Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2026 – 10:14 AM EST

PDB ID	:	36KM / pdb_000036km
Title	:	Crystal structure of Danio rerio histone deacetylase 6 catalytic domain 2 in complex with spirocyclic inhibitor 15
Authors	:	Eafa, A.; Goulart Stollmaier, J.; Christianson, D.W.
Deposited on	:	2026-06-15
Resolution	:	2.07 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

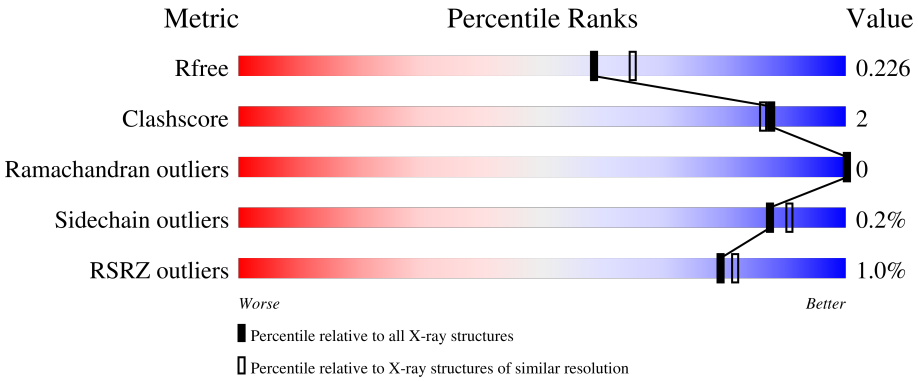
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.07 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	1081	31% · 67%
1	B	1081	31% · 67%

2 Entry composition

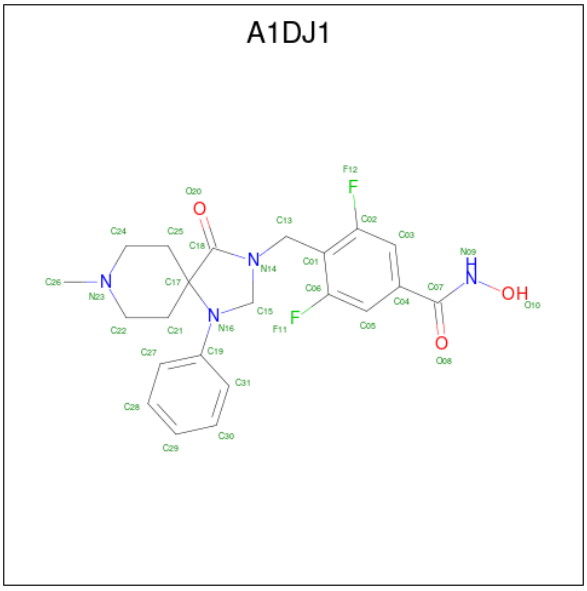
There are 6 unique types of molecules in this entry. The entry contains 11099 atoms, of which 5233 are hydrogens and 0 are deuteriums.

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 Protein deacetylase HDAC6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	352	Total	C	H	N	O	S	0	0	0
			5310	1714	2584	486	508	18			
1	B	353	Total	C	H	N	O	S	0	0	0
			5324	1718	2589	490	509	18			

- Molecule 2 is 3,5-difluoro-N-hydroxy-4-[(8-methyl-4-oxo-1-phenyl-1,3,8-triazaspiro[4.5]decan-3-yl)methyl]benzamide (CCD ID: A1DJ1) (formula: $C_{22}H_{24}F_2N_4O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	H	N	O	0	0
			55	22	2	24	4	3		
2	B	1	Total	C	F	H	N	O	0	0
			55	22	2	24	4	3		

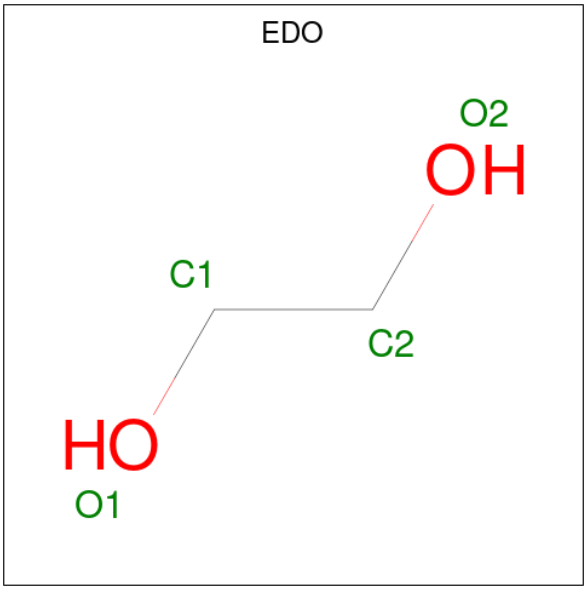
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is POTASSIUM ION (CCD ID: 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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C H O 10 2 6 2	0	0
5	B	1	Total C H O 10 2 6 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	162	Total O 162 162	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	167	Total 167	O 167	0	0

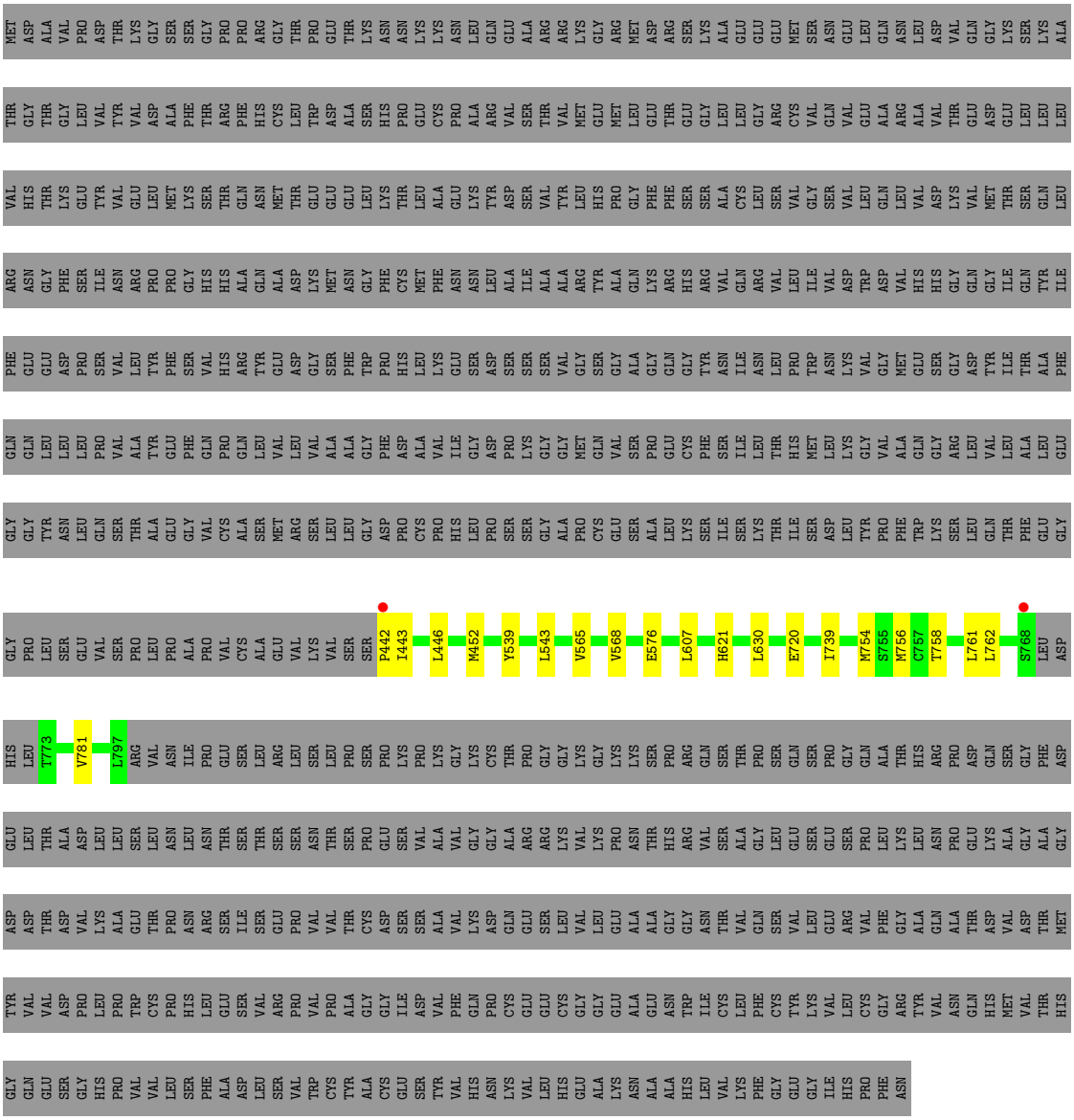
3 Residue-property plots (i)

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: Protein deacetylase HDAC6

Chain A:

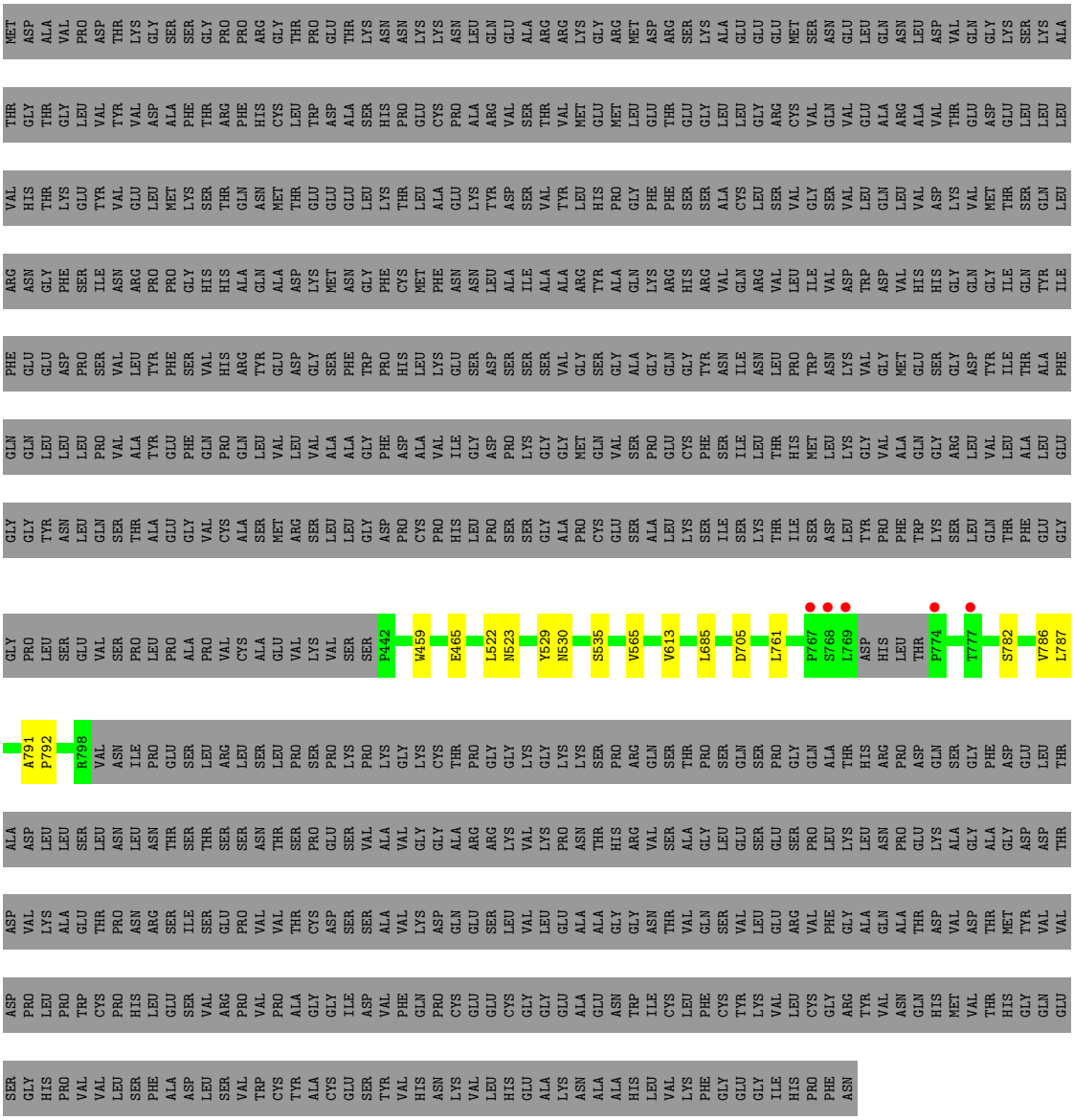




- Molecule 1: Protein deacetylase HDAC6

Chain B:


31%
67%


MET ASP ALA VAL PRO ASP THR LYS GLY SER SER GLY PRO PRO ARG GLY THR PRO GLU THR LYS ASN ASN LYS LYS ASN LEU GLN GLU ALA ARG ARG LYS GLY ARG MET ASP ARG SER LYS ALA GLU GLU GLU MET SER ASN GLU LEU GLN ASN LEU ASP VAL GLN GLY LYS SER LYS ALA
THR GLY THR GLY LEU VAL TYR VAL ASP ALA PHE THR ARG PHE HIS CYS LEU TRP ASP ALA SER HIS PRO GLU CYS PRO ALA ARG VAL SER THR VAL MET GLU MET LEU GLU THR GLU GLY LEU LEU GLY ARG CYS VAL GLN VAL GLU ALA ARG ALA VAL THR GLU ASP GLU LEU LEU LEU
VAL HIS THR LYS GLU TYR VAL GLU LEU MET LYS SER THR GLN ASN MET THR GLU GLU GLU LEU LYS THR LEU ALA GLU GLN LYS TYR ASP SER VAL TYR LEU HIS PRO GLY PHE PHE SER SER ALA CYS LEU SER VAL GLY SER VAL LEU GLN LEU VAL ASP LYS VAL MET THR SER GLN LEU
ARG ASN GLY PHE SER ILE ASN ARG PRO PRO GLY HIS HIS ALA GLN ALA ASP LYS MET ASN GLY PHE CYS MET PHE ASN ASN LEU ALA ILE ALA ARG TYR ALA VAL GLY SER ASP SER SER VAL GLY SER GLY ALA GLN LYS ARG HIS ARG VAL GLN ARG VAL LEU LEU ILE VAL ASP TRP ASP VAL HIS HIS GLY GLN GLY ILE GLN TYR ILE
PHE GLU GLU ASP PRO SER VAL LEU TYR PHE SER VAL HIS ARG TYR GLU ASP GLY SER PHE TRP PRO HIS LEU LYS GLU SER ASP SER SER SER VAL GLY SER GLY ALA GLY GLN GLY TYR ASN ILE ASN LEU PRO TRP ASN LYS VAL GLY MET GLU SER GLY ASP TYR THR ILE THR ALA PHE
GLN GLN LEU LEU LEU PRO VAL ALA TYR GLU PHE GLN PRO GLN LEU VAL LEU VAL ALA ALA GLY PHE ASP ALA VAL ILE GLY ASP PRO LYS GLY GLY GLY MET GLN VAL SER PRO GLU CYS PHE SER ILE LEU SER LYS THR HIS MET LEU LYS GLY VAL ALA GLN GLY SER LEU GLU
GLY GLY TYR ASN LEU GLN SER THR ALA GLU GLY VAL CYS ALA SER MET ARG SER LEU LEU GLY ASP PRO CYS PRO HIS LEU PRO SER SER GLY ALA PRO CYS GLU SER ILE SER LYS THR ILE SER ASP LEU TYR PRO PHE TRP LYS SER LEU GLN THR PHE GLU GLY
GLY PRO LEU SER GLU VAL SER PRO LEU PRO ALA PRO VAL CYS ALA GLU VAL LYS VAL SER SER P442 W459 E465 L522 N523 Y529 N530 S535 V565 V613 L685 D705 L761 P767 S768 L769 ASP HIS LEU THR P774 T777 S782 V786 L787
A791 P792 R798 VAL ASN ILE PRO GLU SER LEU ARG LEU SER LEU PRO SER PRO LYS PRO LYS GLY GLY LYS CYS THR PRO GLY GLY LYS GLY LYS LYS SER PRO ARG GLN SER THR PRO SER GLN SER PRO GLY GLN ALA THR HIS ARG PRO ASP GLN SER GLY PHE ASP GLU LEU THR
ALA ASP LEU LEU SER LEU ASN LEU ASN THR SER THR SER SER ASN THR SER PRO GLU SER VAL ALA VAL GLY GLY ALA ARG ARG LYS VAL LYS PRO ASN THR HIS ARG VAL SER ALA GLY LEU GLU SER GLU SER PRO LEU LYS LEU ASN PRO GLU LYS ALA GLY ASP ASP THR
ASP VAL LYS ALA THR PRO VAL ASN ARG SER ILE SER GLU PRO VAL THR CYS ASP SER SER ALA VAL LYS ASP GLN GLU SER LEU VAL LEU GLU GLU ALA ALA GLY GLY ASN THR VAL GLN SER VAL LEU GLU ARG VAL PHE GLY ALA GLN ALA THR ASP VAL ASP THR MET TYR VAL VAL
ASP PRO LEU PRO TRP CYS PRO HIS LEU GLU GLU SER VAL ARG PRO VAL PRO ALA GLY GLY ILE ASP VAL PHE GLN PRO CYS GLU GLU CYS GLY GLY GLU ALA LYS ASN ALA GLU ASN TRP ILE CYS LEU PHE CYS TYR LYS VAL LEU CYS GLY GLY TYR VAL ASN GLN HIS MET VAL THR HIS GLY GLN GLU
SER GLY HIS PRO VAL VAL LEU SER PHE ALA ASP LEU SER VAL TRP CYS TYR ALA CYS GLU SER TYR VAL HIS ASN LYS VAL LEU HIS GLU ALA LYS ASN ALA ALA HIS LEU VAL LYS PHE GLY GLU GLY ILE HIS PRO PHE ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	48.00Å 55.00Å 75.47Å 69.30° 87.83° 84.09°	Depositor
Resolution (Å)	29.45 – 2.07 29.45 – 2.07	Depositor EDS
% Data completeness (in resolution range)	94.8 (29.45-2.07) 94.8 (29.45-2.07)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.186 , 0.225 0.187 , 0.226	Depositor DCC
R_{free} test set	2003 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å^2)	15.4	Xtriage
Anisotropy	0.615	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 28.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.001 for -h,-k,-k+l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11099	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: ZN, K, EDO, A1DJ1

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	0.30	0/2794	0.40	0/3792
1	B	0.29	0/2802	0.40	0/3801
All	All	0.30	0/5596	0.40	0/7593

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	2726	2584	2617	13	0
1	B	2735	2589	2625	9	0
2	A	31	24	0	0	0
2	B	31	24	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	B	8	12	12	1	0
6	A	162	0	0	0	0
6	B	167	0	0	0	0
All	All	5866	5233	5254	22	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 (22) 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:459:TRP:CZ2	1:B:523:ASN:HB2	2.35	0.61
1:A:565:VAL:CG2	1:A:754:MET:HE2	2.35	0.57
1:A:781:VAL:HG22	5:B:1102:EDO:H21	1.91	0.51
1:A:758:THR:O	1:A:762:LEU:HD23	2.12	0.49
1:B:565:VAL:CG1	1:B:761:LEU:HD12	2.44	0.48
1:A:452:MET:HE1	1:A:568:VAL:HG12	1.96	0.48
1:B:522:LEU:HD13	1:B:535:SER:HA	1.96	0.47
1:B:685:LEU:HD21	1:B:787:LEU:HG	1.96	0.47
1:A:758:THR:HG22	1:A:762:LEU:HD23	1.97	0.47
1:A:442:PRO:C	1:A:443:ILE:HD12	2.39	0.47
1:A:739:ILE:HD12	1:A:761:LEU:HD11	1.96	0.46
1:B:782:SER:O	1:B:786:VAL:HG23	2.16	0.46
1:A:443:ILE:HD12	1:A:443:ILE:N	2.31	0.45
1:A:607:LEU:HD13	1:A:630:LEU:HD23	2.01	0.43
1:B:565:VAL:HG13	1:B:761:LEU:HD12	2.01	0.43
1:B:791:ALA:N	1:B:792:PRO:CD	2.82	0.43
1:A:446:LEU:C	1:A:446:LEU:HD23	2.44	0.42
1:B:613:VAL:HG12	1:B:705:ASP:CG	2.45	0.42
1:A:720:GLU:HA	1:A:756:MET:HE3	2.02	0.42
1:B:529:TYR:O	1:B:530:ASN:HB2	2.20	0.41
1:A:576:GLU:CD	1:A:621:HIS:HD1	2.28	0.41
1:A:539:TYR:CZ	1:A:543:LEU:HD11	2.55	0.41

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	348/1081 (32%)	336 (97%)	12 (3%)	0	100	100
1	B	349/1081 (32%)	340 (97%)	9 (3%)	0	100	100
All	All	697/2162 (32%)	676 (97%)	21 (3%)	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	291/915 (32%)	291 (100%)	0	100	100
1	B	291/915 (32%)	290 (100%)	1 (0%)	86	89
All	All	582/1830 (32%)	581 (100%)	1 (0%)	87	91

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	465	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	487	HIS
1	A	727	HIS
1	B	450	GLN
1	B	462	HIS
1	B	554	GLN
1	B	645	ASN
1	B	727	HIS

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 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
5	EDO	B	1103	-	3,3,3	0.47	0	2,2,2	0.52	0
2	A1DJ1	A	1101	3	33,34,34	3.88	9 (27%)	48,50,50	3.02	18 (37%)
5	EDO	B	1102	-	3,3,3	0.45	0	2,2,2	0.25	0
2	A1DJ1	B	1101	3	33,34,34	4.66	8 (24%)	48,50,50	5.53	22 (45%)

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
5	EDO	B	1103	-	-	1/1/1/1	-
2	A1DJ1	A	1101	3	-	4/14/46/46	0/4/4/4
5	EDO	B	1102	-	-	0/1/1/1	-
2	A1DJ1	B	1101	3	-	3/14/46/46	0/4/4/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	A1DJ1	C21-C17	-14.52	1.38	1.54
2	B	1101	A1DJ1	C25-C17	-13.05	1.40	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	A1DJ1	C26-N23	-11.00	1.20	1.46
2	B	1101	A1DJ1	C26-N23	-10.80	1.20	1.46
2	B	1101	A1DJ1	C07-N09	10.61	1.46	1.32
2	A	1101	A1DJ1	C07-N09	10.24	1.45	1.32
2	A	1101	A1DJ1	C25-C17	-8.51	1.45	1.54
2	A	1101	A1DJ1	C21-C17	-7.36	1.46	1.54
2	B	1101	A1DJ1	C18-N14	-7.32	1.28	1.34
2	A	1101	A1DJ1	C18-N14	-7.06	1.28	1.34
2	A	1101	A1DJ1	C17-N16	6.44	1.54	1.48
2	B	1101	A1DJ1	C15-N14	5.24	1.55	1.45
2	A	1101	A1DJ1	C15-N14	4.80	1.54	1.45
2	A	1101	A1DJ1	O20-C18	-2.61	1.18	1.22
2	A	1101	A1DJ1	C19-N16	2.60	1.47	1.41
2	B	1101	A1DJ1	O20-C18	-2.33	1.18	1.22
2	B	1101	A1DJ1	O08-C07	-2.23	1.18	1.23

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1101	A1DJ1	C25-C24-N23	-24.74	93.29	110.81
2	B	1101	A1DJ1	C21-C22-N23	-12.07	102.26	110.81
2	B	1101	A1DJ1	C21-C17-N16	-10.77	105.22	112.87
2	B	1101	A1DJ1	C25-C17-N16	10.08	120.03	112.87
2	B	1101	A1DJ1	C24-C25-C17	9.88	121.43	113.05
2	A	1101	A1DJ1	C21-C17-N16	8.90	119.19	112.87
2	B	1101	A1DJ1	C15-N16-C17	-8.18	104.46	111.64
2	A	1101	A1DJ1	C03-C02-C01	-7.47	118.89	124.45
2	B	1101	A1DJ1	C05-C06-C01	-7.13	119.14	124.45
2	A	1101	A1DJ1	C15-N16-C17	-7.12	105.39	111.64
2	B	1101	A1DJ1	C01-C13-N14	6.73	123.34	112.55
2	A	1101	A1DJ1	C25-C17-N16	6.26	117.32	112.87
2	B	1101	A1DJ1	C15-N16-C19	6.26	128.99	118.74
2	A	1101	A1DJ1	C05-C06-C01	-6.10	119.92	124.45
2	A	1101	A1DJ1	C24-C25-C17	-5.86	108.09	113.05
2	B	1101	A1DJ1	C03-C02-C01	-5.83	120.11	124.45
2	A	1101	A1DJ1	C06-C01-C02	4.71	120.89	114.54
2	B	1101	A1DJ1	C18-C17-N16	4.67	109.04	101.66
2	B	1101	A1DJ1	C17-N16-C19	-4.26	120.94	127.02
2	B	1101	A1DJ1	C06-C01-C02	4.25	120.27	114.54
2	A	1101	A1DJ1	C21-C17-C18	-3.57	98.98	108.61
2	A	1101	A1DJ1	C25-C17-C18	-3.53	99.11	108.61
2	A	1101	A1DJ1	C15-N16-C19	3.18	123.95	118.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1101	A1DJ1	C25-C17-C21	-3.09	107.59	110.86
2	B	1101	A1DJ1	C26-N23-C22	-3.08	104.77	110.63
2	A	1101	A1DJ1	F12-C02-C01	2.89	121.25	117.64
2	B	1101	A1DJ1	C15-N14-C18	-2.87	110.64	113.53
2	B	1101	A1DJ1	C22-N23-C24	-2.85	104.99	109.54
2	A	1101	A1DJ1	C13-N14-C15	2.78	126.81	121.65
2	A	1101	A1DJ1	C13-N14-C18	-2.59	121.26	123.43
2	A	1101	A1DJ1	C17-N16-C19	2.54	130.65	127.02
2	B	1101	A1DJ1	C13-N14-C15	2.50	126.28	121.65
2	B	1101	A1DJ1	F11-C06-C01	2.40	120.63	117.64
2	A	1101	A1DJ1	C21-C22-N23	-2.38	109.12	110.81
2	B	1101	A1DJ1	C26-N23-C24	-2.35	106.16	110.63
2	A	1101	A1DJ1	C04-C07-N09	2.32	119.84	116.26
2	B	1101	A1DJ1	O10-N09-C07	2.32	125.53	119.73
2	A	1101	A1DJ1	C18-C17-N16	2.25	105.21	101.66
2	B	1101	A1DJ1	C25-C17-C18	-2.18	102.74	108.61
2	A	1101	A1DJ1	O08-C07-N09	-2.08	119.08	122.90

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	A1DJ1	C31-C19-N16-C17
2	A	1101	A1DJ1	C31-C19-N16-C15
2	A	1101	A1DJ1	C27-C19-N16-C17
2	A	1101	A1DJ1	C27-C19-N16-C15
2	B	1101	A1DJ1	C27-C19-N16-C17
2	B	1101	A1DJ1	C27-C19-N16-C15
2	B	1101	A1DJ1	C31-C19-N16-C17
5	B	1103	EDO	O1-C1-C2-O2

There are no ring outliers.

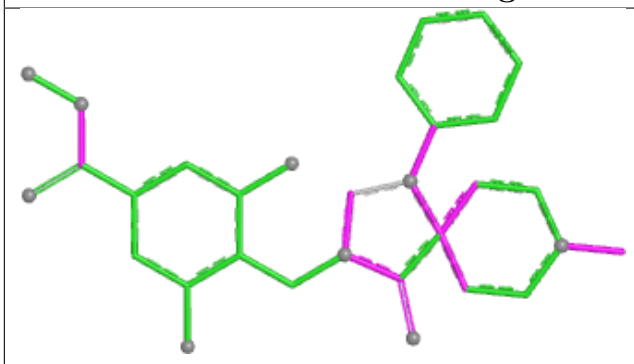
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1102	EDO	1	0

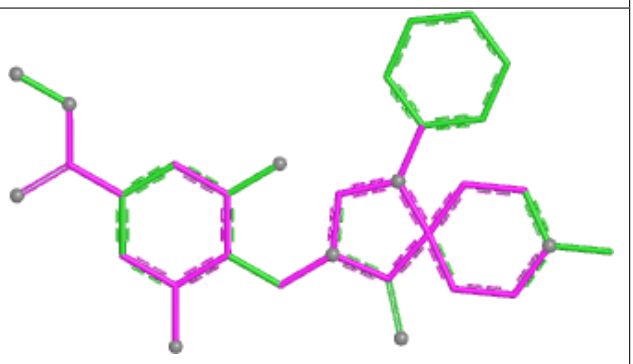
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

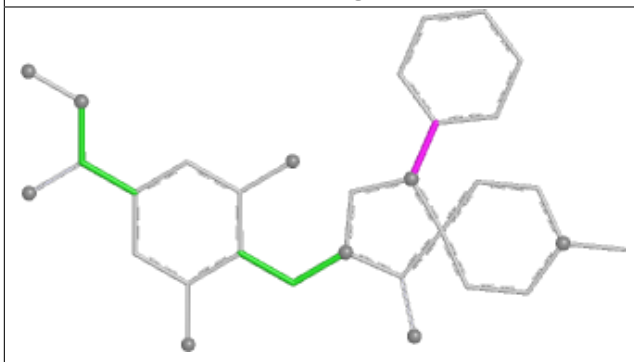
Ligand A1DJ1 A 1101



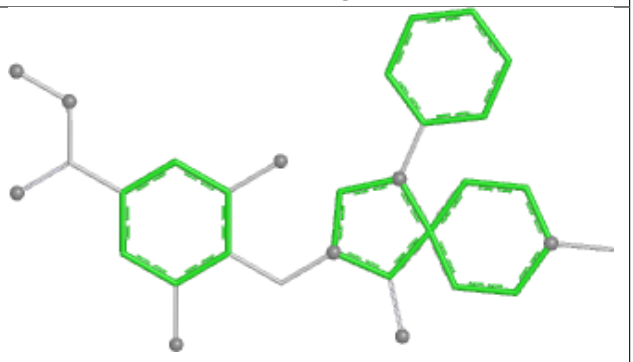
Bond lengths



Bond angles

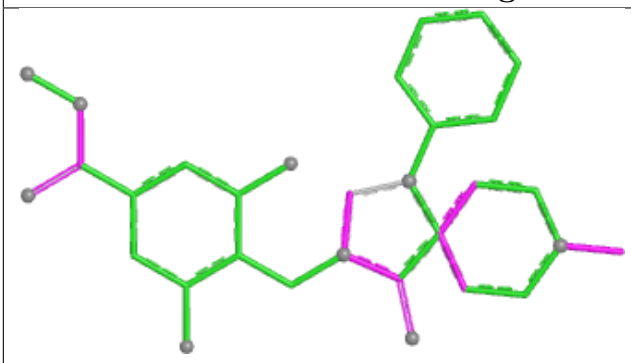


Torsions

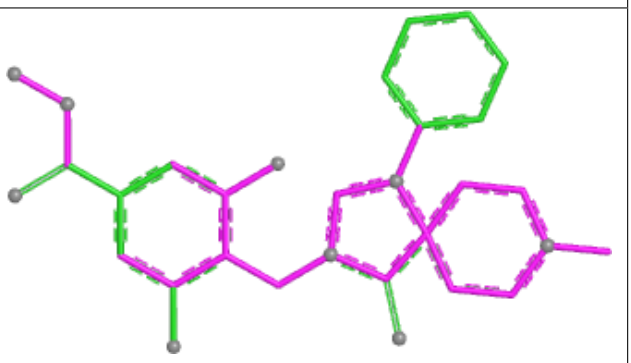


Rings

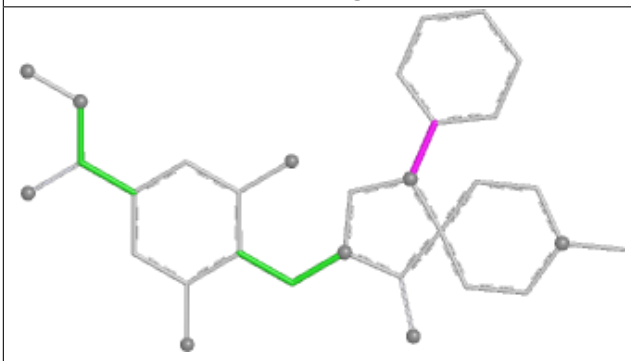
Ligand A1DJ1 B 1101



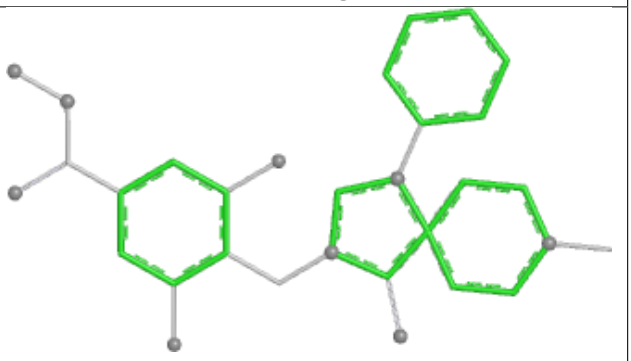
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	352/1081 (32%)	-0.18	2 (0%)	85	88	13, 18, 27, 50	1 (0%)
1	B	353/1081 (32%)	-0.14	5 (1%)	73	75	14, 19, 30, 49	1 (0%)
All	All	705/2162 (32%)	-0.16	7 (0%)	79	82	13, 19, 29, 50	2 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	769	LEU	3.7
1	B	777	THR	3.0
1	B	774	PRO	2.4
1	B	767	PRO	2.3
1	A	442	PRO	2.2
1	A	768	SER	2.1
1	B	768	SER	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 oligosaccharides in this entry.

6.4 Ligands

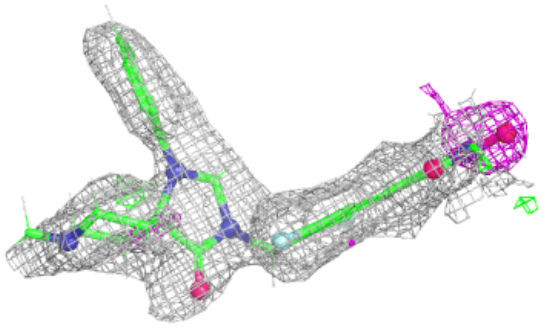
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

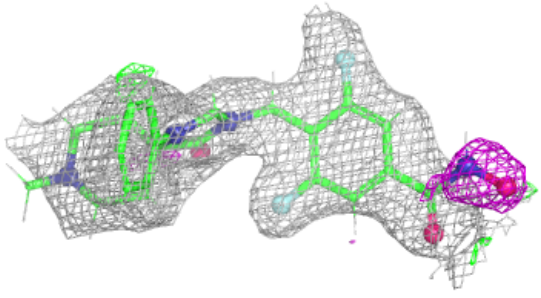
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	A1DJ1	A	1101	31/31	0.78	0.14	22,33,44,49	0
2	A1DJ1	B	1101	31/31	0.79	0.14	19,30,37,39	0
5	EDO	B	1103	4/4	0.81	0.21	18,30,36,42	0
5	EDO	B	1102	4/4	0.87	0.14	16,20,26,26	0
4	K	B	1105	1/1	0.99	0.02	11,11,11,11	0
4	K	B	1106	1/1	0.99	0.04	12,12,12,12	0
3	ZN	B	1104	1/1	0.99	0.02	13,13,13,13	0
4	K	A	1103	1/1	0.99	0.03	12,12,12,12	0
3	ZN	A	1102	1/1	1.00	0.02	14,14,14,14	0
4	K	A	1104	1/1	1.00	0.02	11,11,11,11	0

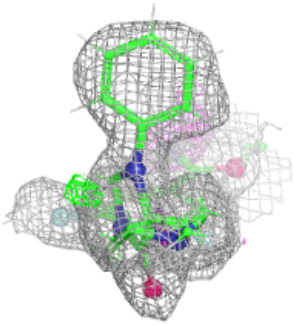
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1DJ1 A 1101:

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

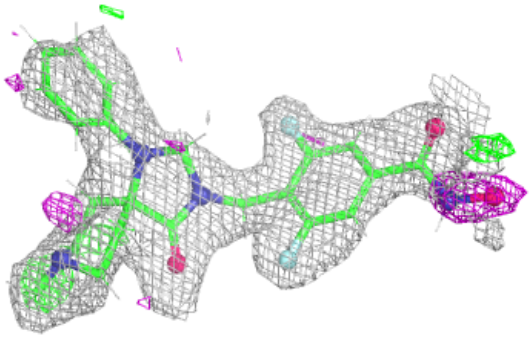


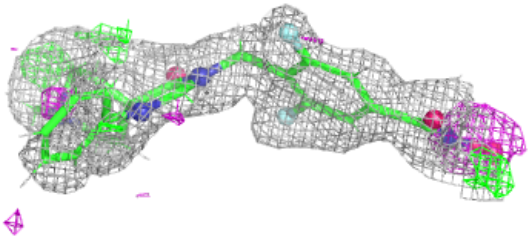


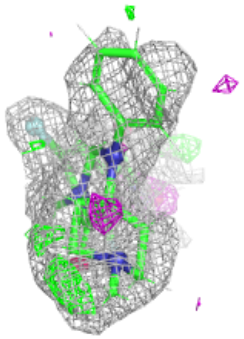


Electron density around A1DJ1 B 1101:

$2mF_o$-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

There are no such residues in this entry.