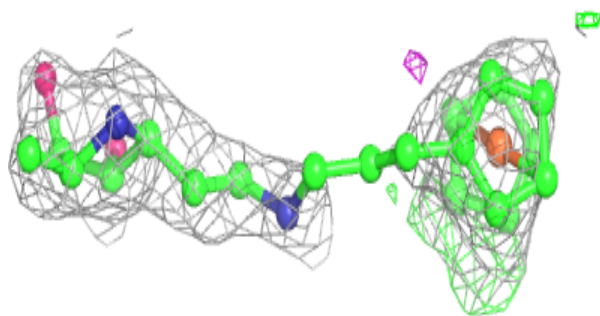
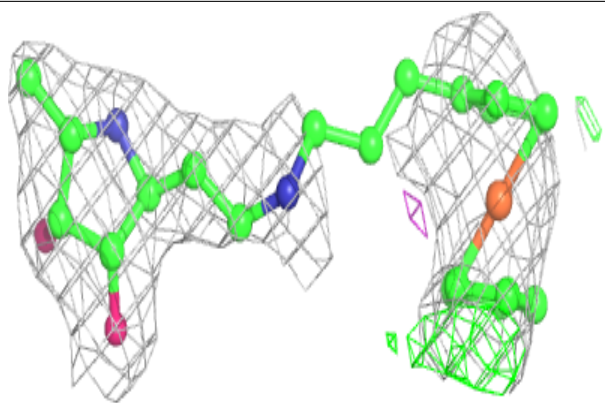
**Electron density around H58 A 501:**

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

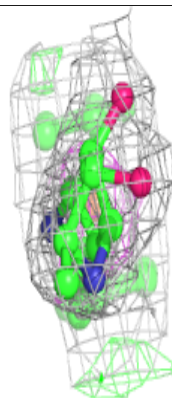
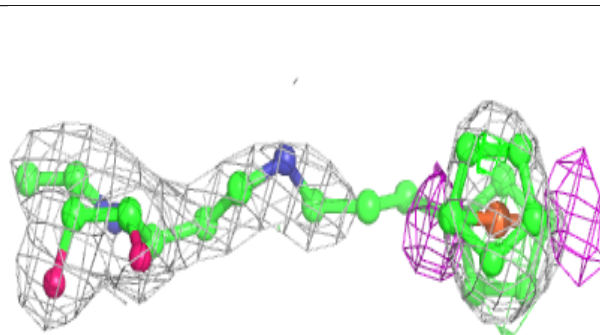
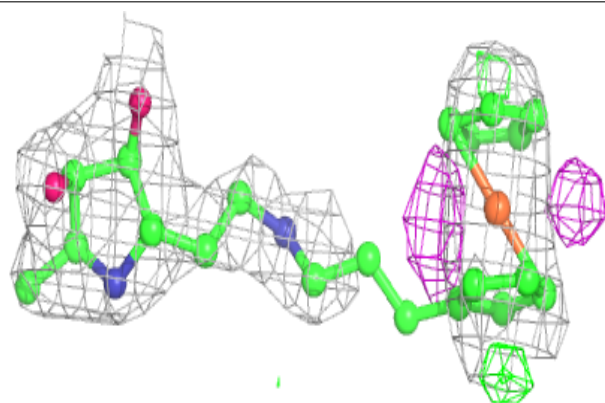


Electron density around H58 D 501:

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

**Electron density around H58 C 501:**

$2mF_o-DF_c$ (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.