



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 09:54 pm BST

PDB ID : 5TKB
Title : CRYSTAL STRUCTURE OF HUMAN PHOSPHODIESTERASE 4D IN
COMPLEX WITH A TETRAFLUORANILINE COMPOUND
Authors : Sack, J.S.
Deposited on : 2016-10-06
Resolution : 2.16 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

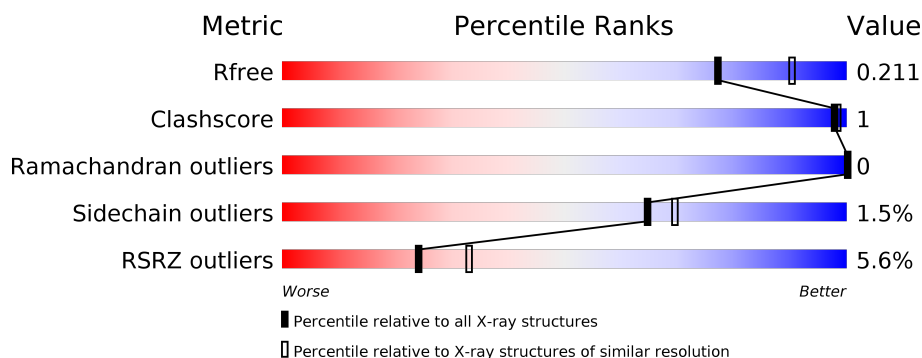
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	381	<div> <div>4%</div> <div>84%</div> <div>14%</div> </div>
1	B	381	<div> <div>6%</div> <div>81%</div> <div>15%</div> </div>
1	C	381	<div> <div>7%</div> <div>81%</div> <div>15%</div> </div>
1	D	381	<div> <div>3%</div> <div>83%</div> <div>15%</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11083 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 cAMP-specific 3',5'-cyclic phosphodiesterase 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2622	1662	446	500	14			
1	B	323	Total	C	N	O	S	0	0	0
			2593	1642	439	498	14			
1	C	323	Total	C	N	O	S	0	0	0
			2609	1649	445	501	14			
1	D	325	Total	C	N	O	S	0	0	0
			2617	1657	446	500	14			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	243	MET	-	initiating methionine	UNP Q08499
A	579	ALA	SER	engineered mutation	UNP Q08499
A	581	ALA	SER	engineered mutation	UNP Q08499
A	618	HIS	-	expression tag	UNP Q08499
A	619	HIS	-	expression tag	UNP Q08499
A	620	HIS	-	expression tag	UNP Q08499
A	621	HIS	-	expression tag	UNP Q08499
A	622	HIS	-	expression tag	UNP Q08499
A	623	HIS	-	expression tag	UNP Q08499
B	243	MET	-	initiating methionine	UNP Q08499
B	579	ALA	SER	engineered mutation	UNP Q08499
B	581	ALA	SER	engineered mutation	UNP Q08499
B	618	HIS	-	expression tag	UNP Q08499
B	619	HIS	-	expression tag	UNP Q08499
B	620	HIS	-	expression tag	UNP Q08499
B	621	HIS	-	expression tag	UNP Q08499
B	622	HIS	-	expression tag	UNP Q08499
B	623	HIS	-	expression tag	UNP Q08499
C	243	MET	-	initiating methionine	UNP Q08499
C	579	ALA	SER	engineered mutation	UNP Q08499
C	581	ALA	SER	engineered mutation	UNP Q08499

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Chain	Residue	Modelled	Actual	Comment	Reference
C	618	HIS	-	expression tag	UNP Q08499
C	619	HIS	-	expression tag	UNP Q08499
C	620	HIS	-	expression tag	UNP Q08499
C	621	HIS	-	expression tag	UNP Q08499
C	622	HIS	-	expression tag	UNP Q08499
C	623	HIS	-	expression tag	UNP Q08499
D	243	MET	-	initiating methionine	UNP Q08499
D	579	ALA	SER	engineered mutation	UNP Q08499
D	581	ALA	SER	engineered mutation	UNP Q08499
D	618	HIS	-	expression tag	UNP Q08499
D	619	HIS	-	expression tag	UNP Q08499
D	620	HIS	-	expression tag	UNP Q08499
D	621	HIS	-	expression tag	UNP Q08499
D	622	HIS	-	expression tag	UNP Q08499
D	623	HIS	-	expression tag	UNP Q08499

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

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

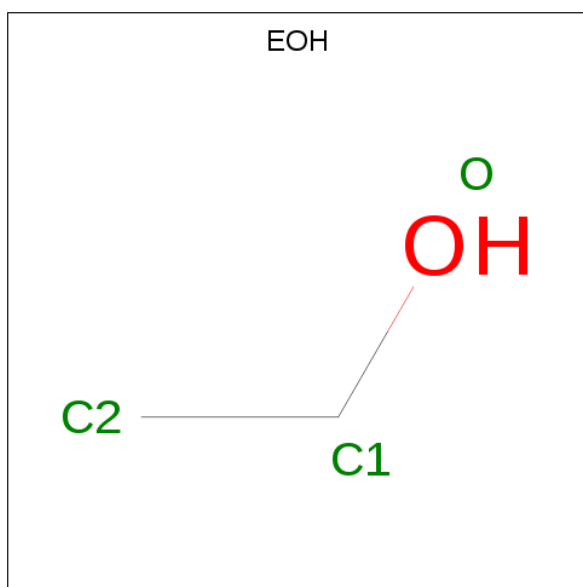
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 5 is ETHANOL (three-letter code: EOH) (formula: C₂H₆O).



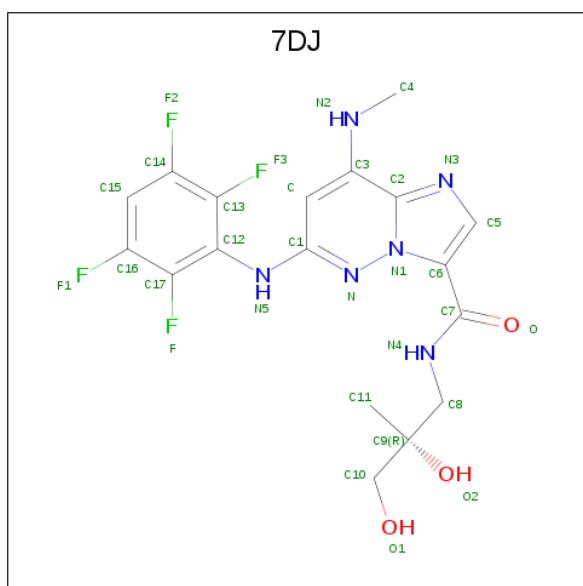
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	2	1		

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

- Molecule 6 is N-[(2R)-2,3-dihydroxy-2-methylpropyl]-8-(methylamino)-6-[(2,3,5,6-tetrafluorophenyl)amino]imidazo[1,2-b]pyridazine-3-carboxamide (three-letter code: 7DJ) (formula: C₁₈H₁₈F₄N₆O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	F	N	O	0	0
			31	18	4	6	3		
6	B	1	Total	C	F	N	O	0	0
			31	18	4	6	3		
6	C	1	Total	C	F	N	O	0	0
			31	18	4	6	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	F	N	O	0	0
			31	18	4	6	3		

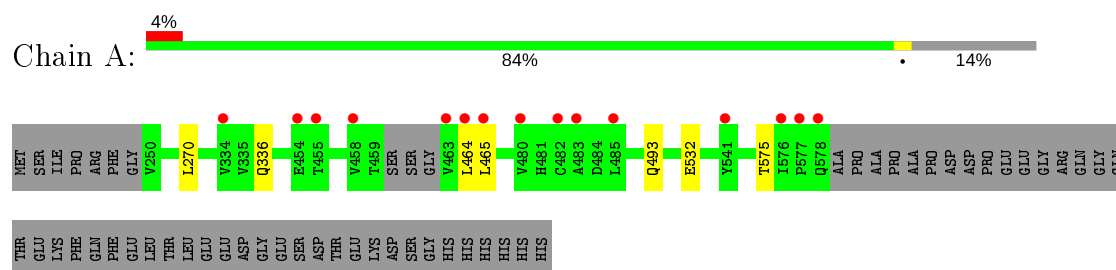
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	128	Total	O	0	0
			128	128		
7	B	90	Total	O	0	0
			90	90		
7	C	104	Total	O	0	0
			104	104		
7	D	149	Total	O	0	0
			149	149		

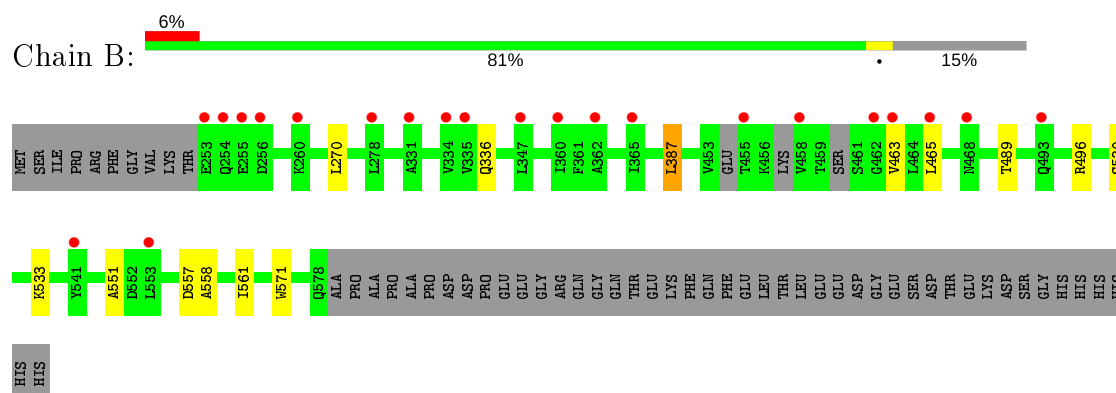
3 Residue-property plots [i](#)

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.

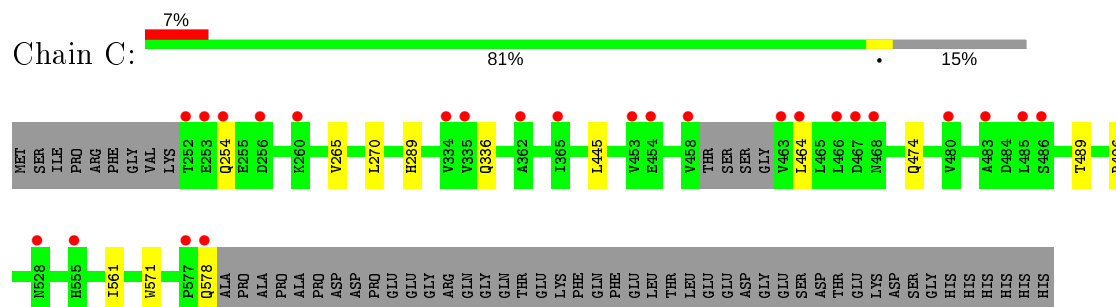
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



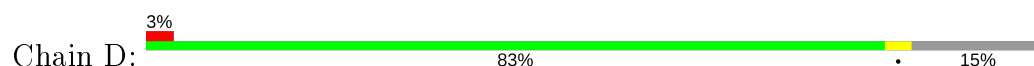
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

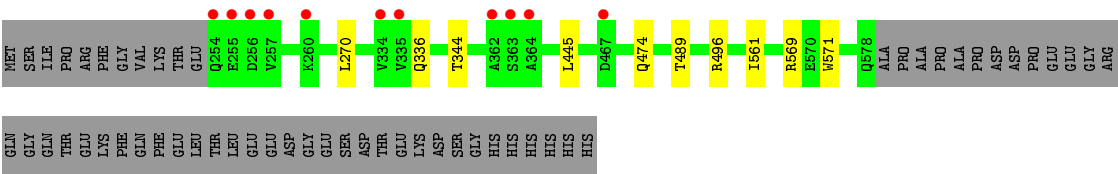


- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.00Å 112.70Å 159.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.62 – 2.16 31.10 – 2.16	Depositor EDS
% Data completeness (in resolution range)	100.0 (31.62-2.16) 100.0 (31.10-2.16)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.16Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.188 , 0.209 0.190 , 0.211	Depositor DCC
R_{free} test set	4770 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.4	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	11083	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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: ZN, MG, EOH, 7DJ, 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	0.50	0/2675	0.57	0/3638
1	B	0.49	0/2644	0.59	0/3594
1	C	0.49	0/2662	0.58	0/3620
1	D	0.51	0/2671	0.57	0/3631
All	All	0.50	0/10652	0.58	0/14483

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 [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	2622	0	2562	3	0
1	B	2593	0	2519	6	0
1	C	2609	0	2536	3	0
1	D	2617	0	2565	3	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
5	A	9	0	18	0	0
5	B	9	0	18	0	0
5	C	3	0	6	0	0
5	D	3	0	6	0	0
6	A	31	0	0	0	0
6	B	31	0	0	0	0
6	C	31	0	0	0	0
6	D	31	0	0	0	0
7	A	128	0	0	1	0
7	B	90	0	0	1	0
7	C	104	0	0	0	0
7	D	149	0	0	0	0
All	All	11083	0	10230	15	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 1.

All (15) 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:532:GLU:HG2	1:A:575:THR:HG22	1.73	0.68
1:B:387:LEU:HG	7:B:879:HOH:O	2.00	0.61
1:B:489:THR:HB	1:B:561:ILE:HG23	1.89	0.54
1:C:496:ARG:HD3	1:C:571:TRP:CH2	2.48	0.48
1:D:496:ARG:HD3	1:D:571:TRP:CH2	2.49	0.47
1:B:496:ARG:HD3	1:B:571:TRP:CH2	2.50	0.47
1:A:270:LEU:HD22	1:A:336:GLN:HG3	1.97	0.46
1:B:270:LEU:HD22	1:B:336:GLN:HG3	1.98	0.46
1:C:270:LEU:HD22	1:C:336:GLN:HG3	1.99	0.43
1:D:489:THR:HB	1:D:561:ILE:HG23	2.00	0.43
1:B:551:ALA:HA	1:B:558:ALA:HB3	1.99	0.43
1:B:530:SER:HB3	1:B:533:LYS:HB2	2.01	0.42
1:C:489:THR:HB	1:C:561:ILE:HG23	2.00	0.42
1:D:270:LEU:HD22	1:D:336:GLN:HG3	2.00	0.42
1:A:493:GLN:HG3	7:A:961:HOH:O	2.21	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	322/381 (84%)	316 (98%)	6 (2%)	0	100	100
1	B	315/381 (83%)	310 (98%)	5 (2%)	0	100	100
1	C	319/381 (84%)	314 (98%)	5 (2%)	0	100	100
1	D	323/381 (85%)	318 (98%)	5 (2%)	0	100	100
All	All	1279/1524 (84%)	1258 (98%)	21 (2%)	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	293/345 (85%)	291 (99%)	2 (1%)	84	89
1	B	290/345 (84%)	286 (99%)	4 (1%)	67	72
1	C	292/345 (85%)	285 (98%)	7 (2%)	49	51
1	D	294/345 (85%)	290 (99%)	4 (1%)	67	72
All	All	1169/1380 (85%)	1152 (98%)	17 (2%)	65	69

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

Mol	Chain	Res	Type
1	A	464	LEU
1	A	465	LEU
1	B	387	LEU
1	B	463	VAL
1	B	465	LEU
1	B	557	ASP
1	C	254	GLN
1	C	265	VAL
1	C	289	HIS
1	C	445	LEU
1	C	464	LEU
1	C	474	GLN
1	C	578	GLN
1	D	344	THR
1	D	445	LEU
1	D	474	GLN
1	D	569	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	293	GLN
1	A	535	GLN
1	B	293	GLN
1	B	474	GLN
1	B	535	GLN
1	C	424	GLN
1	C	478	ASN
1	C	535	GLN
1	D	289	HIS
1	D	293	GLN
1	D	474	GLN
1	D	478	ASN
1	D	535	GLN

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 ⓘ

Of 23 ligands modelled in this entry, 8 are monoatomic - leaving 15 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$
6	7DJ	A	807	-	28,33,33	1.25	2 (7%)	29,49,49	0.83	3 (10%)
5	EOH	A	806	-	2,2,2	0.37	0	1,1,1	0.98	0
5	EOH	B	705	-	2,2,2	0.48	0	1,1,1	0.67	0
4	SO4	C	703	-	4,4,4	0.07	0	6,6,6	0.35	0
5	EOH	B	706	-	2,2,2	0.50	0	1,1,1	0.79	0
4	SO4	B	703	-	4,4,4	0.22	0	6,6,6	0.17	0
6	7DJ	B	707	-	28,33,33	1.21	4 (14%)	29,49,49	0.85	2 (6%)
5	EOH	A	805	-	2,2,2	0.61	0	1,1,1	0.62	0
5	EOH	A	804	-	2,2,2	0.51	0	1,1,1	0.77	0
5	EOH	D	703	-	2,2,2	0.52	0	1,1,1	0.75	0
5	EOH	B	704	-	2,2,2	0.68	0	1,1,1	0.64	0
6	7DJ	C	705	-	28,33,33	1.38	4 (14%)	29,49,49	0.91	3 (10%)
6	7DJ	D	704	-	28,33,33	1.29	4 (14%)	29,49,49	0.67	2 (6%)
5	EOH	C	704	-	2,2,2	0.51	0	1,1,1	0.74	0
4	SO4	A	803	-	4,4,4	0.36	0	6,6,6	0.29	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
6	7DJ	A	807	-	-	0/15/19/19	0/3/3/3
6	7DJ	D	704	-	-	0/15/19/19	0/3/3/3
6	7DJ	B	707	-	-	2/15/19/19	0/3/3/3
6	7DJ	C	705	-	-	2/15/19/19	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	705	7DJ	C3-C2	5.25	1.51	1.42
6	D	704	7DJ	C3-C2	4.69	1.50	1.42
6	A	807	7DJ	C3-C2	4.49	1.50	1.42
6	B	707	7DJ	C3-C2	3.97	1.49	1.42
6	A	807	7DJ	C-C1	3.84	1.49	1.39
6	B	707	7DJ	C-C1	3.36	1.48	1.39
6	D	704	7DJ	C-C1	3.11	1.47	1.39
6	C	705	7DJ	C-C1	3.11	1.47	1.39
6	D	704	7DJ	C1-N5	2.49	1.43	1.38
6	B	707	7DJ	C10-C9	2.49	1.57	1.51
6	C	705	7DJ	C1-N	2.45	1.39	1.33
6	C	705	7DJ	C10-C9	2.12	1.56	1.51
6	D	704	7DJ	C10-C9	2.07	1.56	1.51
6	B	707	7DJ	C1-N5	2.06	1.42	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	705	7DJ	C4-N2-C3	2.88	127.14	122.39
6	B	707	7DJ	C4-N2-C3	2.53	126.57	122.39
6	B	707	7DJ	C2-C3-N2	-2.34	115.22	116.78
6	C	705	7DJ	C2-C3-N2	-2.24	115.29	116.78
6	C	705	7DJ	C8-N4-C7	2.18	126.50	122.89
6	A	807	7DJ	C4-N2-C3	2.13	125.91	122.39
6	D	704	7DJ	C8-N4-C7	2.08	126.33	122.89
6	A	807	7DJ	C8-N4-C7	2.06	126.29	122.89
6	D	704	7DJ	C4-N2-C3	2.05	125.78	122.39
6	A	807	7DJ	C2-C3-N2	-2.01	115.44	116.78

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	707	7DJ	O1-C10-C9-C8

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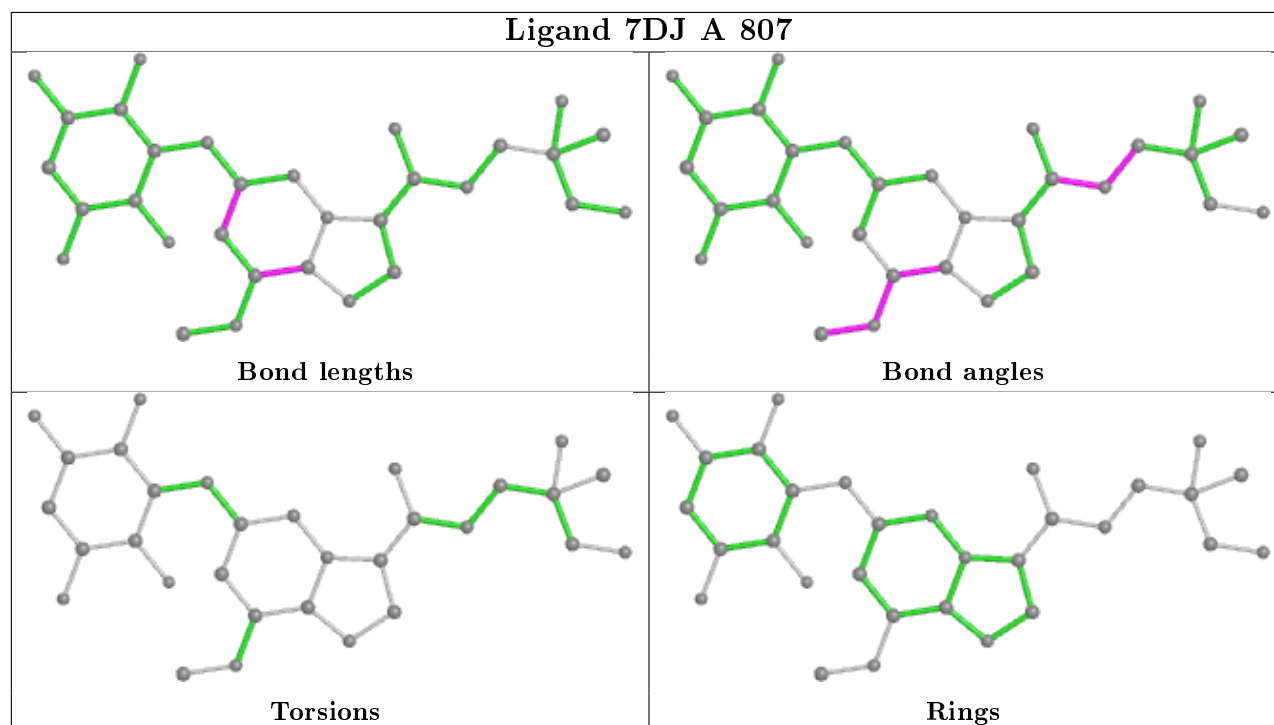
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Mol	Chain	Res	Type	Atoms
6	C	705	7DJ	O1-C10-C9-C8
6	B	707	7DJ	C6-C7-N4-C8
6	C	705	7DJ	O1-C10-C9-O2

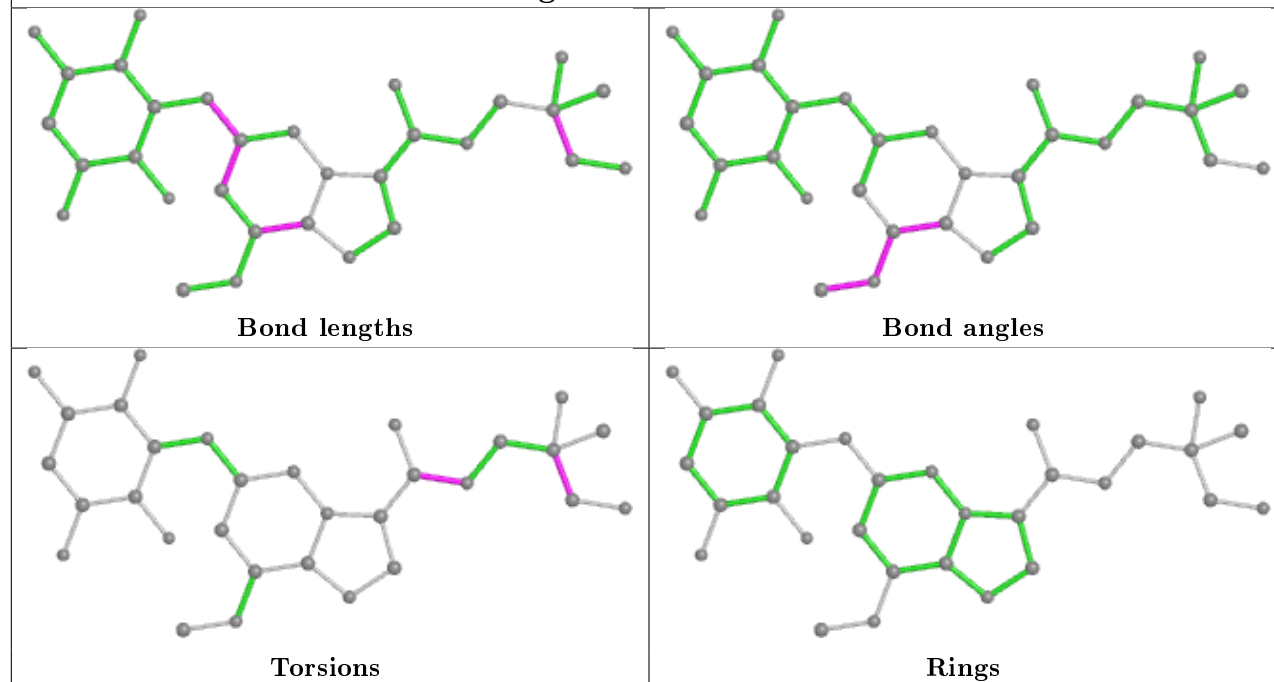
There are no ring outliers.

No monomer is involved in short contacts.

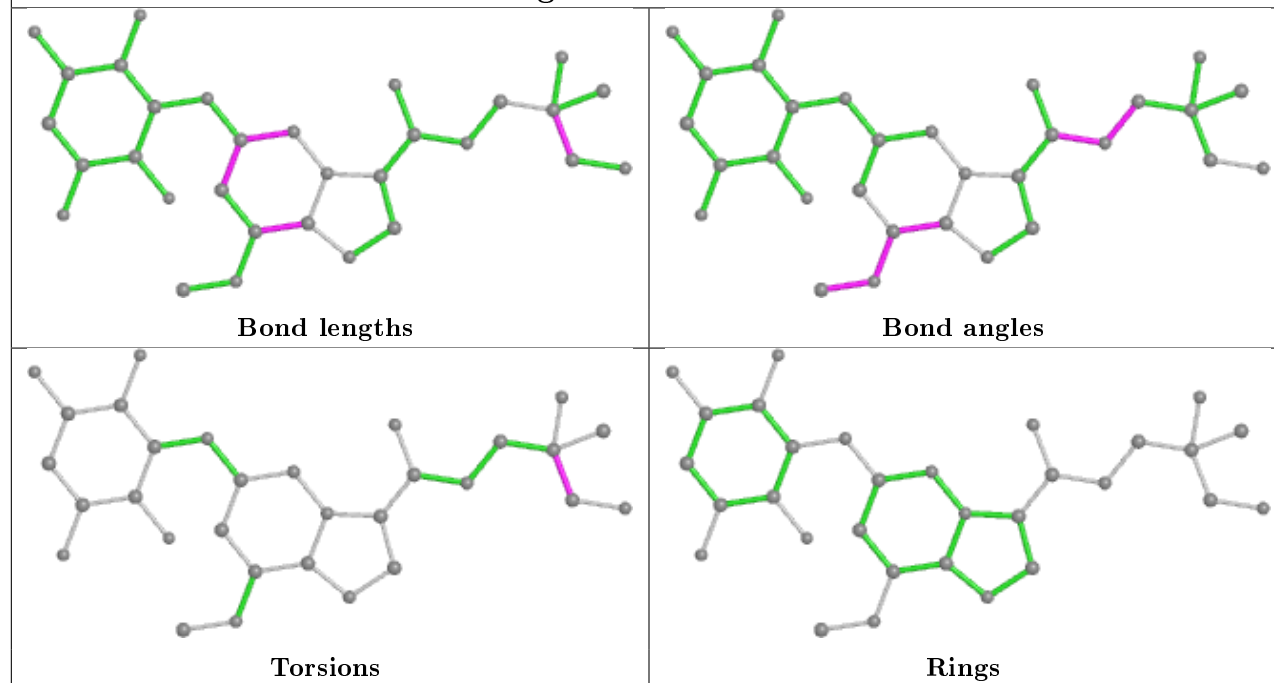
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

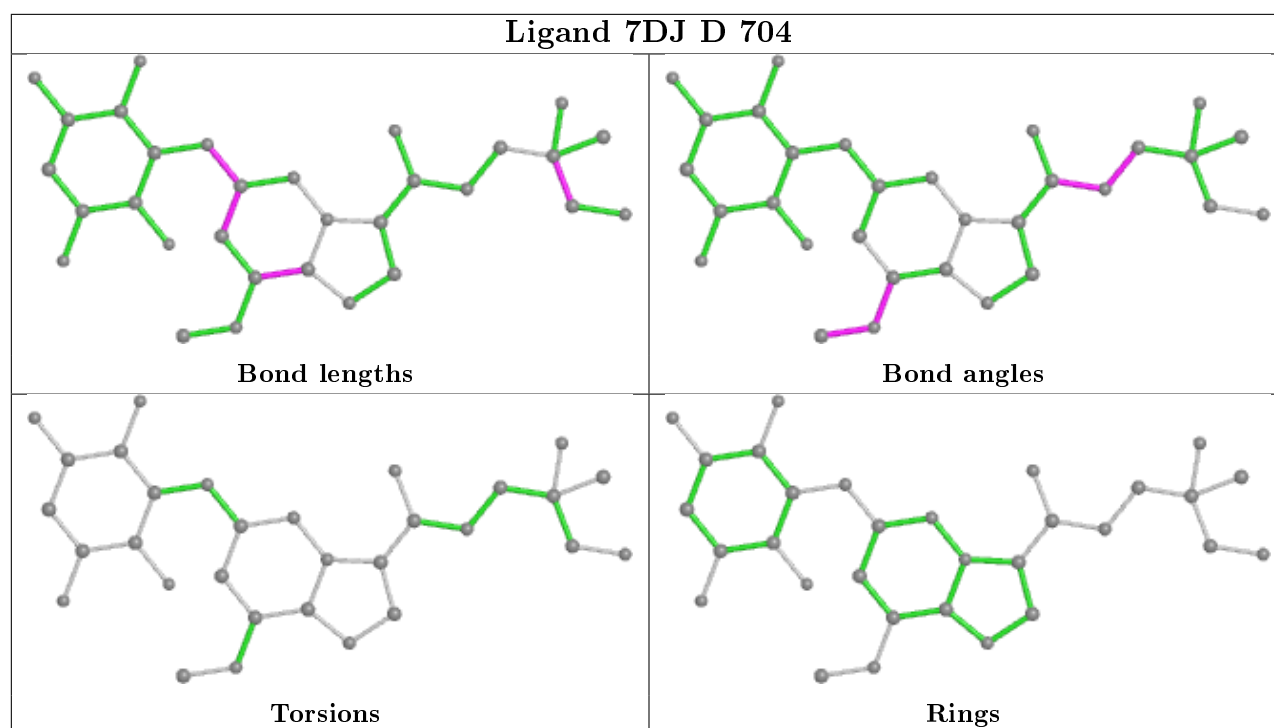


Ligand 7DJ B 707



Ligand 7DJ C 705





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	326/381 (85%)	-0.02	15 (4%) 32 42	24, 34, 59, 117	0
1	B	323/381 (84%)	0.32	22 (6%) 17 24	25, 43, 68, 112	0
1	C	323/381 (84%)	0.16	25 (7%) 13 18	22, 38, 70, 115	0
1	D	325/381 (85%)	-0.07	11 (3%) 45 53	20, 33, 54, 92	0
All	All	1297/1524 (85%)	0.10	73 (5%) 24 33	20, 37, 66, 117	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	253	GLU	5.6
1	A	578	GLN	5.6
1	C	458	VAL	5.3
1	B	462	GLY	5.1
1	A	577	PRO	4.7
1	B	254	GLN	4.7
1	C	253	GLU	4.1
1	C	467	ASP	3.8
1	C	463	VAL	3.8
1	B	334	VAL	3.6
1	C	334	VAL	3.6
1	D	256	ASP	3.6
1	A	458	VAL	3.6
1	D	260	LYS	3.5
1	B	255	GLU	3.5
1	D	254	GLN	3.4
1	B	458	VAL	3.4
1	A	483	ALA	3.3
1	A	334	VAL	3.2
1	B	455	THR	3.2
1	C	252	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	335	VAL	3.1
1	B	335	VAL	3.0
1	B	256	ASP	3.0
1	B	362	ALA	2.9
1	C	555	HIS	2.9
1	C	528	ASN	2.9
1	B	365	ILE	2.9
1	C	254	GLN	2.8
1	C	577	PRO	2.8
1	C	480	VAL	2.8
1	A	485	LEU	2.7
1	C	464	LEU	2.7
1	C	578	GLN	2.7
1	B	553	LEU	2.7
1	A	463	VAL	2.7
1	D	362	ALA	2.7
1	B	260	LYS	2.6
1	B	463	VAL	2.6
1	B	541	TYR	2.6
1	D	334	VAL	2.6
1	A	576	ILE	2.6
1	C	454	GLU	2.6
1	B	465	LEU	2.6
1	A	464	LEU	2.6
1	D	467	ASP	2.5
1	C	260	LYS	2.5
1	D	364	ALA	2.5
1	D	257	VAL	2.4
1	C	365	ILE	2.4
1	C	485	LEU	2.4
1	C	468	ASN	2.4
1	A	480	VAL	2.4
1	A	482	CYS	2.4
1	C	362	ALA	2.4
1	A	455	THR	2.3
1	B	360	ILE	2.3
1	D	255	GLU	2.3
1	C	453	VAL	2.3
1	C	483	ALA	2.3
1	A	465	LEU	2.3
1	C	256	ASP	2.3
1	A	541	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	454	GLU	2.3
1	B	278	LEU	2.2
1	B	347	LEU	2.2
1	B	493	GLN	2.2
1	B	331	ALA	2.2
1	D	335	VAL	2.1
1	D	363	SER	2.1
1	B	468	ASN	2.1
1	C	486	SER	2.1
1	C	466	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 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(Å ²)	Q<0.9
5	EOH	C	704	3/3	0.80	0.14	31,31,35,37	0
5	EOH	A	805	3/3	0.84	0.21	45,45,48,51	0
4	SO4	B	703	5/5	0.84	0.23	93,96,97,98	0
5	EOH	B	704	3/3	0.86	0.17	37,37,39,39	0
6	7DJ	C	705	31/31	0.86	0.16	49,60,70,70	0
6	7DJ	A	807	31/31	0.87	0.17	44,53,62,67	0
5	EOH	D	703	3/3	0.88	0.27	27,27,33,37	0
6	7DJ	D	704	31/31	0.90	0.14	44,54,65,67	0
6	7DJ	B	707	31/31	0.90	0.14	50,63,73,75	0
4	SO4	C	703	5/5	0.90	0.17	65,75,77,79	0
5	EOH	A	804	3/3	0.92	0.11	30,30,37,42	0
5	EOH	B	706	3/3	0.92	0.13	35,35,39,41	0
5	EOH	A	806	3/3	0.93	0.24	38,38,39,41	0

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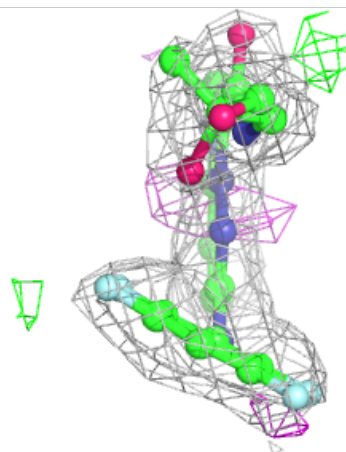
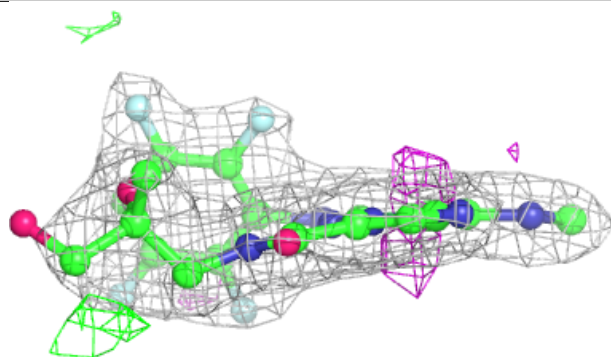
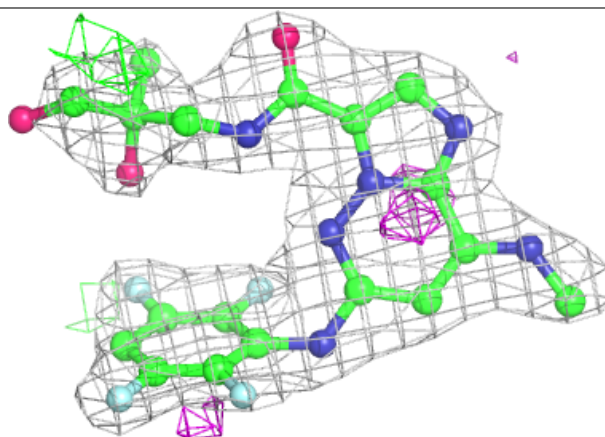
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EOH	B	705	3/3	0.95	0.20	43,43,43,44	0
4	SO4	A	803	5/5	0.96	0.14	49,59,63,64	0
3	MG	C	702	1/1	0.98	0.12	25,25,25,25	0
3	MG	D	702	1/1	0.99	0.13	24,24,24,24	0
3	MG	B	702	1/1	0.99	0.09	27,27,27,27	0
2	ZN	B	701	1/1	0.99	0.09	35,35,35,35	0
3	MG	A	802	1/1	0.99	0.11	25,25,25,25	0
2	ZN	A	801	1/1	1.00	0.10	29,29,29,29	0
2	ZN	C	701	1/1	1.00	0.10	32,32,32,32	0
2	ZN	D	701	1/1	1.00	0.11	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.

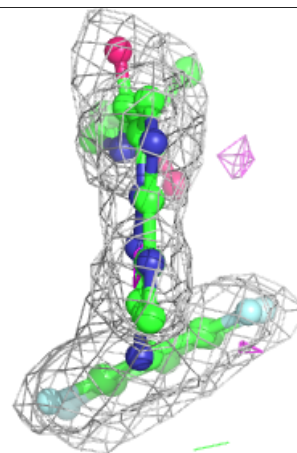
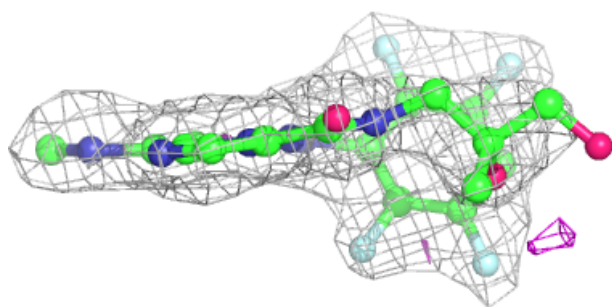
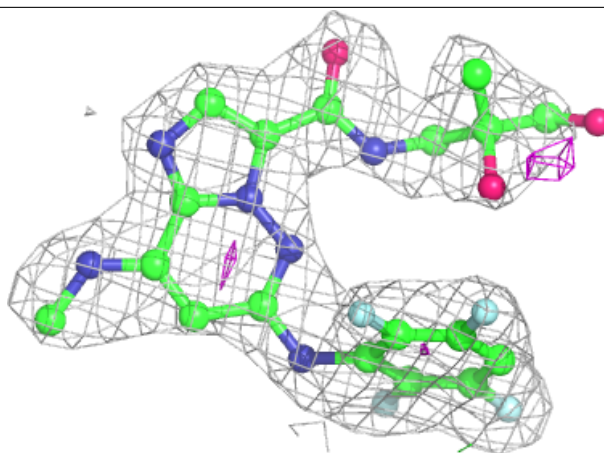
Electron density around 7DJ C 705:

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



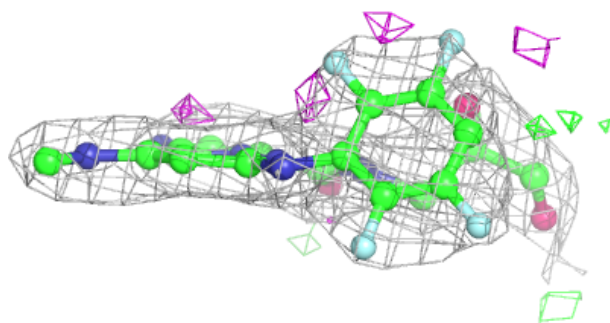
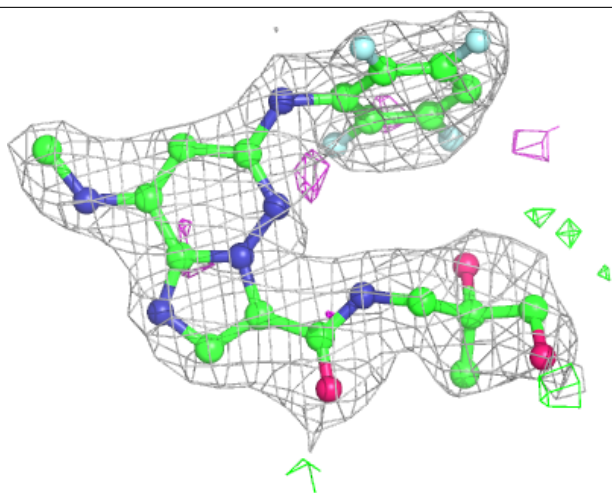
Electron density around 7DJ A 807:

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



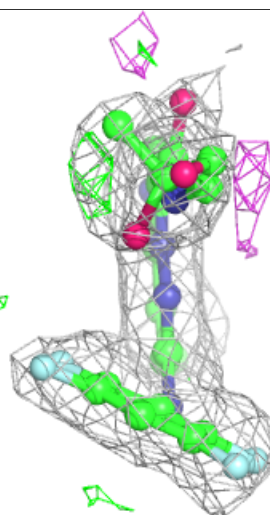
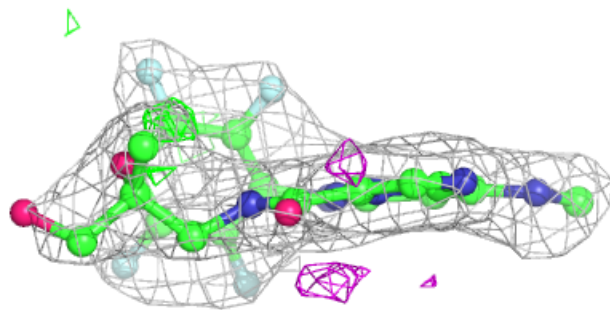
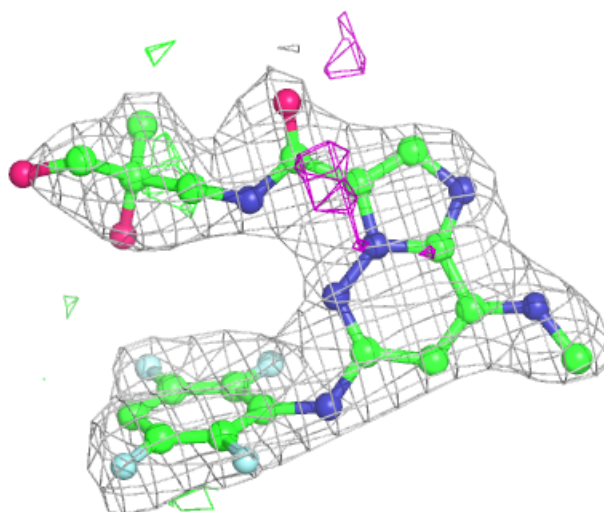
Electron density around 7DJ D 704:

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



Electron density around 7DJ B 707:

$2mF_o-DF_c$ (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.