



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2026 – 12:52 AM UTC

PDB ID : 5OTD / pdb_00005otd
Title : The crystal structure of CK2alpha in complex with compound 25
Authors : Brear, P.; De Fusco, C.; Iegre, J.; Yoshida, M.; Mitchell, S.; Rossmann, M.; Carro, L.; Sore, H.; Hyvonen, M.; Spring, D.
Deposited on : 2017-08-21
Resolution : 1.57 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

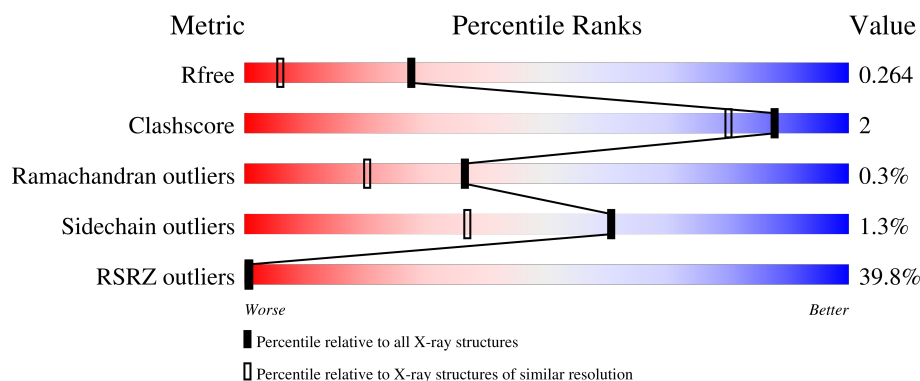
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.57 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	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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	352	15% 86% 7% 7%
1	B	352	59% 87% 5% 8%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PEG	A	406	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6092 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 Casein kinase II subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	324	Total	C	N	O	S	0	3	0
			2763	1770	485	497	11			
1	A	327	Total	C	N	O	S	0	5	0
			2797	1789	493	504	11			

There are 50 discrepancies between the modelled and reference sequences:

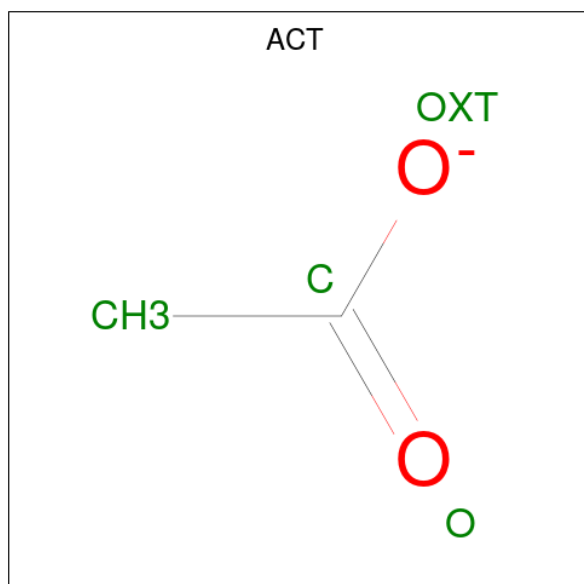
Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	GLY	-	expression tag	UNP P68400
B	-21	SER	-	expression tag	UNP P68400
B	-20	MET	-	expression tag	UNP P68400
B	-19	ASP	-	expression tag	UNP P68400
B	-18	ILE	-	expression tag	UNP P68400
B	-17	GLU	-	expression tag	UNP P68400
B	-16	PHE	-	expression tag	UNP P68400
B	-15	ASP	-	expression tag	UNP P68400
B	-14	ASP	-	expression tag	UNP P68400
B	-13	ASP	-	expression tag	UNP P68400
B	-12	ALA	-	expression tag	UNP P68400
B	-11	ASP	-	expression tag	UNP P68400
B	-10	ASP	-	expression tag	UNP P68400
B	-9	ASP	-	expression tag	UNP P68400
B	-8	GLY	-	expression tag	UNP P68400
B	-7	SER	-	expression tag	UNP P68400
B	-6	GLY	-	expression tag	UNP P68400
B	-5	SER	-	expression tag	UNP P68400
B	-4	GLY	-	expression tag	UNP P68400
B	-3	SER	-	expression tag	UNP P68400
B	-2	GLY	-	expression tag	UNP P68400
B	-1	SER	-	expression tag	UNP P68400
B	0	GLY	-	expression tag	UNP P68400
B	1	SER	-	expression tag	UNP P68400
B	21	SER	ARG	engineered mutation	UNP P68400

Continued on next page...

Continued from previous page...

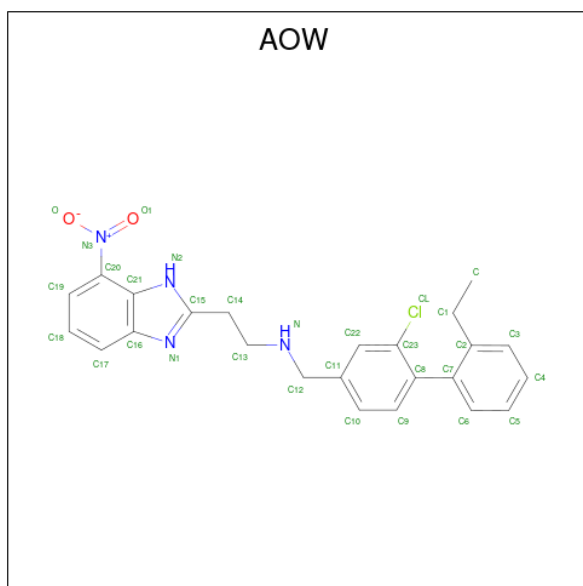
Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	GLY	-	expression tag	UNP P68400
A	-21	SER	-	expression tag	UNP P68400
A	-20	MET	-	expression tag	UNP P68400
A	-19	ASP	-	expression tag	UNP P68400
A	-18	ILE	-	expression tag	UNP P68400
A	-17	GLU	-	expression tag	UNP P68400
A	-16	PHE	-	expression tag	UNP P68400
A	-15	ASP	-	expression tag	UNP P68400
A	-14	ASP	-	expression tag	UNP P68400
A	-13	ASP	-	expression tag	UNP P68400
A	-12	ALA	-	expression tag	UNP P68400
A	-11	ASP	-	expression tag	UNP P68400
A	-10	ASP	-	expression tag	UNP P68400
A	-9	ASP	-	expression tag	UNP P68400
A	-8	GLY	-	expression tag	UNP P68400
A	-7	SER	-	expression tag	UNP P68400
A	-6	GLY	-	expression tag	UNP P68400
A	-5	SER	-	expression tag	UNP P68400
A	-4	GLY	-	expression tag	UNP P68400
A	-3	SER	-	expression tag	UNP P68400
A	-2	GLY	-	expression tag	UNP P68400
A	-1	SER	-	expression tag	UNP P68400
A	0	GLY	-	expression tag	UNP P68400
A	1	SER	-	expression tag	UNP P68400
A	21	SER	ARG	engineered mutation	UNP P68400

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 3 is N-[[[(1M)-2-chloro-2'-ethyl[1,1'-biphenyl]-4-yl]methyl}-2-(7-nitro-1H-1,3-benzimidazol-2-yl)ethan-1-amine (CCD ID: AOW) (formula: C₂₄H₂₃ClN₄O₂) (labeled as "Ligand of Interest" by depositor).



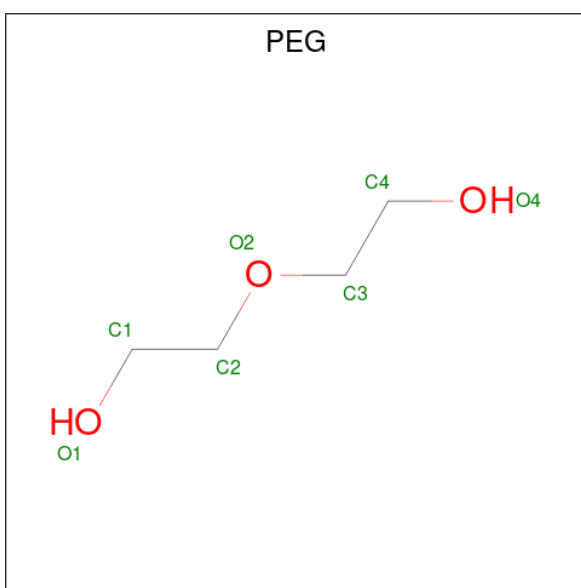
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	Cl	N	O	0	0
			31	24	1	4	2		
3	A	1	Total	C	Cl	N	O	0	1
			62	48	2	8	4		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).

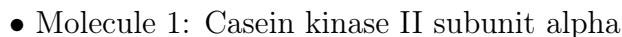


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	115	Total 115	O 115	0	0
6	A	291	Total 291	O 291	0	0

- Molecule 1: Casein kinase II subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	65.59Å 69.25Å 337.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	168.75 – 1.57 168.75 – 1.57	Depositor EDS
% Data completeness (in resolution range)	97.4 (168.75-1.57) 97.4 (168.75-1.57)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 1.57Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.248 , 0.261 0.251 , 0.264	Depositor DCC
R_{free} test set	5404 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6092	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.59% 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: AOW, PEG, ACT, PO4

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	0.98	2/2872 (0.1%)	1.06	2/3885 (0.1%)
1	B	0.85	0/2838	1.14	7/3839 (0.2%)
All	All	0.92	2/5710 (0.0%)	1.10	9/7724 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	137	MET	SD-CE	-6.00	1.64	1.79
1	A	150	MET	SD-CE	-5.49	1.65	1.79

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	TRP	N-CA-C	5.77	120.47	113.38
1	B	257	TYR	CA-C-N	5.32	127.27	120.56
1	B	257	TYR	C-N-CA	5.32	127.27	120.56
1	B	175	ASP	N-CA-C	5.22	117.02	110.91
1	B	13	THR	N-CA-C	5.21	116.64	111.07
1	B	245	ILE	N-CA-C	-5.20	105.33	111.00
1	B	124	LEU	CA-C-N	5.14	131.35	121.54
1	B	124	LEU	C-N-CA	5.14	131.35	121.54
1	A	130	ASP	CA-CB-CG	5.10	117.70	112.60

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	2797	0	2734	15	0
1	B	2763	0	2702	5	0
2	A	12	0	9	0	0
2	B	4	0	3	0	0
3	A	62	0	0	2	0
3	B	31	0	0	1	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	7	0	10	4	0
6	A	291	0	0	4	0
6	B	115	0	0	0	0
All	All	6092	0	5458	22	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (22) 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:225:MET:HE2	1:A:225:MET:HA	1.61	0.82
1:A:32:GLU:OE2	6:A:501:HOH:O	2.16	0.62
3:A:404[A]:AOW:C	3:A:404[A]:AOW:CL	2.90	0.56
1:A:125:TYR:HA	1:A:128:LEU:HD12	1.91	0.51
1:A:225:MET:HA	1:A:225:MET:CE	2.40	0.50
1:B:162:VAL:HG11	3:B:402:AOW:CL	2.48	0.50
1:A:230:GLU:HG2	5:A:406:PEG:H41	1.94	0.48
1:B:47:ARG:HG3	1:B:52:GLU:HG2	1.96	0.47
1:A:32:GLU:HG2	6:A:501:HOH:O	2.13	0.47
1:A:196:TYR:HD2	5:A:406:PEG:H21	1.78	0.47
1:A:47:ARG:HG3	1:A:52:GLU:HG2	1.96	0.47
1:B:89:ARG:HH21	1:B:97:LEU:HD23	1.80	0.46
1:A:286:HIS:HE1	6:A:761:HOH:O	2.00	0.46
1:A:89:ARG:HH21	1:A:97:LEU:HD23	1.81	0.45
1:A:236:HIS:HE1	6:A:724:HOH:O	2.02	0.43
1:A:196:TYR:CD2	5:A:406:PEG:H21	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:PHE:HZ	5:A:406:PEG:H31	1.85	0.42
1:A:96:THR:H	1:A:114:GLU:HG2	1.83	0.41
1:B:303:LYS:HB3	1:B:313:LEU:HG	2.02	0.41
3:A:404[A]:AOW:C	3:A:404[A]:AOW:C23	2.99	0.41
1:B:50:TYR:HA	1:B:71:LYS:HD2	2.03	0.41
1:A:50:TYR:HA	1:A:71:LYS:HD2	2.04	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	330/352 (94%)	323 (98%)	6 (2%)	1 (0%)	36	20
1	B	325/352 (92%)	319 (98%)	5 (2%)	1 (0%)	36	20
All	All	655/704 (93%)	642 (98%)	11 (2%)	2 (0%)	36	20

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	125	TYR
1	A	193	ALA

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	306/319 (96%)	302 (99%)	4 (1%)	61	37
1	B	302/319 (95%)	298 (99%)	4 (1%)	61	37
All	All	608/638 (95%)	600 (99%)	8 (1%)	61	37

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	21	SER
1	B	57	ILE
1	B	73	VAL
1	B	262	ASN
1	A	57	ILE
1	A	73	VAL
1	A	122	LYS
1	A	225	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	62	ASN
1	B	115	HIS
1	B	160	HIS
1	B	186	GLN
1	B	207	GLN
1	B	234	HIS
1	B	270	ASN
1	A	62	ASN
1	A	160	HIS
1	A	168	HIS
1	A	186	GLN
1	A	234	HIS
1	A	236	HIS
1	A	270	ASN
1	A	286	HIS

5.3.3 RNA ⓘ

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](#)

10 ligands are modelled in this entry.

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	ACT	A	402	-	3,3,3	0.84	0	3,3,3	0.76	0
3	AOW	A	404[A]	-	34,34,34	0.64	0	40,47,47	1.53	3 (7%)
4	PO4	B	403	-	4,4,4	2.57	2 (50%)	6,6,6	0.48	0
3	AOW	B	402	-	34,34,34	0.60	0	40,47,47	1.43	4 (10%)
2	ACT	B	401	-	3,3,3	0.82	0	3,3,3	0.73	0
2	ACT	A	401	-	3,3,3	1.44	1 (33%)	3,3,3	0.94	0
2	ACT	A	403	-	3,3,3	0.83	0	3,3,3	0.72	0
4	PO4	A	405	-	4,4,4	2.60	3 (75%)	6,6,6	0.74	0
3	AOW	A	404[B]	-	34,34,34	0.61	1 (2%)	40,47,47	1.45	3 (7%)
5	PEG	A	406	-	6,6,6	0.20	0	5,5,5	0.17	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
3	AOW	A	404[A]	-	-	3/15/17/17	0/4/4/4
3	AOW	B	402	-	-	0/15/17/17	0/4/4/4
3	AOW	A	404[B]	-	-	1/15/17/17	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	A	406	-	-	2/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	403	PO4	P-O1	4.29	1.60	1.50
4	A	405	PO4	P-O1	4.26	1.60	1.50
2	A	401	ACT	CH3-C	2.10	1.57	1.49
4	A	405	PO4	P-O2	2.10	1.60	1.54
4	A	405	PO4	P-O3	2.05	1.60	1.54
3	A	404[B]	AOW	C15-N1	2.04	1.35	1.32
4	B	403	PO4	P-O3	2.00	1.60	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	404[A]	AOW	C21-C16-N1	-6.63	105.38	109.91
3	A	404[B]	AOW	C21-C16-N1	-6.51	105.46	109.91
3	B	402	AOW	C21-C16-N1	-6.23	105.65	109.91
3	A	404[A]	AOW	C16-C21-N2	4.89	109.47	105.40
3	A	404[B]	AOW	C16-C21-N2	4.38	109.05	105.40
3	B	402	AOW	C16-C21-N2	3.97	108.71	105.40
3	A	404[A]	AOW	C17-C16-C21	3.37	123.32	120.24
3	B	402	AOW	C17-C16-C21	3.21	123.18	120.24
3	A	404[B]	AOW	C17-C16-C21	3.05	123.04	120.24
3	B	402	AOW	C20-C21-N2	2.03	135.40	133.21

There are no chirality outliers.

All (6) torsion outliers are listed below:

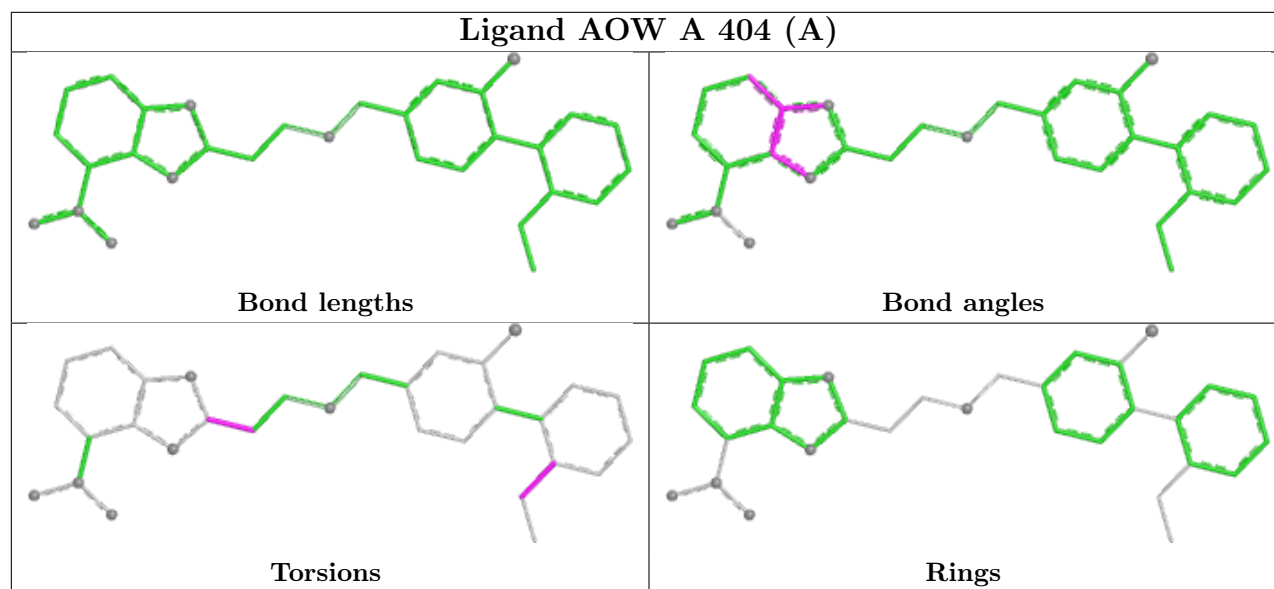
Mol	Chain	Res	Type	Atoms
3	A	404[A]	AOW	C-C1-C2-C3
3	A	404[A]	AOW	C-C1-C2-C7
5	A	406	PEG	C1-C2-O2-C3
5	A	406	PEG	C4-C3-O2-C2
3	A	404[A]	AOW	C13-C14-C15-N1
3	A	404[B]	AOW	C13-C14-C15-N1

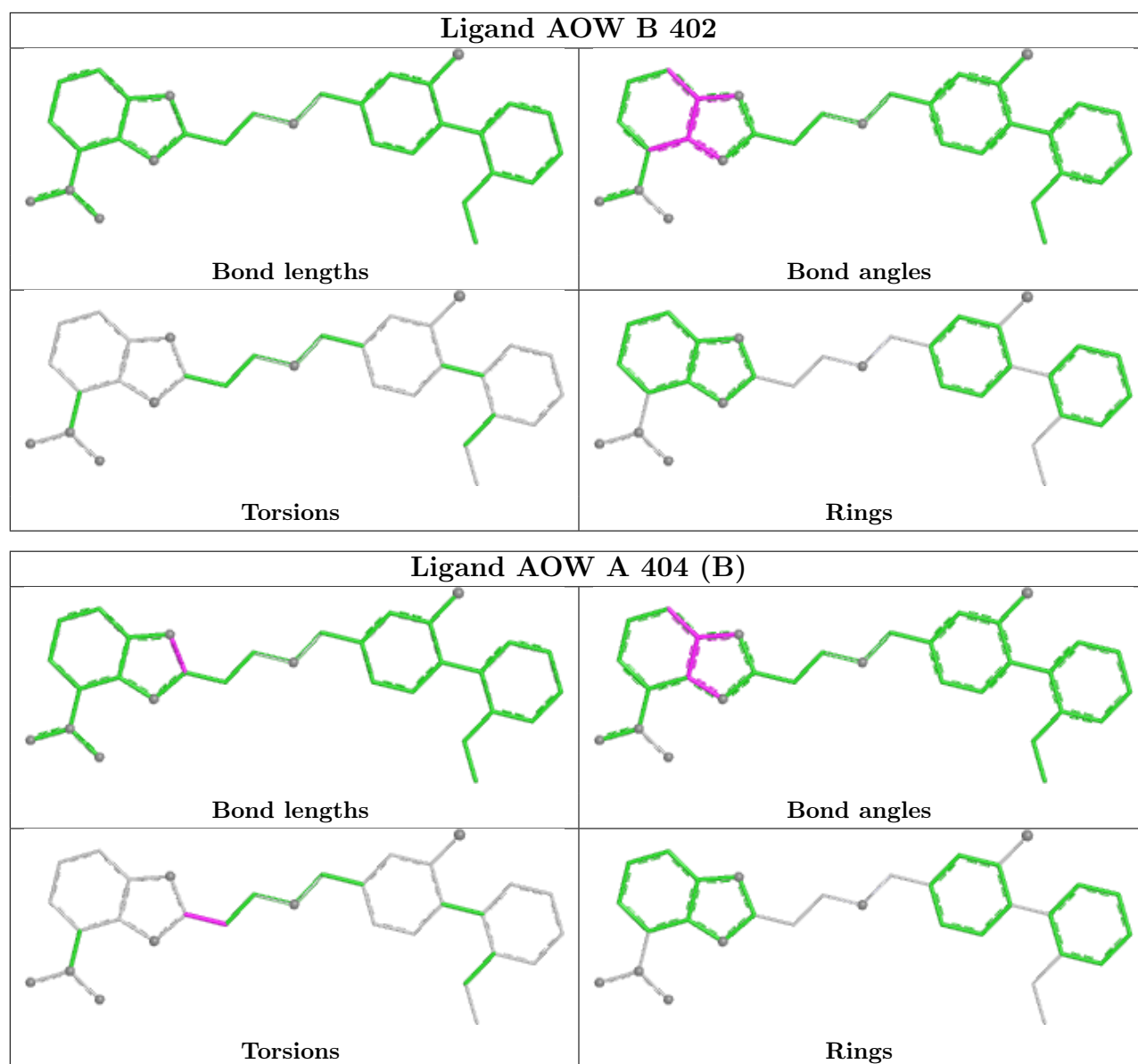
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	404[A]	AOW	2	0
3	B	402	AOW	1	0
5	A	406	PEG	4	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	327/352 (92%)	0.79	53 (16%) 4 8	8, 23, 55, 84	5 (1%)
1	B	324/352 (92%)	2.66	206 (63%) 0 0	17, 45, 83, 109	3 (0%)
All	All	651/704 (92%)	1.72	259 (39%) 1 1	8, 33, 75, 109	8 (1%)

All (259) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	124	LEU	12.0
1	B	327	VAL	8.4
1	A	125	TYR	8.0
1	A	50	TYR	7.8
1	B	124	LEU	7.6
1	A	121	PHE	7.6
1	B	307	TYR	7.0
1	B	281	TRP	6.8
1	B	121	PHE	6.8
1	B	273	LEU	6.8
1	B	272	ILE	6.3
1	A	328	VAL	6.1
1	B	257	TYR	6.1
1	B	293	VAL	6.1
1	B	233	PHE	6.1
1	B	53	VAL	6.1
1	B	45	LEU	5.9
1	B	116	VAL	5.9
1	B	305	LEU	5.8
1	B	269	PHE	5.7
1	B	284	PHE	5.7
1	B	216	TRP	5.7
1	B	265	LEU	5.7
1	B	125	TYR	5.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	292	LEU	5.7
1	B	128	LEU	5.6
1	B	249	LEU	5.6
1	B	298	LEU	5.6
1	B	255	TYR	5.5
1	B	248	VAL	5.3
1	B	73	VAL	5.3
1	B	254	LEU	5.2
1	B	227	PHE	5.2
1	B	129	THR	5.2
1	B	263	ILE	5.2
1	B	285	VAL	5.1
1	B	5	VAL	5.1
1	B	42	VAL	5.1
1	B	50	TYR	5.0
1	B	46	GLY	5.0
1	B	323	TYR	5.0
1	B	4	PRO	4.9
1	B	300	PHE	4.9
1	B	251	THR	4.7
1	B	245	ILE	4.7
1	B	226	ILE	4.7
1	A	73	VAL	4.7
1	B	258	ILE	4.7
1	B	325	TYR	4.6
1	B	279	LYS	4.6
1	B	72	PRO	4.5
1	B	232	PHE	4.5
1	B	222	LEU	4.4
1	B	119	THR	4.3
1	B	204	VAL	4.3
1	B	48	GLY	4.3
1	B	274	GLY	4.3
1	B	239	TYR	4.2
1	B	282	GLU	4.1
1	B	206	TYR	4.1
1	B	57	ILE	4.1
1	B	74	LYS	4.1
1	B	54	PHE	4.1
1	A	105	VAL	4.1
1	B	49	LYS	4.0
1	B	122	LYS	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	324	PHE	4.0
1	A	49	LYS	4.0
1	B	59	ILE	4.0
1	B	291	HIS	4.0
1	B	31	VAL	4.0
1	B	267	PRO	4.0
1	B	297	ALA	4.0
1	A	33	TRP	3.9
1	B	127	THR	3.9
1	B	123	GLN	3.9
1	B	30	VAL	3.9
1	B	126	GLN	3.9
1	B	301	LEU	3.9
1	B	261	TYR	3.8
1	B	295	PRO	3.8
1	A	74	LYS	3.8
1	A	2	SER	3.8
1	A	31	VAL	3.8
1	A	118	ASN	3.8
1	A	127	THR	3.7
1	B	280	ARG	3.7
1	B	131	TYR	3.7
1	B	41	LEU	3.7
1	B	202	LEU	3.7
1	B	11	VAL	3.7
1	B	224	SER	3.6
1	B	289	ASN	3.6
1	B	133	ILE	3.6
1	A	59	ILE	3.6
1	B	288	GLU	3.6
1	B	304	LEU	3.6
1	A	116	VAL	3.6
1	B	242	LEU	3.5
1	B	275	ARG	3.5
1	B	287	SER	3.5
1	B	256	ASP	3.5
1	B	266	ASP	3.5
1	B	51	SER	3.4
1	B	66	VAL	3.4
1	B	71	LYS	3.4
1	B	318	ALA	3.4
1	B	276	HIS	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	70	LEU	3.4
1	B	203	LEU	3.3
1	A	123	GLN	3.3
1	B	69	ILE	3.3
1	B	33	TRP	3.2
1	A	117	ASN	3.2
1	A	71	LYS	3.2
1	B	320	GLU	3.2
1	B	286	HIS	3.2
1	A	126	GLN	3.2
1	B	228	ARG	3.2
1	A	122	LYS	3.2
1	B	17	THR	3.1
1	B	44	LYS	3.1
1	B	278	ARG	3.1
1	B	277	SER	3.1
1	B	134	ARG	3.1
1	B	283	ARG	3.1
1	A	48	GLY	3.1
1	A	191	ARG	3.1
1	B	302	ASP	3.1
1	B	225	MET	3.1
1	B	213	LEU	3.1
1	A	30	VAL	3.0
1	B	313	LEU	3.0
1	B	299	ASP	3.0
1	B	75	LYS	3.0
1	B	120	ASP	3.0
1	B	268	ARG	3.0
1	B	247	LYS	3.0
1	B	260	LYS	3.0
1	B	105	VAL	3.0
1	B	205	ASP	3.0
1	B	326	THR	3.0
1	B	246	ALA	2.9
1	A	288	GLU	2.9
1	B	229	LYS	2.9
1	B	43	ARG	2.9
1	A	107[A]	ARG	2.9
1	B	60	THR	2.9
1	B	182	TYR	2.9
1	B	311[A]	SER	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	308	ASP	2.8
1	B	290	GLN	2.8
1	B	78	ILE	2.8
1	B	130	ASP	2.8
1	B	117	ASN	2.8
1	B	18	HIS	2.8
1	A	89	ARG	2.8
1	B	253	ASP	2.8
1	B	76	LYS	2.8
1	B	219	GLY	2.7
1	B	89	ARG	2.7
1	B	294	SER	2.7
1	B	185	GLY	2.7
1	B	135	PHE	2.7
1	B	259	ASP	2.7
1	B	191	ARG	2.7
1	B	306	ARG	2.7
1	B	186	GLN	2.7
1	B	322	PRO	2.7
1	B	56	ALA	2.6
1	B	113	PHE	2.6
1	B	196	TYR	2.6
1	A	60	THR	2.6
1	B	190	VAL	2.6
1	A	75	LYS	2.6
1	B	6	PRO	2.6
1	B	223	ALA	2.6
1	B	169	ARG	2.6
1	B	22	GLU	2.5
1	A	72	PRO	2.5
1	B	98	ALA	2.5
1	B	171	LEU	2.5
1	B	250	GLY	2.5
1	B	252	GLU	2.5
1	A	114	GLU	2.5
1	B	170	LYS	2.5
1	A	283	ARG	2.5
1	B	243	VAL	2.5
1	B	296	GLU	2.4
1	B	82	ILE	2.4
1	A	268	ARG	2.4
1	B	271	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	200	PRO	2.4
1	B	231	PRO	2.4
1	B	316	ARG	2.4
1	B	238	ASN	2.4
1	A	57	ILE	2.4
1	B	303	LYS	2.4
1	A	128	LEU	2.4
1	B	26	TYR	2.4
1	B	199	GLY	2.4
1	B	270	ASN	2.4
1	B	264	GLU	2.4
1	B	166	HIS	2.3
1	B	64	LYS	2.3
1	B	52	GLU	2.3
1	A	265	LEU	2.3
1	B	118	ASN	2.3
1	A	271	ASP	2.3
1	B	115	HIS	2.3
1	B	236	HIS	2.3
1	B	315	ALA	2.3
1	B	197	PHE	2.3
1	B	28	SER	2.3
1	A	70	LEU	2.3
1	B	321	HIS	2.3
1	B	27	GLU	2.3
1	B	230	GLU	2.3
1	A	280	ARG	2.3
1	A	100	ILE	2.3
1	B	220	CYS	2.2
1	B	19[A]	ARG	2.2
1	B	309	HIS	2.2
1	B	164	ILE	2.2
1	A	258	ILE	2.2
1	B	109	PRO	2.2
1	A	168	HIS	2.2
1	B	141	LEU	2.2
1	B	14	ASP	2.2
1	B	168	HIS	2.2
1	A	34	GLY	2.1
1	B	47	ARG	2.1
1	A	47	ARG	2.1
1	B	310	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	46	GLY	2.1
1	B	62	ASN	2.1
1	A	27	GLU	2.1
1	A	325	TYR	2.1
1	B	68	LYS	2.1
1	B	8	ARG	2.1
1	A	42	VAL	2.1
1	A	104	PRO	2.1
1	B	314	THR	2.1
1	B	188	TYR	2.1
1	B	55	GLU	2.1
1	B	262	ASN	2.1
1	A	120	ASP	2.1
1	B	184	PRO	2.1
1	B	79	LYS	2.0
1	A	170	LYS	2.0
1	B	136	TYR	2.0
1	B	194[A]	SER	2.0
1	B	108	THR	2.0
1	B	24	TRP	2.0
1	B	65	VAL	2.0
1	B	192	VAL	2.0
1	B	97	LEU	2.0
1	A	41	LEU	2.0
1	A	28	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

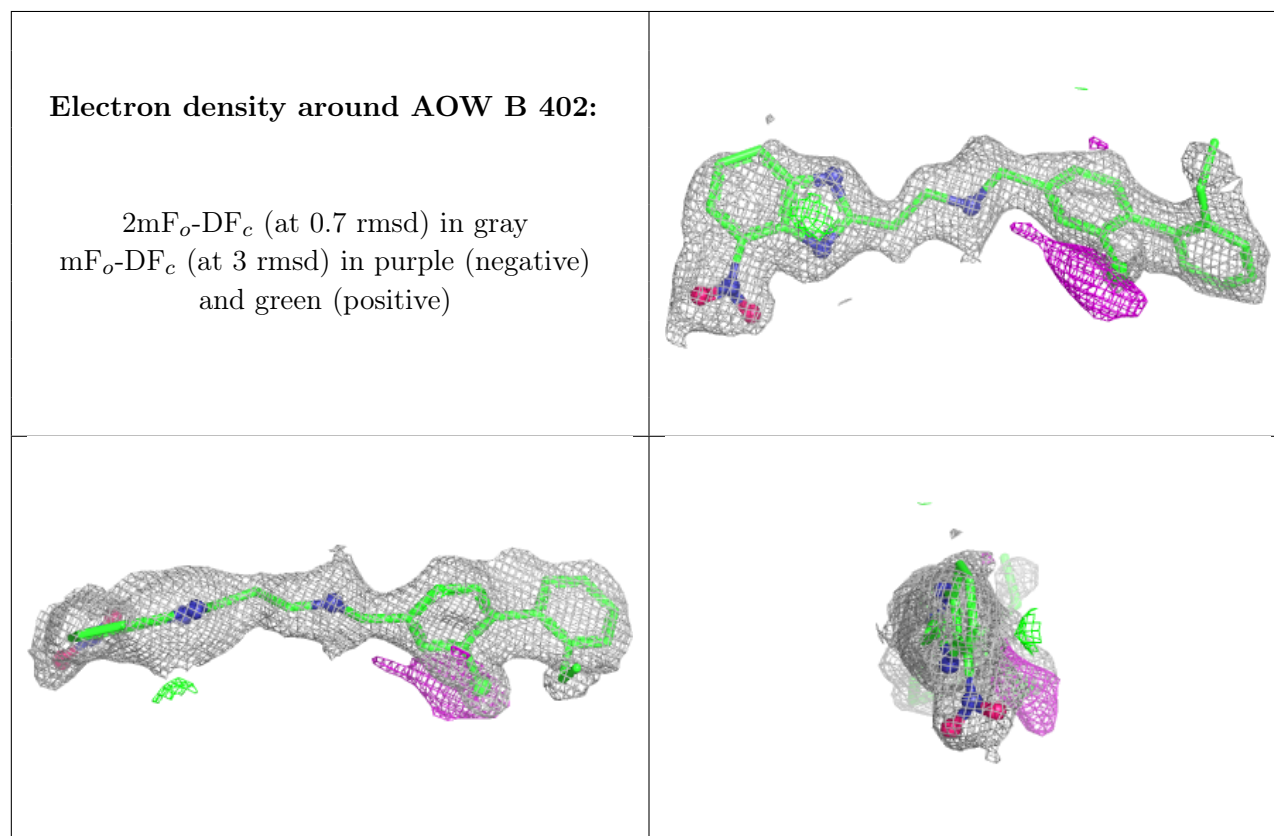
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

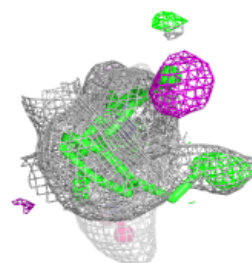
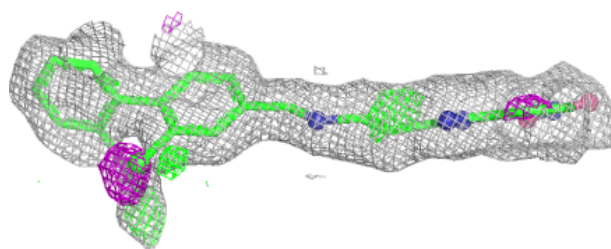
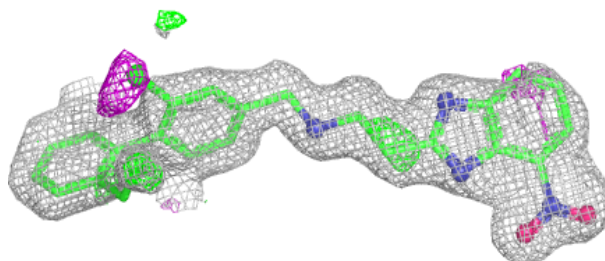
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	AOW	B	402	31/31	0.73	0.20	59,64,65,69	0
3	AOW	A	404[A]	31/31	0.73	0.24	41,47,54,55	31
3	AOW	A	404[B]	31/31	0.73	0.24	10,20,33,36	31
5	PEG	A	406	7/7	0.81	0.16	26,35,41,43	0
4	PO4	B	403	5/5	0.84	0.12	51,53,53,54	0
4	PO4	A	405	5/5	0.87	0.11	37,38,40,41	0
2	ACT	B	401	4/4	0.90	0.11	33,34,35,36	0
2	ACT	A	403	4/4	0.93	0.11	37,38,39,39	0
2	ACT	A	402	4/4	0.96	0.08	26,30,31,32	0
2	ACT	A	401	4/4	0.96	0.07	21,22,22,24	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.

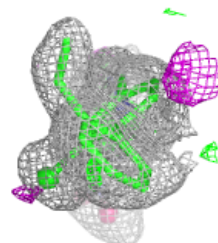
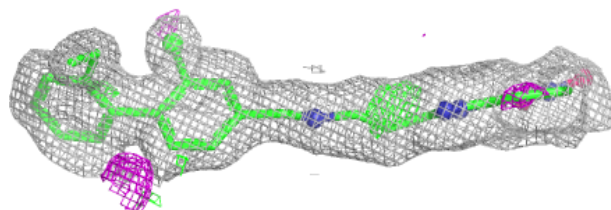
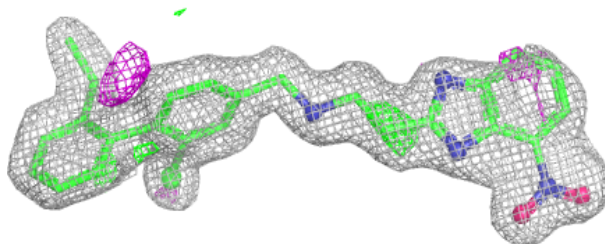


Electron density around AOW A 404 (A):

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

**Electron density around AOW A 404 (B):**

$2mF_o-DF_c$ (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.