



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:16 PM UTC

PDB ID : 5TKB / pdb_00005tkb
Title : CRYSTAL STRUCTURE OF HUMAN PHOSPHODIESTERASE 4D IN COMPLEX WITH A TETRAFLUORANLINE 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 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 Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

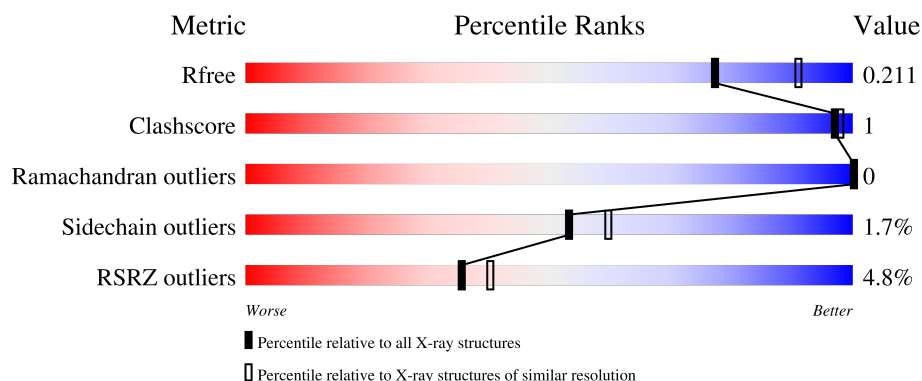
1 Overall quality at a glance

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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (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 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 $\leq 5\%$. 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	3% 83% • 14%
1	B	381	9% 80% 5% • 15%
1	C	381	4% 81% • 15%
1	D	381	0% 81% • 15%

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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

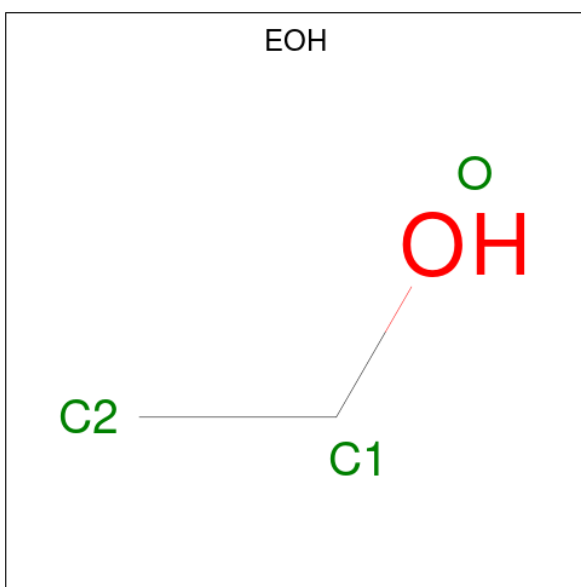
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

- Molecule 4 is SULFATE ION (CCD ID: 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 (CCD ID: EOH) (formula: C₂H₆O).



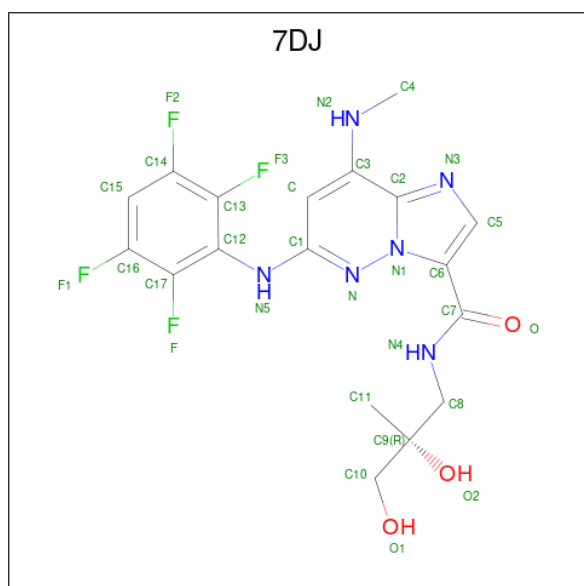
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	2	1		

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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 (CCD ID: 7DJ) (formula: $C_{18}H_{18}F_4N_6O_3$).



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		

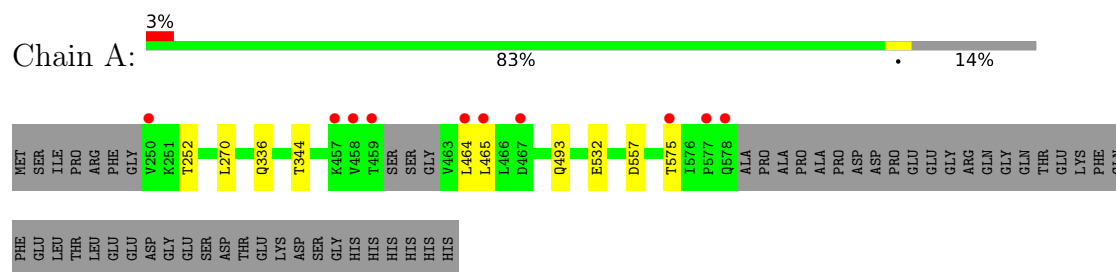
- Molecule 7 is water.

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		

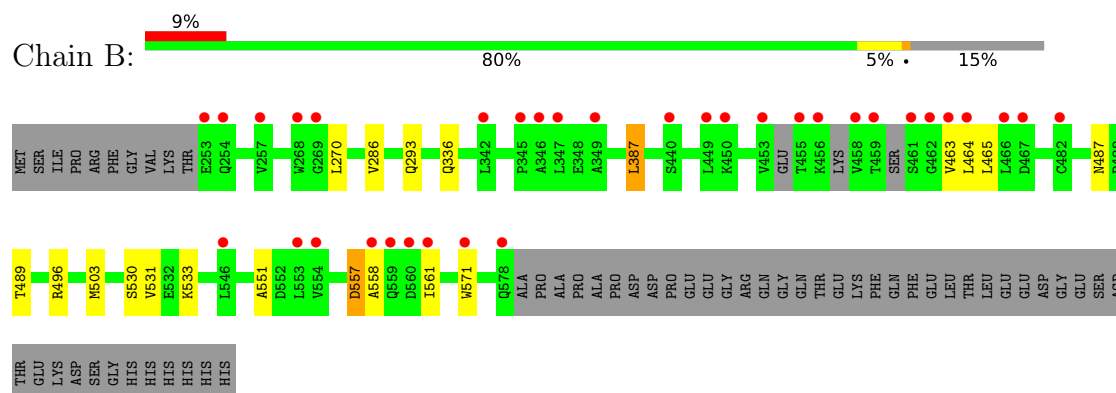
3 Residue-property plots

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.

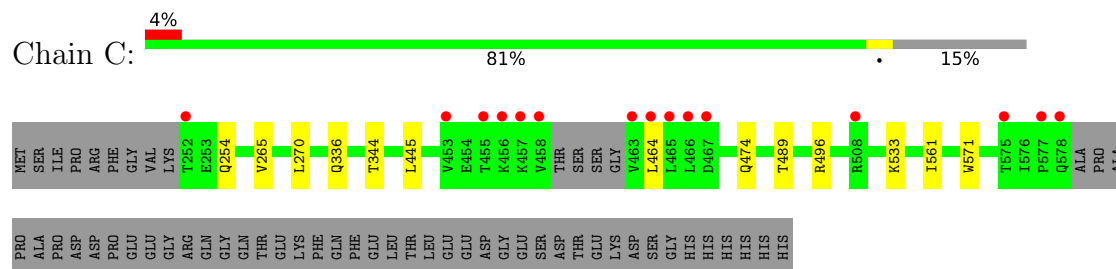
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



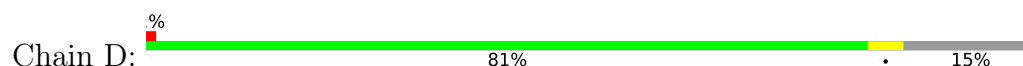
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

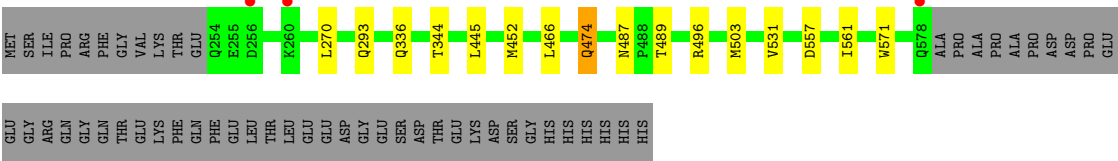


- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



- 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 31.62 – 2.16	Depositor EDS
% Data completeness (in resolution range)	100.0 (31.62-2.16) 99.9 (31.62-2.16)	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 , 32.8	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	0.95	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 7DJ, ZN, EOH, MG, 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	0.86	0/2675	1.25	1/3638 (0.0%)
1	B	0.85	0/2644	1.30	4/3594 (0.1%)
1	C	0.84	0/2662	1.28	0/3620
1	D	0.87	0/2671	1.25	6/3631 (0.2%)
All	All	0.86	0/10652	1.27	11/14483 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	557	ASP	CA-CB-CG	6.73	119.33	112.60
1	D	466	LEU	CA-C-N	5.94	129.34	120.31
1	D	466	LEU	C-N-CA	5.94	129.34	120.31
1	D	487	ASN	CA-CB-CG	5.33	117.93	112.60
1	B	293	GLN	CA-C-N	5.18	127.22	120.28
1	B	293	GLN	C-N-CA	5.18	127.22	120.28
1	D	557	ASP	CA-CB-CG	5.15	117.75	112.60
1	B	487	ASN	CA-CB-CG	5.14	117.74	112.60
1	A	557	ASP	CA-CB-CG	5.06	117.66	112.60
1	D	293	GLN	CA-C-N	5.04	127.04	120.28
1	D	293	GLN	C-N-CA	5.04	127.04	120.28

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	2622	0	2562	3	0
1	B	2593	0	2519	7	0
1	C	2609	0	2536	3	0
1	D	2617	0	2565	5	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
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	18	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 (18) 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:503:MET:HE2	1:B:531:VAL:HG22	1.83	0.61
1:B:489:THR:HB	1:B:561:ILE:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:503:MET:HE2	1:D:531:VAL:HG22	1.93	0.49
1:D:452:MET:HE3	1:D:474:GLN:HE21	1.77	0.49
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 ⓘ

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%)	289 (99%)	4 (1%)	59	66
1	B	290/345 (84%)	284 (98%)	6 (2%)	47	52
1	C	292/345 (85%)	285 (98%)	7 (2%)	43	47
1	D	294/345 (85%)	291 (99%)	3 (1%)	68	75
All	All	1169/1380 (85%)	1149 (98%)	20 (2%)	53	60

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	252	THR
1	A	344	THR
1	A	464	LEU
1	A	465	LEU
1	B	286	VAL
1	B	387	LEU
1	B	463	VAL
1	B	464	LEU
1	B	465	LEU
1	B	557	ASP
1	C	254	GLN
1	C	265	VAL
1	C	344	THR
1	C	445	LEU
1	C	464	LEU
1	C	474	GLN
1	C	533	LYS
1	D	344	THR
1	D	445	LEU
1	D	474	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	293	GLN
1	A	376	GLN
1	A	424	GLN
1	A	535	GLN
1	B	293	GLN
1	B	376	GLN
1	B	474	GLN
1	B	493	GLN
1	B	535	GLN
1	C	376	GLN
1	C	424	GLN
1	C	478	ASN
1	C	535	GLN
1	D	254	GLN
1	D	289	HIS
1	D	293	GLN
1	D	474	GLN
1	D	478	ASN
1	D	487	ASN
1	D	535	GLN
1	D	573	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 oligosaccharides 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	C	705	-	31,33,33	1.56	5 (16%)	34,49,49	1.01	3 (8%)
6	7DJ	A	807	-	31,33,33	1.42	4 (12%)	34,49,49	0.89	1 (2%)
5	EOH	C	704	-	2,2,2	0.52	0	1,1,1	0.75	0
5	EOH	B	706	-	2,2,2	0.50	0	1,1,1	0.81	0
6	7DJ	D	704	-	31,33,33	1.45	5 (16%)	34,49,49	0.89	2 (5%)
6	7DJ	B	707	-	31,33,33	1.46	5 (16%)	34,49,49	0.84	1 (2%)
4	SO4	B	703	-	4,4,4	0.33	0	6,6,6	0.17	0
5	EOH	A	805	-	2,2,2	0.62	0	1,1,1	0.63	0
5	EOH	B	705	-	2,2,2	0.48	0	1,1,1	0.69	0
5	EOH	D	703	-	2,2,2	0.53	0	1,1,1	0.77	0
5	EOH	B	704	-	2,2,2	0.69	0	1,1,1	0.65	0
4	SO4	A	803	-	4,4,4	0.29	0	6,6,6	0.31	0
5	EOH	A	806	-	2,2,2	0.37	0	1,1,1	1.00	0
4	SO4	C	703	-	4,4,4	0.13	0	6,6,6	0.37	0
5	EOH	A	804	-	2,2,2	0.52	0	1,1,1	0.78	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	-	-	1/19/19/19	0/3/3/3
6	7DJ	C	705	-	-	2/19/19/19	0/3/3/3
6	7DJ	D	704	-	-	2/19/19/19	0/3/3/3
6	7DJ	B	707	-	-	3/19/19/19	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	705	7DJ	C1-N	5.99	1.39	1.30
6	A	807	7DJ	C-C1	4.49	1.49	1.42
6	B	707	7DJ	C3-N2	4.43	1.40	1.34
6	D	704	7DJ	C3-N2	4.37	1.40	1.34
6	A	807	7DJ	C3-N2	4.31	1.40	1.34
6	D	704	7DJ	C1-N	4.21	1.36	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	707	7DJ	C1-N	4.08	1.36	1.30
6	C	705	7DJ	C3-N2	3.77	1.39	1.34
6	B	707	7DJ	C-C1	3.72	1.48	1.42
6	A	807	7DJ	C1-N	3.51	1.35	1.30
6	D	704	7DJ	C1-N5	3.45	1.43	1.37
6	D	704	7DJ	C-C1	3.33	1.47	1.42
6	C	705	7DJ	C-C1	3.32	1.47	1.42
6	B	707	7DJ	C1-N5	2.98	1.42	1.37
6	C	705	7DJ	C1-N5	2.86	1.42	1.37
6	A	807	7DJ	C1-N5	2.72	1.41	1.37
6	B	707	7DJ	C10-C9	2.45	1.57	1.51
6	C	705	7DJ	C10-C9	2.07	1.56	1.51
6	D	704	7DJ	C10-C9	2.01	1.56	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	705	7DJ	C8-N4-C7	2.97	126.50	122.73
6	D	704	7DJ	C8-N4-C7	2.83	126.33	122.73
6	A	807	7DJ	C8-N4-C7	2.81	126.29	122.73
6	C	705	7DJ	C5-C6-C7	-2.56	127.21	131.01
6	D	704	7DJ	C5-C6-C7	-2.30	127.60	131.01
6	B	707	7DJ	C5-C6-C7	-2.24	127.68	131.01
6	C	705	7DJ	C4-N2-C3	2.05	127.14	123.98

There are no chirality outliers.

All (8) torsion outliers are listed below:

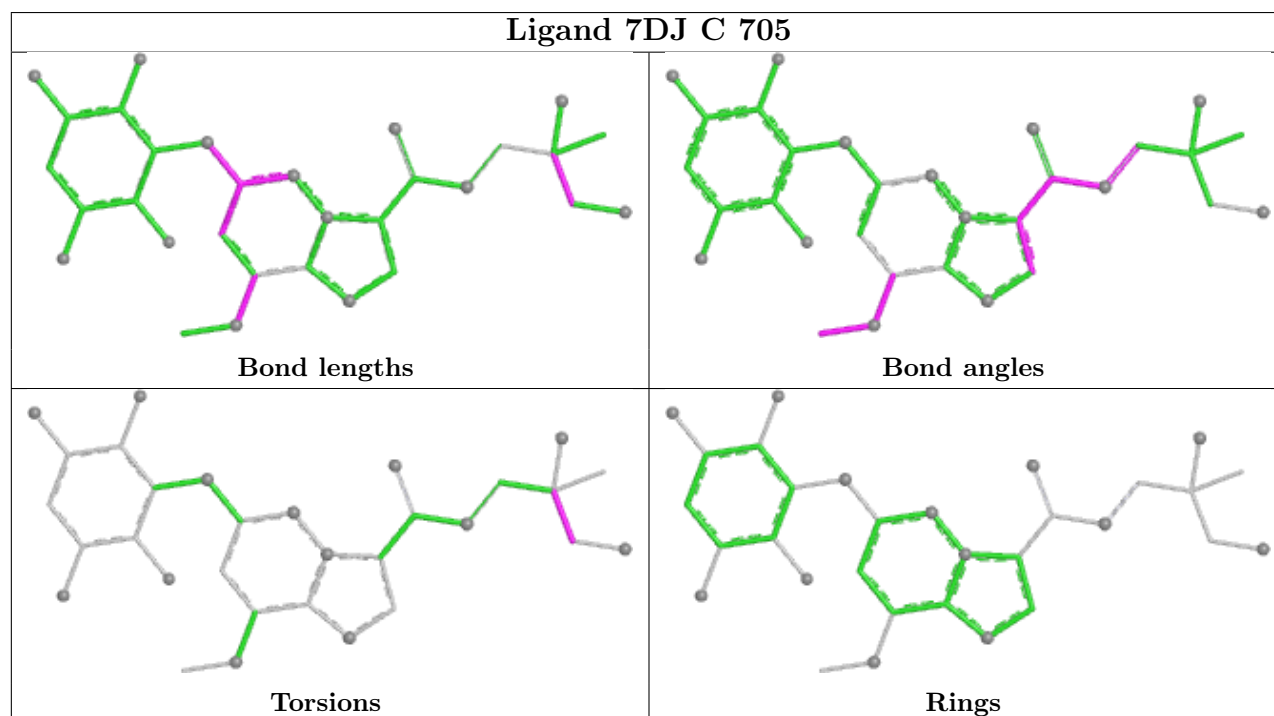
Mol	Chain	Res	Type	Atoms
6	D	704	7DJ	N1-C6-C7-O
6	B	707	7DJ	O1-C10-C9-C8
6	C	705	7DJ	O1-C10-C9-C8
6	A	807	7DJ	N1-C6-C7-O
6	B	707	7DJ	N1-C6-C7-O
6	D	704	7DJ	N1-C6-C7-N4
6	C	705	7DJ	O1-C10-C9-O2
6	B	707	7DJ	C6-C7-N4-C8

There are no ring outliers.

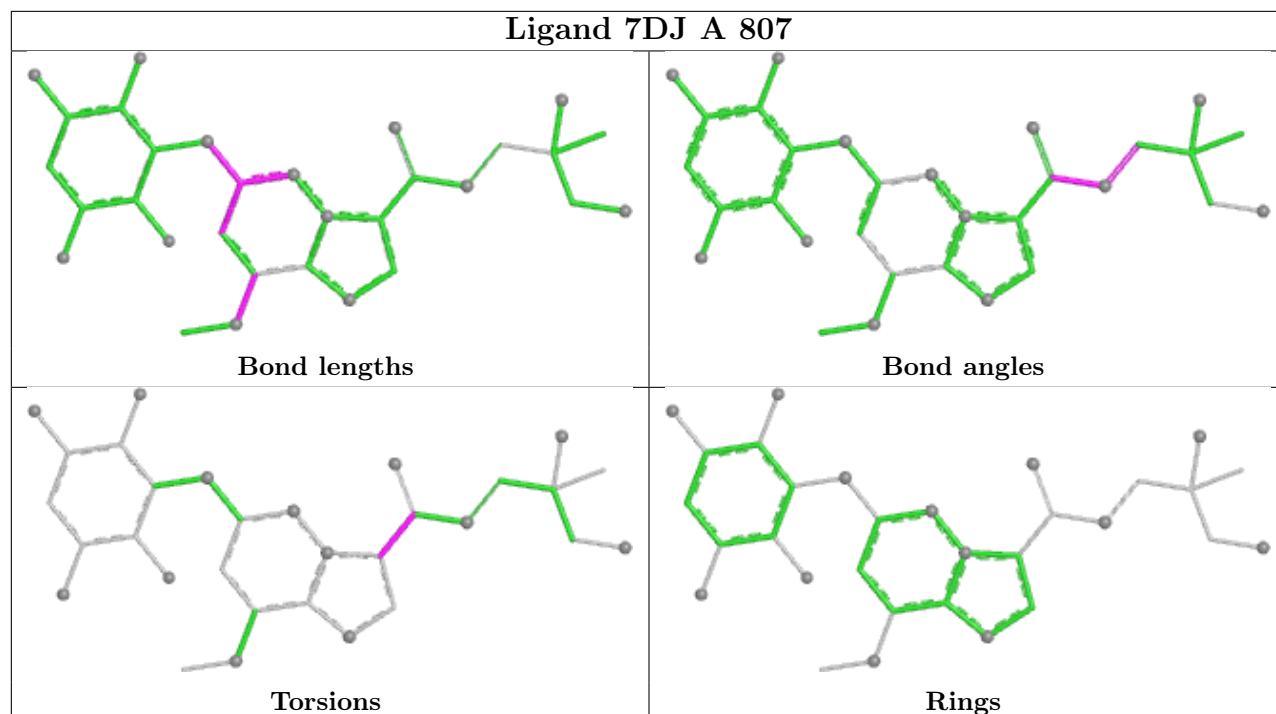
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

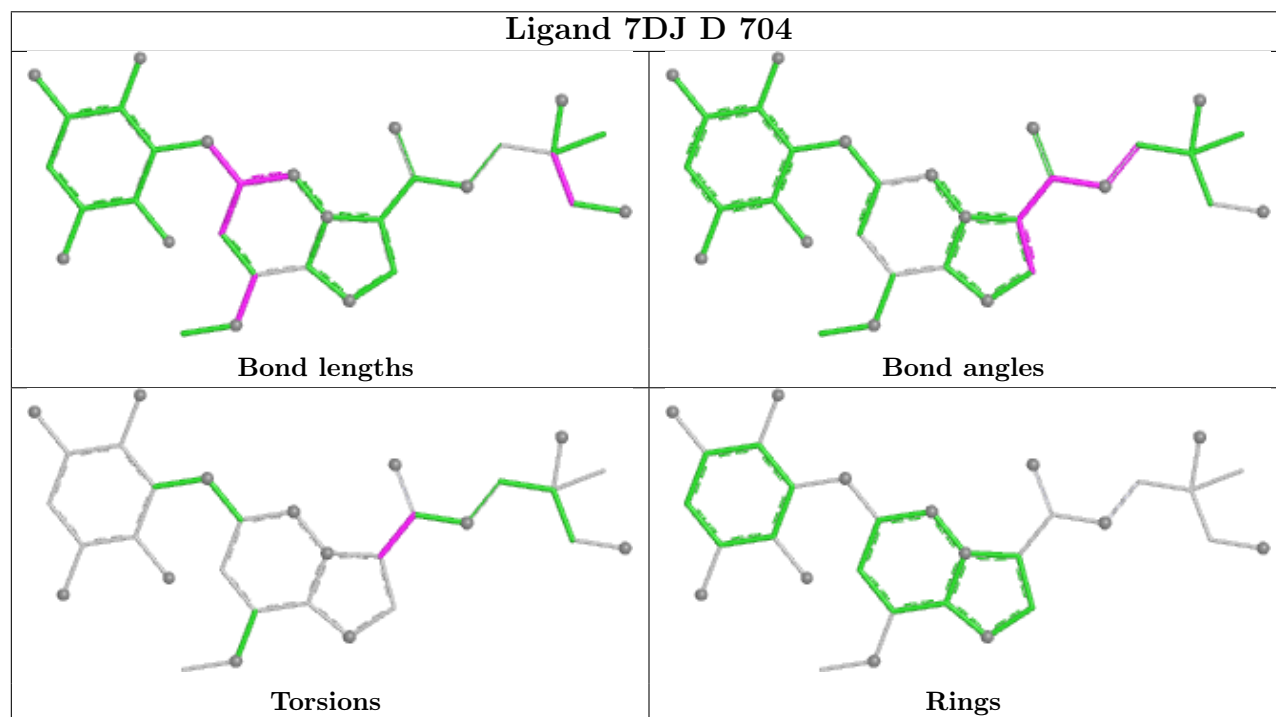
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

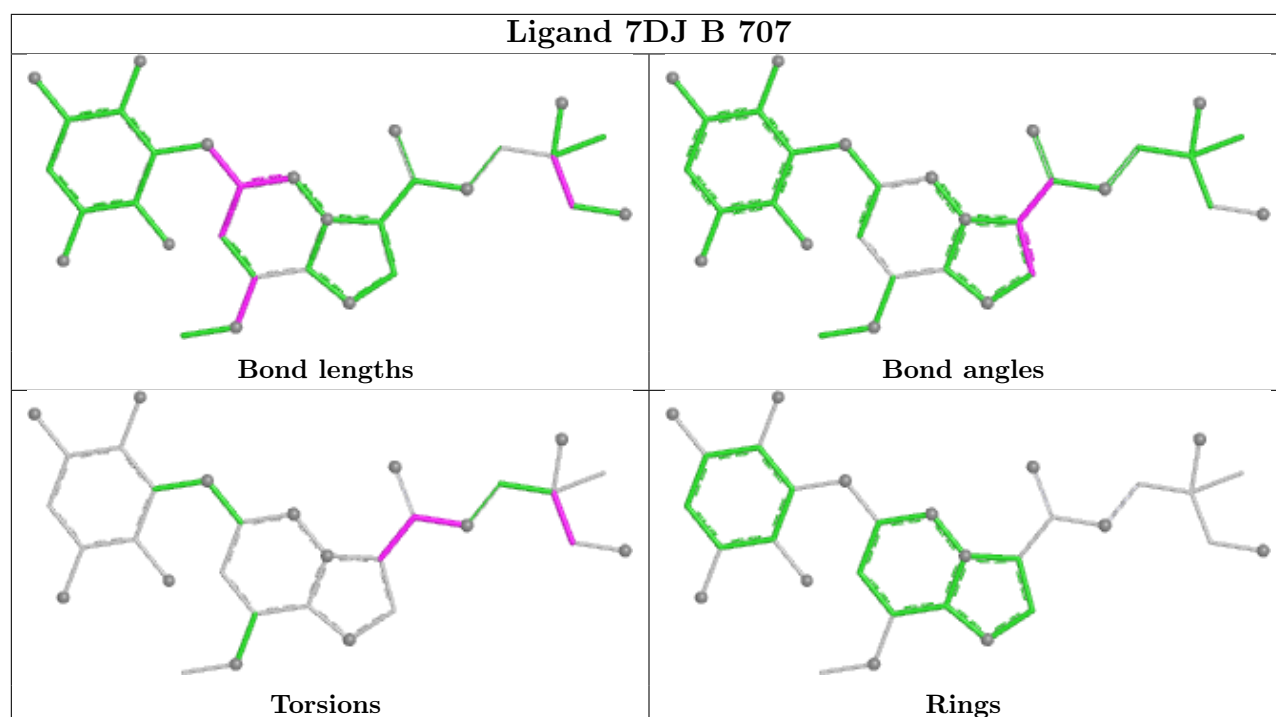


Ligand 7DJ A 807



Ligand 7DJ D 704





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%)	-0.12	10 (3%) 51 55	24, 34, 59, 117	0
1	B	323/381 (84%)	0.64	34 (10%) 11 13	25, 43, 68, 112	0
1	C	323/381 (84%)	0.14	15 (4%) 37 42	22, 38, 70, 115	0
1	D	325/381 (85%)	-0.22	3 (0%) 81 83	20, 33, 54, 92	0
All	All	1297/1524 (85%)	0.11	62 (4%) 35 40	20, 37, 66, 117	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	453	VAL	6.6
1	B	462	GLY	6.1
1	C	458	VAL	5.6
1	B	458	VAL	4.9
1	C	463	VAL	4.8
1	D	578	GLN	4.8
1	A	459	THR	4.5
1	B	463	VAL	4.2
1	B	459	THR	4.1
1	C	464	LEU	4.0
1	C	252	THR	4.0
1	B	461	SER	3.9
1	B	347	LEU	3.9
1	B	553	LEU	3.9
1	C	578	GLN	3.6
1	A	578	GLN	3.5
1	B	561	ILE	3.5
1	B	578	GLN	3.5
1	B	467	ASP	3.4
1	A	577	PRO	3.4
1	B	254	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	456	LYS	3.3
1	B	257	VAL	3.3
1	B	558	ALA	3.3
1	B	346	ALA	3.2
1	C	577	PRO	2.9
1	A	250	VAL	2.8
1	B	554	VAL	2.8
1	B	268	TRP	2.7
1	A	465	LEU	2.6
1	B	466	LEU	2.6
1	C	465	LEU	2.6
1	C	457	LYS	2.5
1	A	457	LYS	2.5
1	B	482	CYS	2.5
1	A	458	VAL	2.4
1	C	456	LYS	2.4
1	C	453	VAL	2.4
1	B	253	GLU	2.4
1	B	560	ASP	2.4
1	B	464	LEU	2.3
1	A	575	THR	2.3
1	B	455	THR	2.3
1	C	467	ASP	2.3
1	B	450	LYS	2.3
1	A	464	LEU	2.3
1	C	508	ARG	2.3
1	A	467	ASP	2.3
1	B	449	LEU	2.2
1	C	575	THR	2.2
1	C	455	THR	2.2
1	B	269	GLY	2.1
1	B	345	PRO	2.1
1	B	559	GLN	2.1
1	B	440	SER	2.1
1	B	546	LEU	2.1
1	D	260	LYS	2.1
1	B	342	LEU	2.0
1	C	466	LEU	2.0
1	D	256	ASP	2.0
1	B	349	ALA	2.0
1	B	571	TRP	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

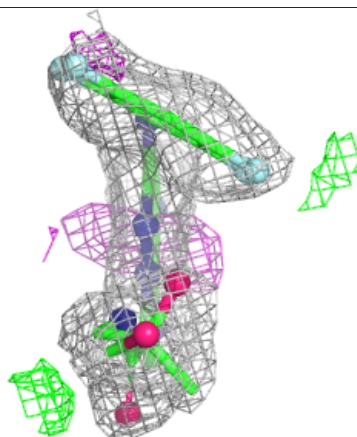
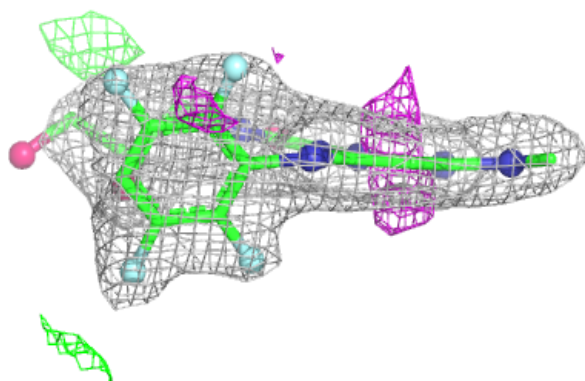
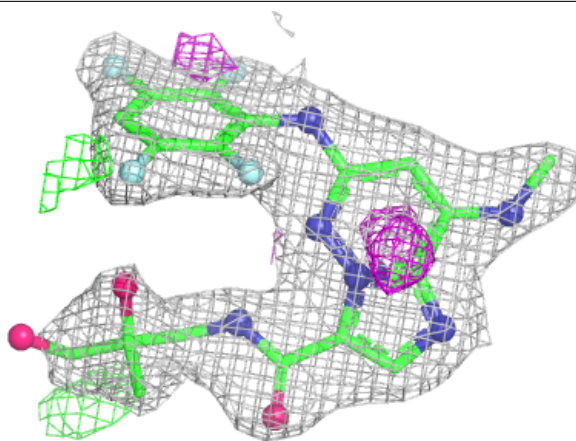
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EOH	B	704	3/3	0.75	0.18	37,37,39,39	0
5	EOH	D	703	3/3	0.79	0.20	27,27,33,37	0
5	EOH	C	704	3/3	0.81	0.12	31,31,35,37	0
5	EOH	A	805	3/3	0.82	0.18	45,45,48,51	0
4	SO4	B	703	5/5	0.83	0.15	93,96,97,98	0
6	7DJ	C	705	31/31	0.84	0.14	49,60,70,70	0
4	SO4	C	703	5/5	0.85	0.14	65,75,77,79	0
6	7DJ	B	707	31/31	0.86	0.13	50,63,73,75	0
5	EOH	B	706	3/3	0.86	0.12	35,35,39,41	0
6	7DJ	D	704	31/31	0.86	0.13	44,54,65,67	0
6	7DJ	A	807	31/31	0.88	0.12	44,53,62,67	0
5	EOH	A	806	3/3	0.89	0.17	38,38,39,41	0
5	EOH	B	705	3/3	0.90	0.16	43,43,43,44	0
5	EOH	A	804	3/3	0.92	0.13	30,30,37,42	0
4	SO4	A	803	5/5	0.93	0.12	49,59,63,64	0
3	MG	C	702	1/1	0.99	0.04	25,25,25,25	0
2	ZN	B	701	1/1	0.99	0.02	35,35,35,35	0
3	MG	B	702	1/1	1.00	0.01	27,27,27,27	0
2	ZN	A	801	1/1	1.00	0.02	29,29,29,29	0
3	MG	D	702	1/1	1.00	0.03	24,24,24,24	0
2	ZN	C	701	1/1	1.00	0.02	32,32,32,32	0
2	ZN	D	701	1/1	1.00	0.04	28,28,28,28	0
3	MG	A	802	1/1	1.00	0.02	25,25,25,25	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.

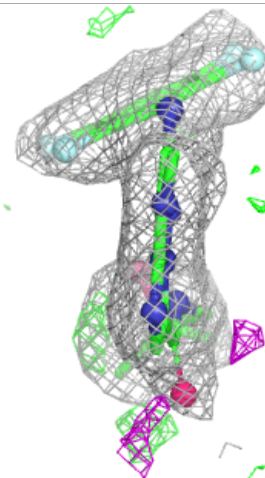
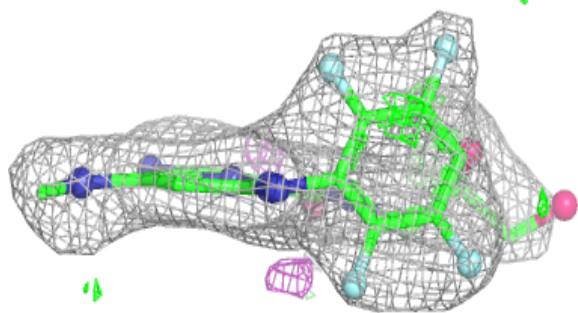
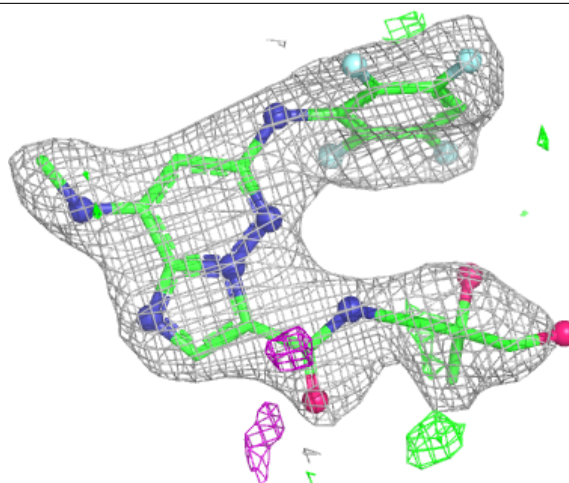
Electron density around 7DJ C 705:

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



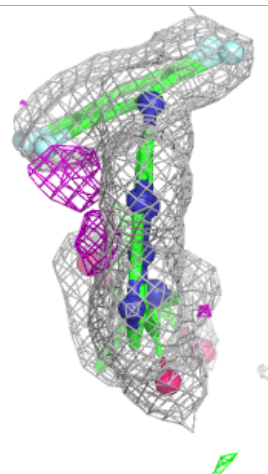
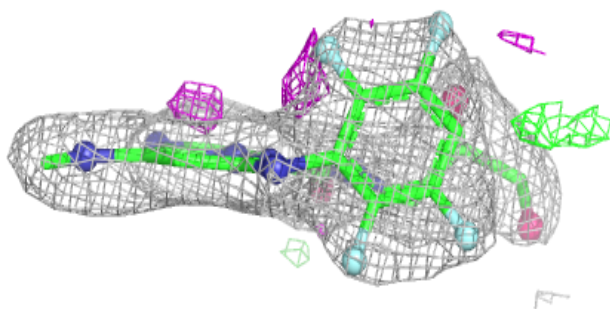
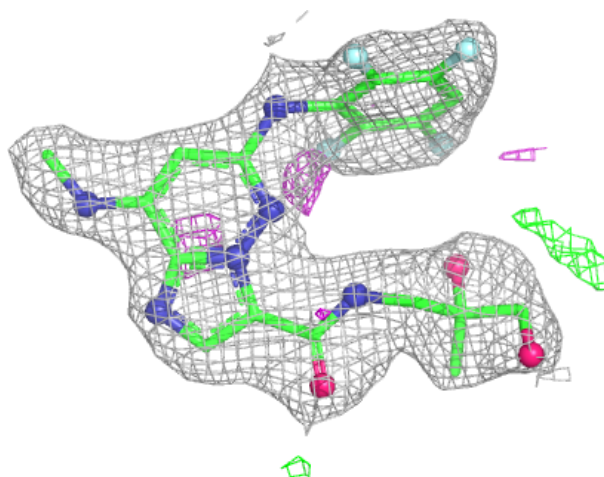
Electron density around 7DJ B 707:

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



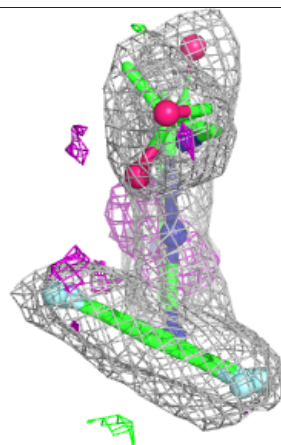
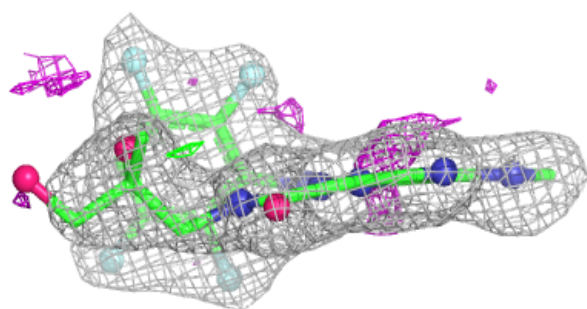
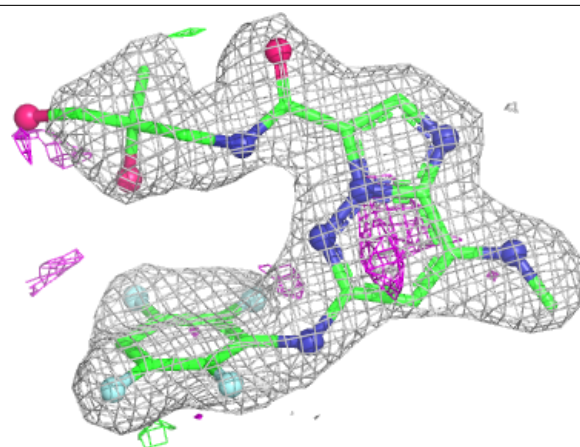
Electron density around 7DJ D 704:

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



Electron density around 7DJ 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.