



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:21 PM UTC

PDB ID : 8K4H / pdb_00008k4h
Title : Crystal structure of PDE4D complexed with benzbromarone
Authors : Liu, J.Y.; Li, M.J.; Xu, Y.C.
Deposited on : 2023-07-18
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

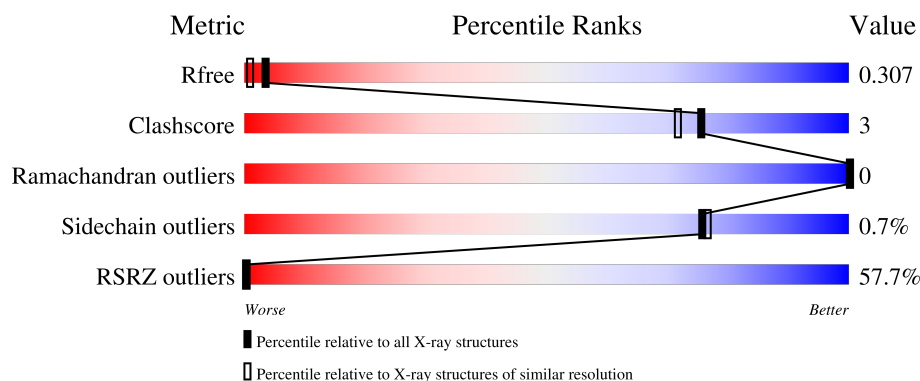
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	349	39% 89% 5% 7%
1	B	349	69% 84% 9% 7%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5326 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
			2597	1644	442	497	14			
1	B	326	Total	C	N	O	S	0	0	0
			2540	1609	430	488	13			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	65	MET	-	expression tag	UNP Q08499
A	66	GLY	-	expression tag	UNP Q08499
A	67	SER	-	expression tag	UNP Q08499
A	68	SER	-	expression tag	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	-	expression tag	UNP Q08499
A	76	SER	-	expression tag	UNP Q08499
A	77	GLY	-	expression tag	UNP Q08499
A	78	LEU	-	expression tag	UNP Q08499
A	79	VAL	-	expression tag	UNP Q08499
A	80	PRO	-	expression tag	UNP Q08499
A	81	ARG	-	expression tag	UNP Q08499
A	82	GLY	-	expression tag	UNP Q08499
A	83	SER	-	expression tag	UNP Q08499
A	84	HIS	-	expression tag	UNP Q08499
A	85	MET	-	expression tag	UNP Q08499
B	65	MET	-	expression tag	UNP Q08499
B	66	GLY	-	expression tag	UNP Q08499
B	67	SER	-	expression tag	UNP Q08499
B	68	SER	-	expression tag	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	-	expression tag	UNP Q08499
B	76	SER	-	expression tag	UNP Q08499
B	77	GLY	-	expression tag	UNP Q08499
B	78	LEU	-	expression tag	UNP Q08499
B	79	VAL	-	expression tag	UNP Q08499
B	80	PRO	-	expression tag	UNP Q08499
B	81	ARG	-	expression tag	UNP Q08499
B	82	GLY	-	expression tag	UNP Q08499
B	83	SER	-	expression tag	UNP Q08499
B	84	HIS	-	expression tag	UNP Q08499
B	85	MET	-	expression tag	UNP Q08499

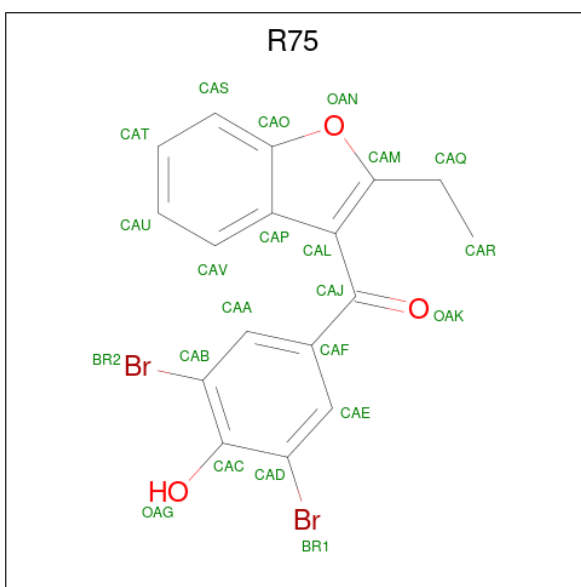
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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

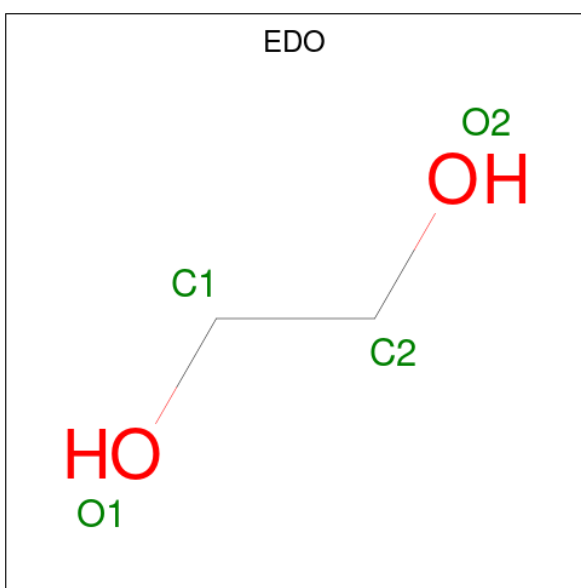
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0

- Molecule 4 is [3,5-bis(bromanyl)-4-oxidanyl-phenyl]-(2-ethyl-1-benzofuran-3-yl)methanone (CCD ID: R75) (formula: C₁₇H₁₂Br₂O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Br	C	O	0	0
			22	2	17	3		
4	B	1	Total	Br	C	O	0	0
			22	2	17	3		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: 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		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	89	Total 89	O 89	0	0
6	B	44	Total 44	O 44	0	0

E401	E402	E403	E404	Y405	Y406	Q407	S408	T409	T410	P411	GLN	SER
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.51Å 79.81Å 162.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.45 – 1.95 40.45 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.45-1.95) 100.0 (40.45-1.95)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 1.95Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660)	Depositor
R, R_{free}	0.247 , 0.279 0.290 , 0.307	Depositor DCC
R_{free} test set	2883 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.2	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	0.90	EDS
Total number of atoms	5326	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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: EDO, ZN, R75, 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	0.14	0/2651	0.34	0/3611
1	B	0.14	0/2594	0.32	0/3544
All	All	0.14	0/5245	0.33	0/7155

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	2597	0	2516	9	0
1	B	2540	0	2401	21	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	22	0	0	1	0
4	B	22	0	0	3	0
5	A	8	0	12	0	0
6	A	89	0	0	0	0
6	B	44	0	0	0	0
All	All	5326	0	4929	30	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 3.

All (30) 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:354:ILE:HG21	1:B:359:ASP:HB2	1.74	0.69
1:B:178:THR:HG21	1:B:388:VAL:HG11	1.75	0.68
1:B:348:ARG:HG3	1:B:354:ILE:HD11	1.79	0.63
1:B:388:VAL:HG12	1:B:388:VAL:O	2.08	0.54
1:B:345:ASP:OD1	1:B:348:ARG:NH2	2.41	0.53
1:B:336:ILE:HD11	4:B:503:R75:BR1	2.64	0.52
1:A:160:HIS:ND1	1:A:339:GLU:OE2	2.34	0.49
1:B:347:GLU:HA	1:B:352:MET:HG3	1.94	0.49
1:B:160:HIS:HE1	4:B:503:R75:BR1	2.53	0.47
1:A:410:ILE:HB	1:A:411:PRO:HD3	1.97	0.47
1:A:354:ILE:HG21	1:A:359:ASP:HB2	1.98	0.46
1:B:321:ASN:HB2	1:B:322:PRO:HD3	1.97	0.46
1:A:132:LEU:HD22	1:A:139:VAL:HG22	1.98	0.45
1:B:180:ALA:HB3	1:B:388:VAL:HG13	1.99	0.45
1:B:406:TYR:O	1:B:409:THR:OG1	2.32	0.45
1:A:347:GLU:OE1	1:A:355:SER:OG	2.28	0.45
1:B:280:LEU:O	1:B:284:LYS:HG2	2.16	0.45
1:B:389:HIS:HA	1:B:390:PRO:HA	1.64	0.44
1:A:336:ILE:HD11	4:A:503:R75:BR1	2.72	0.44
1:B:273:MET:SD	1:B:315:HIS:HE1	2.41	0.44
1:B:116:ARG:NH1	1:B:151:ASP:OD1	2.47	0.43
1:B:388:VAL:HG12	1:B:391:ASP:HB2	1.99	0.43
1:A:321:ASN:HB2	1:A:322:PRO:HD3	2.00	0.42
1:B:192:ALA:HB2	1:B:263:MET:HE3	2.02	0.42
1:B:167:ASP:OD1	1:B:324:LYS:NZ	2.53	0.42
1:B:135:PHE:HB3	1:B:252:LEU:HD11	2.02	0.41
1:B:160:HIS:CE1	4:B:503:R75:BR1	3.28	0.41
1:A:181:LEU:HD21	1:A:298:LEU:HD12	2.02	0.41
1:A:373:ILE:HA	1:A:377:VAL:HB	2.03	0.41
1:B:326:LEU:HD21	1:B:405:TRP:CD2	2.56	0.41

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	324/349 (93%)	317 (98%)	7 (2%)	0	100	100
1	B	324/349 (93%)	313 (97%)	11 (3%)	0	100	100
All	All	648/698 (93%)	630 (97%)	18 (3%)	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	288/318 (91%)	288 (100%)	0	100	100
1	B	273/318 (86%)	269 (98%)	4 (2%)	57	54
All	All	561/636 (88%)	557 (99%)	4 (1%)	76	76

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	297	VAL
1	B	352	MET
1	B	354	ILE
1	B	389	HIS

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

Mol	Chain	Res	Type
1	A	250	GLN
1	B	250	GLN
1	B	369	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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	A	505	-	3,3,3	0.41	0	2,2,2	0.45	0
4	R75	A	503	-	24,24,24	0.42	0	33,35,35	0.79	1 (3%)
5	EDO	A	504	-	3,3,3	0.42	0	2,2,2	0.36	0
4	R75	B	503	-	24,24,24	0.43	0	33,35,35	0.77	1 (3%)

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	A	505	-	-	0/1/1/1	-
4	R75	A	503	-	-	2/10/10/10	0/3/3/3
5	EDO	A	504	-	-	0/1/1/1	-
4	R75	B	503	-	-	2/10/10/10	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	R75	CAT-CAS-CAO	-2.11	115.76	119.60
4	B	503	R75	CAT-CAS-CAO	-2.11	115.77	119.60

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	R75	CAL-CAM-CAQ-CAR
4	A	503	R75	OAN-CAM-CAQ-CAR
4	B	503	R75	CAL-CAM-CAQ-CAR
4	B	503	R75	OAN-CAM-CAQ-CAR

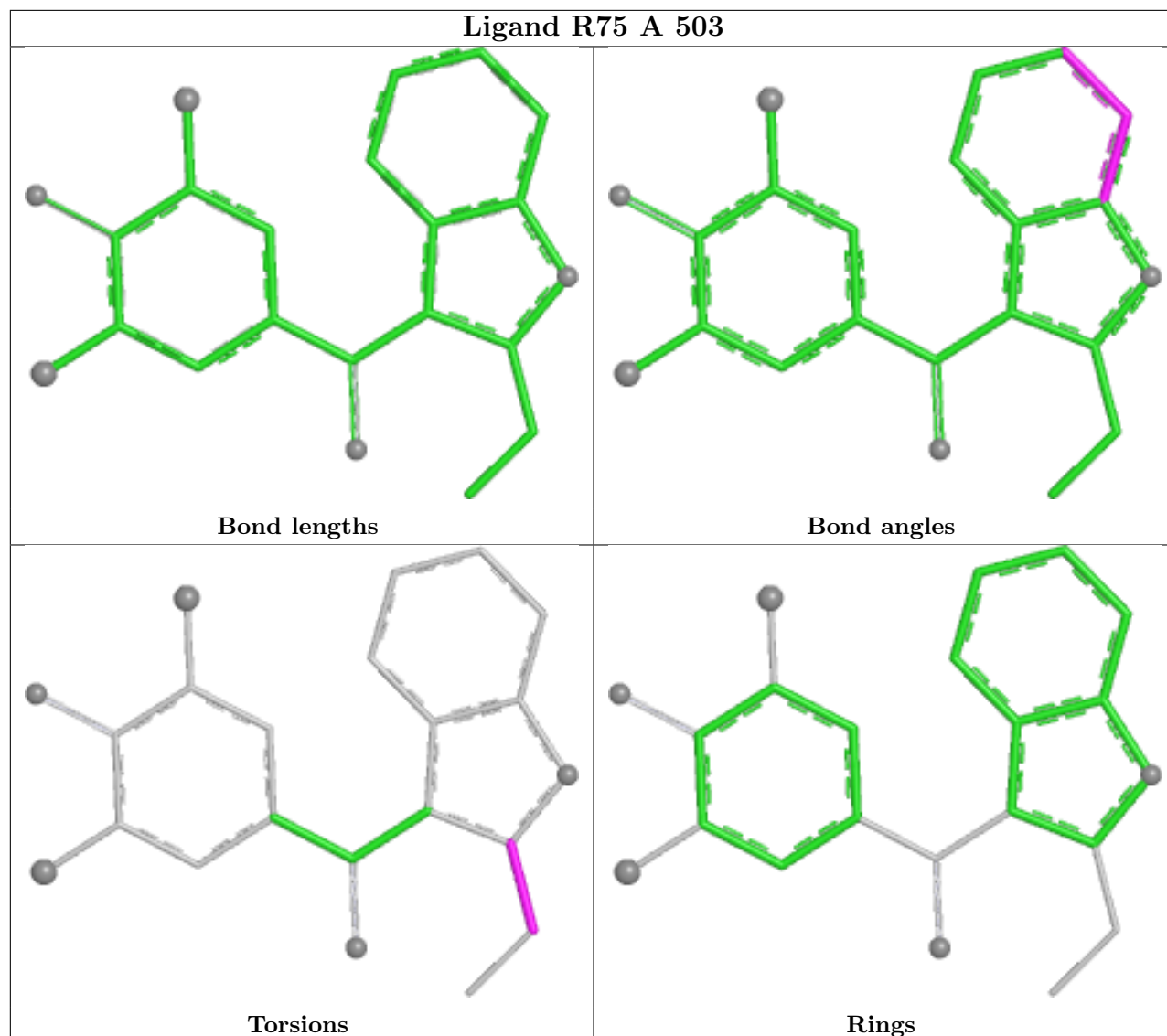
There are no ring outliers.

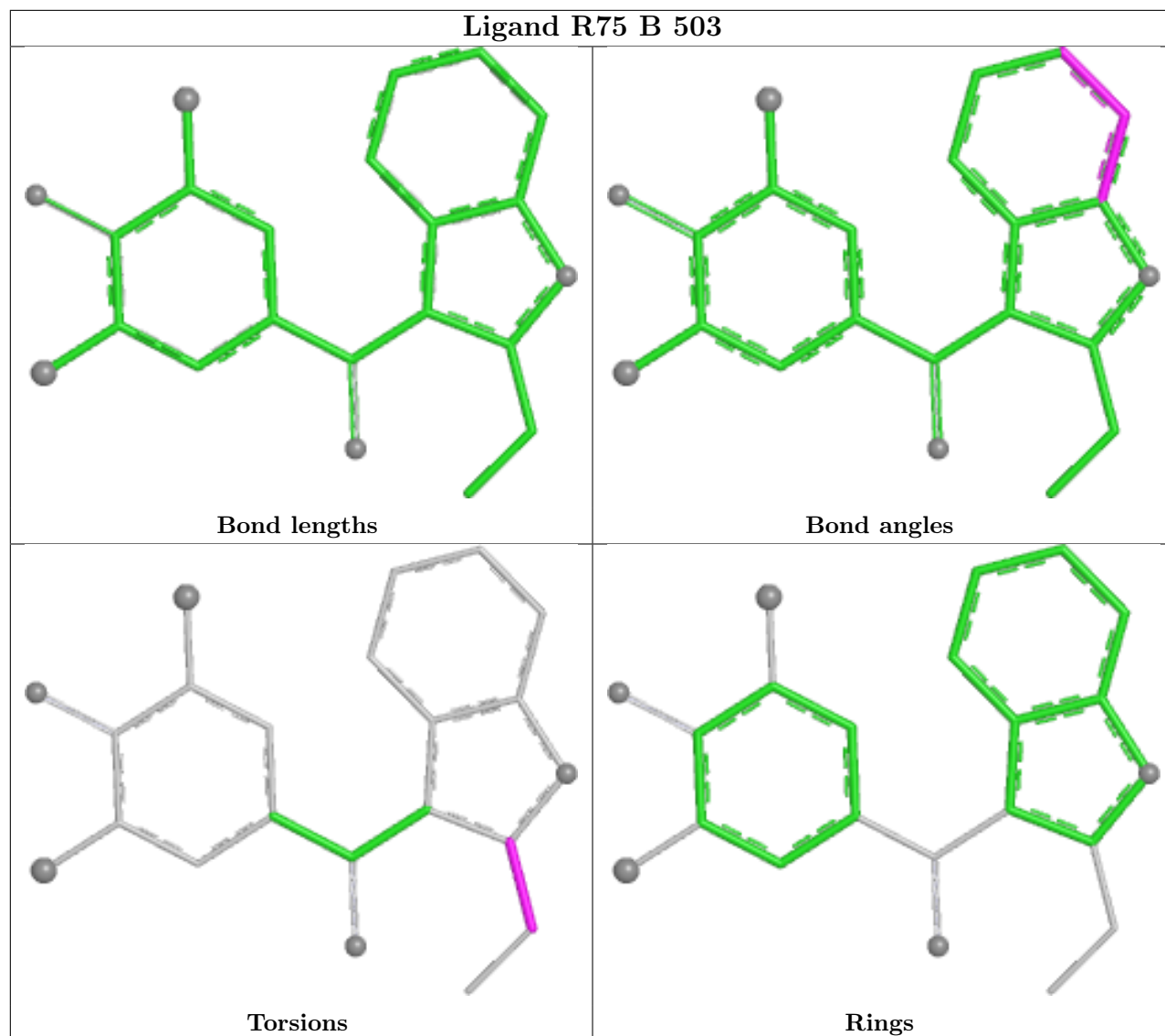
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	R75	1	0
4	B	503	R75	3	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 R75 A 503





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	326/349 (93%)	1.89	135 (41%) 0 0	27, 41, 65, 125	0
1	B	326/349 (93%)	3.25	241 (73%) 0 0	31, 61, 102, 170	0
All	All	652/698 (93%)	2.57	376 (57%) 0 0	27, 48, 93, 170	0

All (376) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	183	ALA	8.5
1	B	387	LEU	8.5
1	B	99	VAL	8.2
1	B	295	SER	7.6
1	B	139	VAL	7.6
1	B	184	VAL	7.6
1	B	135	PHE	7.5
1	B	96	LEU	7.5
1	B	180	ALA	7.2
1	B	292	VAL	7.1
1	B	297	VAL	7.1
1	B	296	GLY	7.1
1	B	102	TRP	6.9
1	B	181	LEU	6.8
1	B	190	ILE	6.8
1	B	93	ALA	6.7
1	B	132	LEU	6.7
1	B	142	LEU	6.6
1	B	176	LEU	6.6
1	B	130	ASP	6.4
1	B	104	LEU	6.3
1	B	86	THR	6.2
1	B	92	LEU	6.2
1	B	143	ILE	6.2

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Mol	Chain	Res	Type	RSRZ
1	B	87	GLU	6.1
1	B	179	PRO	5.9
1	B	112	LEU	5.9
1	B	124	THR	5.9
1	B	125	ILE	5.8
1	A	86	THR	5.8
1	B	90	ASP	5.7
1	B	298	LEU	5.7
1	B	120	VAL	5.6
1	B	137	ILE	5.6
1	B	388	VAL	5.3
1	B	94	LYS	5.3
1	B	191	LEU	5.2
1	B	396	LEU	5.2
1	B	294	SER	5.2
1	B	126	PHE	5.1
1	B	254	LYS	5.1
1	B	136	LYS	5.1
1	B	395	ILE	5.1
1	B	141	THR	5.1
1	B	289	THR	5.1
1	B	185	PHE	5.0
1	B	91	VAL	5.0
1	B	246	CYS	4.9
1	B	309	VAL	4.9
1	B	178	THR	4.9
1	B	299	LEU	4.8
1	A	244	GLU	4.8
1	B	287	VAL	4.8
1	B	393	GLN	4.8
1	B	375	TYR	4.8
1	B	384	TRP	4.8
1	B	182	GLU	4.8
1	B	103	GLY	4.8
1	B	129	ARG	4.7
1	B	411	PRO	4.7
1	B	356	PRO	4.7
1	B	174	VAL	4.7
1	B	186	THR	4.7
1	B	291	LYS	4.7
1	B	385	ALA	4.6
1	B	123	HIS	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	121	ILE	4.6
1	B	110	ALA	4.6
1	B	354	ILE	4.6
1	B	300	LEU	4.6
1	B	378	HIS	4.5
1	B	193	ALA	4.5
1	B	310	LEU	4.5
1	A	363	ALA	4.5
1	B	293	THR	4.5
1	B	89	GLU	4.5
1	B	394	ASP	4.4
1	B	131	LEU	4.4
1	B	109	ILE	4.4
1	B	248	ILE	4.4
1	B	175	LEU	4.4
1	B	353	GLU	4.4
1	B	134	THR	4.4
1	B	307	ILE	4.3
1	B	171	SER	4.3
1	B	168	VAL	4.3
1	B	133	LYS	4.3
1	B	399	LEU	4.2
1	B	170	GLN	4.2
1	B	188	LEU	4.2
1	B	111	GLU	4.2
1	B	380	LEU	4.2
1	B	146	LEU	4.1
1	A	353	GLU	4.1
1	B	114	GLY	4.1
1	B	262	LYS	4.1
1	B	286	MET	4.1
1	B	281	ALA	4.1
1	B	390	PRO	4.1
1	B	308	GLN	4.1
1	B	290	LYS	4.0
1	A	87	GLU	4.0
1	B	389	HIS	4.0
1	B	245	ASN	4.0
1	B	251	ASN	3.9
1	B	138	PRO	3.9
1	B	194	ILE	3.9
1	B	372	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	90	ASP	3.9
1	B	105	HIS	3.8
1	A	147	MET	3.8
1	B	327	GLN	3.8
1	B	101	LYS	3.8
1	A	375	TYR	3.8
1	B	116	ARG	3.8
1	B	155	ALA	3.8
1	B	392	ALA	3.8
1	B	127	GLN	3.8
1	B	363	ALA	3.8
1	A	255	LYS	3.8
1	A	91	VAL	3.7
1	B	100	ASN	3.7
1	B	257	ARG	3.7
1	B	304	SER	3.7
1	B	351	GLY	3.7
1	B	88	GLN	3.7
1	A	298	LEU	3.6
1	B	244	GLU	3.6
1	A	273	MET	3.6
1	B	236	VAL	3.6
1	A	362	ASN	3.5
1	B	371	GLY	3.5
1	B	376	ILE	3.5
1	B	192	ALA	3.5
1	B	283	LEU	3.5
1	B	173	HIS	3.5
1	A	89	GLU	3.5
1	A	277	MET	3.5
1	B	222	MET	3.5
1	B	314	VAL	3.5
1	B	348	ARG	3.5
1	B	113	SER	3.4
1	A	356	PRO	3.4
1	A	157	VAL	3.4
1	B	166	ALA	3.4
1	B	362	ASN	3.4
1	B	108	ARG	3.4
1	A	292	VAL	3.4
1	B	301	ASP	3.4
1	A	92	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	364	SER	3.4
1	B	383	THR	3.4
1	B	145	TYR	3.4
1	B	260	LEU	3.4
1	A	286	MET	3.4
1	B	274	SER	3.3
1	B	202	VAL	3.3
1	B	342	ARG	3.3
1	B	325	PRO	3.3
1	B	306	ARG	3.3
1	A	295	SER	3.3
1	B	302	ASN	3.3
1	B	303	TYR	3.3
1	B	213	ILE	3.3
1	A	99	VAL	3.3
1	A	181	LEU	3.3
1	A	411	PRO	3.3
1	A	222	MET	3.2
1	B	284	LYS	3.2
1	B	106	VAL	3.2
1	B	386	ASP	3.2
1	B	122	MET	3.2
1	A	105	HIS	3.2
1	B	98	ASP	3.2
1	A	121	ILE	3.2
1	B	398	THR	3.2
1	A	88	GLN	3.2
1	B	350	ARG	3.2
1	B	391	ASP	3.2
1	A	354	ILE	3.1
1	A	390	PRO	3.1
1	B	337	MET	3.1
1	A	94	LYS	3.1
1	B	172	THR	3.1
1	B	285	THR	3.1
1	A	348	ARG	3.1
1	A	139	VAL	3.1
1	B	144	THR	3.1
1	B	247	ASP	3.1
1	B	280	LEU	3.1
1	B	107	PHE	3.1
1	B	147	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	189	GLU	3.1
1	B	149	LEU	3.0
1	B	228	VAL	3.0
1	A	108	ARG	3.0
1	A	191	LEU	3.0
1	A	352	MET	3.0
1	B	252	LEU	3.0
1	B	326	LEU	3.0
1	B	177	SER	3.0
1	A	114	GLY	3.0
1	A	133	LYS	3.0
1	A	155	ALA	3.0
1	B	273	MET	3.0
1	B	277	MET	3.0
1	A	376	ILE	3.0
1	B	140	ASP	3.0
1	B	349	GLU	3.0
1	A	387	LEU	2.9
1	A	409	THR	2.9
1	B	97	GLU	2.9
1	B	115	ASN	2.9
1	A	132	LEU	2.9
1	A	218	GLU	2.9
1	B	128	GLU	2.9
1	B	381	TRP	2.9
1	A	351	GLY	2.9
1	B	312	ASN	2.9
1	B	397	ASP	2.9
1	A	300	LEU	2.9
1	B	328	LEU	2.9
1	B	340	PHE	2.8
1	A	118	LEU	2.8
1	A	410	ILE	2.8
1	B	279	LEU	2.8
1	B	365	VAL	2.8
1	B	357	MET	2.8
1	B	323	THR	2.8
1	A	143	ILE	2.8
1	A	245	ASN	2.7
1	B	249	PHE	2.7
1	B	243	GLU	2.7
1	B	352	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	169	VAL	2.7
1	B	162	ASN	2.7
1	A	93	ALA	2.7
1	B	187	ASP	2.7
1	A	226	SER	2.7
1	A	257	ARG	2.7
1	A	308	GLN	2.7
1	B	316	CYS	2.7
1	B	305	ASP	2.7
1	B	341	PHE	2.7
1	B	240	LEU	2.7
1	B	322	PRO	2.7
1	A	296	GLY	2.6
1	B	119	THR	2.6
1	A	112	LEU	2.6
1	A	248	ILE	2.6
1	A	357	MET	2.6
1	B	148	THR	2.6
1	A	137	ILE	2.6
1	B	377	VAL	2.6
1	B	379	PRO	2.6
1	A	185	PHE	2.6
1	B	250	GLN	2.6
1	A	301	ASP	2.6
1	A	180	ALA	2.6
1	A	281	ALA	2.6
1	A	403	ARG	2.5
1	A	406	TYR	2.5
1	B	167	ASP	2.5
1	A	287	VAL	2.5
1	A	297	VAL	2.5
1	B	370	VAL	2.5
1	B	117	PRO	2.5
1	A	107	PHE	2.5
1	A	372	PHE	2.5
1	A	384	TRP	2.5
1	B	373	ILE	2.5
1	A	177	SER	2.5
1	B	164	HIS	2.5
1	B	258	GLN	2.5
1	A	313	MET	2.5
1	A	388	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	382	GLU	2.5
1	A	104	LEU	2.5
1	A	213	ILE	2.5
1	A	349	GLU	2.5
1	A	183	ALA	2.5
1	A	207	VAL	2.5
1	B	403	ARG	2.4
1	A	408	SER	2.4
1	B	332	TRP	2.4
1	A	184	VAL	2.4
1	B	95	GLU	2.4
1	B	288	GLU	2.4
1	B	361	HIS	2.4
1	A	340	PHE	2.4
1	A	186	THR	2.4
1	B	404	GLU	2.4
1	A	361	HIS	2.4
1	A	389	HIS	2.4
1	A	304	SER	2.4
1	A	212	LEU	2.4
1	A	319	LEU	2.4
1	B	406	TYR	2.4
1	A	98	ASP	2.4
1	A	135	PHE	2.4
1	A	116	ARG	2.4
1	B	165	ALA	2.4
1	B	400	GLU	2.4
1	A	331	GLN	2.4
1	A	342	ARG	2.3
1	B	118	LEU	2.3
1	B	195	PHE	2.3
1	B	410	ILE	2.3
1	B	207	VAL	2.3
1	A	350	ARG	2.3
1	A	246	CYS	2.3
1	B	358	CYS	2.3
1	B	219	LEU	2.3
1	B	319	LEU	2.3
1	A	341	PHE	2.3
1	B	216	ASN	2.3
1	A	290	LYS	2.3
1	B	346	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	188	LEU	2.3
1	A	279	LEU	2.3
1	A	326	LEU	2.3
1	A	293	THR	2.3
1	B	209	ASN	2.3
1	B	153	TYR	2.3
1	A	193	ALA	2.3
1	A	325	PRO	2.3
1	A	113	SER	2.3
1	A	404	GLU	2.3
1	B	214	ASN	2.3
1	A	291	LYS	2.3
1	B	226	SER	2.2
1	A	407	GLN	2.2
1	A	120	VAL	2.2
1	A	358	CYS	2.2
1	A	138	PRO	2.2
1	B	196	ALA	2.2
1	B	163	ILE	2.2
1	B	267	ILE	2.2
1	B	255	LYS	2.2
1	A	169	VAL	2.2
1	B	253	THR	2.2
1	A	229	LEU	2.2
1	A	299	LEU	2.2
1	B	229	LEU	2.2
1	A	140	ASP	2.2
1	B	368	SER	2.2
1	A	322	PRO	2.2
1	B	402	ASN	2.2
1	A	110	ALA	2.2
1	A	154	HIS	2.1
1	B	278	ASN	2.1
1	B	329	TYR	2.1
1	A	405	TRP	2.1
1	A	271	THR	2.1
1	A	252	LEU	2.1
1	A	280	LEU	2.1
1	A	338	GLU	2.1
1	A	194	ILE	2.1
1	B	374	ASP	2.1
1	A	148	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	409	THR	2.1
1	A	106	VAL	2.1
1	A	131	LEU	2.1
1	A	380	LEU	2.1
1	B	407	GLN	2.1
1	B	218	GLU	2.1
1	A	127	GLN	2.1
1	A	179	PRO	2.1
1	A	346	ARG	2.1
1	A	294	SER	2.0
1	A	264	VAL	2.0
1	B	313	MET	2.0
1	A	103	GLY	2.0
1	A	144	THR	2.0
1	B	242	GLN	2.0
1	A	309	VAL	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(Å ²)	Q<0.9
5	EDO	A	505	4/4	0.86	0.49	93,94,98,103	0
5	EDO	A	504	4/4	0.87	0.14	39,40,42,42	0
4	R75	B	503	22/22	0.93	0.28	21,60,69,74	0
4	R75	A	503	22/22	0.95	0.28	7,50,59,60	0
3	MG	B	502	1/1	0.96	0.16	15,15,15,15	0
3	MG	A	502	1/1	0.97	0.06	21,21,21,21	0
2	ZN	B	501	1/1	0.99	0.24	11,11,11,11	0

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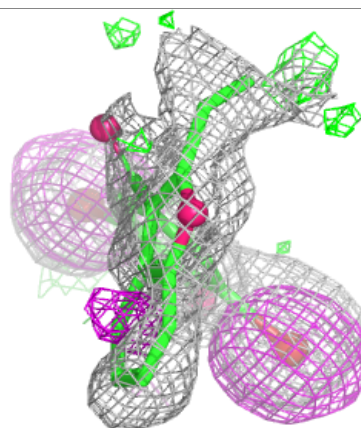
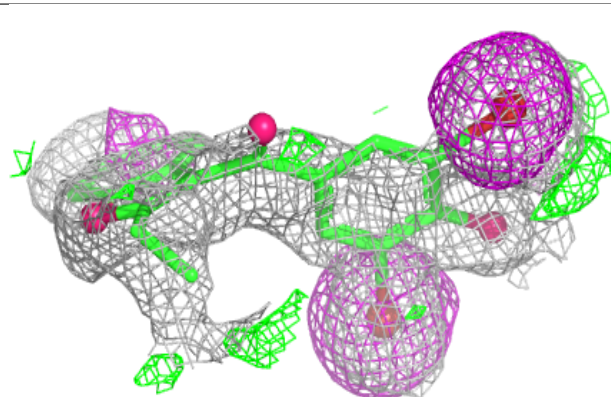
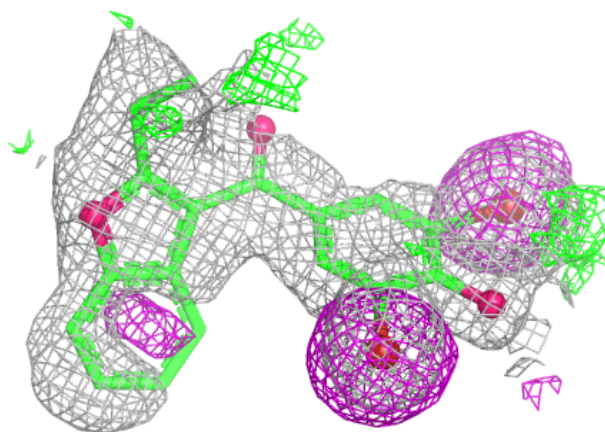
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	501	1/1	1.00	0.07	19,19,19,19	0

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.

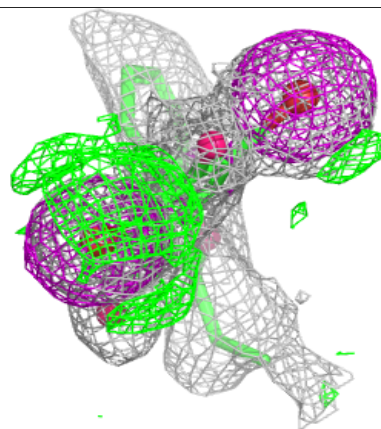
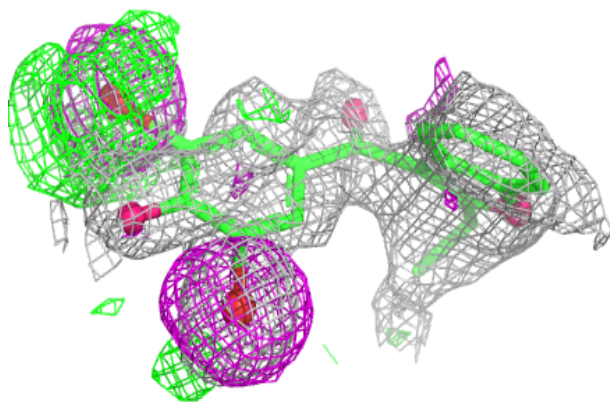
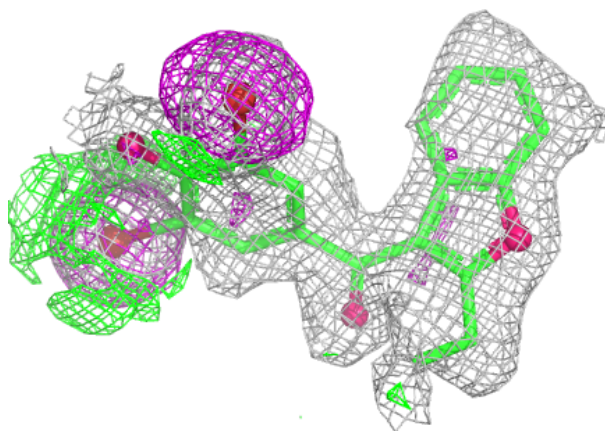
Electron density around R75 B 503:

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 R75 A 503:

$2mF_o-DF_c$ (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.