



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:33 am BST

PDB ID : 1Y2K
Title : Catalytic Domain Of Human Phosphodiesterase 4D In Complex With 3,5-di methyl-1-(3-nitro-phenyl)-1H-pyrazole-4-carboxylic acid ethyl ester
Authors : Card, G.L.; Blasdel, L.; England, B.P.; Zhang, C.; Suzuki, Y.; Gillette, S.; Fong, D.; Ibrahim, P.N.; Artis, D.R.; Bollag, G.; Milburn, M.V.; Kim, S.-H.; Schlessinger, J.; Zhang, K.Y.J.
Deposited on : 2004-11-22
Resolution : 1.36 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

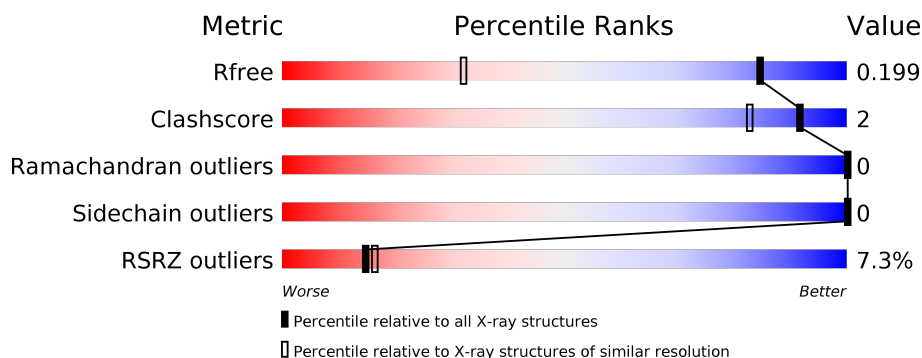
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.36 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	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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	349	<div> <div>6%</div> <div>89%</div> <div>5%</div> <div>7%</div> </div>
1	B	349	<div> <div>7%</div> <div>90%</div> <div>•</div> <div>8%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	A	731	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5927 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	4	5	0
			2654	1677	450	511	16			
1	B	322	Total	C	N	O	S	4	6	0
			2636	1668	446	506	16			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	65	MET	-	INITIATING METHIONINE	UNP Q08499
A	66	GLY	-	CLONING ARTIFACT	UNP Q08499
A	67	SER	-	CLONING ARTIFACT	UNP Q08499
A	68	SER	-	CLONING ARTIFACT	UNP Q08499
A	69	HIS	-	EXPRESSION TAG	UNP Q08499
A	70	HIS	-	EXPRESSION TAG	UNP Q08499
A	71	HIS	-	EXPRESSION TAG	UNP Q08499
A	72	HIS	-	EXPRESSION TAG	UNP Q08499
A	73	HIS	-	EXPRESSION TAG	UNP Q08499
A	74	HIS	-	EXPRESSION TAG	UNP Q08499
A	75	SER	-	CLONING ARTIFACT	UNP Q08499
A	76	SER	-	CLONING ARTIFACT	UNP Q08499
A	77	GLY	-	CLONING ARTIFACT	UNP Q08499
A	78	LEU	-	CLONING ARTIFACT	UNP Q08499
A	79	VAL	-	CLONING ARTIFACT	UNP Q08499
A	80	PRO	-	CLONING ARTIFACT	UNP Q08499
A	81	ARG	-	CLONING ARTIFACT	UNP Q08499
A	82	GLY	-	CLONING ARTIFACT	UNP Q08499
A	83	SER	-	CLONING ARTIFACT	UNP Q08499
A	84	HIS	-	CLONING ARTIFACT	UNP Q08499
A	85	MET	-	CLONING ARTIFACT	UNP Q08499
B	65	MET	-	INITIATING METHIONINE	UNP Q08499
B	66	GLY	-	CLONING ARTIFACT	UNP Q08499
B	67	SER	-	CLONING ARTIFACT	UNP Q08499
B	68	SER	-	CLONING ARTIFACT	UNP Q08499

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Chain	Residue	Modelled	Actual	Comment	Reference
B	69	HIS	-	EXPRESSION TAG	UNP Q08499
B	70	HIS	-	EXPRESSION TAG	UNP Q08499
B	71	HIS	-	EXPRESSION TAG	UNP Q08499
B	72	HIS	-	EXPRESSION TAG	UNP Q08499
B	73	HIS	-	EXPRESSION TAG	UNP Q08499
B	74	HIS	-	EXPRESSION TAG	UNP Q08499
B	75	SER	-	CLONING ARTIFACT	UNP Q08499
B	76	SER	-	CLONING ARTIFACT	UNP Q08499
B	77	GLY	-	CLONING ARTIFACT	UNP Q08499
B	78	LEU	-	CLONING ARTIFACT	UNP Q08499
B	79	VAL	-	CLONING ARTIFACT	UNP Q08499
B	80	PRO	-	CLONING ARTIFACT	UNP Q08499
B	81	ARG	-	CLONING ARTIFACT	UNP Q08499
B	82	GLY	-	CLONING ARTIFACT	UNP Q08499
B	83	SER	-	CLONING ARTIFACT	UNP Q08499
B	84	HIS	-	CLONING ARTIFACT	UNP Q08499
B	85	MET	-	CLONING ARTIFACT	UNP Q08499

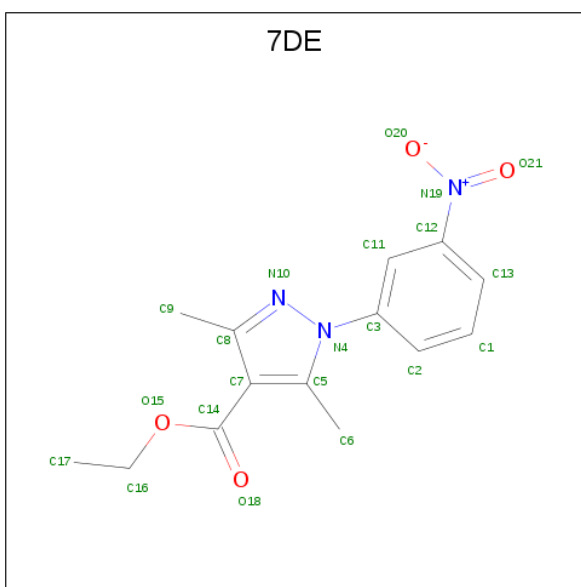
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

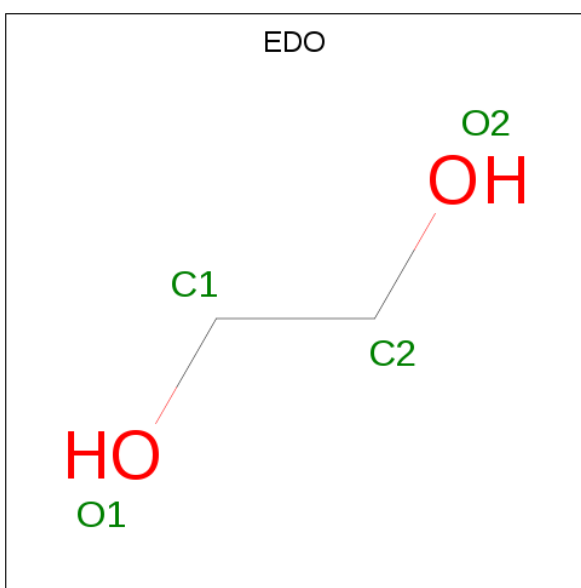
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 3,5-DIMETHYL-1-(3-NITROPHENYL)-1H-PYRAZOLE-4-CARBOXYLIC ACID ETHYL ESTER (three-letter code: 7DE) (formula: C₁₄H₁₅N₃O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			21	14	3	4		
4	B	1	Total	C	N	O	0	0
			21	14	3	4		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

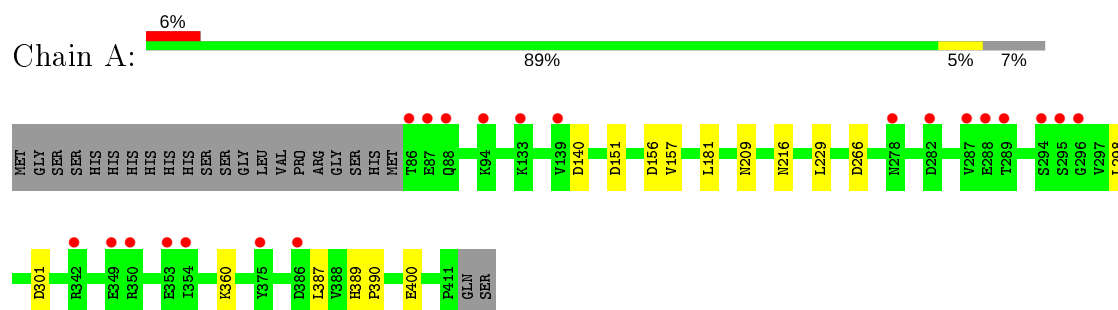
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	234	Total O 234 234	0	0
6	B	225	Total O 225 225	0	0

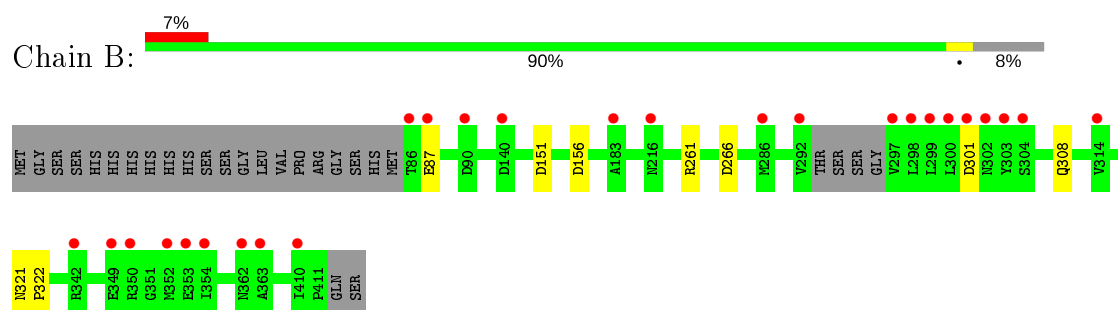
3 Residue-property plots [i](#)

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: 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	60.35Å 78.89Å 164.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.65 – 1.36 44.93 – 1.36	Depositor EDS
% Data completeness (in resolution range)	89.6 (81.65-1.36) 89.6 (44.93-1.36)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 1.36Å)	Xtriage
Refinement program	REFMAC 5.1.25	Depositor
R, R_{free}	0.175 , 0.188 0.184 , 0.199	Depositor DCC
R_{free} test set	7536 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	14.4	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5927	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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: MG, EDO, ZN, 7DE

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	0.29	0/2730	0.70	5/3708 (0.1%)
1	B	0.34	1/2715 (0.0%)	0.70	4/3686 (0.1%)
All	All	0.32	1/5445 (0.0%)	0.70	9/7394 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	87	GLU	CB-CG	9.24	1.69	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	ASP	CB-CG-OD2	6.44	124.09	118.30
1	A	156	ASP	CB-CG-OD2	6.37	124.04	118.30
1	A	301	ASP	CB-CG-OD2	5.77	123.50	118.30
1	B	156	ASP	CB-CG-OD2	5.77	123.49	118.30
1	A	140	ASP	CB-CG-OD2	5.72	123.44	118.30
1	A	151	ASP	CB-CG-OD2	5.63	123.37	118.30
1	B	301	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	266	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	266	ASP	CB-CG-OD2	5.10	122.89	118.30

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	2654	0	2602	10	0
1	B	2636	0	2583	6	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	21	0	15	0	0
4	B	21	0	15	0	0
5	A	72	0	108	7	0
5	B	60	0	90	4	0
6	A	234	0	0	1	0
6	B	225	0	0	1	0
All	All	5927	0	5413	17	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 (17) 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)
5:B:726:EDO:H22	6:B:2132:HOH:O	1.82	0.80
5:A:732:EDO:H22	1:B:261:ARG:NH2	2.04	0.73
1:A:157:VAL:HG22	5:A:729:EDO:H21	1.85	0.58
5:A:732:EDO:H22	1:B:261:ARG:CZ	2.33	0.57
1:A:400:GLU:HB2	5:A:738:EDO:H11	1.88	0.55
1:B:308:GLN:HE22	5:B:737:EDO:H11	1.71	0.55
1:A:209:ASN:ND2	5:A:723:EDO:H12	2.26	0.50
1:B:308:GLN:NE2	5:B:737:EDO:H11	2.28	0.49
1:B:261:ARG:HD3	5:B:718:EDO:H12	1.96	0.48
1:A:229:LEU:HD12	5:A:723:EDO:H11	1.98	0.46
1:B:321:ASN:HB2	1:B:322:PRO:HD3	1.98	0.45
1:A:181:LEU:HD21	1:A:298:LEU:HD12	1.99	0.44
1:A:181:LEU:CD2	1:A:298:LEU:HD12	2.49	0.43
1:A:298:LEU:HD11	1:A:387:LEU:HG	2.00	0.42
1:A:216:ASN:HA	6:A:1040:HOH:O	2.19	0.42
1:A:360:LYS:CE	5:A:736:EDO:H22	2.50	0.41
1:A:389:HIS:HA	1:A:390:PRO:HA	1.87	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	329/349 (94%)	324 (98%)	5 (2%)	0	100	100
1	B	324/349 (93%)	321 (99%)	3 (1%)	0	100	100
All	All	653/698 (94%)	645 (99%)	8 (1%)	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	303/318 (95%)	303 (100%)	0	100	100
1	B	301/318 (95%)	301 (100%)	0	100	100
All	All	604/636 (95%)	604 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	308	GLN
1	B	123	HIS
1	B	389	HIS

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 39 ligands modelled in this entry, 4 are monoatomic - leaving 35 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	709	-	3,3,3	0.27	0	2,2,2	0.29	0
5	EDO	A	736	-	3,3,3	0.29	0	2,2,2	0.34	0
5	EDO	B	708	-	3,3,3	0.29	0	2,2,2	0.28	0
5	EDO	B	730	-	3,3,3	0.28	0	2,2,2	0.36	0
5	EDO	A	733	-	3,3,3	0.29	0	2,2,2	0.38	0
5	EDO	A	738	-	3,3,3	0.28	0	2,2,2	0.34	0
5	EDO	A	731	-	3,3,3	0.28	0	2,2,2	0.40	0
5	EDO	A	707	-	3,3,3	0.28	0	2,2,2	0.49	0
5	EDO	B	734	-	3,3,3	0.27	0	2,2,2	0.37	0
5	EDO	B	718	-	3,3,3	0.28	0	2,2,2	0.39	0
4	7DE	B	601	-	19,22,22	1.53	4 (21%)	23,31,31	1.28	2 (8%)
5	EDO	B	726	-	3,3,3	0.30	0	2,2,2	0.41	0
5	EDO	A	739	-	3,3,3	0.28	0	2,2,2	0.38	0
5	EDO	B	740	-	3,3,3	0.29	0	2,2,2	0.39	0
5	EDO	B	701	-	3,3,3	0.26	0	2,2,2	0.33	0
5	EDO	B	727	-	3,3,3	0.27	0	2,2,2	0.40	0
5	EDO	B	728	-	3,3,3	0.27	0	2,2,2	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	A	704	-	3,3,3	0.27	0	2,2,2	0.32	0
5	EDO	B	717	-	3,3,3	0.28	0	2,2,2	0.37	0
5	EDO	A	724	-	3,3,3	0.29	0	2,2,2	0.41	0
5	EDO	A	712	-	3,3,3	0.28	0	2,2,2	0.36	0
5	EDO	A	720	-	3,3,3	0.28	0	2,2,2	0.39	0
5	EDO	B	706	-	3,3,3	0.29	0	2,2,2	0.40	0
5	EDO	A	729	-	3,3,3	0.28	0	2,2,2	0.32	0
5	EDO	B	725	-	3,3,3	0.27	0	2,2,2	0.31	0
5	EDO	A	732	-	3,3,3	0.28	0	2,2,2	0.54	0
5	EDO	A	702	-	3,3,3	0.26	0	2,2,2	0.34	0
5	EDO	B	737	-	3,3,3	0.28	0	2,2,2	0.39	0
5	EDO	A	719	-	3,3,3	0.28	0	2,2,2	0.20	0
5	EDO	A	722	-	3,3,3	0.27	0	2,2,2	0.49	0
4	7DE	A	602	-	19,22,22	1.52	4 (21%)	23,31,31	1.27	2 (8%)
5	EDO	A	723	-	3,3,3	0.26	0	2,2,2	0.33	0
5	EDO	A	716	-	3,3,3	0.29	0	2,2,2	0.38	0
5	EDO	B	735	-	3,3,3	0.28	0	2,2,2	0.42	0
5	EDO	A	715	-	3,3,3	0.24	0	2,2,2	0.40	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
5	EDO	B	709	-	-	1/1/1/1	-
5	EDO	A	736	-	-	1/1/1/1	-
5	EDO	B	708	-	-	1/1/1/1	-
5	EDO	B	730	-	-	0/1/1/1	-
5	EDO	A	733	-	-	0/1/1/1	-
5	EDO	A	738	-	-	0/1/1/1	-
5	EDO	A	731	-	-	0/1/1/1	-
5	EDO	A	707	-	-	0/1/1/1	-
5	EDO	B	734	-	-	1/1/1/1	-
5	EDO	B	718	-	-	1/1/1/1	-
4	7DE	B	601	-	-	0/13/15/15	0/2/2/2
5	EDO	B	726	-	-	0/1/1/1	-
5	EDO	A	739	-	-	1/1/1/1	-
5	EDO	B	740	-	-	1/1/1/1	-
5	EDO	B	701	-	-	0/1/1/1	-
5	EDO	B	727	-	-	1/1/1/1	-
5	EDO	B	728	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	704	-	-	0/1/1/1	-
5	EDO	B	717	-	-	0/1/1/1	-
5	EDO	A	724	-	-	0/1/1/1	-
5	EDO	A	712	-	-	1/1/1/1	-
5	EDO	A	720	-	-	0/1/1/1	-
5	EDO	B	706	-	-	0/1/1/1	-
5	EDO	A	729	-	-	0/1/1/1	-
5	EDO	B	725	-	-	0/1/1/1	-
5	EDO	A	732	-	-	1/1/1/1	-
5	EDO	A	702	-	-	0/1/1/1	-
5	EDO	B	737	-	-	1/1/1/1	-
5	EDO	A	719	-	-	1/1/1/1	-
5	EDO	A	722	-	-	0/1/1/1	-
4	7DE	A	602	-	-	0/13/15/15	0/2/2/2
5	EDO	A	723	-	-	1/1/1/1	-
5	EDO	A	716	-	-	1/1/1/1	-
5	EDO	B	735	-	-	0/1/1/1	-
5	EDO	A	715	-	-	0/1/1/1	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	7DE	C12-N19	-3.38	1.37	1.45
4	B	601	7DE	C12-N19	-3.36	1.37	1.45
4	B	601	7DE	C8-N10	-2.87	1.26	1.33
4	A	602	7DE	C8-N10	-2.79	1.26	1.33
4	B	601	7DE	C3-N4	-2.59	1.36	1.44
4	A	602	7DE	C3-N4	-2.58	1.36	1.44
4	A	602	7DE	N10-N4	-2.35	1.35	1.39
4	B	601	7DE	N10-N4	-2.33	1.35	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	7DE	C11-C12-N19	3.12	121.50	118.75
4	A	602	7DE	C11-C12-N19	2.99	121.38	118.75
4	A	602	7DE	O15-C14-C7	2.39	117.71	112.33
4	B	601	7DE	O15-C14-C7	2.20	117.28	112.33

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	734	EDO	O1-C1-C2-O2
5	B	709	EDO	O1-C1-C2-O2
5	B	740	EDO	O1-C1-C2-O2
5	A	732	EDO	O1-C1-C2-O2
5	B	718	EDO	O1-C1-C2-O2
5	B	737	EDO	O1-C1-C2-O2
5	A	723	EDO	O1-C1-C2-O2
5	A	739	EDO	O1-C1-C2-O2
5	A	736	EDO	O1-C1-C2-O2
5	B	727	EDO	O1-C1-C2-O2
5	A	712	EDO	O1-C1-C2-O2
5	A	716	EDO	O1-C1-C2-O2
5	B	708	EDO	O1-C1-C2-O2
5	A	719	EDO	O1-C1-C2-O2

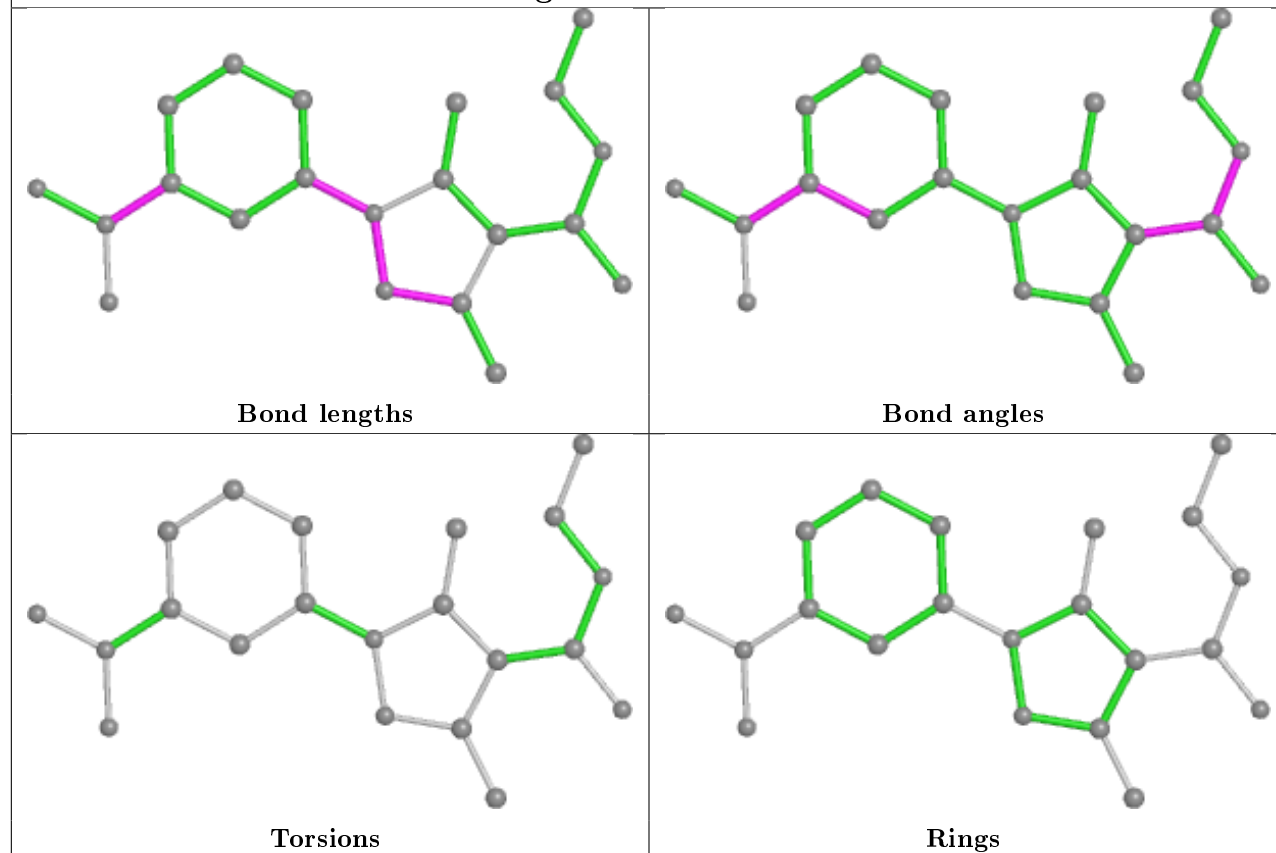
There are no ring outliers.

8 monomers are involved in 11 short contacts:

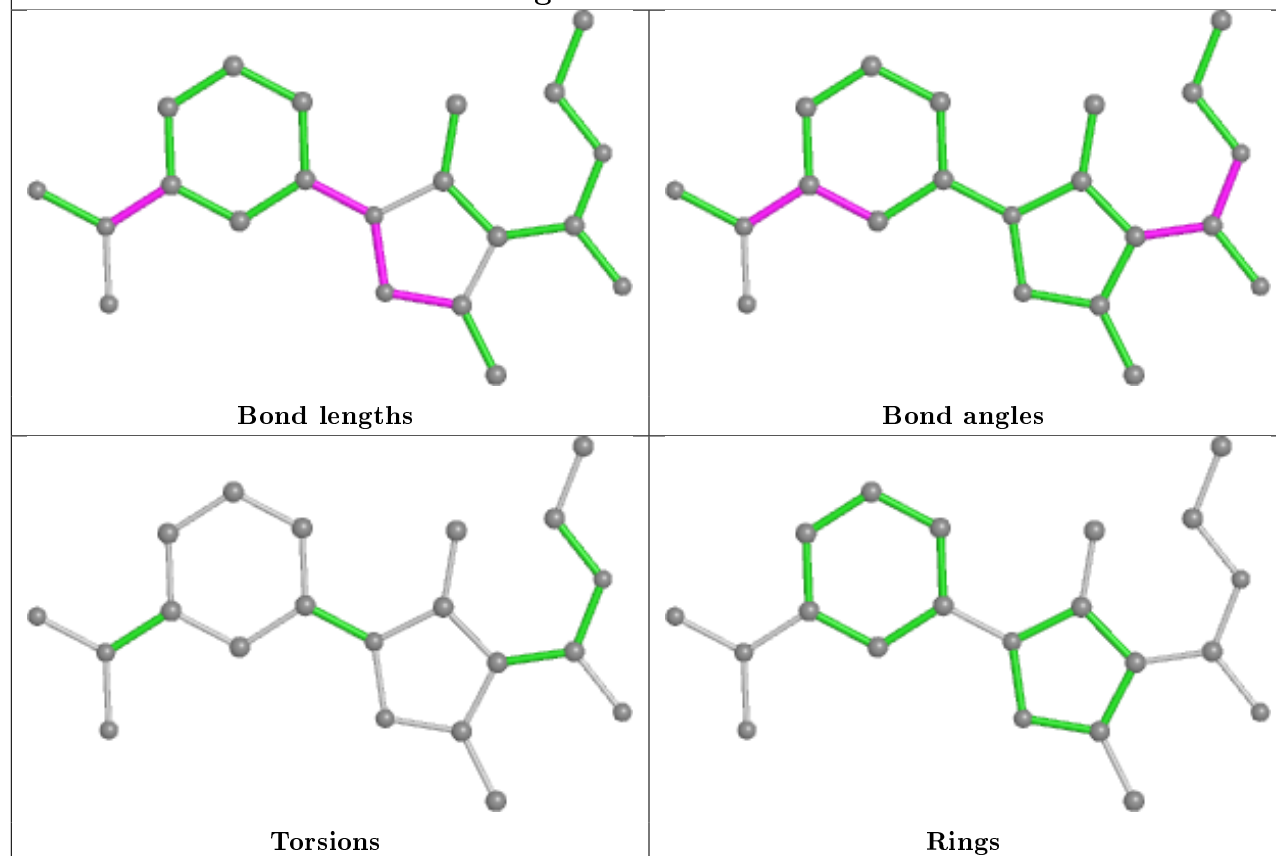
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	736	EDO	1	0
5	A	738	EDO	1	0
5	B	718	EDO	1	0
5	B	726	EDO	1	0
5	A	729	EDO	1	0
5	A	732	EDO	2	0
5	B	737	EDO	2	0
5	A	723	EDO	2	0

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 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 7DE B 601



Ligand 7DE A 602



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, 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	326/349 (93%)	0.57	21 (6%)	19 21	4, 10, 17, 23	1 (0%)
1	B	322/349 (92%)	0.75	26 (8%)	12 13	5, 9, 19, 26	2 (0%)
All	All	648/698 (92%)	0.66	47 (7%)	15 16	4, 10, 18, 26	3 (0%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	301	ASP	9.2
1	B	299	LEU	7.3
1	A	289	THR	6.2
1	B	86	THR	5.3
1	A	375	TYR	5.1
1	B	298	LEU	5.0
1	A	86	THR	4.6
1	A	294	SER	4.3
1	B	349	GLU	4.2
1	B	354	ILE	4.1
1	B	303	TYR	4.1
1	B	300	LEU	4.0
1	B	87	GLU	3.9
1	B	297	VAL	3.7
1	B	410	ILE	3.7
1	B	362	ASN	3.6
1	A	295	SER	3.5
1	A	353	GLU	3.5
1	A	287	VAL	3.4
1	B	292	VAL	3.2
1	B	302	ASN	3.2
1	B	353	GLU	3.2
1	B	90	ASP	3.0
1	B	183	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	342	ARG	2.8
1	A	133	LYS	2.7
1	B	216	ASN	2.7
1	B	350	ARG	2.6
1	A	94	LYS	2.6
1	A	296	GLY	2.4
1	A	288	GLU	2.4
1	B	342	ARG	2.3
1	A	349	GLU	2.3
1	A	282	ASP	2.3
1	A	386[A]	ASP	2.3
1	A	87	GLU	2.2
1	A	139	VAL	2.2
1	A	88	GLN	2.2
1	A	354	ILE	2.1
1	B	314	VAL	2.1
1	B	352	MET	2.1
1	A	350	ARG	2.1
1	B	363	ALA	2.1
1	B	286	MET	2.0
1	B	140	ASP	2.0
1	A	278	ASN	2.0
1	B	304	SER	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.

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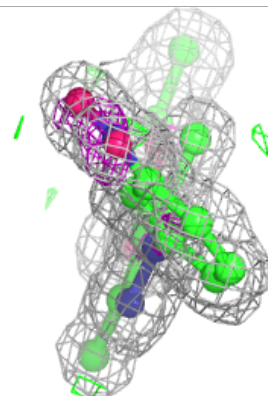
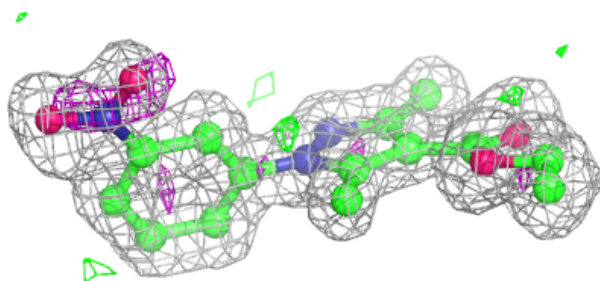
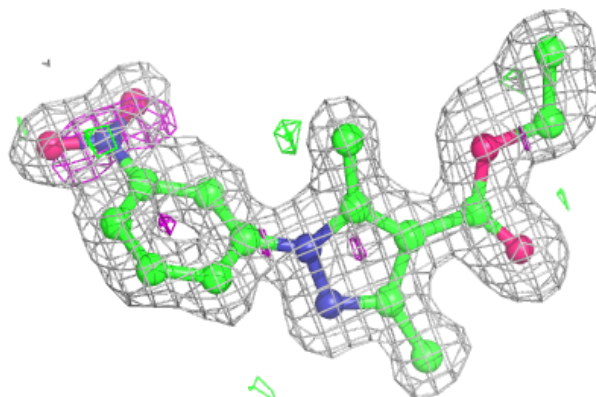
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EDO	A	729	4/4	0.64	0.30	38,40,40,40	0
5	EDO	A	739	4/4	0.65	0.23	46,47,47,47	0
5	EDO	A	712	4/4	0.67	0.22	46,46,46,46	0
5	EDO	B	734	4/4	0.67	0.17	40,40,40,41	0
5	EDO	A	733	4/4	0.68	0.17	34,35,36,37	0
5	EDO	B	730	4/4	0.72	0.29	33,36,36,37	0
5	EDO	A	736	4/4	0.74	0.26	42,43,43,43	0
5	EDO	B	737	4/4	0.74	0.37	44,44,44,44	0
5	EDO	B	708	4/4	0.75	0.11	39,39,39,40	0
5	EDO	A	716	4/4	0.75	0.15	28,30,30,31	0
5	EDO	B	728	4/4	0.77	0.14	26,27,28,30	0
5	EDO	A	731	4/4	0.80	0.43	41,41,41,41	0
5	EDO	B	709	4/4	0.80	0.21	39,40,40,40	0
5	EDO	B	717	4/4	0.80	0.11	31,31,31,32	0
5	EDO	A	724	4/4	0.80	0.22	38,39,39,40	0
5	EDO	B	740	4/4	0.81	0.22	38,39,39,39	0
5	EDO	A	715	4/4	0.83	0.16	31,32,32,34	0
5	EDO	A	704	4/4	0.84	0.12	28,29,30,32	0
4	7DE	A	602	21/21	0.85	0.14	18,21,25,27	0
5	EDO	A	738	4/4	0.85	0.23	35,36,36,37	0
5	EDO	B	735	4/4	0.85	0.14	41,41,41,41	0
5	EDO	A	719	4/4	0.85	0.16	33,34,35,35	0
5	EDO	A	707	4/4	0.87	0.14	31,31,31,32	0
5	EDO	B	725	4/4	0.87	0.10	28,28,28,28	0
5	EDO	A	732	4/4	0.87	0.24	24,28,29,29	0
5	EDO	A	723	4/4	0.88	0.16	21,25,25,25	0
5	EDO	A	720	4/4	0.88	0.12	31,31,31,32	0
5	EDO	A	722	4/4	0.89	0.09	25,25,26,27	0
5	EDO	B	706	4/4	0.89	0.09	26,27,27,28	0
5	EDO	B	726	4/4	0.89	0.13	24,27,27,29	0
5	EDO	B	727	4/4	0.90	0.14	34,35,35,35	0
5	EDO	B	701	4/4	0.91	0.14	22,25,26,28	0
4	7DE	B	601	21/21	0.91	0.13	17,19,25,26	0
5	EDO	A	702	4/4	0.92	0.09	22,23,24,24	0
5	EDO	B	718	4/4	0.93	0.17	39,39,39,40	0
2	ZN	A	1001	1/1	0.99	0.07	13,13,13,13	0
2	ZN	B	1001	1/1	1.00	0.07	12,12,12,12	0
3	MG	B	1002	1/1	1.00	0.13	8,8,8,8	0
3	MG	A	1002	1/1	1.00	0.15	8,8,8,8	0

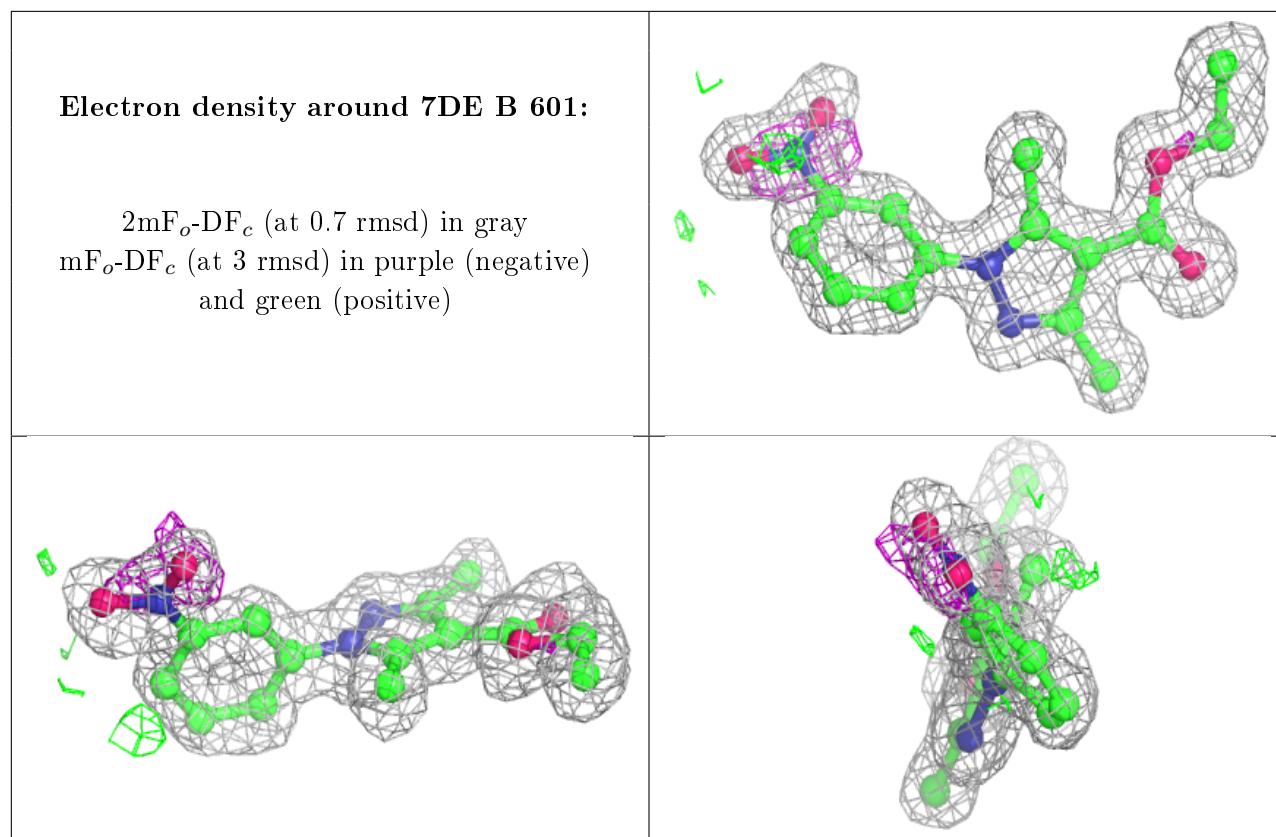
The following is a graphical depiction of the model fit to experimental electron density of all

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 7DE A 602:

$2mF_o-DF_c$ (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.