



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:13 AM UTC

PDB ID : 6F8W / pdb_00006f8w
Title : Crystal structure of the PDE4D catalytic domain in complex with GEBR-18a
Authors : Prosdocimi, T.; Donini, S.; Parisini, E.
Deposited on : 2017-12-13
Resolution : 1.60 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

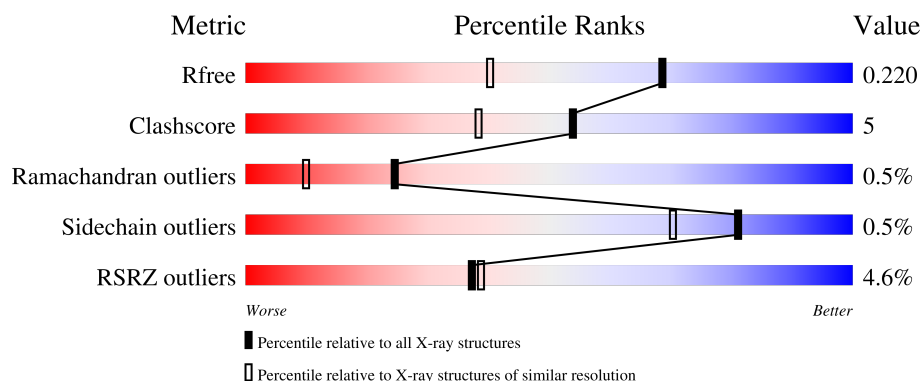
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	343	4% 86% 8% 6%
1	B	343	5% 84% 12% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5977 atoms, of which 58 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	322	Total	C	N	O	S	0	9	0
			2662	1691	457	497	17			
1	B	331	Total	C	N	O	S	0	8	0
			2700	1713	457	514	16			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	243	MET	-	initiating methionine	UNP Q08499
A	579	ALA	-	expression tag	UNP Q08499
A	580	HIS	-	expression tag	UNP Q08499
A	581	HIS	-	expression tag	UNP Q08499
A	582	HIS	-	expression tag	UNP Q08499
A	583	HIS	-	expression tag	UNP Q08499
A	584	HIS	-	expression tag	UNP Q08499
A	585	HIS	-	expression tag	UNP Q08499
B	243	MET	-	initiating methionine	UNP Q08499
B	579	ALA	-	expression tag	UNP Q08499
B	580	HIS	-	expression tag	UNP Q08499
B	581	HIS	-	expression tag	UNP Q08499
B	582	HIS	-	expression tag	UNP Q08499
B	583	HIS	-	expression tag	UNP Q08499
B	584	HIS	-	expression tag	UNP Q08499
B	585	HIS	-	expression tag	UNP Q08499

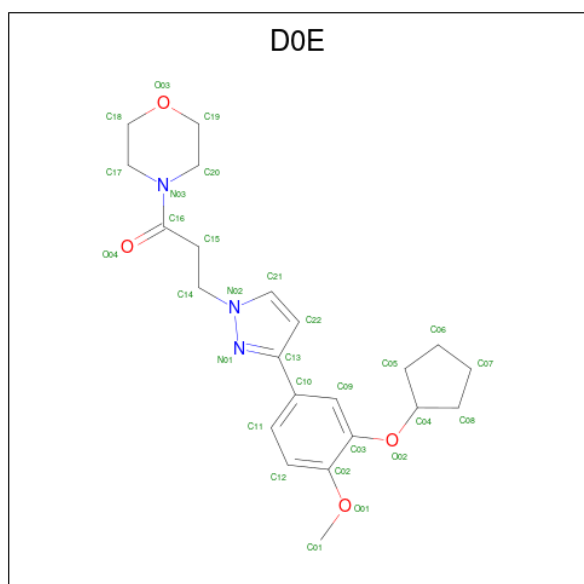
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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

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

- Molecule 4 is 3-[3-(3-cyclopentyloxy-4-methoxy-phenyl)pyrazol-1-yl]-1-morpholin-4-ylpropan-1-one (CCD ID: D0E) (formula: C₂₂H₂₉N₃O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			58	22	29	3	4		
4	B	1	Total	C	H	N	O	0	0
			58	22	29	3	4		

- Molecule 5 is water.

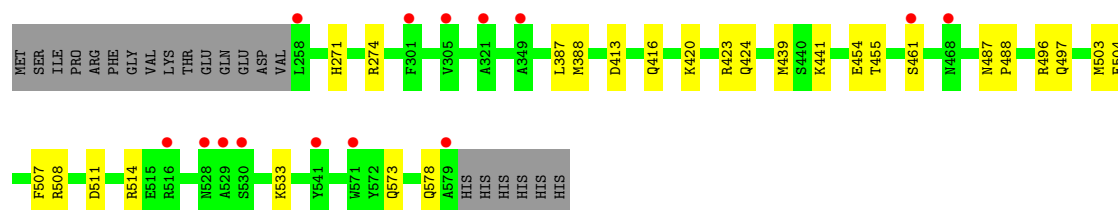
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	244	Total	O	0	0
			244	244		
5	B	248	Total	O	0	0
			248	248		

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.

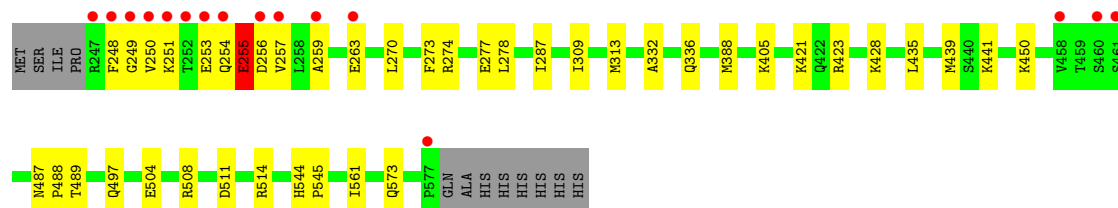
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

Chain A: 



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

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.04Å 98.72Å 120.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.69 – 1.60 45.69 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (45.69-1.60) 99.9 (45.69-1.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.191 , 0.219 0.194 , 0.220	Depositor DCC
R_{free} test set	5147 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.6	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	5977	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: D0E, MG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.40	0/2745	0.67	0/3725
1	B	0.41	0/2779	0.67	0/3773
All	All	0.41	0/5524	0.67	0/7498

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	2662	0	2653	28	0
1	B	2700	0	2665	28	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
4	A	29	29	0	1	0
4	B	29	29	0	1	0
5	A	244	0	0	11	0
5	B	248	0	0	4	0
All	All	5919	58	5318	53	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (53) 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:504:GLU:OE2	1:B:508:ARG:NH2	2.11	0.84
1:B:428[B]:LYS:NZ	5:B:702:HOH:O	2.11	0.81
1:B:511:ASP:OD1	1:B:514:ARG:NH2	2.14	0.79
1:A:274:ARG:NH2	5:A:702:HOH:O	2.15	0.79
1:A:511:ASP:OD1	1:A:514:ARG:NH2	2.16	0.78
1:A:423[B]:ARG:NH1	5:A:704:HOH:O	2.18	0.76
1:B:254:GLN:HB3	1:B:257:VAL:HG12	1.69	0.73
1:B:508:ARG:NH1	5:B:703:HOH:O	2.20	0.73
1:A:441:LYS:HD2	5:A:833:HOH:O	1.98	0.62
1:A:504:GLU:OE2	1:A:508[A]:ARG:NH2	2.34	0.60
1:A:413:ASP:OD2	1:A:423[B]:ARG:NH2	2.36	0.59
1:B:487:ASN:HB2	1:B:488:PRO:HD3	1.85	0.59
1:A:388[B]:MET:SD	1:B:388[B]:MET:SD	3.02	0.57
1:A:487:ASN:HB2	1:A:488:PRO:HD3	1.87	0.57
1:A:461:SER:HB3	5:A:712:HOH:O	2.05	0.56
1:B:489:THR:HB	1:B:561:ILE:HG23	1.88	0.56
1:B:273:PHE:CZ	1:B:497:GLN:HG2	2.41	0.54
1:B:248:PHE:O	1:B:250:VAL:N	2.33	0.54
1:B:439:MET:HG2	4:B:604:D0E:O04	2.09	0.53
1:B:423:ARG:NH1	5:B:712:HOH:O	2.37	0.53
1:A:388[A]:MET:SD	1:B:388[A]:MET:SD	3.06	0.53
1:B:254:GLN:HG3	1:B:256:ASP:H	1.72	0.52
1:B:277[A]:GLU:HG3	1:B:278:LEU:N	2.25	0.52
1:A:420:LYS:NZ	5:A:714:HOH:O	2.32	0.52
1:A:423[A]:ARG:NH1	5:A:721:HOH:O	2.43	0.51
1:B:544:HIS:HB3	1:B:545:PRO:HD3	1.92	0.51
1:A:454:GLU:HG3	1:A:455:THR:HG23	1.93	0.50
1:A:508[B]:ARG:HH21	1:A:508[B]:ARG:HB3	1.77	0.49
1:B:254:GLN:HG3	1:B:255:GLU:N	2.25	0.49
1:A:271:HIS:CG	1:A:274:ARG:HG3	2.47	0.49
1:B:274:ARG:O	1:B:277[A]:GLU:HG3	2.12	0.49
1:A:441:LYS:NZ	5:A:726:HOH:O	2.47	0.48
1:A:387:LEU:HD21	1:B:405:LYS:HD3	1.95	0.47
1:A:439:MET:HG2	4:A:605:D0E:O04	2.15	0.47
1:A:573:GLN:HE21	1:A:578:GLN:HE22	1.61	0.46
1:A:416:GLN:HA	1:A:423[B]:ARG:HH21	1.80	0.46
1:A:497[B]:GLN:HE21	1:A:497[B]:GLN:HA	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:LYS:NZ	5:B:709:HOH:O	2.33	0.46
1:B:435:LEU:O	1:B:441:LYS:HE2	2.15	0.46
1:B:270:LEU:HD22	1:B:336:GLN:HG3	1.98	0.46
1:B:287:ILE:HD12	1:B:332:ALA:HB1	1.98	0.45
1:B:259:ALA:O	1:B:263:GLU:HG3	2.17	0.45
1:B:277[A]:GLU:HG3	1:B:278:LEU:H	1.81	0.45
1:A:496:ARG:NH2	5:A:707:HOH:O	2.23	0.44
1:A:503:MET:HE3	1:A:507:PHE:CZ	2.53	0.44
1:B:253:GLU:HA	1:B:254:GLN:HA	1.77	0.44
1:A:508[A]:ARG:NH1	5:A:722:HOH:O	2.43	0.44
1:B:274:ARG:HA	1:B:277[A]:GLU:HG2	2.00	0.43
1:A:496:ARG:HD3	5:A:738:HOH:O	2.18	0.43
1:A:573:GLN:HG2	1:A:578:GLN:OE1	2.18	0.42
1:A:533:LYS:HE3	1:A:533:LYS:HB2	1.55	0.42
1:B:309:ILE:O	1:B:313[B]:MET:HG3	2.20	0.42
1:A:424:GLN:OE1	5:A:706:HOH:O	2.22	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	329/343 (96%)	325 (99%)	4 (1%)	0	100	100
1	B	337/343 (98%)	329 (98%)	5 (2%)	3 (1%)	14	3
All	All	666/686 (97%)	654 (98%)	9 (1%)	3 (0%)	24	10

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	255	GLU
1	B	249	GLY

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Mol	Chain	Res	Type
1	B	251	LYS

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	302/313 (96%)	302 (100%)	0	100	100
1	B	306/313 (98%)	303 (99%)	3 (1%)	68	50
All	All	608/626 (97%)	605 (100%)	3 (0%)	81	70

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	255	GLU
1	B	421	LYS
1	B	573	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	289	HIS
1	A	487	ASN
1	A	527	HIS
1	A	573	GLN
1	B	487	ASN
1	B	535	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 7 are monoatomic - leaving 2 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	$\# Z > 2$
4	D0E	B	604	-	32,32,32	1.96	10 (31%)	43,43,43	2.42	16 (37%)
4	D0E	A	605	-	32,32,32	1.89	10 (31%)	43,43,43	2.53	18 (41%)

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
4	D0E	B	604	-	-	4/19/34/34	0/4/4/4
4	D0E	A	605	-	-	4/19/34/34	0/4/4/4

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	605	D0E	C13-N01	-5.69	1.27	1.34
4	B	604	D0E	C13-N01	-5.61	1.27	1.34
4	B	604	D0E	C11-C10	-3.21	1.34	1.39
4	A	605	D0E	C11-C10	-3.17	1.34	1.39
4	A	605	D0E	N02-N01	-3.11	1.32	1.35
4	B	604	D0E	N02-N01	-3.07	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	604	D0E	C03-C02	-2.97	1.34	1.40
4	A	605	D0E	C03-C02	-2.93	1.34	1.40
4	B	604	D0E	O01-C02	-2.92	1.32	1.37
4	B	604	D0E	O01-C01	-2.79	1.35	1.42
4	A	605	D0E	O01-C01	-2.55	1.35	1.42
4	B	604	D0E	O02-C03	-2.54	1.33	1.37
4	B	604	D0E	C21-N02	-2.38	1.30	1.34
4	A	605	D0E	O02-C03	-2.33	1.33	1.37
4	A	605	D0E	C08-C04	-2.33	1.40	1.52
4	B	604	D0E	C08-C04	-2.31	1.40	1.52
4	B	604	D0E	C12-C02	-2.23	1.35	1.39
4	A	605	D0E	C21-N02	-2.20	1.31	1.34
4	A	605	D0E	C10-C13	-2.18	1.44	1.47
4	A	605	D0E	C12-C02	-2.12	1.35	1.39

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	604	D0E	C14-N02-N01	6.80	126.44	119.56
4	A	605	D0E	C14-N02-N01	6.37	126.00	119.56
4	A	605	D0E	C15-C14-N02	5.39	117.85	111.89
4	A	605	D0E	O02-C03-C09	-4.63	113.48	123.87
4	B	604	D0E	O02-C03-C09	-4.61	113.54	123.87
4	B	604	D0E	C13-N01-N02	4.34	109.64	104.70
4	A	605	D0E	C13-N01-N02	4.25	109.55	104.70
4	B	604	D0E	C22-C13-N01	-4.25	106.65	110.87
4	A	605	D0E	O02-C03-C02	4.24	129.24	116.70
4	B	604	D0E	O02-C03-C02	4.19	129.09	116.70
4	B	604	D0E	C01-O01-C02	4.02	123.41	117.51
4	A	605	D0E	C15-C16-N03	3.82	123.87	118.09
4	A	605	D0E	O01-C02-C03	-3.67	110.43	115.40
4	A	605	D0E	C22-C13-N01	-3.65	107.25	110.87
4	A	605	D0E	C01-O01-C02	3.61	122.81	117.51
4	A	605	D0E	O01-C02-C12	3.17	129.65	124.30
4	B	604	D0E	C15-C14-N02	3.05	115.26	111.89
4	B	604	D0E	C15-C16-N03	3.04	122.69	118.09
4	A	605	D0E	C18-C17-N03	2.97	116.07	109.82
4	B	604	D0E	C10-C13-N01	2.97	124.40	120.49
4	B	604	D0E	O01-C02-C03	-2.90	111.47	115.40
4	B	604	D0E	C18-C17-N03	2.57	115.23	109.82
4	A	605	D0E	O02-C04-C08	-2.47	100.20	108.71
4	A	605	D0E	C10-C13-N01	2.46	123.73	120.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	604	D0E	O02-C04-C08	-2.46	100.25	108.71
4	A	605	D0E	O02-C04-C05	2.45	117.16	108.71
4	B	604	D0E	C14-N02-C21	-2.36	123.11	128.66
4	A	605	D0E	C14-C15-C16	-2.33	107.93	111.22
4	B	604	D0E	O01-C02-C12	2.31	128.19	124.30
4	B	604	D0E	C14-C15-C16	-2.19	108.13	111.22
4	A	605	D0E	C07-C08-C04	-2.11	96.57	104.33
4	A	605	D0E	C14-N02-C21	-2.08	123.76	128.66
4	A	605	D0E	C10-C09-C03	2.03	122.32	119.60
4	B	604	D0E	O02-C04-C05	2.01	115.62	108.71

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	605	D0E	C05-C04-O02-C03
4	A	605	D0E	C08-C04-O02-C03
4	B	604	D0E	C05-C04-O02-C03
4	B	604	D0E	C08-C04-O02-C03
4	A	605	D0E	C02-C03-O02-C04
4	B	604	D0E	C02-C03-O02-C04
4	B	604	D0E	C14-C15-C16-O04
4	A	605	D0E	C09-C03-O02-C04

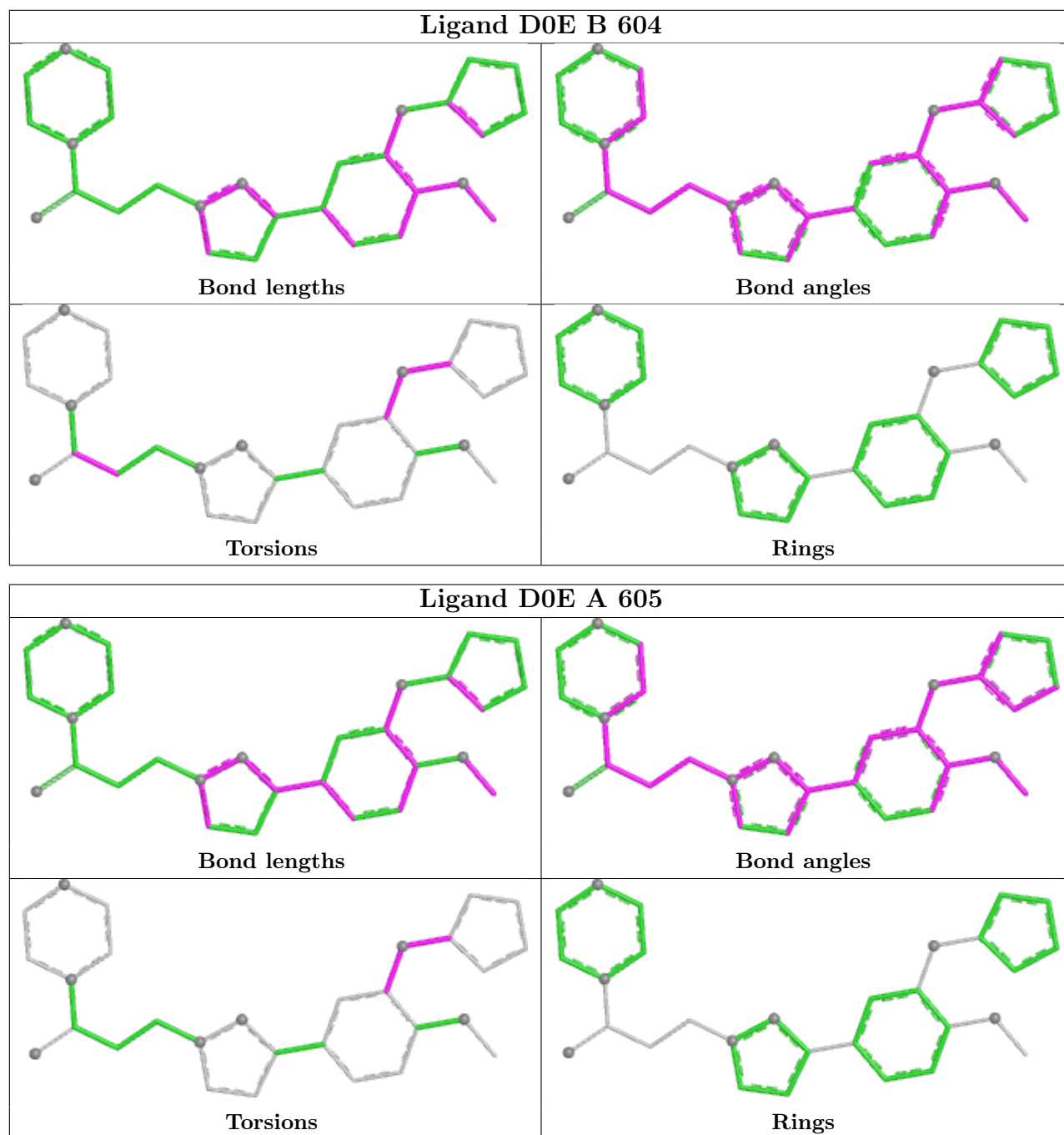
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	604	D0E	1	0
4	A	605	D0E	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 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.



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	322/343 (93%)	0.43	14 (4%) 40 41	12, 27, 44, 57	9 (2%)
1	B	331/343 (96%)	0.38	16 (4%) 35 37	11, 25, 39, 60	15 (4%)
All	All	653/686 (95%)	0.40	30 (4%) 37 39	11, 26, 42, 60	24 (3%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	250	VAL	6.1
1	B	253	GLU	5.9
1	B	248	PHE	5.6
1	B	249	GLY	4.6
1	B	252	THR	4.2
1	B	257	VAL	4.0
1	A	530	SER	3.8
1	B	460	SER	3.7
1	A	571[A]	TRP	3.6
1	A	258	LEU	3.6
1	A	529	ALA	3.3
1	B	577	PRO	3.1
1	A	579	ALA	3.1
1	B	461	SER	3.1
1	A	349	ALA	3.0
1	A	461	SER	3.0
1	B	254	GLN	2.9
1	B	251	LYS	2.7
1	B	259	ALA	2.6
1	B	247	ARG	2.6
1	B	256	ASP	2.3
1	A	541	TYR	2.2
1	B	263	GLU	2.2
1	A	516[A]	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	305	VAL	2.2
1	A	301	PHE	2.1
1	A	528	ASN	2.1
1	B	458	VAL	2.1
1	A	321	ALA	2.0
1	A	468	ASN	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](#)

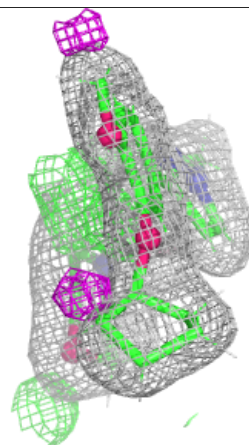
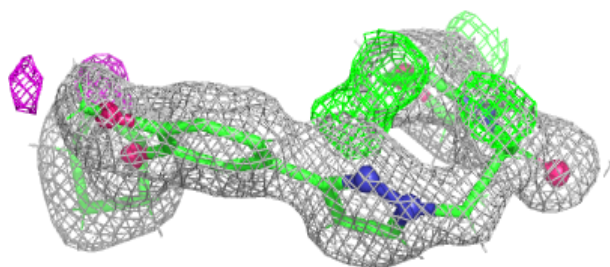
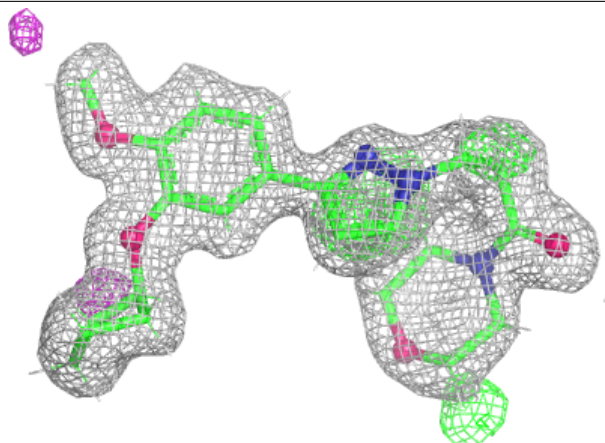
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	D0E	B	604	29/29	0.87	0.11	18,27,35,35	58
4	D0E	A	605	29/29	0.91	0.10	17,26,40,42	58
3	MG	A	603	1/1	0.91	0.18	44,44,44,44	0
3	MG	A	604	1/1	0.95	0.09	41,41,41,41	0
3	MG	B	603	1/1	0.97	0.18	30,30,30,30	0
3	MG	B	602	1/1	1.00	0.03	15,15,15,15	0
3	MG	A	602	1/1	1.00	0.03	15,15,15,15	0
2	ZN	A	601	1/1	1.00	0.02	21,21,21,21	0
2	ZN	B	601	1/1	1.00	0.03	20,20,20,20	0

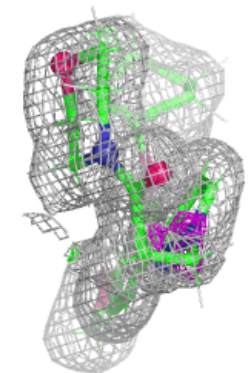
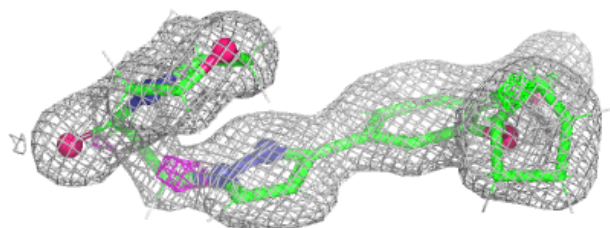
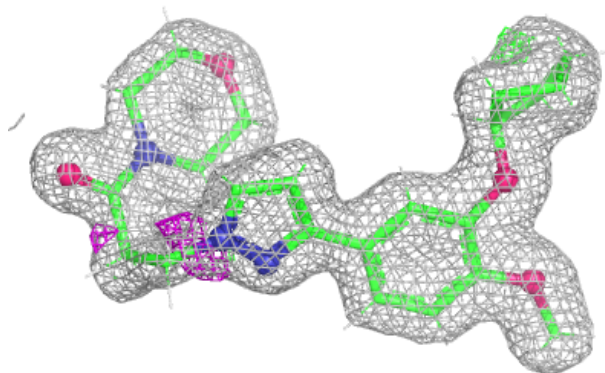
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around D0E B 604:

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

**Electron density around D0E A 605:**

$2mF_o-DF_c$ (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.