Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2024 – 08:22 PM EST

PDB ID	:	9EFX
Title	:	Crystal structure of Danio rerio histone deacetylase 6 catalytic domain 2 complexed with TO-584
Authors	:	Erdogan, F.; Seo, H.-S.; Dhe-Paganon, S.
Deposited on	:	2024-11-20
Resolution	:	1.26 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:

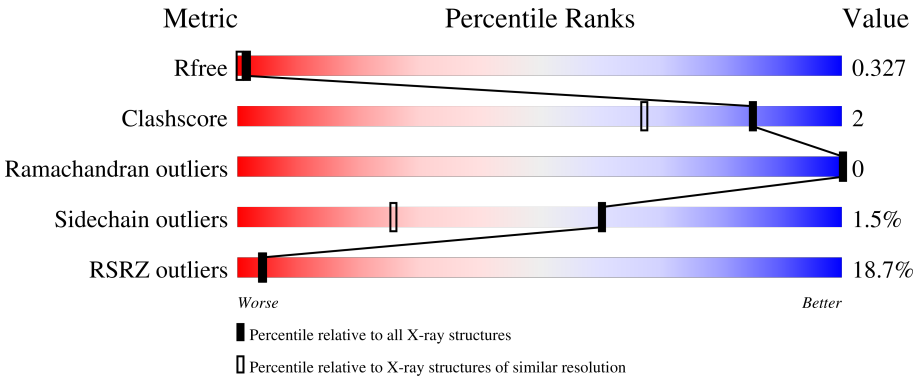
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (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 1.26 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	1447 (1.28-1.24)
Clashscore	180529	1571 (1.28-1.24)
Ramachandran outliers	177936	1538 (1.28-1.24)
Sidechain outliers	177891	1537 (1.28-1.24)
RSRZ outliers	164620	1447 (1.28-1.24)

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% 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	357	21% 93% 6%
1	B	357	15% 93% 6%
1	C	357	19% 93% 6%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	B	801	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8799 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.

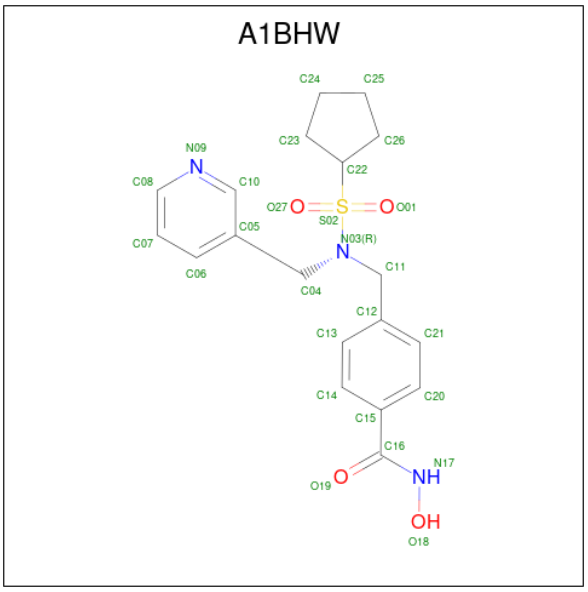
- Molecule 1 is a protein called Hdac6 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	0	0
			2771	1742	497	514	18			
1	B	354	Total	C	N	O	S	0	3	0
			2775	1745	496	516	18			
1	C	355	Total	C	N	O	S	0	0	0
			2771	1742	497	514	18			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 4-({(cyclopentanesulfonyl)[(pyridin-3-yl)methyl]amino}methyl)-N-hydroxybenzamide (three-letter code: A1BHW) (formula: $C_{19}H_{23}N_3O_4S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 27 19 3 4 1	0	0
3	B	1	Total C N O S 27 19 3 4 1	0	0
3	C	1	Total C N O S 27 19 3 4 1	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total K 2 2	0	0
4	B	2	Total K 2 2	0	0
4	C	1	Total K 1 1	0	0

- Molecule 5 is water.

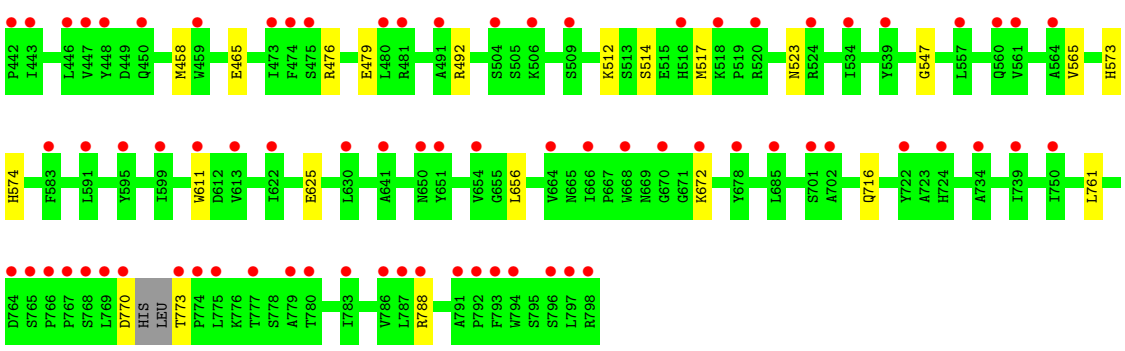
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	110	Total O 110 110	0	0
5	B	130	Total O 130 130	0	0
5	C	153	Total O 153 153	0	0

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.

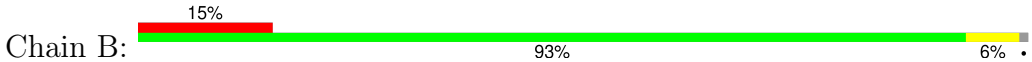
• Molecule 1: Hdac6 protein

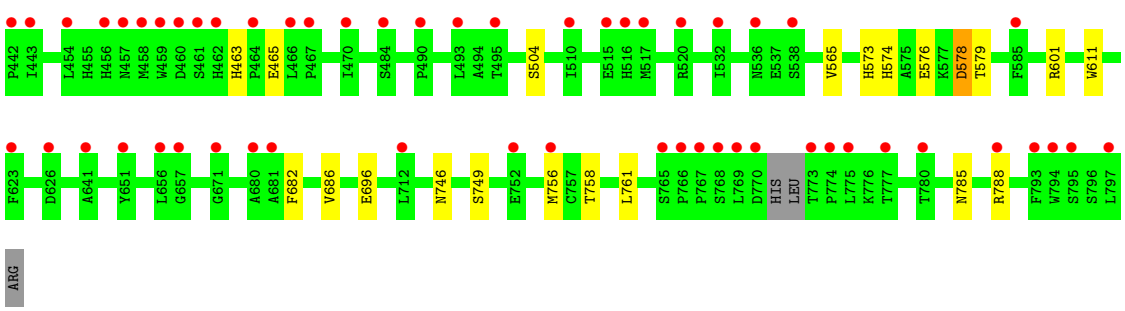
Chain A:



• Molecule 1: Hdac6 protein

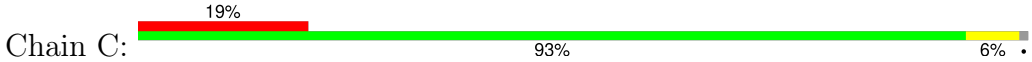
Chain B:

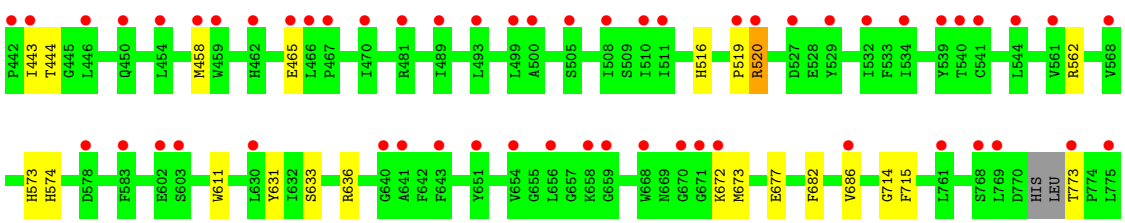


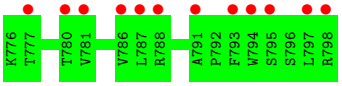


• Molecule 1: Hdac6 protein

Chain C:






K776
T777
T780
V781
V786
L787
R788
A791
P792
F793
W794
S795
S796
L797
R798

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	91.77Å 82.57Å 105.82Å 90.00° 115.13° 90.00°	Depositor
Resolution (Å)	58.57 – 1.26 58.57 – 1.26	Depositor EDS
% Data completeness (in resolution range)	73.5 (58.57-1.26) 73.5 (58.57-1.26)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.99 (at 1.26Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.303 , (Not available) 0.303 , 0.327	Depositor DCC
R_{free} test set	115082 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	16.5	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 36.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.008 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	8799	wwPDB-VP
Average B, all atoms (Å^2)	20.0	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 23.59 % 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 4.5248e-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: A1BHW, K, ZN

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	0.36	0/2840	0.57	0/3851
1	B	0.39	0/2847	0.58	0/3861
1	C	0.37	0/2840	0.57	0/3851
All	All	0.37	0/8527	0.57	0/11563

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	2771	0	2689	13	0
1	B	2775	0	2684	10	0
1	C	2771	0	2689	12	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	27	0	0	1	0
3	B	27	0	0	1	0
3	C	27	0	0	1	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2	0	0	0	0
4	C	1	0	0	0	0
5	A	110	0	0	3	0
5	B	130	0	0	1	0
5	C	153	0	0	2	0
All	All	8799	0	8062	34	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 (34) 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:A:476:ARG:NH1	1:A:479:GLU:OE1	2.19	0.75
1:C:458:MET:HE1	1:C:519:PRO:HB3	1.83	0.60
1:C:773:THR:N	5:C:902:HOH:O	2.35	0.60
1:A:512:LYS:NZ	5:A:902:HOH:O	2.34	0.58
1:C:562:ARG:NH1	5:C:903:HOH:O	2.38	0.56
1:A:770:ASP:OD1	1:A:773:THR:OG1	2.26	0.53
1:B:504:SER:OG	1:B:578[A]:ASP:OD1	2.26	0.53
1:B:601:ARG:NH2	1:B:696:GLU:OE1	2.33	0.52
1:B:746:ASN:HB3	1:B:749:SER:HB2	1.93	0.50
1:B:785:ASN:OD1	1:B:788:ARG:NH1	2.45	0.50
1:C:520:ARG:HE	1:C:520:ARG:H	1.60	0.49
1:C:443:ILE:HG12	1:C:444:THR:H	1.78	0.48
1:B:565:VAL:HG13	1:B:761:LEU:HD12	1.95	0.48
1:A:565:VAL:HG13	1:A:761:LEU:HD12	1.96	0.47
1:A:574:HIS:NE2	3:A:802:A1BHW:N17	2.62	0.47
1:C:574:HIS:NE2	3:C:802:A1BHW:N17	2.63	0.47
1:A:625:GLU:HG2	1:A:656:LEU:HB2	1.99	0.45
1:A:788:ARG:NH1	1:C:516:HIS:HA	2.32	0.45
1:B:463:HIS:HB3	5:B:993:HOH:O	2.17	0.44
1:B:682:PHE:HA	1:B:686:VAL:HB	2.00	0.44
1:A:492:ARG:O	1:A:547:GLY:HA3	2.19	0.42
1:B:574:HIS:NE2	3:B:802:A1BHW:N17	2.68	0.42
1:A:773:THR:N	5:A:901:HOH:O	2.53	0.42
1:A:514:SER:HA	1:A:517:MET:HG3	2.01	0.42
1:A:512:LYS:HZ2	1:A:512:LYS:HG3	1.77	0.42
1:A:458:MET:HG3	5:A:926:HOH:O	2.20	0.41
1:A:672:LYS:HG2	1:A:716:GLN:HG2	2.01	0.41
1:C:631:TYR:CZ	1:C:633:SER:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:682:PHE:HA	1:C:686:VAL:HB	2.02	0.41
1:B:565:VAL:HG11	1:B:758:THR:OG1	2.21	0.40
1:C:673:MET:SD	1:C:677:GLU:HG2	2.61	0.40
1:B:576:GLU:HB2	1:B:579:THR:HG22	2.03	0.40
1:C:636:ARG:HD2	1:C:715:PHE:CE1	2.57	0.40
1:C:672:LYS:HG3	1:C:714:GLY:O	2.22	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	351/357 (98%)	340 (97%)	11 (3%)	0	100	100
1	B	353/357 (99%)	339 (96%)	14 (4%)	0	100	100
1	C	351/357 (98%)	338 (96%)	13 (4%)	0	100	100
All	All	1055/1071 (98%)	1017 (96%)	38 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	299/301 (99%)	295 (99%)	4 (1%)	65	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	299/301 (99%)	293 (98%)	6 (2%)	50 15
1	C	299/301 (99%)	295 (99%)	4 (1%)	65 30
All	All	897/903 (99%)	883 (98%)	14 (2%)	60 23

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	465	GLU
1	A	523	ASN
1	A	573	HIS
1	A	611	TRP
1	B	465	GLU
1	B	573	HIS
1	B	578[A]	ASP
1	B	578[B]	ASP
1	B	611	TRP
1	B	756	MET
1	C	465	GLU
1	C	520	ARG
1	C	573	HIS
1	C	611	TRP

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)

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 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 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	A1BHW	B	802	2	27,29,29	4.10	9 (33%)	33,40,40	3.13	5 (15%)
3	A1BHW	C	802	2	27,29,29	4.03	8 (29%)	33,40,40	3.22	7 (21%)
3	A1BHW	A	802	2	27,29,29	4.02	9 (33%)	33,40,40	2.96	11 (33%)

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	A1BHW	B	802	2	-	0/24/33/33	0/3/3/3
3	A1BHW	C	802	2	-	1/24/33/33	0/3/3/3
3	A1BHW	A	802	2	-	1/24/33/33	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	802	A1BHW	C26-C22	-13.07	1.37	1.54
3	A	802	A1BHW	C26-C22	-12.96	1.37	1.54
3	B	802	A1BHW	C26-C22	-12.94	1.38	1.54
3	B	802	A1BHW	C16-N17	11.04	1.46	1.32
3	C	802	A1BHW	C16-N17	11.03	1.46	1.32
3	A	802	A1BHW	C16-N17	10.66	1.46	1.32
3	B	802	A1BHW	C23-C22	10.08	1.66	1.54
3	A	802	A1BHW	C23-C22	9.74	1.66	1.54
3	C	802	A1BHW	C23-C22	9.74	1.66	1.54
3	A	802	A1BHW	C24-C23	-3.56	1.37	1.51
3	B	802	A1BHW	C24-C23	-3.46	1.37	1.51
3	C	802	A1BHW	C24-C23	-3.41	1.38	1.51
3	B	802	A1BHW	C11-C12	3.20	1.57	1.51
3	B	802	A1BHW	O27-S02	3.15	1.46	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	A1BHW	C15-C16	2.93	1.56	1.50
3	A	802	A1BHW	O01-S02	2.82	1.45	1.43
3	C	802	A1BHW	C15-C16	2.73	1.56	1.50
3	A	802	A1BHW	C15-C16	2.72	1.56	1.50
3	A	802	A1BHW	C11-C12	2.68	1.56	1.51
3	C	802	A1BHW	O19-C16	-2.64	1.17	1.23
3	C	802	A1BHW	C11-C12	2.50	1.55	1.51
3	B	802	A1BHW	C04-C05	2.28	1.55	1.51
3	C	802	A1BHW	C25-C26	2.22	1.60	1.51
3	A	802	A1BHW	O19-C16	-2.19	1.18	1.23
3	B	802	A1BHW	C25-C26	2.08	1.60	1.51
3	A	802	A1BHW	O27-S02	2.07	1.45	1.43

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	802	A1BHW	O27-S02-O01	-16.34	106.86	119.17
3	C	802	A1BHW	O27-S02-O01	-15.52	107.48	119.17
3	A	802	A1BHW	O27-S02-O01	-14.32	108.39	119.17
3	C	802	A1BHW	C08-N09-C10	4.48	124.70	116.85
3	C	802	A1BHW	O01-S02-C22	4.22	113.20	107.82
3	A	802	A1BHW	O01-S02-C22	3.82	112.68	107.82
3	B	802	A1BHW	C08-N09-C10	3.47	122.93	116.85
3	C	802	A1BHW	C15-C16-N17	2.91	120.75	116.26
3	A	802	A1BHW	C15-C16-N17	2.74	120.49	116.26
3	C	802	A1BHW	O27-S02-N03	2.63	110.10	107.44
3	C	802	A1BHW	C05-C10-N09	-2.62	118.74	123.75
3	A	802	A1BHW	C20-C15-C14	2.59	121.86	118.57
3	B	802	A1BHW	O27-S02-C22	2.52	111.04	107.82
3	A	802	A1BHW	C21-C12-C13	2.52	121.97	118.23
3	A	802	A1BHW	C07-C06-C05	-2.31	117.36	120.61
3	A	802	A1BHW	C04-N03-C11	2.26	120.91	116.27
3	A	802	A1BHW	C21-C20-C15	-2.25	118.39	120.80
3	B	802	A1BHW	O01-S02-C22	2.22	110.65	107.82
3	A	802	A1BHW	C08-N09-C10	2.17	120.66	116.85
3	B	802	A1BHW	C05-C10-N09	-2.11	119.72	123.75
3	A	802	A1BHW	O01-S02-N03	2.09	109.55	107.44
3	C	802	A1BHW	C21-C12-C13	2.06	121.30	118.23
3	A	802	A1BHW	C06-C05-C10	2.02	120.07	117.10

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	802	A1BHW	C05-C04-N03-C11
3	A	802	A1BHW	C05-C04-N03-C11

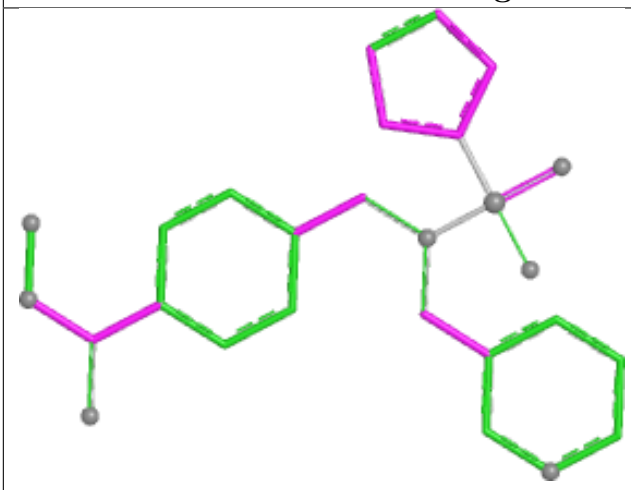
There are no ring outliers.

3 monomers are involved in 3 short contacts:

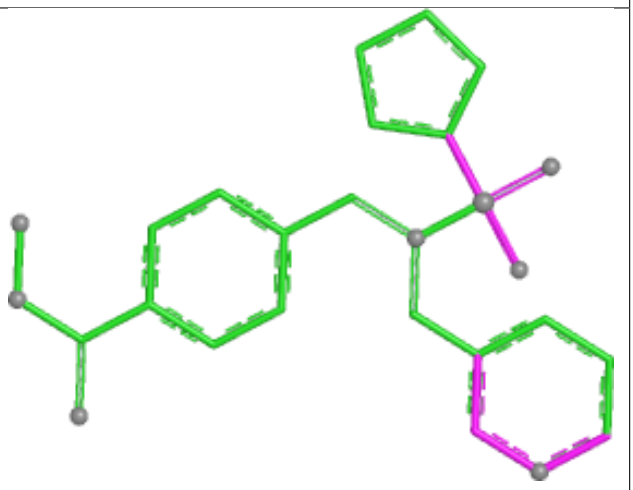
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	802	A1BHW	1	0
3	C	802	A1BHW	1	0
3	A	802	A1BHW	1	0

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 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.

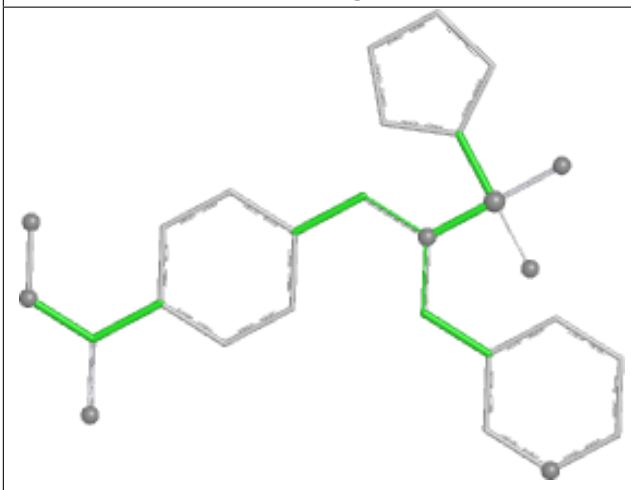
Ligand A1BHW B 802



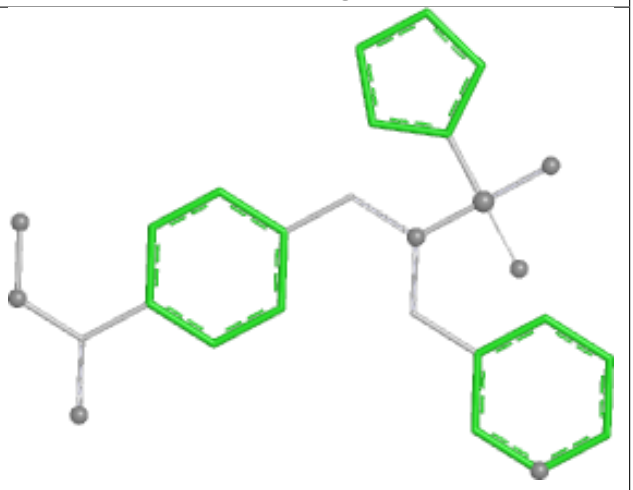
Bond lengths



Bond angles

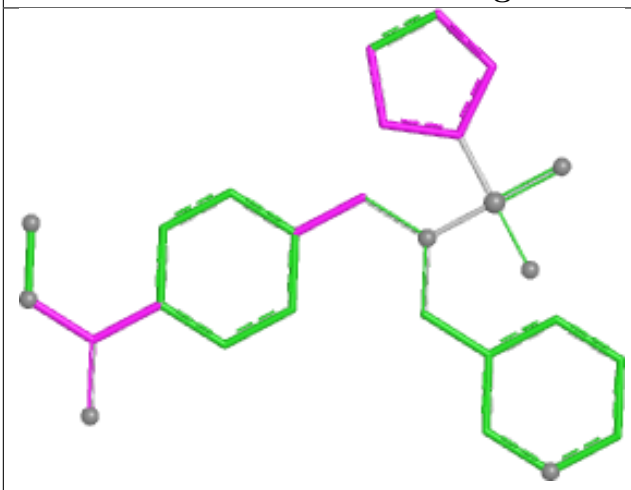


Torsions

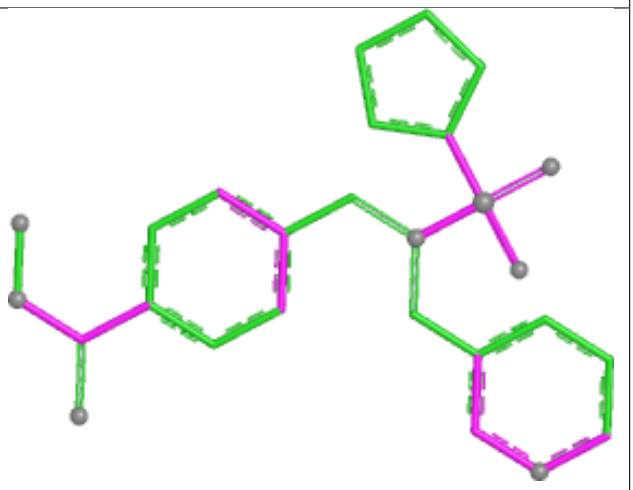


Rings

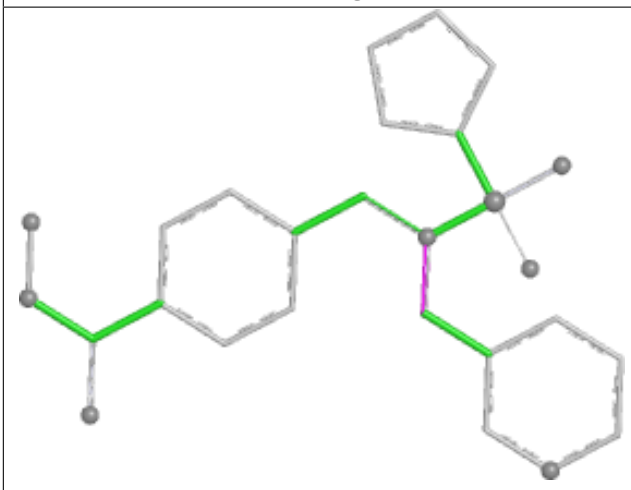
Ligand A1BHW C 802



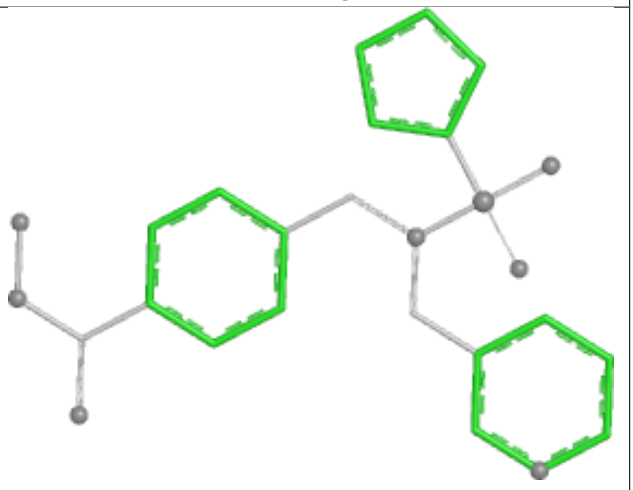
Bond lengths



Bond angles

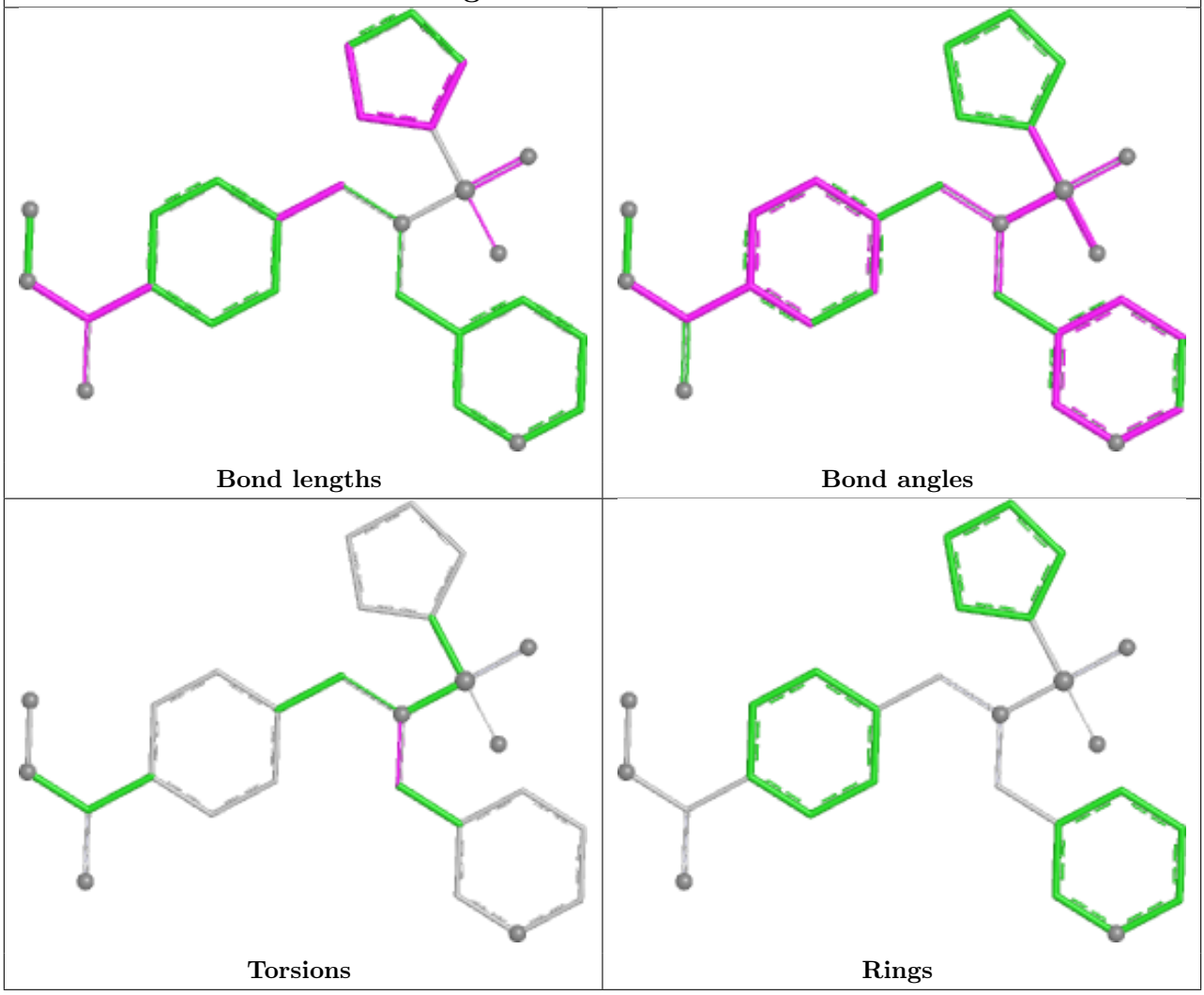


Torsions



Rings

Ligand A1BHW A 802



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, 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	355/357 (99%)	1.40	76 (21%)	3	3	13, 19, 30, 56	0
1	B	354/357 (99%)	1.29	55 (15%)	6	6	10, 17, 29, 52	3 (0%)
1	C	355/357 (99%)	1.35	68 (19%)	4	4	13, 19, 29, 42	0
All	All	1064/1071 (99%)	1.35	199 (18%)	4	4	10, 18, 30, 56	3 (0%)

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	443	ILE	6.9
1	B	459	TRP	6.7
1	C	443	ILE	6.4
1	A	769	LEU	6.2
1	B	462	HIS	5.9
1	B	773	THR	5.5
1	C	442	PRO	5.5
1	B	442	PRO	5.0
1	A	768	SER	4.9
1	B	516	HIS	4.8
1	A	442	PRO	4.7
1	B	769	LEU	4.6
1	B	458	MET	4.5
1	A	773	THR	4.2
1	B	641	ALA	4.2
1	A	767	PRO	4.0
1	B	461	SER	4.0
1	B	657	GLY	3.9
1	A	797	LEU	3.9
1	A	668	TRP	3.9
1	C	787	LEU	3.9
1	C	658	LYS	3.8
1	C	510	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	641	ALA	3.8
1	A	443	ILE	3.7
1	A	670	GLY	3.7
1	B	767	PRO	3.7
1	A	473	ILE	3.6
1	B	457	ASN	3.6
1	B	766	PRO	3.6
1	A	770	ASP	3.5
1	A	798	ARG	3.5
1	A	779	ALA	3.5
1	A	666	ILE	3.4
1	B	712	LEU	3.4
1	C	670	GLY	3.4
1	A	774	PRO	3.4
1	B	797	LEU	3.4
1	B	536	ASN	3.3
1	A	793	PHE	3.3
1	A	775	LEU	3.2
1	B	515	GLU	3.2
1	C	499	LEU	3.2
1	A	651	TYR	3.2
1	B	770	ASP	3.1
1	C	795	SER	3.1
1	A	518	LYS	3.1
1	C	651	TYR	3.1
1	B	777	THR	3.1
1	C	511	ILE	3.1
1	C	467	PRO	3.1
1	A	561	VAL	3.0
1	B	454	LEU	3.0
1	C	777	THR	3.0
1	B	626	ASP	3.0
1	C	500	ALA	3.0
1	C	797	LEU	3.0
1	C	450	GLN	3.0
1	B	623	PHE	3.0
1	A	524	ARG	3.0
1	A	787	LEU	3.0
1	C	769	LEU	3.0
1	C	781	VAL	3.0
1	C	668	TRP	3.0
1	A	765	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	622	ILE	2.9
1	A	459	TRP	2.9
1	A	480	LEU	2.9
1	C	544	LEU	2.9
1	B	681	ALA	2.9
1	C	791	ALA	2.9
1	B	656	LEU	2.9
1	A	450	GLN	2.8
1	B	794	TRP	2.8
1	C	520	ARG	2.8
1	B	768	SER	2.8
1	A	780	THR	2.8
1	C	641	ALA	2.8
1	B	671	GLY	2.8
1	A	685	LEU	2.8
1	A	786	VAL	2.8
1	C	454	LEU	2.7
1	C	672	LYS	2.7
1	A	534	ILE	2.7
1	B	460	ASP	2.6
1	A	599	ILE	2.6
1	A	448	TYR	2.6
1	A	734	ALA	2.6
1	C	773	THR	2.6
1	C	793	PHE	2.6
1	A	481	ARG	2.6
1	A	788	ARG	2.6
1	A	564	ALA	2.6
1	C	481	ARG	2.6
1	C	654	VAL	2.6
1	B	517	MET	2.6
1	C	532	ILE	2.6
1	A	783	ILE	2.5
1	C	671	GLY	2.5
1	C	780	THR	2.5
1	A	509	SER	2.5
1	B	788	ARG	2.5
1	B	774	PRO	2.5
1	A	474	PHE	2.5
1	B	793	PHE	2.5
1	A	702	ALA	2.5
1	C	798	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	630	LEU	2.5
1	C	462	HIS	2.5
1	A	766	PRO	2.5
1	A	520	ARG	2.4
1	A	796	SER	2.4
1	B	585	PHE	2.4
1	C	794	TRP	2.4
1	B	470	ILE	2.4
1	B	510	ILE	2.4
1	C	529	TYR	2.4
1	C	527	ASP	2.4
1	C	568	VAL	2.4
1	C	465	GLU	2.4
1	B	651	TYR	2.4
1	C	458	MET	2.4
1	C	578	ASP	2.4
1	A	791	ALA	2.4
1	C	519	PRO	2.4
1	A	446	LEU	2.4
1	C	493	LEU	2.4
1	A	654	VAL	2.3
1	C	768	SER	2.3
1	B	490	PRO	2.3
1	C	643	PHE	2.3
1	A	750	ILE	2.3
1	A	722	TYR	2.3
1	B	495	THR	2.3
1	B	780	THR	2.3
1	C	540	THR	2.3
1	C	602	GLU	2.3
1	A	613	VAL	2.3
1	A	792	PRO	2.3
1	A	504	SER	2.3
1	C	446	LEU	2.3
1	C	489	ILE	2.3
1	A	678	TYR	2.3
1	A	560	GLN	2.3
1	B	464	PRO	2.3
1	C	561	VAL	2.3
1	B	538	SER	2.2
1	A	650	ASN	2.2
1	C	583	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	466	LEU	2.2
1	B	532	ILE	2.2
1	C	534	ILE	2.2
1	B	756	MET	2.2
1	A	447	VAL	2.2
1	C	786	VAL	2.2
1	A	516	HIS	2.2
1	A	557	LEU	2.2
1	C	656	LEU	2.2
1	C	775	LEU	2.2
1	A	739	ILE	2.2
1	C	788	ARG	2.2
1	A	506	LYS	2.2
1	A	475	SER	2.2
1	B	765	SER	2.2
1	C	761	LEU	2.2
1	C	541	CYS	2.2
1	B	520	ARG	2.1
1	A	794	TRP	2.1
1	C	686	VAL	2.1
1	B	466	LEU	2.1
1	A	777	THR	2.1
1	B	795	SER	2.1
1	C	505	SER	2.1
1	C	603	SER	2.1
1	A	611	TRP	2.1
1	A	664	VAL	2.1
1	B	680	ALA	2.1
1	A	701	SER	2.1
1	B	484	SER	2.1
1	A	539	TYR	2.1
1	B	456	HIS	2.1
1	B	752	GLU	2.1
1	B	467	PRO	2.1
1	C	459	TRP	2.1
1	A	491	ALA	2.0
1	A	591	LEU	2.0
1	A	724	HIS	2.0
1	A	583	PHE	2.0
1	A	595	TYR	2.0
1	A	672	LYS	2.0
1	C	539	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	470	ILE	2.0
1	C	508	ILE	2.0
1	C	640	GLY	2.0
1	C	659	GLY	2.0
1	A	764	ASP	2.0
1	B	493	LEU	2.0
1	B	775	LEU	2.0
1	C	630	LEU	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, 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.

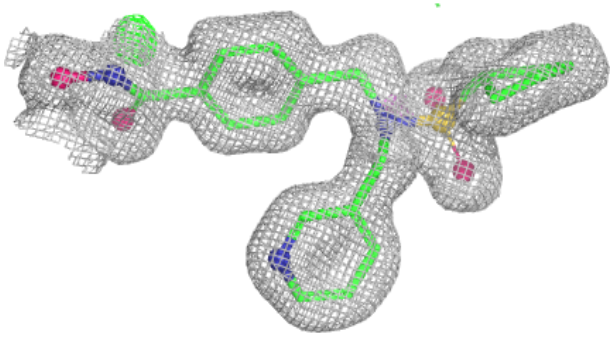
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	B	801	1/1	0.55	0.43	121,121,121,121	0
3	A1BHW	A	802	27/27	0.94	0.10	13,16,21,22	0
3	A1BHW	B	802	27/27	0.95	0.10	13,17,24,37	0
3	A1BHW	C	802	27/27	0.95	0.10	13,18,25,43	0
4	K	C	803	1/1	0.97	0.19	13,13,13,13	1
4	K	B	803	1/1	0.98	0.16	12,12,12,12	1
4	K	A	803	1/1	0.99	0.07	15,15,15,15	1
4	K	A	804	1/1	0.99	0.07	18,18,18,18	0
2	ZN	C	801	1/1	0.99	0.07	24,24,24,24	0
4	K	B	804	1/1	0.99	0.07	14,14,14,14	1
2	ZN	A	801	1/1	0.99	0.03	18,18,18,18	0

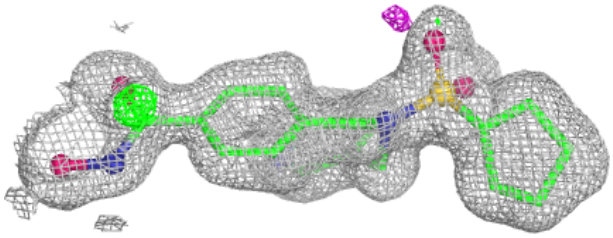
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

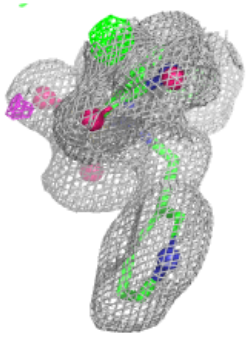
orientation to approximate a three-dimensional view.

Electron density around A1BHW A 802:

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

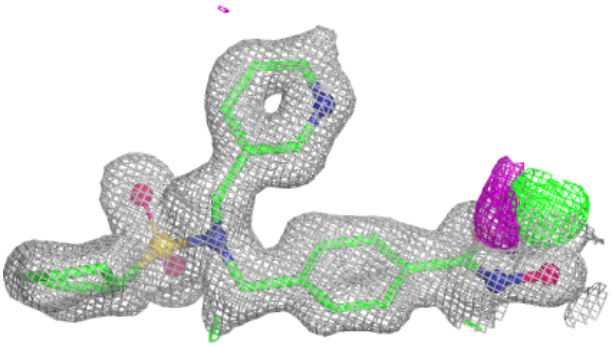


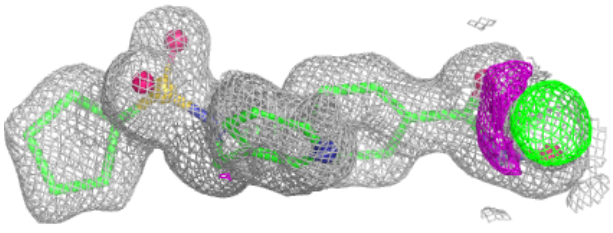


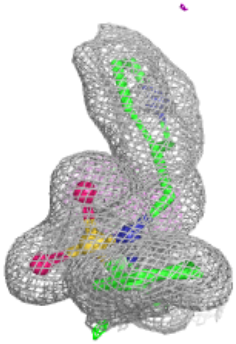


Electron density around A1BHW B 802:

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

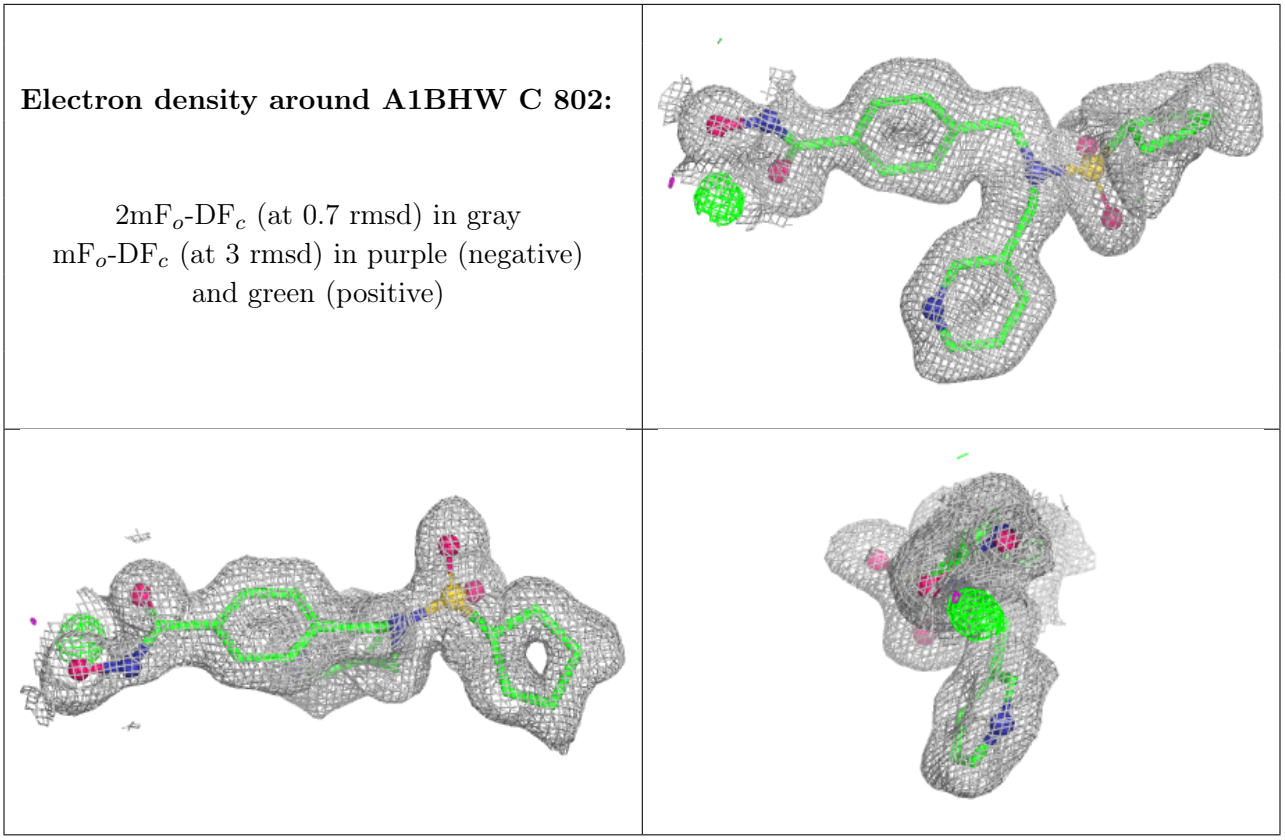






Electron density around A1BHW C 802:

$2mF_o$-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.