



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2022 – 09:42 PM EDT

PDB ID : 3WI2
Title : Crystal structure of PDE10A in complex with inhibitor
Authors : Amano, Y.
Deposited on : 2013-09-04
Resolution : 2.26 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.29
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

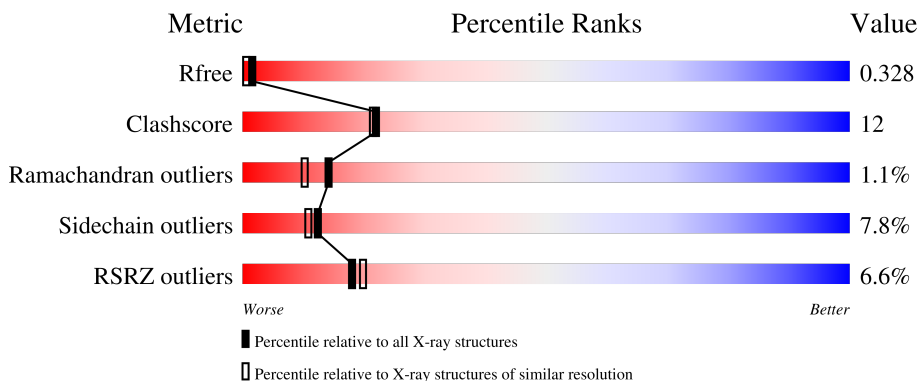
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	345	 8% 66% 26% • 6%
1	B	345	 4% 61% 31% • 6%

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 5335 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 and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	324	2629	1678	447	479	25	0	0	0
1	B	324	2629	1678	447	479	25	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	445	GLY	-	expression tag	UNP Q9Y233
A	446	SER	-	expression tag	UNP Q9Y233
A	447	HIS	-	expression tag	UNP Q9Y233
A	448	MET	-	expression tag	UNP Q9Y233
B	445	GLY	-	expression tag	UNP Q9Y233
B	446	SER	-	expression tag	UNP Q9Y233
B	447	HIS	-	expression tag	UNP Q9Y233
B	448	MET	-	expression tag	UNP Q9Y233

- Molecule 2 is ZINC ION (three-letter code: 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 (three-letter code: MG) (formula: Mg).

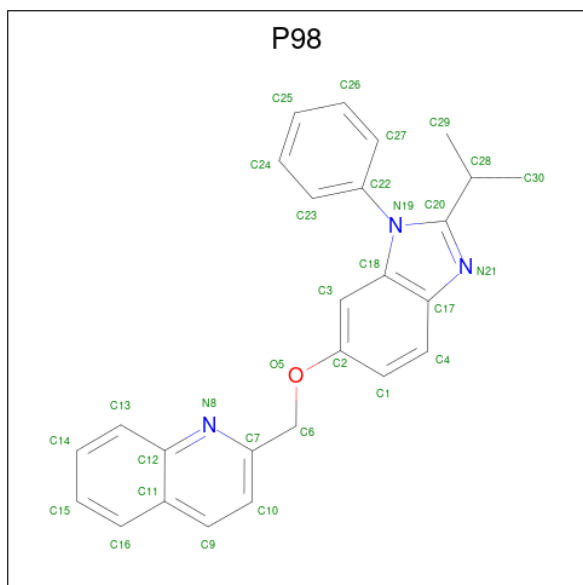
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

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

- Molecule 4 is 2-([1-phenyl-2-(propan-2-yl)-1H-benzimidazol-6-yl]oxy)methylquinoline (three-letter code: P98) (formula: C₂₆H₂₃N₃O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 30 26 3 1	0	0
4	B	1	Total C N O 30 26 3 1	0	0

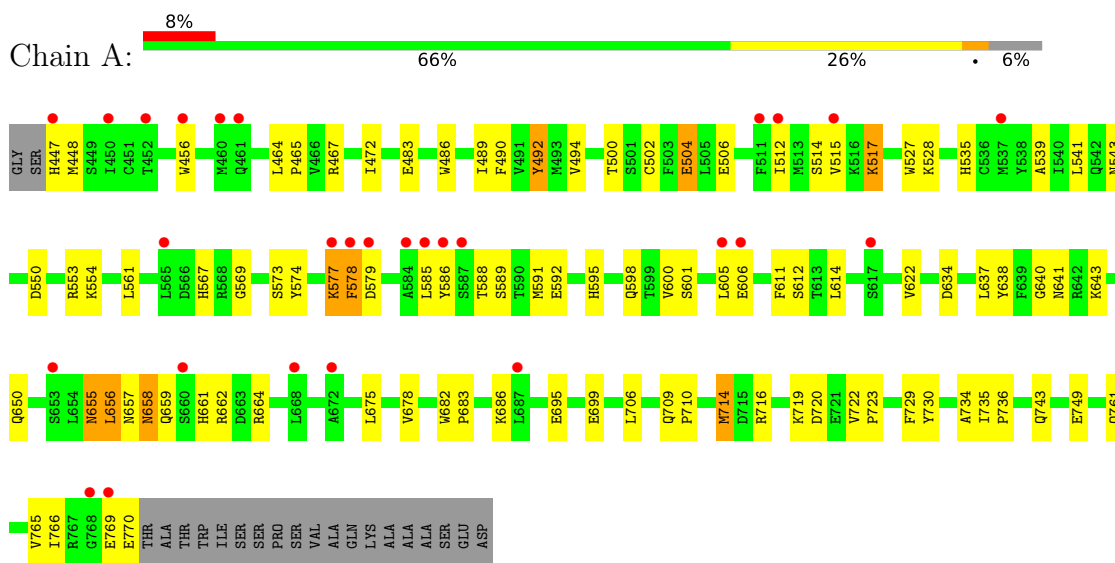
- Molecule 5 is water.

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

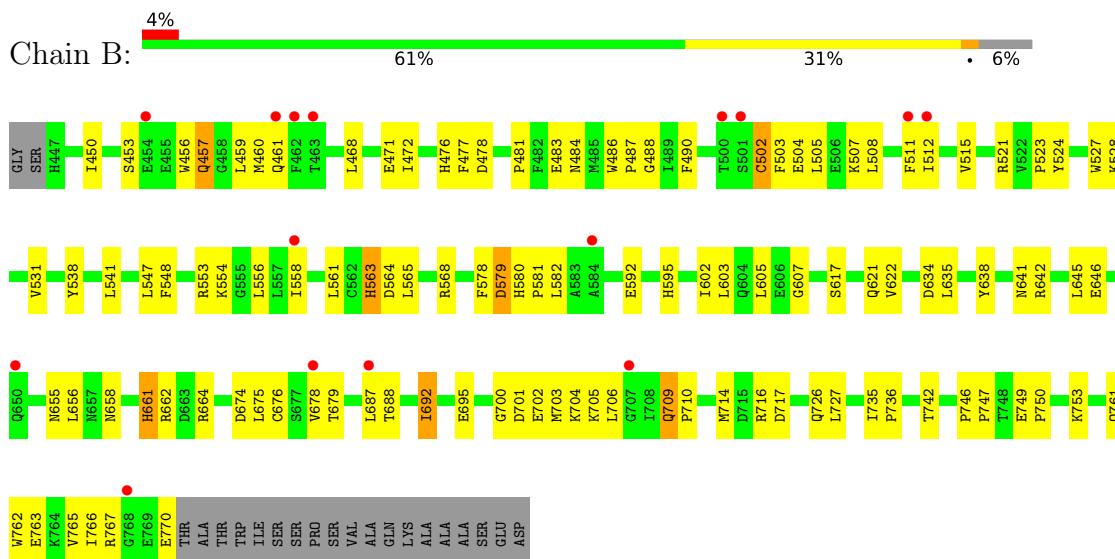
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.12Å 81.63Å 158.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.26 19.96 – 2.26	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.96-2.26) 98.2 (19.96-2.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.26Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.253 , 0.329 0.252 , 0.328	Depositor DCC
R_{free} test set	1542 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	45.2	Xtrriage
Anisotropy	0.319	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5335	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: P98, ZN, 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	0.60	0/2694	0.78	0/3647
1	B	0.66	2/2694 (0.1%)	0.87	4/3647 (0.1%)
All	All	0.63	2/5388 (0.0%)	0.82	4/7294 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	564	ASP	CB-CG	8.05	1.68	1.51
1	B	674	ASP	CB-CG	6.83	1.66	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	564	ASP	CB-CG-OD1	7.15	124.74	118.30
1	B	692	ILE	CG1-CB-CG2	-6.82	96.40	111.40
1	B	662	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	749	GLU	C-N-CD	5.02	138.93	128.40

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	2629	0	2588	58	0
1	B	2629	0	2588	67	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	30	0	23	1	0
4	B	30	0	23	0	0
5	A	5	0	0	0	0
5	B	8	0	0	1	0
All	All	5335	0	5222	124	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 12.

All (124) 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:709:GLN:HE21	1:B:710:PRO:HD2	1.27	0.95
1:A:502:CYS:SG	1:A:554:LYS:HD2	2.12	0.88
1:A:641:ASN:HD22	1:A:664:ARG:HH11	1.11	0.88
1:A:641:ASN:ND2	1:A:664:ARG:HH11	1.72	0.87
1:A:539:ALA:O	1:A:543:ASN:ND2	2.10	0.84
1:B:527:TRP:O	1:B:531:VAL:HG23	1.81	0.80
1:B:554:LYS:O	1:B:558:ILE:HG12	1.84	0.78
1:A:641:ASN:HD22	1:A:664:ARG:NH1	1.81	0.77
1:B:655:ASN:H	1:B:661:HIS:HD2	1.32	0.76
1:B:709:GLN:NE2	1:B:710:PRO:HD2	2.02	0.73
1:A:574:TYR:HB2	1:A:699:GLU:OE2	1.89	0.72
1:A:573:SER:O	1:A:577:LYS:HB2	1.91	0.70
1:A:456:TRP:CH2	1:A:506:GLU:HG3	2.26	0.69
1:B:761:GLN:O	1:B:765:VAL:HG23	1.92	0.68
1:A:550:ASP:O	1:A:554:LYS:HG2	1.93	0.68
1:A:658:ASN:HD22	1:A:661:HIS:H	1.41	0.67
1:B:472:ILE:HG22	1:B:538:TYR:HE2	1.61	0.66
1:A:675:LEU:O	1:A:678:VAL:HG22	1.96	0.65
1:B:704:LYS:C	1:B:706:LEU:H	2.00	0.64
1:B:563:HIS:O	1:B:595:HIS:CD2	2.51	0.64
1:B:602:ILE:HA	1:B:605:LEU:HD12	1.81	0.63
1:B:765:VAL:HG22	1:B:770:GLU:HB3	1.81	0.62
1:A:486:TRP:CZ3	1:A:528:LYS:HB2	2.34	0.62
1:B:468:LEU:O	1:B:471:GLU:N	2.31	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:PHE:O	1:A:494:VAL:HG23	2.00	0.61
1:B:523:PRO:HD2	1:B:695:GLU:HG3	1.82	0.60
1:A:577:LYS:O	1:A:578:PHE:HB3	2.02	0.60
1:B:655:ASN:H	1:B:661:HIS:CD2	2.16	0.60
1:A:578:PHE:CE1	1:A:706:LEU:HD12	2.37	0.59
1:A:761:GLN:O	1:A:765:VAL:HG23	2.03	0.59
1:A:658:ASN:ND2	1:A:661:HIS:H	1.99	0.59
1:B:646:GLU:HA	1:B:646:GLU:OE1	2.03	0.58
1:B:521:ARG:HH11	1:B:521:ARG:HG3	1.67	0.58
1:B:676:CYS:O	1:B:679:THR:OG1	2.07	0.57
1:B:507:LYS:HG2	1:B:607:GLY:O	2.04	0.57
1:A:735:ILE:HG13	1:B:481:PRO:HB3	1.87	0.57
1:B:701:ASP:OD2	1:B:716:ARG:NH2	2.29	0.56
1:A:578:PHE:CG	1:A:578:PHE:O	2.58	0.56
1:B:490:PHE:CD1	1:B:561:LEU:HD13	2.40	0.56
1:B:504:GLU:HG3	1:B:504:GLU:O	2.04	0.56
1:B:702:GLU:O	1:B:706:LEU:HD13	2.07	0.55
1:A:640:GLY:O	1:A:643:LYS:HB3	2.06	0.55
1:A:589:SER:HB3	1:A:592:GLU:HB2	1.90	0.54
1:B:704:LYS:O	1:B:706:LEU:N	2.37	0.53
1:A:448:MET:HG3	1:A:601:SER:HB3	1.89	0.53
1:B:675:LEU:O	1:B:678:VAL:HG22	2.08	0.53
1:B:486:TRP:CH2	1:B:528:LYS:HG3	2.43	0.53
1:B:503:PHE:CE1	1:B:554:LYS:HE2	2.44	0.53
1:B:655:ASN:N	1:B:661:HIS:HD2	2.05	0.52
1:A:578:PHE:O	1:A:578:PHE:CD1	2.62	0.52
1:B:727:LEU:HD13	1:B:766:ILE:HD12	1.91	0.52
1:A:591:MET:O	1:A:595:HIS:CD2	2.63	0.52
1:B:457:GLN:O	1:B:461:GLN:HG3	2.11	0.51
1:B:709:GLN:HE21	1:B:709:GLN:HA	1.76	0.51
1:B:483:GLU:HA	1:B:486:TRP:CE2	2.46	0.50
1:A:515:VAL:HG12	1:A:527:TRP:HZ3	1.76	0.50
1:B:472:ILE:HG22	1:B:538:TYR:CE2	2.45	0.50
1:A:578:PHE:HA	1:A:579:ASP:HB2	1.94	0.49
1:A:595:HIS:O	1:A:598:GLN:HB2	2.12	0.49
1:B:476:HIS:O	1:B:477:PHE:C	2.51	0.49
1:A:730:TYR:HA	1:A:734:ALA:HB3	1.95	0.49
1:B:548:PHE:O	1:B:553:ARG:NH1	2.46	0.49
1:B:688:THR:HG22	1:B:692:ILE:CD1	2.42	0.49
1:A:535:HIS:C	1:A:535:HIS:ND1	2.65	0.49
1:A:567:HIS:HA	1:A:591:MET:CE	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:ARG:HG3	1:B:521:ARG:NH1	2.28	0.48
1:A:541:LEU:HD13	1:A:553:ARG:HG2	1.95	0.48
1:B:735:ILE:N	1:B:736:PRO:HD2	2.27	0.48
1:B:511:PHE:O	1:B:515:VAL:HG23	2.13	0.48
1:A:514:SER:O	1:A:517:LYS:HB2	2.14	0.48
1:B:486:TRP:HB2	1:B:487:PRO:HD3	1.96	0.48
1:A:464:LEU:HD12	1:A:465:PRO:HD2	1.96	0.47
1:B:704:LYS:C	1:B:706:LEU:N	2.67	0.47
1:B:580:HIS:CG	1:B:581:PRO:HD2	2.50	0.47
1:B:700:GLY:HA3	1:B:714:MET:O	2.13	0.47
1:A:472:ILE:HD11	1:A:489:ILE:HG23	1.95	0.47
1:B:524:TYR:CE1	1:B:692:ILE:HD11	2.49	0.47
1:B:645:LEU:HD11	1:B:664:ARG:O	2.15	0.46
1:B:735:ILE:N	1:B:736:PRO:CD	2.78	0.46
1:A:486:TRP:CH2	1:A:528:LYS:HB2	2.50	0.46
1:A:729:PHE:CE2	4:A:803:P98:H11	2.51	0.46
1:A:569:GLY:HA2	1:A:695:GLU:OE2	2.16	0.45
1:B:746:PRO:HD2	1:B:747:PRO:HD3	1.97	0.45
1:B:568:ARG:NH1	1:B:582:LEU:HD11	2.32	0.45
1:B:726:GLN:HG3	1:B:762:TRP:CZ2	2.52	0.45
1:A:719:LYS:O	1:A:722:VAL:HG23	2.17	0.45
1:B:453:SER:O	1:B:457:GLN:HB2	2.17	0.45
1:B:750:PRO:HA	1:B:753:LYS:HB2	1.98	0.44
1:A:655:ASN:ND2	1:A:657:ASN:H	2.16	0.44
1:A:656:LEU:HD22	1:A:656:LEU:N	2.31	0.44
1:B:603:LEU:HD23	1:B:603:LEU:HA	1.90	0.44
1:B:763:GLU:HB3	1:B:767:ARG:HH12	1.82	0.44
1:B:508:LEU:O	1:B:512:ILE:HG13	2.18	0.44
1:B:592:GLU:OE1	1:B:634:ASP:HB2	2.16	0.44
1:A:515:VAL:HG12	1:A:527:TRP:CZ3	2.52	0.44
1:B:502:CYS:SG	1:B:554:LYS:HE3	2.58	0.44
1:A:709:GLN:HE21	1:A:710:PRO:HD2	1.83	0.43
1:A:483:GLU:HA	1:A:486:TRP:CE2	2.52	0.43
1:A:577:LYS:O	1:A:578:PHE:HD2	2.01	0.43
1:A:611:PHE:HB3	1:A:614:LEU:HD12	2.01	0.43
1:B:641:ASN:HD21	1:B:664:ARG:HB3	1.84	0.43
1:A:535:HIS:ND1	1:A:535:HIS:O	2.51	0.43
1:B:687:LEU:HD23	1:B:687:LEU:HA	1.89	0.42
1:A:578:PHE:HA	1:A:579:ASP:CB	2.49	0.42
1:A:656:LEU:HD22	1:A:656:LEU:H	1.83	0.42
1:A:682:TRP:HB3	1:A:683:PRO:HD3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:ASP:HA	5:B:903:HOH:O	2.19	0.42
1:A:504:GLU:H	1:A:504:GLU:HG2	1.48	0.42
1:A:659:GLN:O	1:A:662:ARG:HB2	2.19	0.42
1:B:556:LEU:HD23	1:B:556:LEU:HA	1.82	0.42
1:B:578:PHE:CZ	1:B:703:MET:HG2	2.54	0.42
1:A:723:PRO:HB2	1:A:766:ILE:HG13	2.01	0.42
1:B:515:VAL:HG13	1:B:565:LEU:HD21	2.00	0.42
1:A:735:ILE:HD13	1:A:735:ILE:HA	1.96	0.41
1:A:535:HIS:O	1:A:535:HIS:CG	2.72	0.41
1:A:714:MET:H	1:A:714:MET:HG2	1.50	0.41
1:B:580:HIS:CD2	1:B:581:PRO:HD2	2.56	0.41
1:A:561:LEU:HD12	1:A:561:LEU:HA	1.97	0.41
1:B:456:TRP:HZ3	1:B:460:MET:SD	2.43	0.41
1:B:459:LEU:HD11	1:B:488:GLY:HA2	2.03	0.40
1:A:512:ILE:O	1:A:515:VAL:HB	2.21	0.40
1:B:541:LEU:HD22	1:B:553:ARG:HG2	2.03	0.40
1:B:742:THR:O	1:B:742:THR:HG22	2.21	0.40
1:A:492:TYR:CD2	1:A:492:TYR:C	2.95	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	322/345 (93%)	284 (88%)	35 (11%)	3 (1%)	17 14
1	B	322/345 (93%)	291 (90%)	27 (8%)	4 (1%)	13 9
All	All	644/690 (93%)	575 (89%)	62 (10%)	7 (1%)	14 10

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	578	PHE
1	A	577	LYS
1	B	505	LEU
1	B	705	LYS
1	B	717	ASP
1	A	686	LYS
1	B	579	ASP

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	293/308 (95%)	264 (90%)	29 (10%)	8	5
1	B	293/308 (95%)	276 (94%)	17 (6%)	20	20
All	All	586/616 (95%)	540 (92%)	46 (8%)	12	11

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	447	HIS
1	A	467	ARG
1	A	492	TYR
1	A	500	THR
1	A	504	GLU
1	A	517	LYS
1	A	585	LEU
1	A	586	TYR
1	A	588	THR
1	A	600	VAL
1	A	605	LEU
1	A	606	GLU
1	A	612	SER
1	A	622	VAL
1	A	634	ASP
1	A	637	LEU
1	A	638	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	650	GLN
1	A	655	ASN
1	A	656	LEU
1	A	658	ASN
1	A	714	MET
1	A	716	ARG
1	A	720	ASP
1	A	736	PRO
1	A	743	GLN
1	A	749	GLU
1	A	769	GLU
1	A	770	GLU
1	B	450	ILE
1	B	457	GLN
1	B	484	ASN
1	B	502	CYS
1	B	547	LEU
1	B	563	HIS
1	B	579	ASP
1	B	617	SER
1	B	621	GLN
1	B	622	VAL
1	B	635	LEU
1	B	638	TYR
1	B	642	ARG
1	B	656	LEU
1	B	658	ASN
1	B	661	HIS
1	B	709	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	641	ASN
1	A	655	ASN
1	A	658	ASN
1	A	690	ASN
1	A	709	GLN
1	A	724	GLN
1	B	461	GLN
1	B	484	ASN
1	B	495	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	641	ASN
1	B	650	GLN
1	B	655	ASN
1	B	658	ASN
1	B	661	HIS
1	B	690	ASN
1	B	709	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 monosaccharides 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	P98	A	803	-	34,34,34	1.27	2 (5%)	44,48,48	1.58	8 (18%)
4	P98	B	803	-	34,34,34	1.31	3 (8%)	44,48,48	1.39	5 (11%)

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	P98	A	803	-	-	1/13/13/13	0/5/5/5
4	P98	B	803	-	-	1/13/13/13	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	803	P98	C22-N19	-4.74	1.39	1.45
4	A	803	P98	C22-N19	-4.18	1.40	1.45
4	A	803	P98	C18-N19	-2.49	1.35	1.39
4	B	803	P98	C11-C12	-2.12	1.38	1.42
4	B	803	P98	C4-C17	-2.01	1.38	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803	P98	C3-C18-C17	5.09	125.58	120.54
4	B	803	P98	C3-C18-C17	4.64	125.13	120.54
4	A	803	P98	C1-C4-C17	-4.28	115.46	120.84
4	B	803	P98	C1-C4-C17	-3.18	116.84	120.84
4	A	803	P98	C16-C11-C12	2.95	122.61	118.45
4	A	803	P98	C6-O5-C2	-2.68	111.02	117.65
4	A	803	P98	C4-C1-C2	2.29	123.24	120.17
4	A	803	P98	C2-C3-C18	-2.27	113.49	118.10
4	B	803	P98	C6-O5-C2	-2.27	112.04	117.65
4	A	803	P98	C9-C11-C16	-2.23	117.98	123.19
4	B	803	P98	C4-C1-C2	2.23	123.16	120.17
4	B	803	P98	C14-C13-C12	2.10	123.11	120.08
4	A	803	P98	C10-C9-C11	-2.07	117.61	120.82

There are no chirality outliers.

All (2) torsion outliers are listed below:

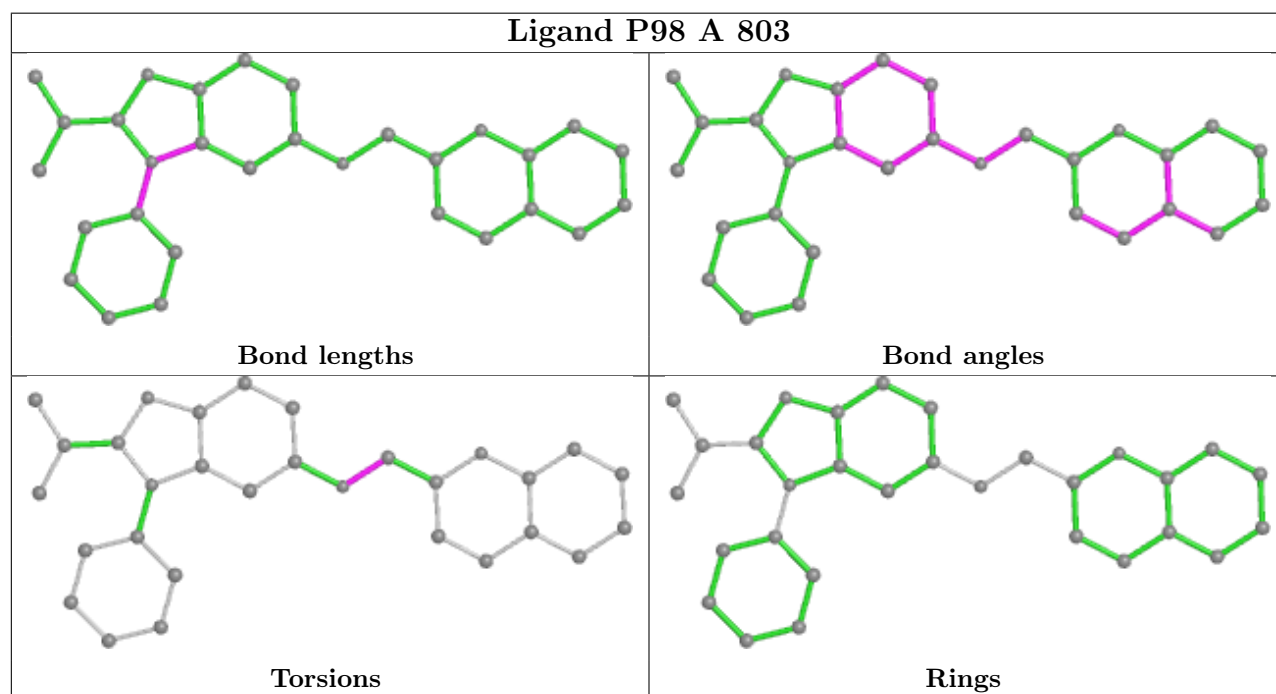
Mol	Chain	Res	Type	Atoms
4	B	803	P98	C7-C6-O5-C2
4	A	803	P98	C7-C6-O5-C2

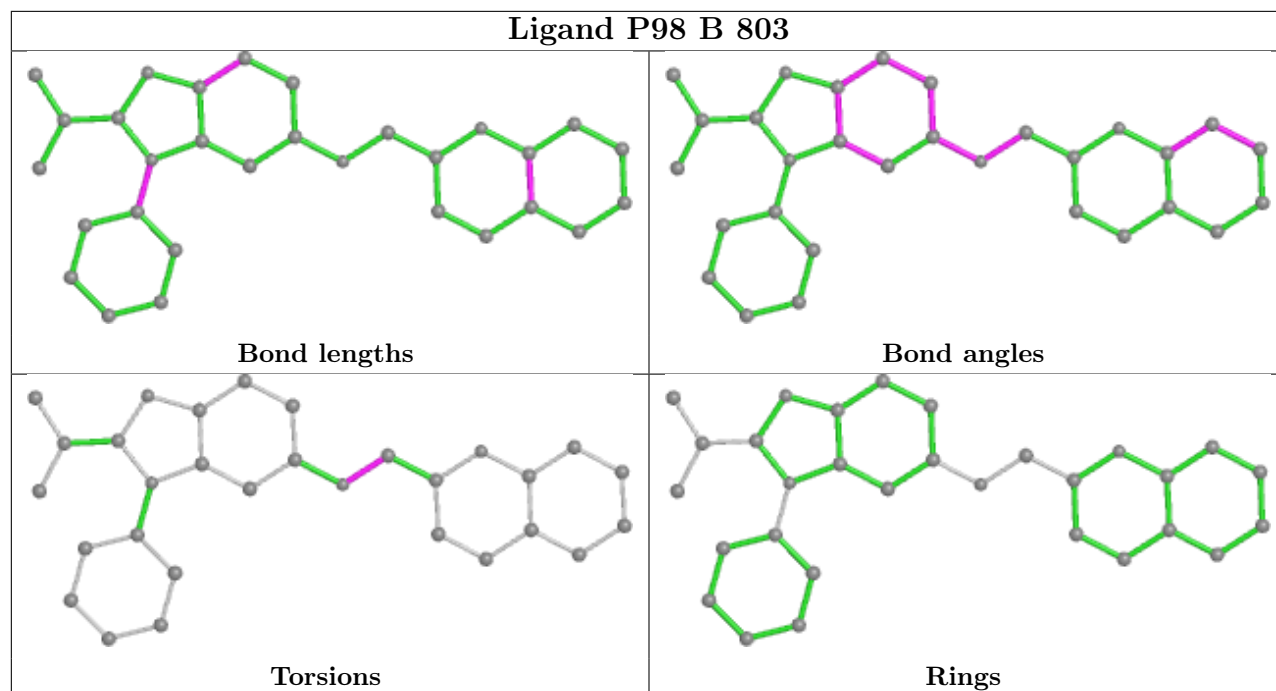
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	803	P98	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	324/345 (93%)	0.52	28 (8%) 10 11	26, 56, 84, 107	0
1	B	324/345 (93%)	0.36	15 (4%) 32 35	26, 52, 79, 97	0
All	All	648/690 (93%)	0.44	43 (6%) 18 20	26, 54, 82, 107	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	585	LEU	6.9
1	A	586	TYR	5.4
1	A	584	ALA	5.3
1	B	501	SER	4.3
1	A	578	PHE	3.5
1	A	587	SER	3.4
1	A	515	VAL	3.3
1	B	512	ILE	3.3
1	B	584	ALA	3.2
1	B	558	ILE	3.2
1	B	454	GLU	3.1
1	A	660	SER	3.0
1	A	456	TRP	2.9
1	A	768	GLY	2.9
1	B	511	PHE	2.9
1	A	653	SER	2.9
1	A	461	GLN	2.9
1	A	687	LEU	2.8
1	B	500	THR	2.8
1	A	447	HIS	2.7
1	A	605	LEU	2.6
1	A	606	GLU	2.6
1	B	462	PHE	2.6
1	A	672	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	577	LYS	2.5
1	A	450	ILE	2.5
1	A	769	GLU	2.4
1	A	452	THR	2.4
1	B	650	GLN	2.3
1	B	461	GLN	2.3
1	B	768	GLY	2.3
1	A	512	ILE	2.3
1	A	668	LEU	2.2
1	B	678	VAL	2.2
1	A	511	PHE	2.2
1	A	617	SER	2.2
1	B	463	THR	2.2
1	A	579	ASP	2.1
1	A	460	MET	2.1
1	B	707	GLY	2.1
1	A	565	LEU	2.0
1	B	687	LEU	2.0
1	A	537	MET	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 monosaccharides 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.

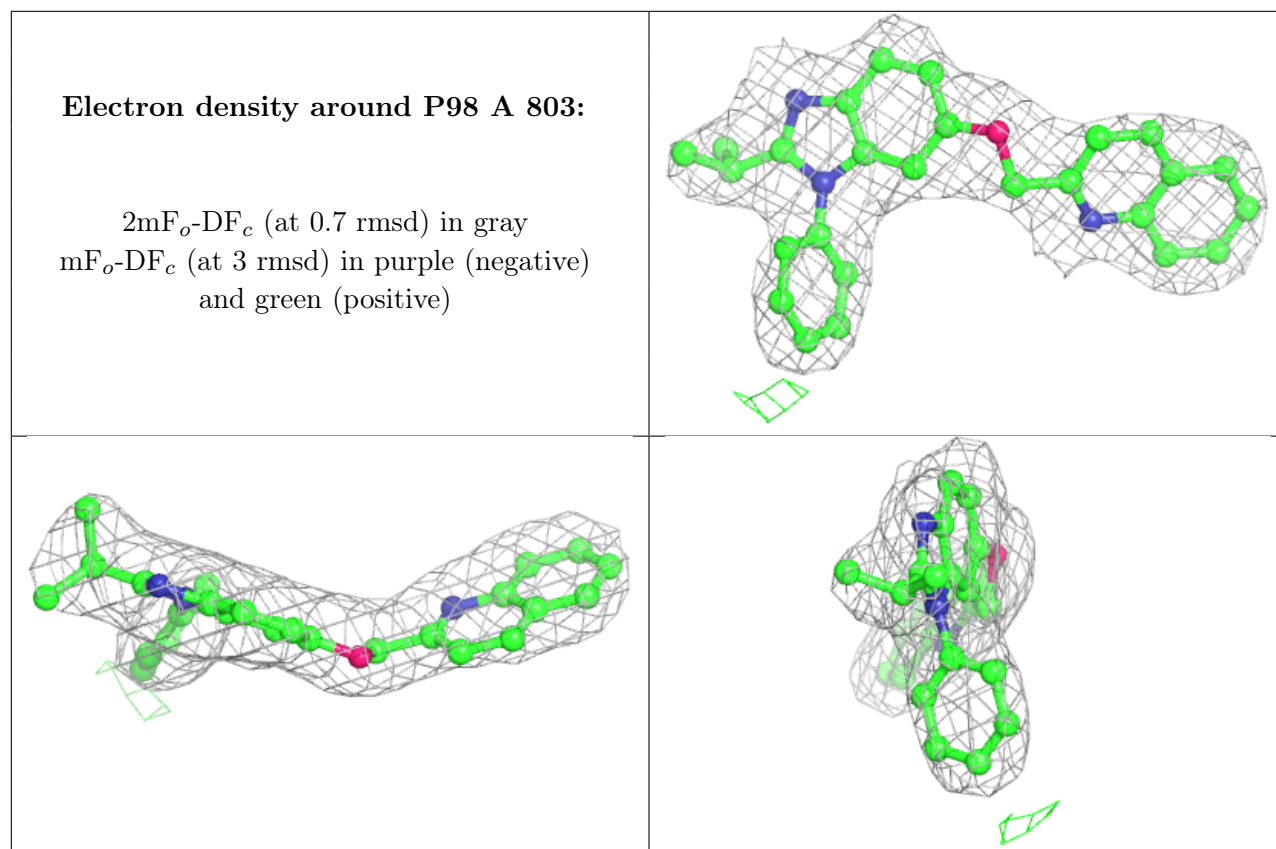
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	A	802	1/1	0.88	0.15	47,47,47,47	0
4	P98	A	803	30/30	0.92	0.13	36,45,54,56	0
4	P98	B	803	30/30	0.93	0.12	31,40,63,65	0
3	MG	B	802	1/1	0.96	0.14	35,35,35,35	0

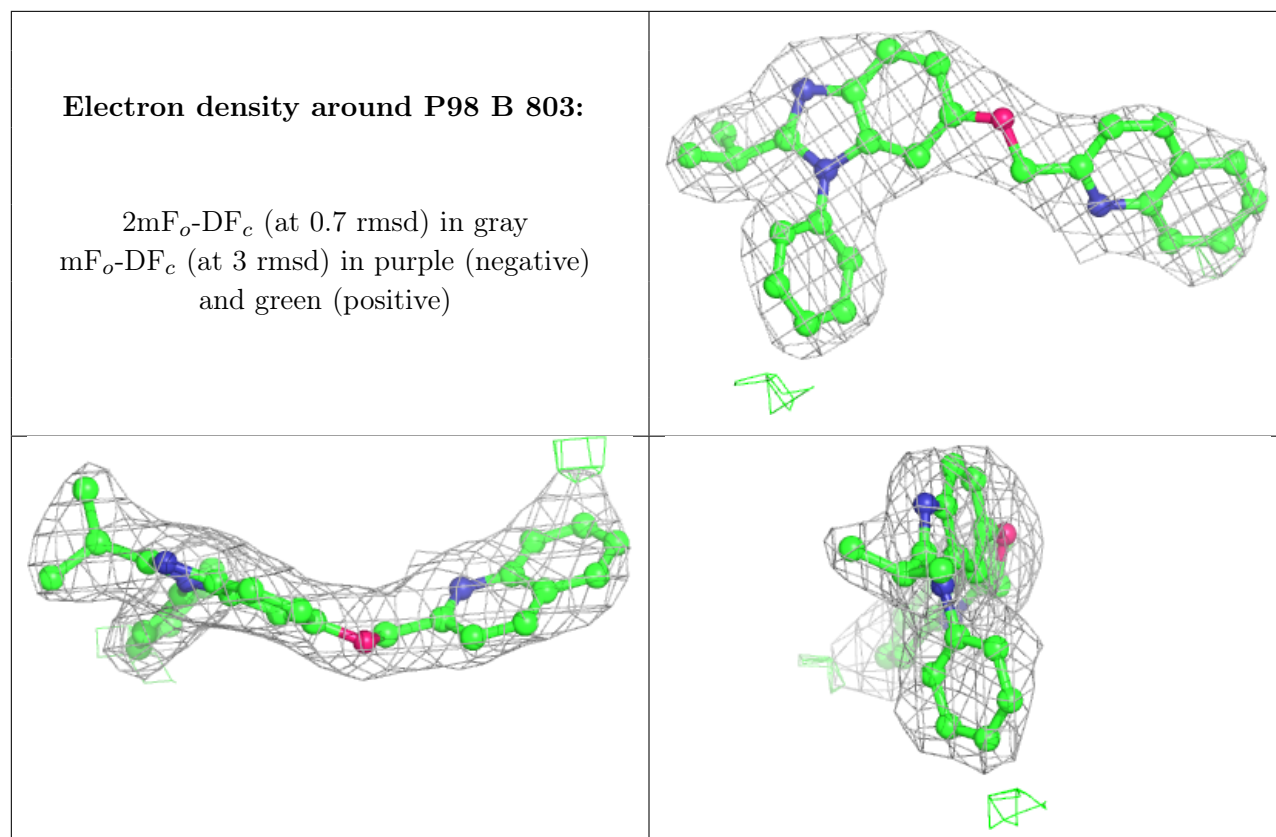
Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	B	801	1/1	0.97	0.05	35,35,35,35	0
2	ZN	A	801	1/1	0.99	0.06	56,56,56,56	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.