Full wwPDB X-ray Structure Validation Report (i)

May 23, 2020 – 10:16 am BST

PDB ID : 4CBT

Title : Design, synthesis, and biological evaluation of potent and selective Class IIa HDAC inhibitors as a potential therapy for Huntington's disease

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Deposited on : 2013-10-16

Resolution : 3.03 Å(reported)

The following versions of software and data (see references (i)) 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 (i)

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

The reported resolution of this entry is 3.03 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.
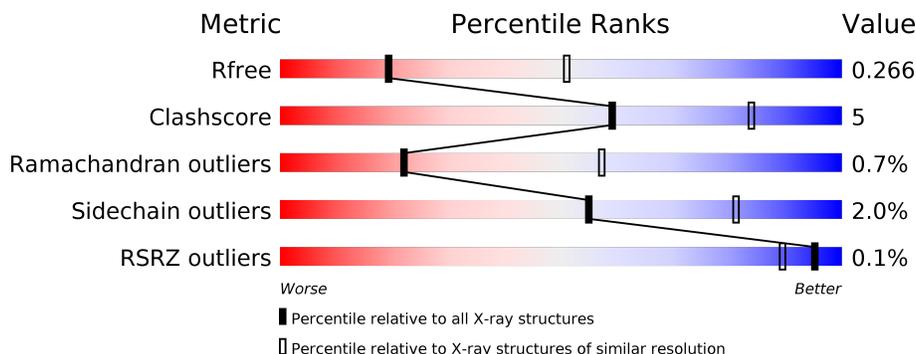
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

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 <=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	395	77% 12% 12%
1	B	395	79% 10% • 11%
1	C	395	75% 12% • 12%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7993 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 HISTONE DEACETYLASE 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	0	0
			2638	1660	465	494	19			
1	B	352	Total	C	N	O	S	0	0	0
			2645	1666	461	499	19			
1	C	346	Total	C	N	O	S	0	0	0
			2616	1650	462	485	19			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	645	MET	-	expression tag	UNP P56524
A	646	GLY	-	expression tag	UNP P56524
A	647	SER	-	expression tag	UNP P56524
A	1034	HIS	-	expression tag	UNP P56524
A	1035	HIS	-	expression tag	UNP P56524
A	1036	HIS	-	expression tag	UNP P56524
A	1037	HIS	-	expression tag	UNP P56524
A	1038	HIS	-	expression tag	UNP P56524
A	1039	HIS	-	expression tag	UNP P56524
B	645	MET	-	expression tag	UNP P56524
B	646	GLY	-	expression tag	UNP P56524
B	647	SER	-	expression tag	UNP P56524
B	1035	HIS	-	expression tag	UNP P56524
B	1036	HIS	-	expression tag	UNP P56524
B	1037	HIS	-	expression tag	UNP P56524
B	1038	HIS	-	expression tag	UNP P56524
B	1039	HIS	-	expression tag	UNP P56524
B	1040	HIS	-	expression tag	UNP P56524
C	645	MET	-	expression tag	UNP P56524
C	646	GLY	-	expression tag	UNP P56524
C	647	SER	-	expression tag	UNP P56524
C	1034	HIS	-	expression tag	UNP P56524
C	1035	HIS	-	expression tag	UNP P56524

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1036	HIS	-	expression tag	UNP P56524
C	1037	HIS	-	expression tag	UNP P56524
C	1038	HIS	-	expression tag	UNP P56524
C	1039	HIS	-	expression tag	UNP P56524

- Molecule 2 is (1R,2R,3R)-2-[4-(5-fluoranylpyrimidin-2-yl)phenyl]-N-oxidanyl-3-phenyl-cyclo propane-1-carboxamide (three-letter code: 9F4) (formula: $C_{20}H_{16}FN_3O_2$).
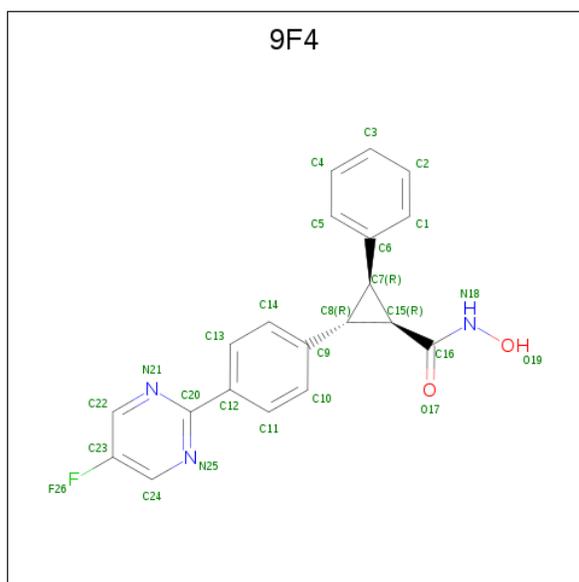
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			26	20	1	3	2		
2	B	1	Total	C	F	N	O	0	0
			26	20	1	3	2		
2	C	1	Total	C	F	N	O	0	0
			26	20	1	3	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is water.

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

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: HISTONE DEACETYLASE 4

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4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	104.41Å 104.41Å 88.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	90.42 – 3.03 90.42 – 3.03	Depositor EDS
% Data completeness (in resolution range)	100.0 (90.42-3.03) 99.8 (90.42-3.03)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.51 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.211 , 0.273 0.211 , 0.266	Depositor DCC
R_{free} test set	1070 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	47.8	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 24.0	EDS
L-test for twinning[2]	$<|L|> = 0.48$, $<L^2> = 0.31$	Xtriage
Estimated twinning fraction	0.011 for -h,-k,l 0.049 for h,-h-k,-l 0.032 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	7993	wwPDB-VP
Average B, all atoms (Å^2)	38.0	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 22.14 % 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 6.0533e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 9F4, 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	0.48	0/2699	0.53	1/3661 (0.0%)
1	B	0.43	0/2707	0.53	2/3679 (0.1%)
1	C	0.52	0/2675	0.54	2/3628 (0.1%)
All	All	0.48	0/8081	0.53	5/10968 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	681	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	C	681	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	A	681	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	B	681	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	C	681	ARG	NE-CZ-NH2	-5.30	117.65	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	899	ASP	Peptide

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	2638	0	2554	25	0
1	B	2645	0	2550	22	0
1	C	2616	0	2537	26	0
2	A	26	0	12	0	0
2	B	26	0	13	0	0
2	C	26	0	12	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
4	A	5	0	0	0	0
4	B	4	0	0	0	0
4	C	1	0	0	0	0
All	All	7993	0	7678	73	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 5.

All (73) 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:785:VAL:HG21	1:B:969:VAL:HG23	1.51	0.91
1:B:785:VAL:HG21	1:B:969:VAL:CG2	2.02	0.88
1:A:825:LEU:HD22	1:A:831:VAL:HG21	1.68	0.73
1:B:916:MET:HE1	1:B:960:LEU:HD23	1.74	0.69
1:B:682:ILE:HD13	1:B:798:ARG:HG2	1.76	0.66
1:C:682:ILE:HD13	1:C:798:ARG:HG2	1.79	0.63
1:C:927:VAL:HB	1:C:968:ILE:HG22	1.80	0.63
1:C:657:VAL:HG12	1:C:795:ALA:HA	1.82	0.60
1:B:717:GLU:O	1:B:720:THR:HG22	2.02	0.59
1:A:892:MET:HE3	1:A:914:VAL:HG11	1.84	0.59
1:A:892:MET:CE	1:A:914:VAL:HG11	2.36	0.56
1:B:785:VAL:HG21	1:B:969:VAL:HG21	1.86	0.56
1:C:836:ILE:HG21	1:C:847:THR:HG21	1.86	0.56
1:B:782:VAL:CG1	1:B:825:LEU:HD11	2.36	0.55
1:C:886:VAL:HG12	1:C:1027:TYR:CE1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:864:ARG:CZ	1:A:898:LEU:HD11	2.36	0.55
1:C:688:ARG:HD2	1:C:982:CYS:HB3	1.89	0.53
1:B:892:MET:HE1	1:B:914:VAL:HG21	1.89	0.53
1:B:865:TYR:OH	1:B:876:ALA:HB2	2.09	0.52
1:A:858:LEU:HD12	1:A:888:PHE:O	2.10	0.52
1:C:711:LEU:HD11	1:C:772:ARG:HG2	1.91	0.52
1:A:682:ILE:HD13	1:A:798:ARG:HG2	1.93	0.51
1:A:711:LEU:HD11	1:A:772:ARG:HG2	1.92	0.51
1:A:916:MET:HE1	1:A:963:LEU:HD11	1.93	0.51
1:B:967:ARG:C	1:B:968:ILE:HD12	2.31	0.50
1:C:892:MET:HE2	1:C:1020:VAL:HG11	1.93	0.50
1:B:789:GLU:O	1:B:790:LEU:HD23	2.11	0.50
1:C:803:HIS:HD2	1:C:845:ASN:OD1	1.95	0.49
1:C:916:MET:HE2	1:C:916:MET:HA	1.94	0.49
1:B:916:MET:CE	1:B:963:LEU:HD11	2.43	0.48
1:A:865:TYR:CB	1:A:893:ALA:HB1	2.43	0.48
1:C:708:LEU:HD21	1:C:725:THR:HG23	1.95	0.48
1:B:907:TYR:CG	1:B:948:LEU:HD21	2.50	0.47
1:C:878:ASP:O	1:C:880:VAL:HG13	2.14	0.46
1:C:883:GLY:O	1:C:886:VAL:HG23	2.16	0.46
1:B:714:VAL:HG23	1:B:820:VAL:HG22	1.98	0.46
1:B:936:VAL:HG12	1:B:937:GLU:N	2.30	0.46
1:A:803:HIS:HB3	1:A:810:MET:HG3	1.97	0.45
1:C:682:ILE:HB	1:C:796:VAL:HG12	1.98	0.45
1:C:834:ILE:HB	1:C:857:VAL:HG22	1.99	0.45
1:C:697:LYS:HD2	1:C:993:LEU:HD13	1.99	0.45
1:A:795:ALA:HB1	1:A:797:VAL:HG13	1.98	0.45
1:C:714:VAL:HG22	1:C:823:LYS:HG3	1.99	0.44
1:A:911:PHE:CD1	1:A:956:LEU:HD22	2.52	0.44
1:A:659:ASP:HB3	1:A:773:LEU:HD21	2.00	0.44
1:B:916:MET:HE2	1:B:963:LEU:HD11	2.00	0.44
1:A:933:PHE:HB2	1:A:981:ILE:HG22	1.99	0.44
1:C:892:MET:HE3	1:C:914:VAL:HG11	2.00	0.43
1:A:911:PHE:CE1	1:A:956:LEU:HD22	2.53	0.43
1:A:760:THR:HG22	1:A:812:PHE:CD1	2.54	0.43
1:C:892:MET:CE	1:C:914:VAL:HG11	2.49	0.43
1:B:682:ILE:HG23	1:B:798:ARG:HD2	2.01	0.43
1:A:957:THR:O	1:A:961:MET:HE2	2.19	0.42
1:A:835:LEU:HD13	1:A:858:LEU:HD23	2.00	0.42
1:A:716:SER:O	1:A:720:THR:HG23	2.19	0.42
1:A:907:TYR:CD1	1:A:948:LEU:HD11	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:781:LEU:HD21	1:C:794:PHE:N	2.34	0.42
1:B:892:MET:HE1	1:B:914:VAL:CG2	2.50	0.42
1:C:878:ASP:HA	1:C:1023:ILE:HD13	2.02	0.42
1:A:898:LEU:CD1	1:A:898:LEU:N	2.83	0.41
1:C:899:ASP:CB	1:C:900:PRO:CD	2.98	0.41
1:B:843:HIS:HB2	1:B:863:HIS:CD2	2.55	0.41
1:A:960:LEU:HB3	1:A:968:ILE:HD12	2.02	0.41
1:B:911:PHE:CD1	1:B:956:LEU:HD22	2.56	0.41
1:C:663:LEU:HD22	1:C:679:ALA:HB1	2.03	0.41
1:C:659:ASP:CG	1:C:773:LEU:HD21	2.41	0.41
1:B:795:ALA:HB3	1:B:971:ALA:HA	2.01	0.41
1:A:659:ASP:CB	1:A:773:LEU:HD21	2.51	0.41
1:A:898:LEU:N	1:A:898:LEU:HD12	2.36	0.40
1:A:892:MET:CE	1:A:914:VAL:HG21	2.52	0.40
1:B:1001:LEU:HD12	1:B:1001:LEU:H	1.87	0.40
1:C:760:THR:HG22	1:C:812:PHE:HD1	1.85	0.40
1:C:977:ASP:HB3	1:C:980:ALA:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	343/395 (87%)	318 (93%)	23 (7%)	2 (1%)	25	60
1	B	346/395 (88%)	325 (94%)	18 (5%)	3 (1%)	17	52
1	C	336/395 (85%)	306 (91%)	28 (8%)	2 (1%)	25	60
All	All	1025/1185 (86%)	949 (93%)	69 (7%)	7 (1%)	22	57

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	652	PHE
1	C	900	PRO
1	A	942	PRO
1	B	994	GLY
1	A	941	THR
1	C	994	GLY
1	B	703	GLY

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	279/322 (87%)	273 (98%)	6 (2%)	52	79
1	B	280/322 (87%)	274 (98%)	6 (2%)	53	80
1	C	275/322 (85%)	270 (98%)	5 (2%)	59	83
All	All	834/966 (86%)	817 (98%)	17 (2%)	55	81

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	759	ASP
1	A	792	ASN
1	A	802	HIS
1	A	829	LEU
1	A	839	TRP
1	A	867	ASP
1	B	726	ASN
1	B	802	HIS
1	B	839	TRP
1	B	867	ASP
1	B	892	MET
1	B	911	PHE
1	C	688	ARG
1	C	802	HIS
1	C	808	THR
1	C	839	TRP

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Mol	Chain	Res	Type
1	C	934	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	678	HIS
1	A	792	ASN
1	A	995	ASN
1	B	683	GLN
1	B	712	GLN
1	B	843	HIS
1	B	869	ASN
1	B	947	ASN
1	B	995	ASN
1	C	803	HIS
1	C	843	HIS
1	C	863	HIS
1	C	1006	GLN
1	C	1032	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 6 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	#$|Z| > 2$
2	9F4	A	2035	3	29,29,29	0.91	2 (6%)	39,41,41	1.03	4 (10%)
2	9F4	B	2034	3	29,29,29	0.85	2 (6%)	39,41,41	0.88	1 (2%)
2	9F4	C	2035	3	29,29,29	0.87	2 (6%)	39,41,41	0.94	3 (7%)

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	9F4	A	2035	3	-	6/18/27/27	0/4/4/4
2	9F4	B	2034	3	-	1/18/27/27	0/4/4/4
2	9F4	C	2035	3	-	2/18/27/27	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2035	9F4	C16-N18	2.53	1.37	1.33
2	C	2035	9F4	C15-C16	-2.44	1.47	1.51
2	A	2035	9F4	C15-C16	-2.37	1.47	1.51
2	C	2035	9F4	C16-N18	2.27	1.36	1.33
2	B	2034	9F4	C15-C16	-2.23	1.47	1.51
2	B	2034	9F4	C16-N18	2.19	1.36	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2034	9F4	C23-C22-N21	3.20	123.38	121.46
2	A	2035	9F4	C6-C7-C8	-3.08	114.14	121.82
2	A	2035	9F4	C23-C22-N21	2.86	123.18	121.46
2	C	2035	9F4	C23-C22-N21	2.84	123.17	121.46
2	C	2035	9F4	C23-C24-N25	2.53	122.98	121.46
2	A	2035	9F4	C23-C24-N25	2.50	122.96	121.46
2	C	2035	9F4	C6-C7-C8	-2.37	115.90	121.82
2	A	2035	9F4	C6-C7-C15	2.04	125.82	121.78

There are no chirality outliers.

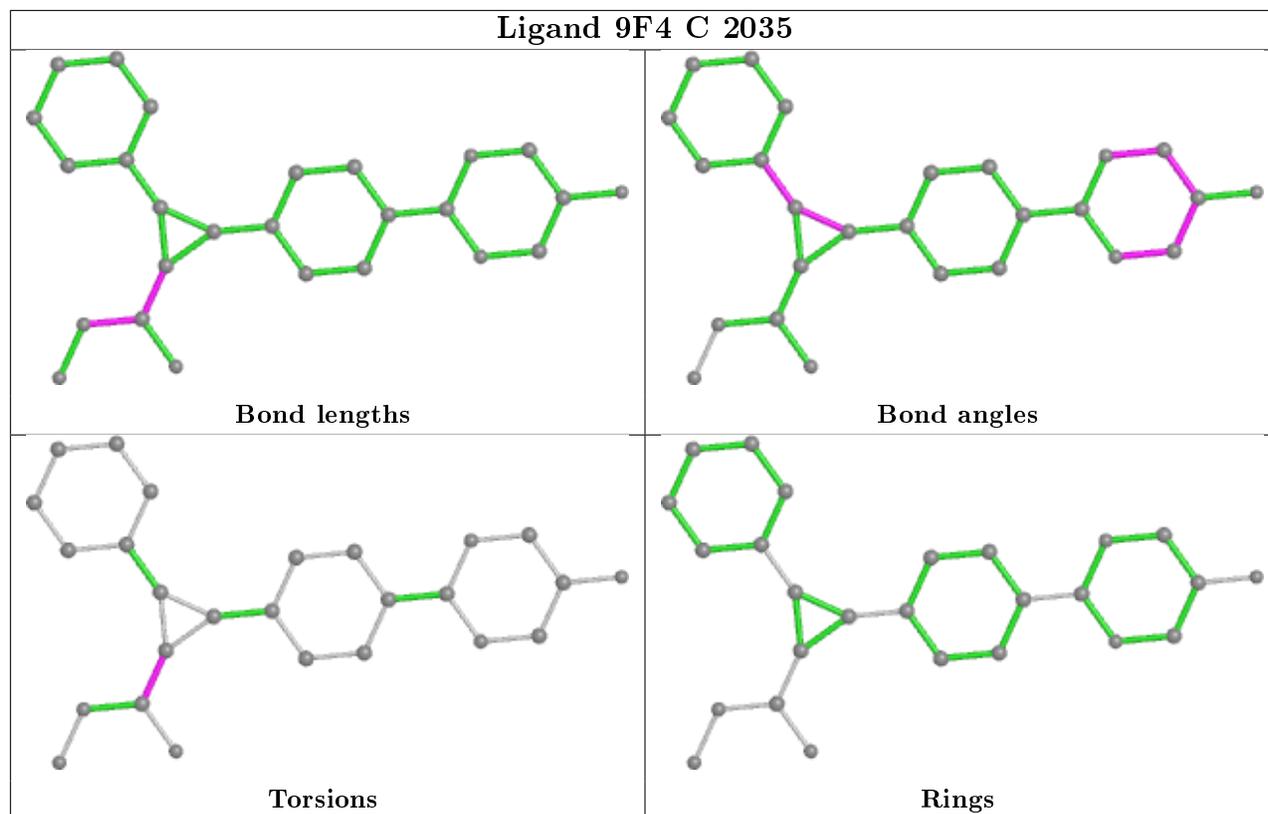All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2034	9F4	C7-C15-C16-O17
2	C	2035	9F4	C7-C15-C16-N18
2	C	2035	9F4	C7-C15-C16-O17
2	A	2035	9F4	C7-C15-C16-N18
2	A	2035	9F4	C7-C15-C16-O17
2	A	2035	9F4	C11-C12-C20-N21
2	A	2035	9F4	C13-C12-C20-N21
2	A	2035	9F4	C11-C12-C20-N25
2	A	2035	9F4	C13-C12-C20-N25

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 9F4 A 2035

Bond lengths

Bond angles

Torsions

Rings

Ligand 9F4 B 2034

Bond lengths

Bond angles

Torsions

Rings

Ligand 9F4 C 2035

Bond lengths

Bond angles

Torsions

Rings
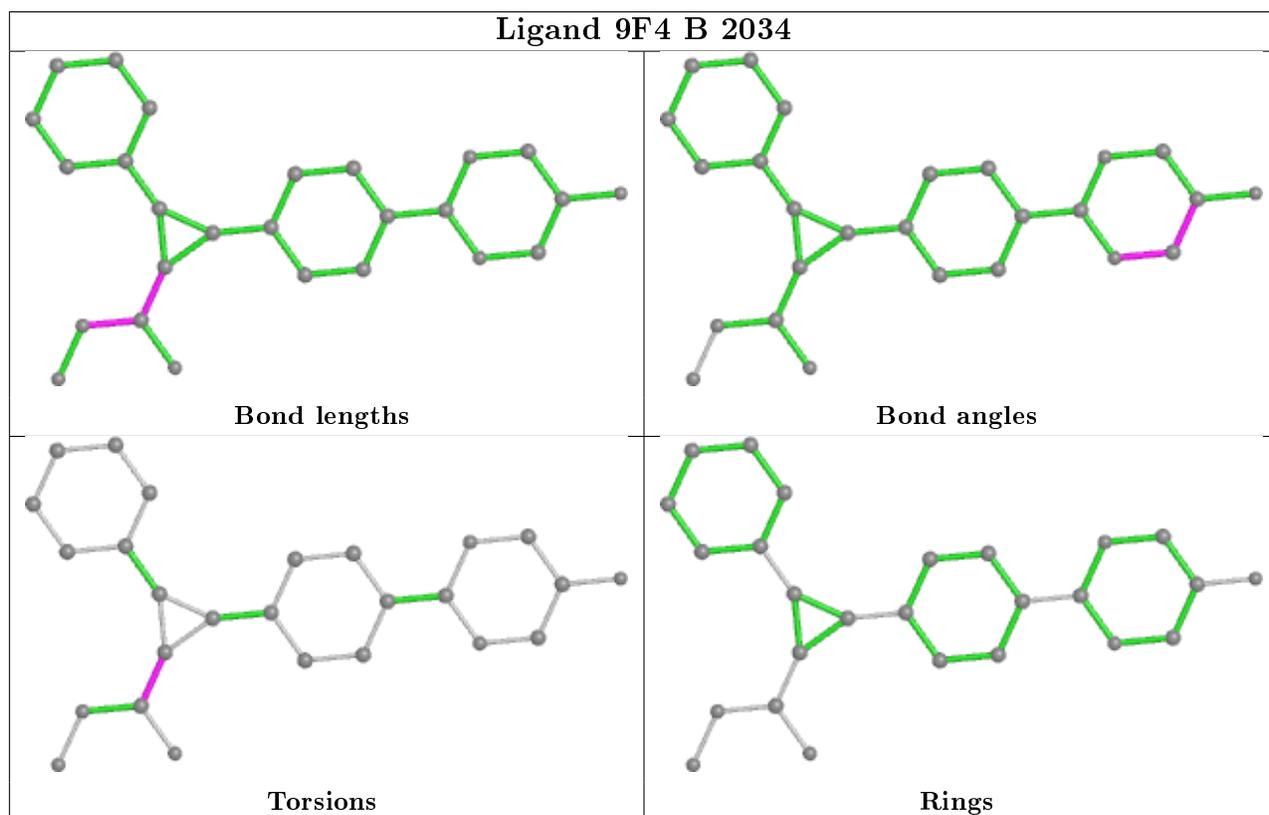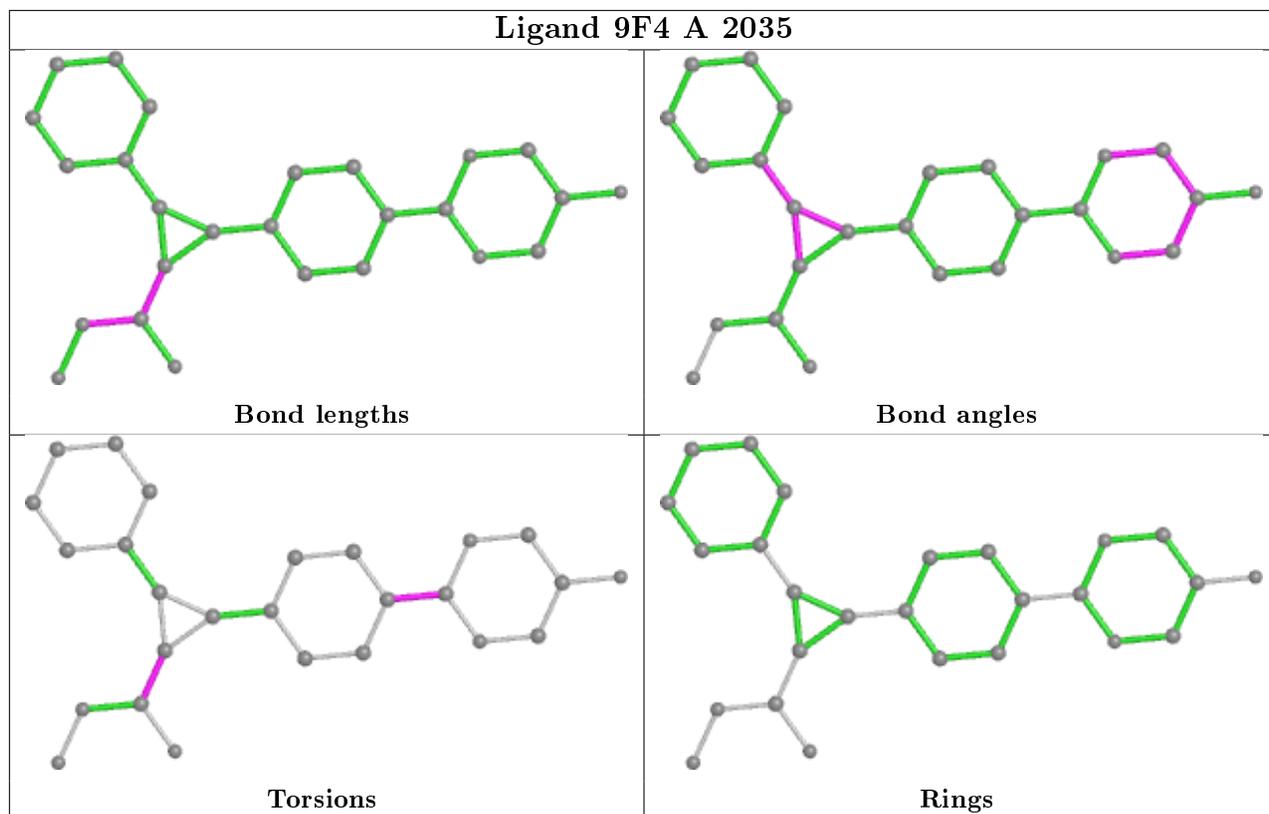
5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	349/395 (88%)	-0.38	1 (0%)	94	83	23, 36, 50, 62	0
1	B	352/395 (89%)	-0.51	0	100	100	24, 34, 46, 48	0
1	C	346/395 (87%)	-0.30	0	100	100	30, 43, 61, 70	0
All	All	1047/1185 (88%)	-0.40	1 (0%)	95	89	23, 38, 54, 70	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	726	ASN	2.2

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 carbohydrates 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.
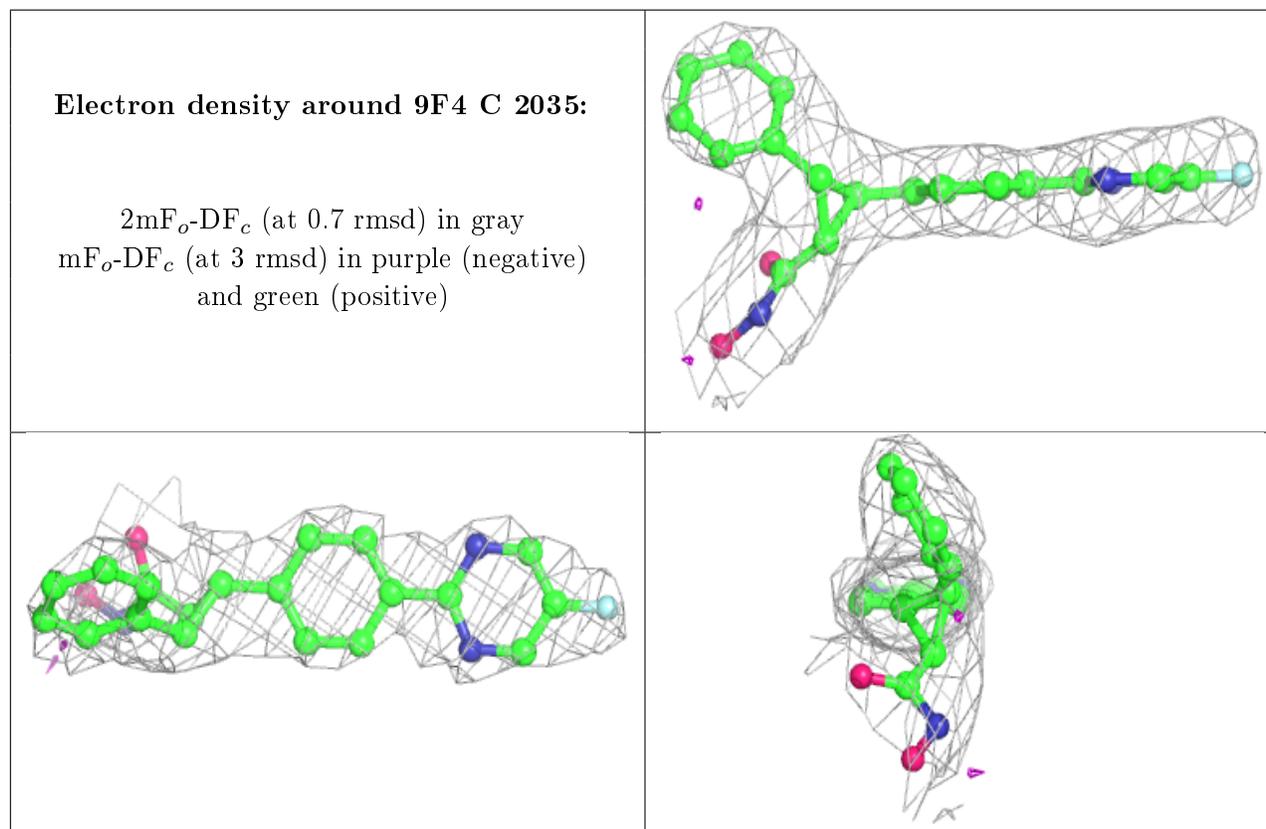
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
2	9F4	C	2035	26/26	0.95	0.23	33,35,38,38	0
3	ZN	B	2036	1/1	0.95	0.10	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	9F4	A	2035	26/26	0.96	0.27	30,31,33,34	0
2	9F4	B	2034	26/26	0.97	0.20	27,28,33,34	0
3	ZN	C	2036	1/1	0.97	0.11	33,33,33,33	0
3	ZN	B	2035	1/1	0.97	0.11	25,25,25,25	0
3	ZN	C	2037	1/1	0.97	0.07	45,45,45,45	0
3	ZN	A	2037	1/1	0.98	0.07	40,40,40,40	0
3	ZN	A	2036	1/1	0.99	0.07	28,28,28,28	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.
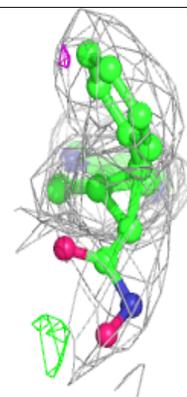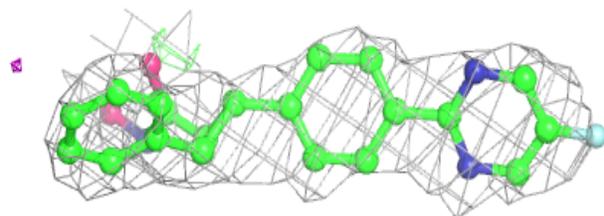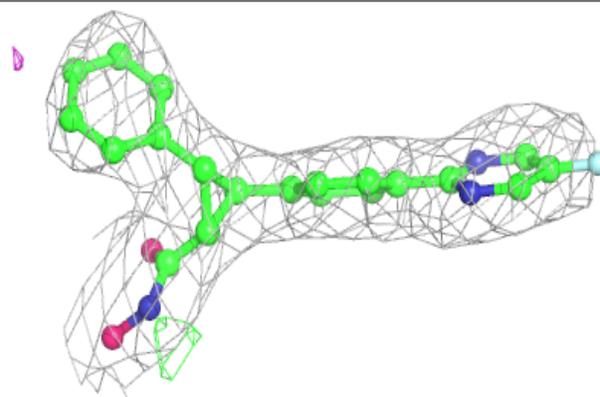
Electron density around 9F4 C 2035:

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

Electron density around 9F4 A 2035:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
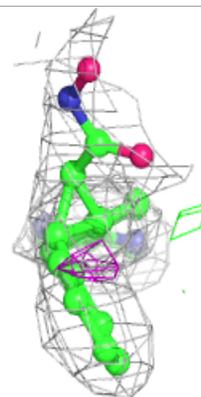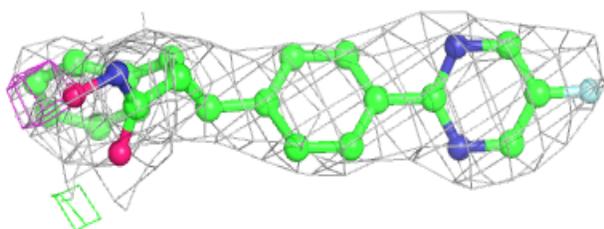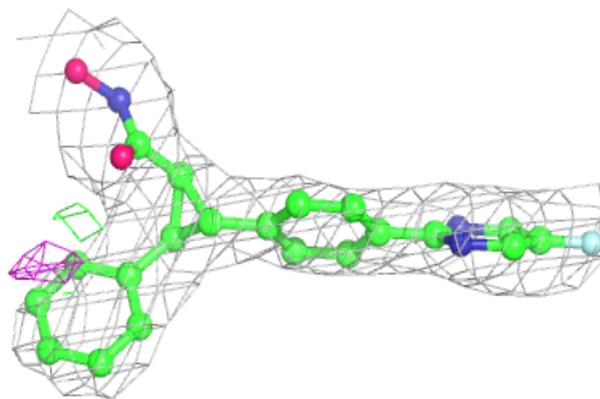
Electron density around 9F4 B 2034:

$2mF_o$-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.