



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:39 AM UTC

PDB ID : 9NAC / pdb_00009nac
Title : Structure of HPK1 with C4 bound at its active site
Authors : Kiefer, J.R.; Wang, W.; Wu, P.; Walters, B.T.; Dou, Y.
Deposited on : 2025-02-11
Resolution : 1.45 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

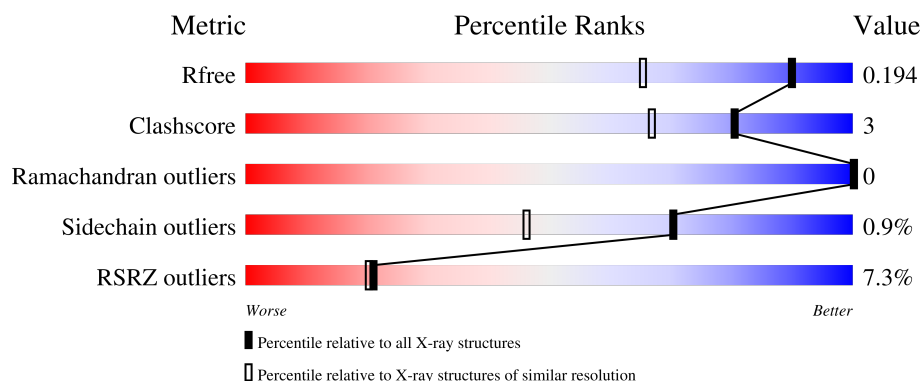
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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	311	5% 87% 7% 6%
1	B	311	8% 86% 5% 8%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5299 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 Mitogen-activated protein kinase kinase kinase kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	7	0
			2333	1499	396	423	15			
1	B	285	Total	C	N	O	S	0	3	0
			2228	1432	381	403	12			

There are 42 discrepancies between the modelled and reference sequences:

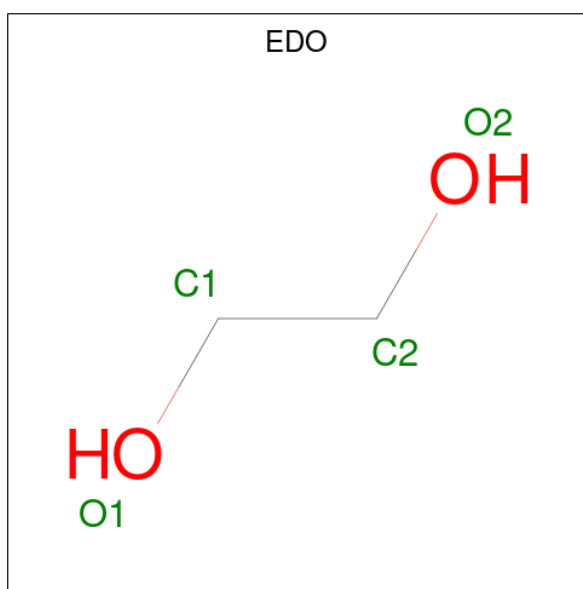
Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	initiating methionine	UNP Q92918
A	-13	HIS	-	expression tag	UNP Q92918
A	-12	HIS	-	expression tag	UNP Q92918
A	-11	HIS	-	expression tag	UNP Q92918
A	-10	HIS	-	expression tag	UNP Q92918
A	-9	HIS	-	expression tag	UNP Q92918
A	-8	HIS	-	expression tag	UNP Q92918
A	-7	GLY	-	expression tag	UNP Q92918
A	-6	GLU	-	expression tag	UNP Q92918
A	-5	ASN	-	expression tag	UNP Q92918
A	-4	LEU	-	expression tag	UNP Q92918
A	-3	TYR	-	expression tag	UNP Q92918
A	-2	PHE	-	expression tag	UNP Q92918
A	-1	GLN	-	expression tag	UNP Q92918
A	0	GLY	-	expression tag	UNP Q92918
A	1	SER	-	expression tag	UNP Q92918
A	165	GLU	THR	conflict	UNP Q92918
A	171	GLU	SER	conflict	UNP Q92918
A	294	GLY	-	expression tag	UNP Q92918
A	295	ASN	-	expression tag	UNP Q92918
A	296	SER	-	expression tag	UNP Q92918
B	-14	MET	-	initiating methionine	UNP Q92918
B	-13	HIS	-	expression tag	UNP Q92918
B	-12	HIS	-	expression tag	UNP Q92918
B	-11	HIS	-	expression tag	UNP Q92918

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	HIS	-	expression tag	UNP Q92918
B	-9	HIS	-	expression tag	UNP Q92918
B	-8	HIS	-	expression tag	UNP Q92918
B	-7	GLY	-	expression tag	UNP Q92918
B	-6	GLU	-	expression tag	UNP Q92918
B	-5	ASN	-	expression tag	UNP Q92918
B	-4	LEU	-	expression tag	UNP Q92918
B	-3	TYR	-	expression tag	UNP Q92918
B	-2	PHE	-	expression tag	UNP Q92918
B	-1	GLN	-	expression tag	UNP Q92918
B	0	GLY	-	expression tag	UNP Q92918
B	1	SER	-	expression tag	UNP Q92918
B	165	GLU	THR	conflict	UNP Q92918
B	171	GLU	SER	conflict	UNP Q92918
B	294	GLY	-	expression tag	UNP Q92918
B	295	ASN	-	expression tag	UNP Q92918
B	296	SER	-	expression tag	UNP Q92918

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



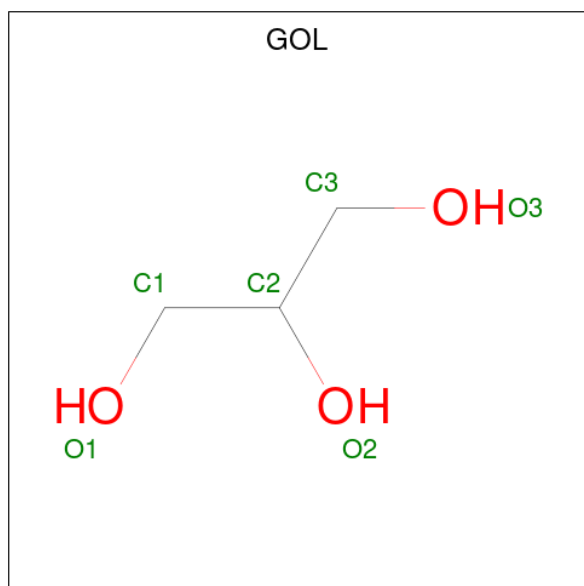
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



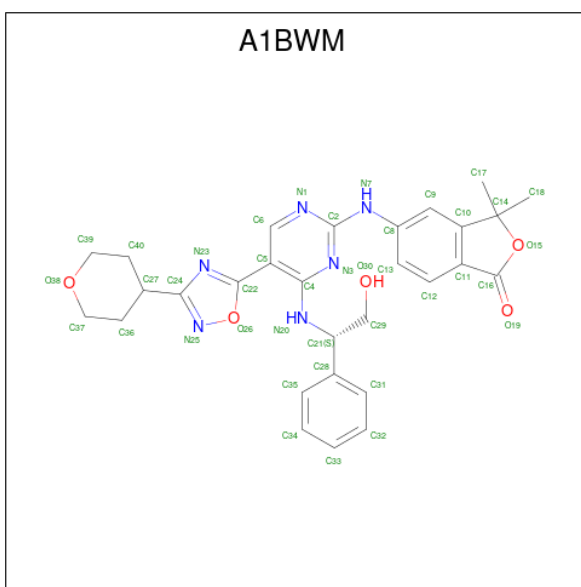
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is 5-[(4-{[(1S)-2-hydroxy-1-phenylethyl]amino}-5-[3-(oxan-4-yl)-1,2,4-oxadiazol-5-yl]pyrimidin-2-yl)amino]-3,3-dimethyl-2-benzofuran-1(3H)-one (CCD ID: A1BWM) (formula: C₂₉H₃₀N₆O₅) (labeled as "Ligand of Interest" by depositor).



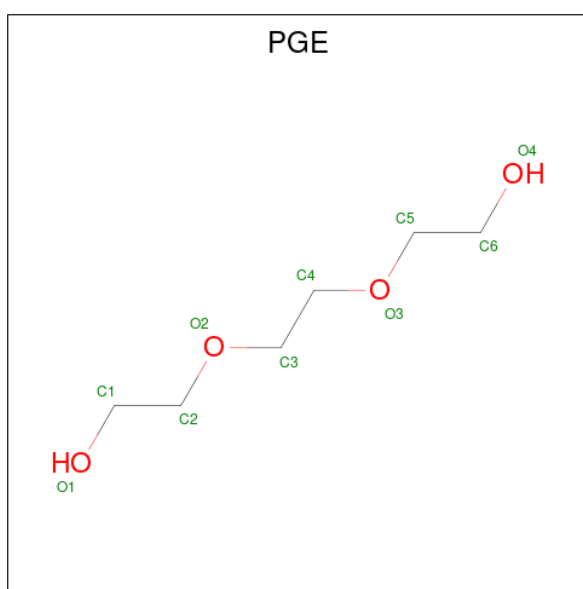
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			40	29	6	5		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		

- Molecule 7 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			10	6	4		

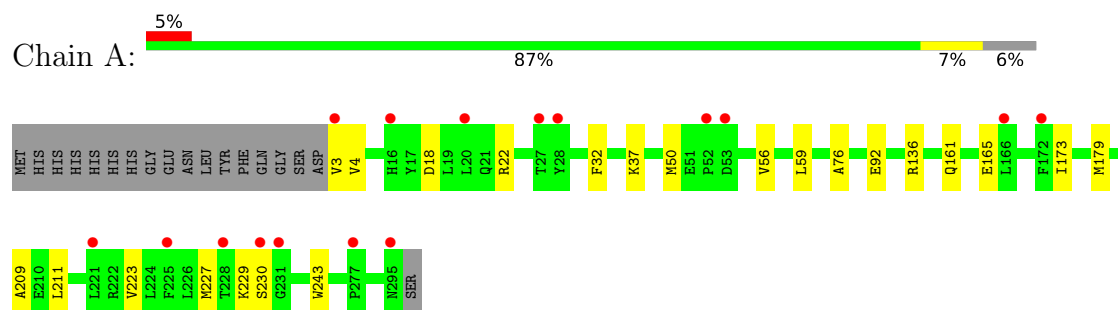
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	319	Total	O	0	5
			324	324		
8	B	243	Total	O	0	0
			243	243		

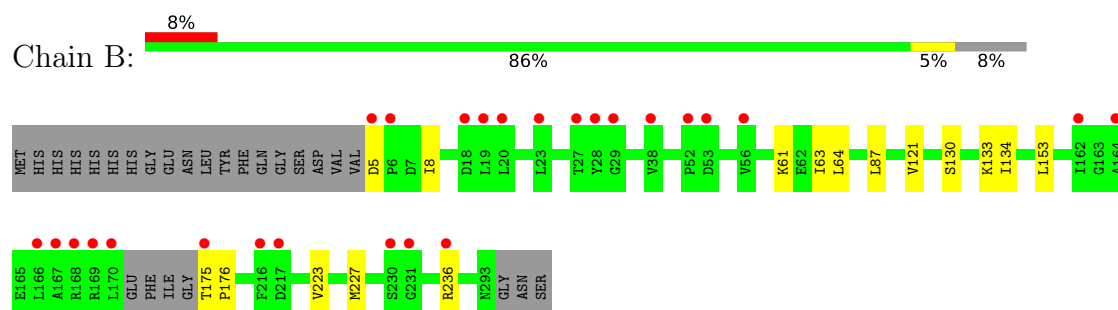
3 Residue-property plots [i](#)

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: Mitogen-activated protein kinase kinase kinase 1



- Molecule 1: Mitogen-activated protein kinase kinase kinase kinase 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	112.63Å 52.34Å 104.41Å 90.00° 104.16° 90.00°	Depositor
Resolution (Å)	33.75 – 1.45 33.75 – 1.45	Depositor EDS
% Data completeness (in resolution range)	94.5 (33.75-1.45) 94.5 (33.75-1.45)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.52 (at 1.45Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.177 , 0.193 0.177 , 0.194	Depositor DCC
R_{free} test set	4789 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	14.8	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.9	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	5299	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.95 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0092e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: A1BWM, EDO, GOL, NA, MES, PGE

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	0.19	0/2383	0.39	0/3229
1	B	0.16	0/2275	0.35	0/3084
All	All	0.17	0/4658	0.37	0/6313

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 [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	2333	0	2332	13	0
1	B	2228	0	2218	11	0
2	A	12	0	18	0	0
2	B	32	0	48	4	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
4	A	12	0	13	1	0
4	B	12	0	13	0	0
5	A	40	0	0	0	0
5	B	40	0	0	0	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	10	0	14	0	0
8	A	324	0	0	1	0
8	B	243	0	0	0	0
All	All	5299	0	4672	24	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 (24) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ILE:HG13	1:A:179[A]:MET:HE1	1.74	0.70
1:B:223:VAL:O	1:B:227:MET:HG3	1.95	0.67
1:B:61:LYS:HE3	1:B:64:LEU:HD23	1.78	0.64
1:B:134:ILE:H	2:B:304:EDO:H21	1.65	0.61
1:B:63:ILE:HD11	1:B:87:LEU:HD21	1.82	0.60
1:A:161:GLN:O	1:A:165:GLU:HG3	2.08	0.54
1:A:223:VAL:O	1:A:227:MET:HG3	2.12	0.50
1:B:130:SER:HA	2:B:301[A]:EDO:H21	1.91	0.50
1:A:50[B]:MET:HE2	1:A:59:LEU:HD12	1.94	0.49
1:B:121:VAL:HG13	1:B:153:LEU:HD21	1.95	0.49
1:B:5:ASP:HB3	1:B:8:ILE:HG13	1.94	0.49
1:A:76:ALA:HB3	1:A:92:GLU:HB2	1.96	0.47
1:A:211:LEU:HD13	4:A:305:MES:H82	1.96	0.47
1:A:4:VAL:HG23	8:A:621:HOH:O	2.15	0.47
1:A:18:ASP:OD1	1:A:37:LYS:NZ	2.42	0.47
1:B:134:ILE:N	2:B:304:EDO:H21	2.30	0.46
1:A:50[B]:MET:HE1	1:A:56:VAL:HG12	1.97	0.46
1:A:22:ARG:HG3	1:A:32:PHE:CE1	2.54	0.43
1:A:229:LYS:HE2	1:A:229:LYS:HB3	1.85	0.42
1:A:4:VAL:HG22	1:A:56:VAL:HB	2.01	0.42
1:B:133:LYS:HA	2:B:304:EDO:H12	2.02	0.42
1:B:61:LYS:HD2	1:B:61:LYS:HA	1.74	0.41
1:B:175:THR:HA	1:B:176:PRO:HD3	1.95	0.41
1:A:209:ALA:HB1	1:A:243:TRP:CZ2	2.56	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	298/311 (96%)	290 (97%)	8 (3%)	0	100	100
1	B	284/311 (91%)	278 (98%)	6 (2%)	0	100	100
All	All	582/622 (94%)	568 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	247/265 (93%)	244 (99%)	3 (1%)	63	33
1	B	232/265 (88%)	231 (100%)	1 (0%)	84	70
All	All	479/530 (90%)	475 (99%)	4 (1%)	70	50

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

Mol	Chain	Res	Type
1	A	3	VAL
1	A	136	ARG
1	A	230	SER
1	B	236	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	233	GLN
1	B	10	ASN
1	B	123	GLN
1	B	212	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 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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	$\# Z > 2$
2	EDO	A	302	-	3,3,3	0.23	0	2,2,2	0.40	0
2	EDO	B	307	-	3,3,3	0.25	0	2,2,2	0.40	0
3	GOL	A	304	-	5,5,5	0.39	0	5,5,5	0.40	0
5	A1BWM	A	306	-	44,45,45	2.09	13 (29%)	59,65,65	2.67	18 (30%)
7	PGE	B	310	-	9,9,9	0.33	0	8,8,8	0.61	0
2	EDO	A	303	-	3,3,3	0.24	0	2,2,2	0.34	0
2	EDO	B	304	-	3,3,3	0.23	0	2,2,2	0.43	0
2	EDO	B	303	-	3,3,3	0.25	0	2,2,2	0.31	0
3	GOL	B	309	-	5,5,5	0.31	0	5,5,5	0.49	0
2	EDO	B	305	-	3,3,3	0.24	0	2,2,2	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MES	A	305	-	12,12,12	1.00	1 (8%)	15,16,16	1.12	2 (13%)
4	MES	B	311	-	12,12,12	1.02	1 (8%)	15,16,16	1.12	2 (13%)
2	EDO	B	301[A]	-	3,3,3	0.24	0	2,2,2	0.20	0
2	EDO	B	302	-	3,3,3	0.25	0	2,2,2	0.38	0
5	A1BWM	B	312	-	44,45,45	2.08	13 (29%)	59,65,65	3.14	18 (30%)
2	EDO	B	306	-	3,3,3	0.24	0	2,2,2	0.41	0
2	EDO	B	308	-	3,3,3	0.24	0	2,2,2	0.39	0
2	EDO	A	301	-	3,3,3	0.25	0	2,2,2	0.41	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
2	EDO	A	302	-	-	1/1/1/1	-
2	EDO	B	307	-	-	0/1/1/1	-
3	GOL	A	304	-	-	0/4/4/4	-
5	A1BWM	A	306	-	-	4/22/45/45	0/6/6/6
7	PGE	B	310	-	-	3/7/7/7	-
2	EDO	A	303	-	-	0/1/1/1	-
2	EDO	B	304	-	-	1/1/1/1	-
2	EDO	B	303	-	-	0/1/1/1	-
3	GOL	B	309	-	-	0/4/4/4	-
2	EDO	B	305	-	-	0/1/1/1	-
4	MES	A	305	-	-	3/6/14/14	0/1/1/1
4	MES	B	311	-	-	0/6/14/14	0/1/1/1
2	EDO	B	301[A]	-	-	0/1/1/1	-
2	EDO	B	302	-	-	1/1/1/1	-
5	A1BWM	B	312	-	-	4/22/45/45	0/6/6/6
2	EDO	B	306	-	-	1/1/1/1	-
2	EDO	B	308	-	-	1/1/1/1	-
2	EDO	A	301	-	-	0/1/1/1	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	306	A1BWM	C4-N20	6.86	1.46	1.35
5	B	312	A1BWM	C4-N20	6.84	1.46	1.35
5	A	306	A1BWM	C5-C22	-4.82	1.38	1.47
5	A	306	A1BWM	O15-C14	-4.58	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	312	A1BWM	C5-C22	-4.27	1.39	1.47
5	B	312	A1BWM	C2-N7	4.21	1.45	1.36
5	B	312	A1BWM	O15-C14	-4.19	1.43	1.47
5	A	306	A1BWM	C2-N7	3.77	1.44	1.36
5	B	312	A1BWM	C24-N23	-3.59	1.32	1.37
5	A	306	A1BWM	C24-N23	-3.21	1.32	1.37
5	A	306	A1BWM	O26-N25	-3.13	1.36	1.42
5	B	312	A1BWM	C11-C10	-2.82	1.34	1.39
5	B	312	A1BWM	O15-C16	2.81	1.41	1.36
5	B	312	A1BWM	C14-C10	2.68	1.55	1.51
5	A	306	A1BWM	C14-C10	2.64	1.55	1.51
5	B	312	A1BWM	C36-C27	-2.59	1.46	1.53
5	A	306	A1BWM	C36-C27	-2.57	1.46	1.53
5	A	306	A1BWM	C5-C4	-2.55	1.39	1.42
5	B	312	A1BWM	O26-N25	-2.54	1.37	1.42
5	B	312	A1BWM	C40-C27	-2.48	1.46	1.53
5	A	306	A1BWM	C40-C27	-2.43	1.46	1.53
4	A	305	MES	C8-S	2.40	1.81	1.77
5	A	306	A1BWM	C11-C10	-2.38	1.35	1.39
5	B	312	A1BWM	C27-C24	2.38	1.53	1.48
4	B	311	MES	C8-S	2.38	1.80	1.77
5	A	306	A1BWM	C27-C24	2.24	1.53	1.48
5	B	312	A1BWM	C5-C4	-2.21	1.39	1.42
5	A	306	A1BWM	O15-C16	2.20	1.40	1.36

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	312	A1BWM	C24-N23-C22	16.19	109.55	102.90
5	A	306	A1BWM	C24-N23-C22	12.67	108.10	102.90
5	B	312	A1BWM	O26-C22-N23	-6.20	108.07	113.29
5	B	312	A1BWM	O15-C14-C10	6.19	106.00	102.56
5	A	306	A1BWM	O15-C14-C10	5.65	105.70	102.56
5	B	312	A1BWM	O15-C16-O19	5.29	126.81	121.12
5	A	306	A1BWM	O26-C22-N23	-5.09	109.00	113.29
5	A	306	A1BWM	N1-C2-N3	-4.72	121.86	126.42
5	B	312	A1BWM	C14-O15-C16	-4.60	109.40	111.48
5	A	306	A1BWM	C6-C5-C4	4.56	119.25	114.67
5	B	312	A1BWM	C6-C5-C4	4.49	119.18	114.67
5	B	312	A1BWM	N1-C2-N3	-4.46	122.11	126.42
5	A	306	A1BWM	O15-C16-O19	4.14	125.57	121.12
5	B	312	A1BWM	O26-C22-C5	4.02	124.78	118.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	306	A1BWM	C5-C4-N3	-3.76	118.07	122.65
5	B	312	A1BWM	C5-C6-N1	-3.70	119.10	124.32
5	B	312	A1BWM	C28-C21-N20	-3.59	108.79	113.50
5	B	312	A1BWM	C5-C4-N3	-3.55	118.32	122.65
5	B	312	A1BWM	C40-C27-C24	-3.46	106.51	112.50
5	B	312	A1BWM	C6-N1-C2	3.44	120.52	115.81
5	A	306	A1BWM	C5-C6-N1	-3.42	119.50	124.32
5	A	306	A1BWM	C6-N1-C2	3.27	120.29	115.81
5	A	306	A1BWM	C40-C27-C24	-3.17	107.02	112.50
5	A	306	A1BWM	C14-O15-C16	-3.08	110.09	111.48
5	A	306	A1BWM	C28-C21-N20	-2.93	109.66	113.50
5	A	306	A1BWM	O26-C22-C5	2.86	122.84	118.05
5	A	306	A1BWM	O15-C14-C18	2.75	109.44	107.30
4	A	305	MES	O2S-S-C8	-2.69	102.67	106.73
5	B	312	A1BWM	O15-C14-C17	2.57	109.30	107.30
4	B	311	MES	O2S-S-C8	-2.51	102.94	106.73
5	B	312	A1BWM	O15-C14-C18	2.47	109.22	107.30
5	B	312	A1BWM	O38-C39-C40	2.40	115.89	111.74
5	A	306	A1BWM	O38-C39-C40	2.36	115.82	111.74
4	A	305	MES	O1S-S-C8	-2.27	103.30	106.73
4	B	311	MES	O1S-S-C8	-2.22	103.38	106.73
5	A	306	A1BWM	C39-O38-C37	2.21	117.04	109.88
5	B	312	A1BWM	C39-O38-C37	2.17	116.91	109.88
5	B	312	A1BWM	C39-C40-C27	2.14	113.89	110.32
5	A	306	A1BWM	C39-C40-C27	2.14	113.88	110.32
5	A	306	A1BWM	C6-C5-C22	-2.01	117.34	120.41

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	305	MES	C7-C8-S-O2S
7	B	310	PGE	O3-C5-C6-O4
4	A	305	MES	C7-C8-S-O3S
5	A	306	A1BWM	C28-C21-N20-C4
5	B	312	A1BWM	C28-C21-N20-C4
2	B	302	EDO	O1-C1-C2-O2
5	B	312	A1BWM	C29-C21-N20-C4
2	A	302	EDO	O1-C1-C2-O2
4	A	305	MES	C7-C8-S-O1S
7	B	310	PGE	C3-C4-O3-C5
5	B	312	A1BWM	N20-C21-C28-C35

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Mol	Chain	Res	Type	Atoms
2	B	306	EDO	O1-C1-C2-O2
5	B	312	A1BWM	N20-C21-C28-C31
5	A	306	A1BWM	C29-C21-N20-C4
5	A	306	A1BWM	N20-C21-C28-C31
5	A	306	A1BWM	N20-C21-C28-C35
7	B	310	PGE	C1-C2-O2-C3
2	B	308	EDO	O1-C1-C2-O2
2	B	304	EDO	O1-C1-C2-O2

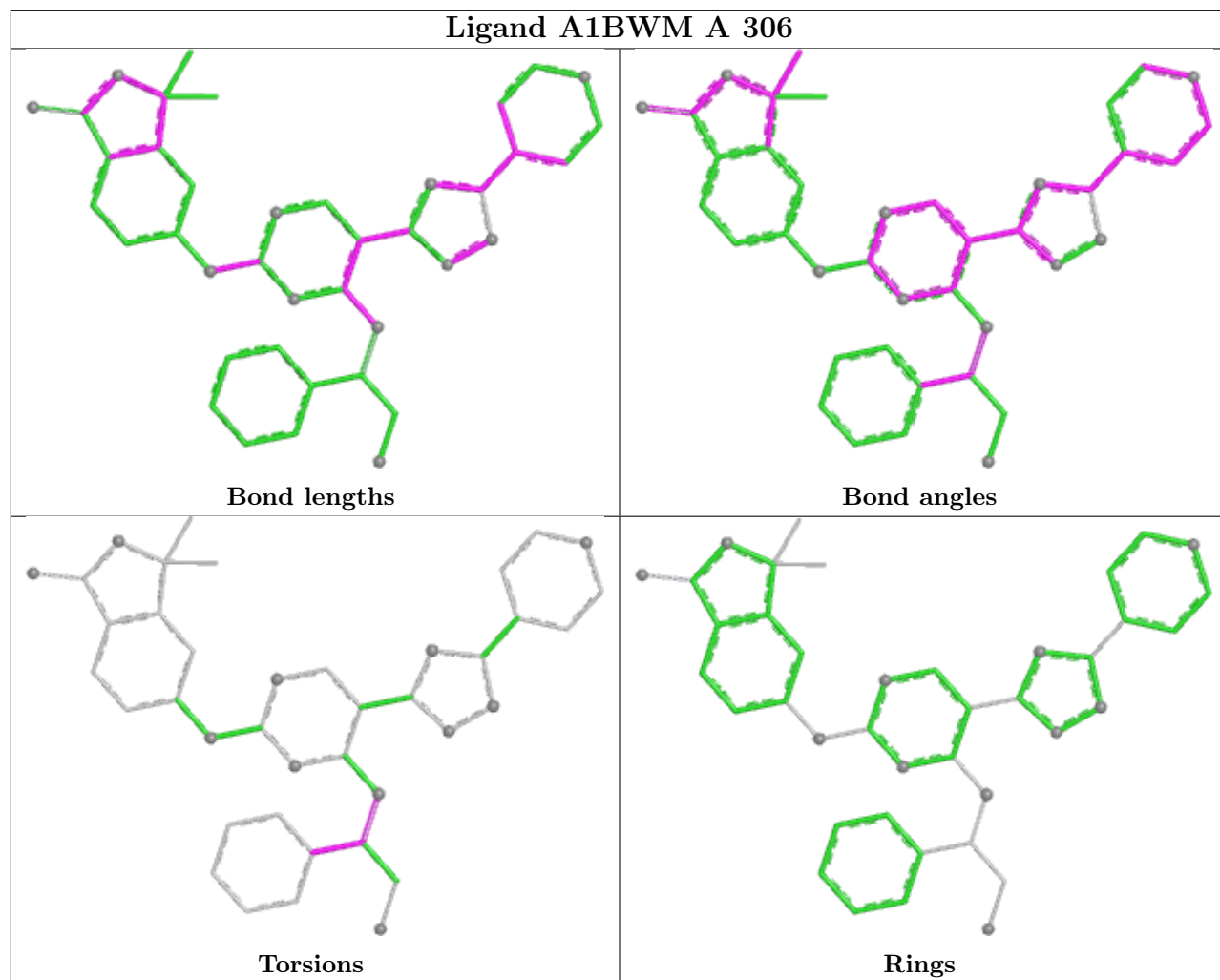
There are no ring outliers.

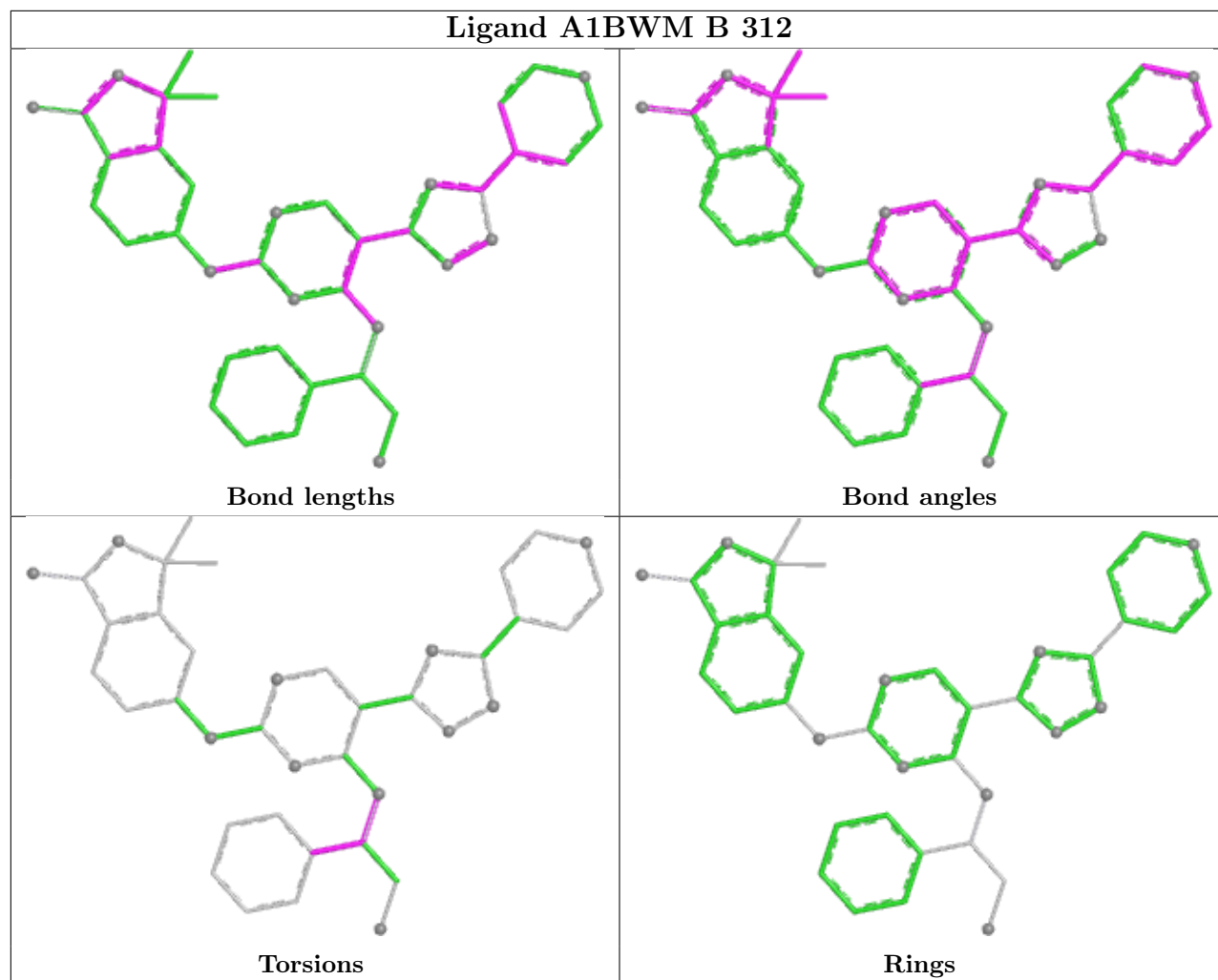
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	304	EDO	3	0
4	A	305	MES	1	0
2	B	301[A]	EDO	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.

Ligand A1BWM A 306





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	293/311 (94%)	0.15	16 (5%) 30 30	6, 15, 33, 52	7 (2%)
1	B	285/311 (91%)	0.50	26 (9%) 15 14	7, 19, 38, 56	3 (1%)
All	All	578/622 (92%)	0.32	42 (7%) 21 20	6, 17, 38, 56	10 (1%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	167	ALA	6.7
1	B	6	PRO	4.4
1	B	170	LEU	4.2
1	A	27	THR	4.1
1	B	166	LEU	4.1
1	A	52	PRO	4.0
1	A	225	PHE	3.9
1	B	19	LEU	3.7
1	B	230	SER	3.6
1	B	216	PHE	3.5
1	B	168	ARG	3.4
1	A	3	VAL	3.3
1	A	28	TYR	3.0
1	B	29	GLY	3.0
1	A	295	ASN	2.9
1	B	28	TYR	2.8
1	A	166	LEU	2.8
1	A	53	ASP	2.7
1	B	20	LEU	2.6
1	A	228	THR	2.6
1	B	175	THR	2.6
1	B	53	ASP	2.6
1	B	162	ILE	2.5
1	B	236	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	221	LEU	2.5
1	A	277	PRO	2.4
1	B	5	ASP	2.4
1	B	217	ASP	2.4
1	B	38	VAL	2.4
1	A	230	SER	2.3
1	B	23	LEU	2.3
1	B	164	ALA	2.3
1	B	231	GLY	2.2
1	A	20	LEU	2.2
1	B	52	PRO	2.2
1	A	16	HIS	2.2
1	A	231	GLY	2.1
1	B	27	THR	2.1
1	A	172	PHE	2.1
1	B	169	ARG	2.1
1	B	56	VAL	2.0
1	B	18	ASP	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
4	MES	B	311	12/12	0.65	0.16	30,43,55,72	0
2	EDO	B	301[A]	4/4	0.68	0.20	18,25,26,35	4
2	EDO	A	301	4/4	0.68	0.18	38,40,44,45	0
2	EDO	A	303	4/4	0.71	0.17	28,33,35,42	0
2	EDO	B	307	4/4	0.74	0.16	36,41,45,48	0

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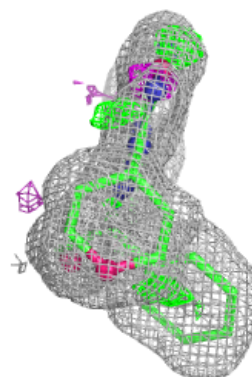
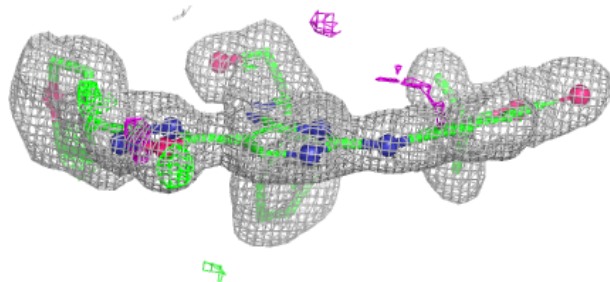
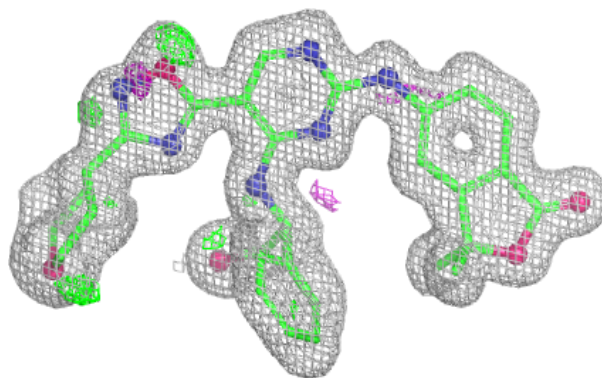
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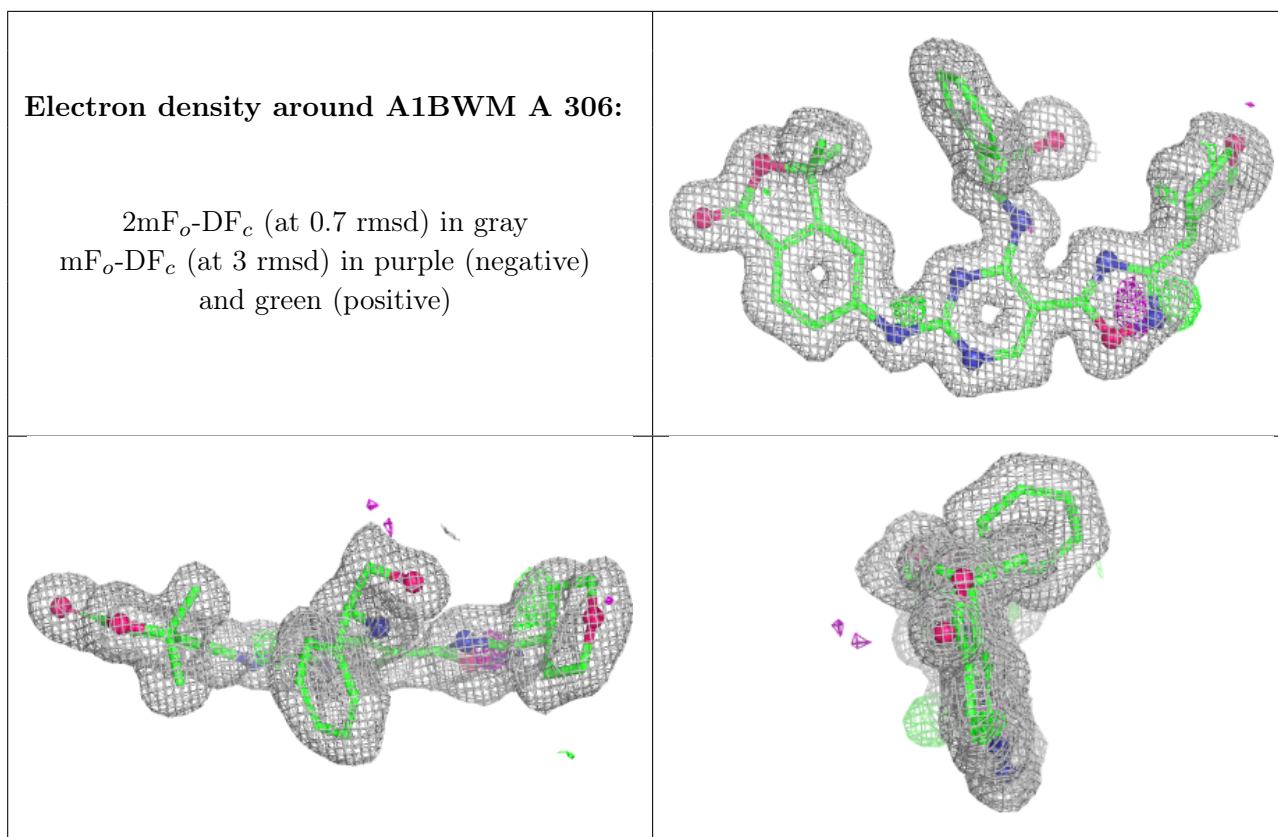
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	B	302	4/4	0.78	0.14	35,40,42,45	0
3	GOL	A	304	6/6	0.79	0.16	31,42,42,47	0
2	EDO	B	304	4/4	0.79	0.15	30,32,35,37	0
2	EDO	B	305	4/4	0.80	0.13	28,35,42,45	0
2	EDO	B	303	4/4	0.81	0.14	38,40,45,46	0
2	EDO	B	308	4/4	0.81	0.13	34,40,41,42	0
7	PGE	B	310	10/10	0.81	0.14	41,44,47,48	0
2	EDO	B	306	4/4	0.82	0.11	31,32,35,43	0
2	EDO	A	302	4/4	0.84	0.12	29,30,39,44	0
4	MES	A	305	12/12	0.84	0.19	19,24,31,33	12
3	GOL	B	309	6/6	0.87	0.13	23,26,30,31	0
6	NA	A	307	1/1	0.92	0.15	41,41,41,41	0
5	A1BWM	B	312	40/40	0.94	0.09	10,16,32,33	0
5	A1BWM	A	306	40/40	0.96	0.07	8,12,31,33	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 A1BWM B 312:

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.