



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:05 PM UTC

PDB ID : 8ZQU / pdb_00008zqu
Title : The crystal structure of PDE4D with isoaurostatin derivatives 2-6
Authors : Huang, Y.-Y.; Luo, H.-B.
Deposited on : 2024-06-03
Resolution : 2.00 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

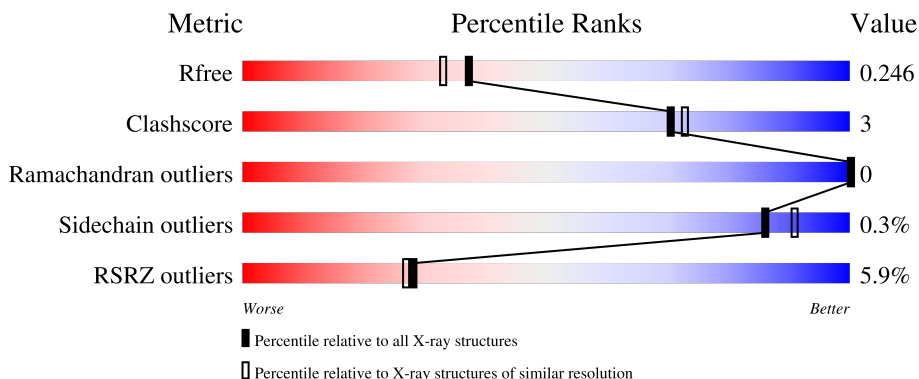
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	506	
1	B	506	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5552 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 3',5'-cyclic-AMP phosphodiesterase 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2624	1659	448	503	14			
1	B	321	Total	C	N	O	S	0	0	0
			2597	1644	444	495	14			

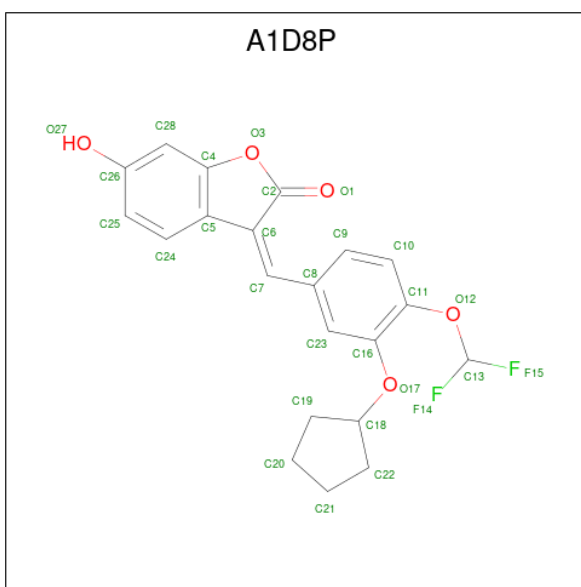
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is (3 {Z})-3-[[4-[bis(fluoranyl)methoxy]-3-cyclopentyloxy-phenyl]methylidene]-6-oxidanyl-1-benzofuran-2-one (CCD ID: A1D8P) (formula: C₂₁H₁₈F₂O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	O	0	0
			28	21	2	5		
4	B	1	Total	C	F	O	0	0
			28	21	2	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	167	Total	O	0	0
			167	167		
5	B	104	Total	O	0	0
			104	104		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.48Å 80.62Å 163.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.64 – 2.00 23.64 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (23.64-2.00) 99.6 (23.64-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 1.99Å)	Xtriage
Refinement program	REFMAC V8, PHENIX 1.10_2155	Depositor
R, R_{free}	0.206 , 0.243 0.212 , 0.246	Depositor DCC
R_{free} test set	2669 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 41.2	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	0.93	EDS
Total number of atoms	5552	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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: ZN, A1D8P, MG

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	0.35	0/2677	0.52	0/3636
1	B	0.32	0/2650	0.49	0/3600
All	All	0.34	0/5327	0.50	0/7236

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	2624	0	2577	12	1
1	B	2597	0	2557	23	1
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	28	0	0	0	0
4	B	28	0	0	0	0
5	A	167	0	0	5	0
5	B	104	0	0	4	0
All	All	5552	0	5134	35	1

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 3.

All (35) 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:207:VAL:HG11	1:B:346:ARG:NH2	1.95	0.81
1:A:254:LYS:HB2	5:A:710:HOH:O	1.84	0.75
1:B:207:VAL:CG1	1:B:346:ARG:NH2	2.51	0.73
1:B:207:VAL:CG1	1:B:346:ARG:HH21	2.03	0.71
1:B:331:GLN:OE1	5:B:701:HOH:O	2.08	0.71
1:B:298:LEU:HD23	1:B:300:LEU:HD21	1.76	0.67
1:A:252:LEU:O	5:A:701:HOH:O	2.14	0.64
1:A:253:THR:OG1	5:A:702:HOH:O	2.15	0.63
1:B:338:GLU:OE2	1:B:342:ARG:NH2	2.33	0.62
1:B:175:LEU:O	1:B:178:THR:HG22	2.01	0.61
1:B:207:VAL:HG13	1:B:346:ARG:HH21	1.64	0.60
1:B:90:ASP:OD2	1:B:91:VAL:N	2.35	0.59
1:B:293:THR:HG23	1:B:297:VAL:O	2.04	0.58
1:B:90:ASP:OD1	5:B:703:HOH:O	2.17	0.57
1:B:143:ILE:O	1:B:147:MET:HG3	2.05	0.56
1:B:396:LEU:O	1:B:400:GLU:HG3	2.06	0.56
1:B:350:ARG:HD3	1:B:352:MET:SD	2.47	0.54
1:A:254:LYS:HE2	1:A:254:LYS:HA	1.91	0.53
1:A:282:ASP:HB3	1:A:308:GLN:NE2	2.24	0.53
1:B:282:ASP:HB3	1:B:308:GLN:OE1	2.08	0.52
1:B:330:ARG:HD2	5:B:798:HOH:O	2.10	0.52
1:B:104:LEU:HD22	1:B:170:GLN:HG3	1.96	0.48
1:A:255:LYS:HD3	5:A:710:HOH:O	2.14	0.48
1:B:293:THR:HG22	1:B:299:LEU:HD21	1.96	0.47
1:A:196:ALA:O	1:A:200:HIS:HB3	2.16	0.45
1:B:321:ASN:HB2	1:B:322:PRO:HD3	2.00	0.44
1:A:298:LEU:HD12	1:A:298:LEU:HA	1.87	0.43
1:B:330:ARG:HD3	1:B:405:TRP:CH2	2.55	0.42
1:B:389:HIS:HA	1:B:390:PRO:HA	1.89	0.42
1:A:255:LYS:NZ	5:A:710:HOH:O	2.50	0.42
1:B:328:LEU:HA	5:B:701:HOH:O	2.20	0.41
1:A:116:ARG:NH2	1:A:151:ASP:OD1	2.44	0.41
1:A:104:LEU:HD22	1:A:170:GLN:HG3	2.01	0.41
1:A:347:GLU:OE2	1:A:355:SER:OG	2.39	0.40
1:B:286:MET:HE2	1:B:286:MET:HB2	1.93	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:GLU:OE1	1:B:295:SER:OG[3_454]	2.15	0.05

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	322/506 (64%)	316 (98%)	6 (2%)	0	100	100
1	B	319/506 (63%)	314 (98%)	5 (2%)	0	100	100
All	All	641/1012 (63%)	630 (98%)	11 (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	296/466 (64%)	295 (100%)	1 (0%)	86	91
1	B	293/466 (63%)	292 (100%)	1 (0%)	86	91
All	All	589/932 (63%)	587 (100%)	2 (0%)	86	91

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	297	VAL
1	B	286	MET

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	88	GLN
1	A	123	HIS
1	A	321	ASN
1	A	369	GLN
1	B	242	GLN
1	B	331	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 6 ligands modelled in this entry, 4 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	A1D8P	A	603	-	31,31,31	0.30	0	43,44,44	0.75	1 (2%)
4	A1D8P	B	603	-	31,31,31	0.25	0	43,44,44	0.71	1 (2%)

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	A1D8P	A	603	-	-	0/12/31/31	0/4/4/4
4	A1D8P	B	603	-	-	0/12/31/31	0/4/4/4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	A1D8P	C5-C6-C7	-2.77	119.27	131.79
4	B	603	A1D8P	C5-C6-C7	-2.67	119.72	131.79

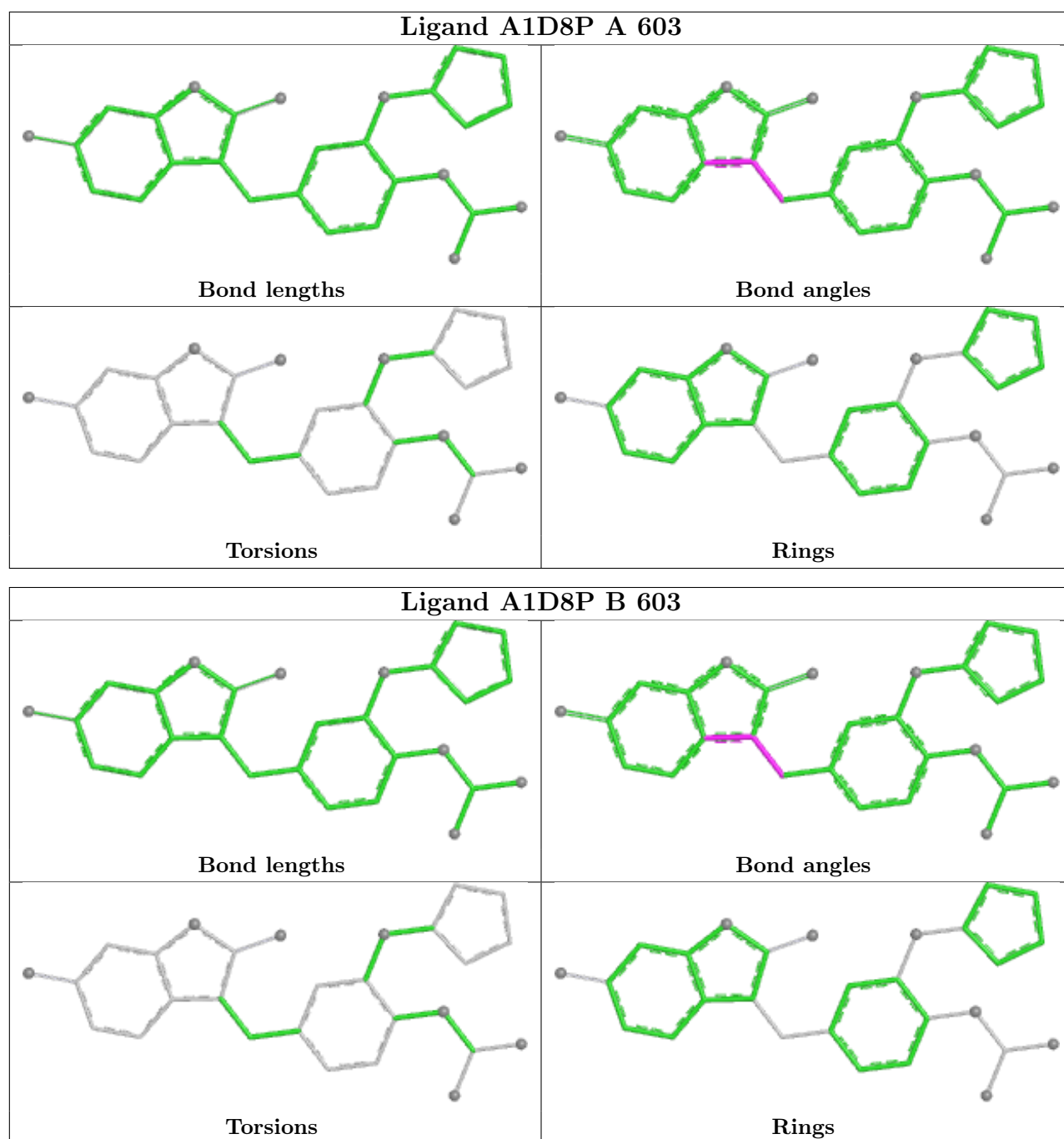
There are no chirality outliers.

There are no torsion outliers.

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.



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	324/506 (64%)	-0.22	11 (3%) 48 47	8, 18, 42, 55	0
1	B	321/506 (63%)	0.40	27 (8%) 17 15	11, 26, 46, 67	0
All	All	645/1012 (63%)	0.08	38 (5%) 28 27	8, 21, 46, 67	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	183	ALA	5.0
1	B	296	GLY	4.0
1	B	293	THR	3.7
1	B	181	LEU	3.6
1	B	295	SER	3.6
1	B	182	GLU	3.5
1	B	297	VAL	3.4
1	A	301	ASP	3.2
1	B	346	ARG	3.0
1	B	389	HIS	3.0
1	B	292	VAL	3.0
1	A	348	ARG	2.9
1	B	184	VAL	2.9
1	A	353	GLU	2.9
1	B	91	VAL	2.9
1	B	298	LEU	2.8
1	A	410	ILE	2.6
1	A	111	GLU	2.6
1	A	354	ILE	2.6
1	A	255	LYS	2.6
1	B	294	SER	2.6
1	B	179	PRO	2.5
1	B	362	ASN	2.5
1	B	93	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	299	LEU	2.4
1	B	178	THR	2.3
1	A	296	GLY	2.3
1	A	356	PRO	2.2
1	B	390	PRO	2.2
1	B	363	ALA	2.2
1	A	351	GLY	2.2
1	A	349	GLU	2.2
1	B	354	ILE	2.2
1	B	133	LYS	2.2
1	B	289	THR	2.1
1	B	127	GLN	2.1
1	B	327	GLN	2.0
1	B	131	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 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.

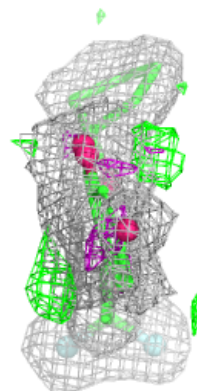
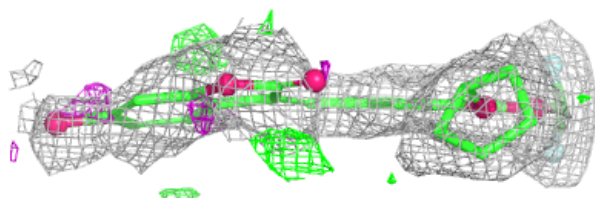
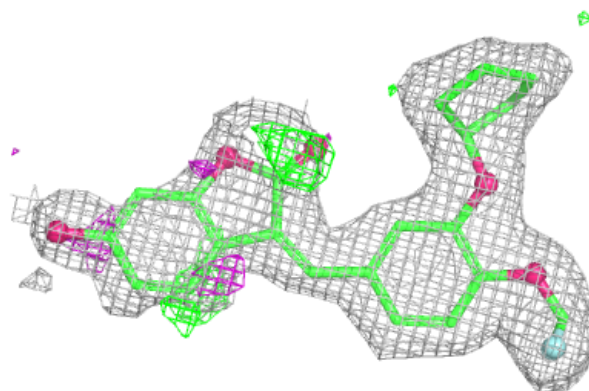
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	A1D8P	B	603	28/28	0.89	0.10	17,26,36,45	0
4	A1D8P	A	603	28/28	0.93	0.09	15,22,33,39	0
3	MG	A	602	1/1	0.98	0.04	7,7,7,7	0
2	ZN	B	601	1/1	0.99	0.02	19,19,19,19	0
3	MG	B	602	1/1	0.99	0.03	11,11,11,11	0
2	ZN	A	601	1/1	1.00	0.01	16,16,16,16	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.

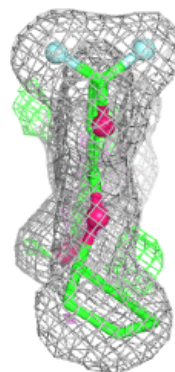
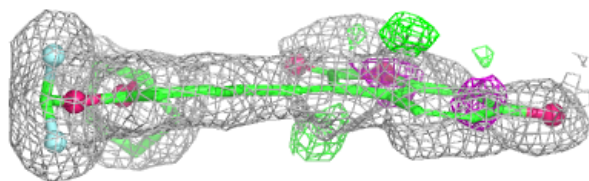
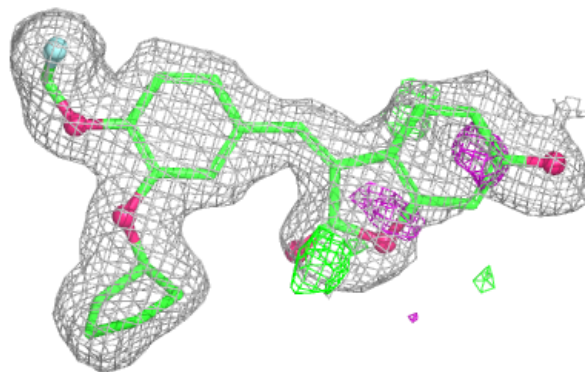
Electron density around A1D8P B 603:

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



Electron density around A1D8P A 603:

$2mF_o-DF_c$ (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.