

Full wwPDB X-ray Structure Validation Report (i)

Oct 5, 2022 – 11:44 AM EDT

PDB ID : 5SGB

Title : Crystal Structure of human phosphodiesterase 10 in complex with 5-(4-chloro

naphthalen-1-yl)oxythiadiazole

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Deposited on : 2022-02-01

Resolution : 2.39 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 (i) 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 (1)) 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 : 2.31.2buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

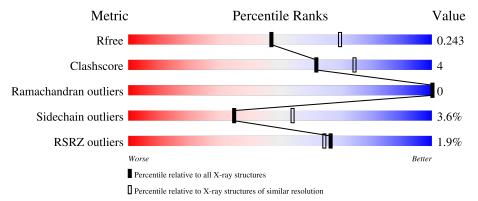
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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 $(\# \mathrm{Entries})$	Similar resolution $(\# \text{Entries, resolution range}(\text{\AA}))$
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	343	80%	10%	• 9%
1	В	343	80%	11%	• 8%
1	С	343	79%	12%	• 9%
1	D	343	79%	12%	10%



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10676 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		
1	٨	313	Total	С	N	О	S	0	0	0
1	A	313	2541	1624	432	461	24	0	0	
1	В	315	Total	С	N	О	S	0	0	0
1	Б	319	2551	1630	434	463	24	0	0	
1	C	212	Total	С	N	О	S	0	0	0
1		313	2541	1624	432	461	24	U	0	
1	D	310	Total	С	N	О	S	0	0	0
1	ש	310	2519	1612	429	454	24	U	U	

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	447	GLY	-	expression tag	UNP Q9Y233
A	448	SER	-	expression tag	UNP Q9Y233
В	447	GLY	-	expression tag	UNP Q9Y233
В	448	SER	-	expression tag	UNP Q9Y233
С	447	GLY	-	expression tag	UNP Q9Y233
С	448	SER	-	expression tag	UNP Q9Y233
D	447	GLY	-	expression tag	UNP Q9Y233
D	448	SER	-	expression tag	UNP Q9Y233

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

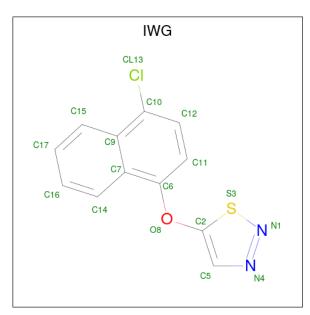
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	В	1	Total Zn 1 1	0	0
2	С	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0



• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

• Molecule 4 is 5-[(4-chloronaphthalen-1-yl)oxy]-1,2,3-thiadiazole (three-letter code: IWG) (formula: $C_{12}H_7ClN_2OS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	A	toms	ZeroOcc	AltConf		
4	Λ	1	Total C	Cl N	О	S	0	0
4	A	1	17 12	1 2	1	1	0	U
1	В	1	Total C	Cl N	О	S	0	0
4	Б	1	17 12	1 2	1	1	0	0
4	C	1	Total C	Cl N	О	S	0	0
4		1	17 12	1 2	1	1	0	0
1	D	1	Total C	Cl N	О	S	0	0
4	ע	1	17 12	1 2	1	1		

• Molecule 5 is water.



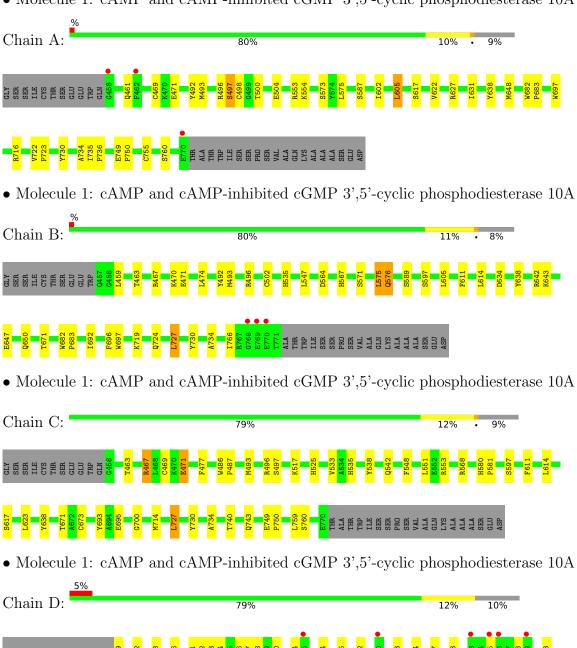
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	122	Total O 122 122	0	0
5	В	136	Total O 136 136	0	0
5	С	132	Total O 132 132	0	0
5	D	58	Total O 58 58	0	0

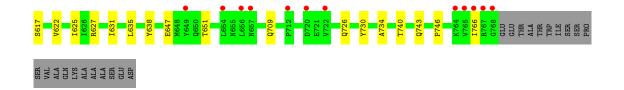


3 Residue-property plots (i)

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







4 Data and refinement statistics (i)

Property	Value	Source
Space group	Н 3	Depositor
Cell constants	135.10Å 135.10Å 234.26Å	Denogitor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.49 - 2.39	Depositor
Resolution (A)	43.49 - 2.39	EDS
% Data completeness	95.5 (43.49-2.39)	Depositor
(in resolution range)	95.5 (43.49-2.39)	EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.32 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
P.P.	0.179 , 0.242	Depositor
R, R_{free}	0.186 , 0.243	DCC
R_{free} test set	3108 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.33, 37.5	EDS
L-test for twinning ²	$< L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.032 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10676	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.81% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: CME, IWG, 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).

Mal	Mol Chain		lengths	Bond angles		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.68	0/2592	0.79	0/3507	
1	В	0.68	0/2602	0.83	0/3521	
1	С	0.68	0/2592	0.81	1/3507~(0.0%)	
1	D	0.71	0/2570	0.79	0/3478	
All	All	0.69	0/10356	0.80	1/14013 (0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Atoms Z		$\operatorname{Ideal}({}^{o})$
1	С	467	ARG	NE-CZ-NH1	5.65	123.13	120.30

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	2541	0	2511	21	0
1	В	2551	0	2515	21	0
1	С	2541	0	2511	27	0
1	D	2519	0	2496	22	0
2	A	1	0	0	0	0
2	В	1	0	0	0	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	С	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	В	1	0	0	0	0
3	С	1	0	0	0	0
3	D	1	0	0	0	0
4	A	17	0	0	0	0
4	В	17	0	0	0	0
4	С	17	0	0	0	0
4	D	17	0	0	1	0
5	A	122	0	0	3	0
5	В	136	0	0	4	0
5	С	132	0	0	4	0
5	D	58	0	0	0	0
All	All	10676	0	10033	90	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 4.

All (90) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance } (\text{\AA}) \end{array}$	Clash overlap (Å)
1:C:553:ARG:NH1	5:C:901:HOH:O	2.11	0.83
1:D:493:MET:O	1:D:497:SER:HB2	1.82	0.78
1:A:602:ILE:HA	1:A:605:LEU:HD22	1.69	0.73
1:A:493:MET:O	1:A:497:SER:HB2	1.91	0.71
1:C:497:SER:HA	1:C:542:GLN:HE22	1.56	0.70
1:A:469:CYS:SG	5:A:1017:HOH:O	2.52	0.68
1:C:469:CYS:SG	5:C:1021:HOH:O	2.51	0.68
1:C:693:TYR:OH	5:C:902:HOH:O	2.11	0.65
1:A:461:GLN:NE2	1:A:461:GLN:HA	2.16	0.61
1:B:727:LEU:HD12	1:B:766:ILE:CD1	2.30	0.61
1:B:724:GLN:NE2	5:B:902:HOH:O	2.28	0.59
1:A:461:GLN:HE22	1:A:500:THR:CG2	2.17	0.58
1:D:766:ILE:HG22	1:D:766:ILE:O	2.04	0.57
1:A:722:VAL:HB	1:A:723:PRO:HD3	1.86	0.57
1:B:470:LYS:HE2	1:D:746:PRO:HG3	1.86	0.57
1:B:576:GLN:HB2	5:B:1006:HOH:O	2.05	0.56
1:C:497:SER:HA	1:C:542:GLN:NE2	2.20	0.56
1:A:469:CYS:SG	5:A:1006:HOH:O	2.58	0.56
1:D:726:GLN:HE22	4:D:803:IWG:C15	2.20	0.55



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Continued from prev		Interatomic	Clash	
Atom-1	Atom-2	${\rm distance}\ (\mathring{\rm A})$	overlap (Å)	
1:A:461:GLN:HE22	1:A:500:THR:HG21	1.73	0.53	
1:C:493:MET:SD	1:C:535:HIS:HA	2.48	0.52	
1:A:492:TYR:CZ	1:A:496:ARG:HD2	2.45	0.52	
1:A:749:GLU:N	1:A:750:PRO:CD	2.72	0.52	
1:C:525:HIS:ND1	1:C:695:GLU:OE1	2.34	0.52	
1:A:648:MET:HE1	5:A:1014:HOH:O	2.10	0.52	
1:C:611:PHE:HB3	1:C:614:LEU:HD22	1.92	0.51	
1:D:497:SER:HA	1:D:542:GLN:NE2	2.26	0.51	
1:C:467:ARG:O	1:C:471:GLU:HB2	2.11	0.50	
1:A:461:GLN:NE2	1:A:500:THR:HG21	2.26	0.50	
1:C:700:GLY:HA3	1:C:714:MET:O	2.12	0.49	
1:D:627:ARG:O	1:D:631:ILE:HG12	2.13	0.49	
1:A:461:GLN:HA	1:A:461:GLN:HE21	1.77	0.49	
1:D:514:SER:HG	1:D:608:HIS:CD2	2.28	0.48	
1:B:727:LEU:HD12	1:B:766:ILE:HD13	1.96	0.48	
1:C:740:THR:HA	1:C:743:GLN:NE2	2.29	0.48	
1:B:643:LYS:HE3	1:B:647:GLU:OE2	2.14	0.48	
1:A:498:CYS:SG	1:A:554:LYS:HG3	2.54	0.47	
1:B:697:TRP:CZ2	1:B:719:LYS:HG2	2.49	0.47	
1:B:492:TYR:OH	5:B:901:HOH:O	2.20	0.47	
1:D:493:MET:SD	1:D:535:HIS:HA	2.55	0.47	
1:A:730:TYR:HA	1:A:734:ALA:HB3	1.97	0.46	
1:D:766:ILE:O	1:D:766:ILE:CG2	2.62	0.46	
1:A:735:ILE:HB	1:A:736:PRO:HD3	1.97	0.46	
1:B:589:SER:OG	1:B:634:ASP:OD2	2.25	0.46	
1:B:730:TYR:HA	1:B:734:ALA:HB3	1.97	0.46	
1:A:735:ILE:HD13	1:A:755:CYS:SG	2.56	0.45	
1:D:730:TYR:HA	1:D:734:ALA:HB3	1.98	0.45	
1:B:611:PHE:HB3	1:B:614:LEU:HD22	1.99	0.45	
1:C:535:HIS:O	1:C:538:TYR:HB3	2.17	0.45	
1:B:467:ARG:O	1:B:471:GLU:HB2	2.16	0.45	
1:B:692:ILE:HG22	1:B:696:PHE:CE2	2.52	0.45	
1:D:497:SER:O	1:D:553:ARG:HD2	2.16	0.45	
1:A:697:TRP:HB3	1:A:716:ARG:HB3	1.98	0.44	
1:A:627:ARG:O	1:A:631:ILE:HG12	2.17	0.44	
1:B:642:ARG:NH2	5:B:907:HOH:O	2.49	0.44	
1:C:749:GLU:HG3	5:C:1006:HOH:O	2.17	0.44	
1:D:493:MET:O	1:D:497:SER:CB	2.60	0.44	
1:C:740:THR:HA	1:C:743:GLN:HE21	1.82	0.44	
1:D:647:GLU:O	1:D:651:THR:HG23	2.19	0.43	
1:C:497:SER:O	1:C:553:ARG:CD	2.66	0.43	



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A J		Interatomic	Clash	
Atom-1	Atom-2	${\rm distance}({\rm \AA})$	overlap (Å)	
1:D:740:THR:O	1:D:743:GLN:HB2	2.19	0.43	
1:D:494:VAL:O	1:D:498:CYS:HB3	2.18	0.43	
1:B:682:TRP:HB3	1:B:683:PRO:HD3	2.01	0.43	
1:D:483:GLU:HA	1:D:486:TRP:CD2	2.54	0.43	
1:D:564:ASP:O	1:D:567:HIS:HB2	2.18	0.43	
1:D:622:VAL:HA	1:D:625:ILE:HD12	2.01	0.42	
1:B:564:ASP:O	1:B:567:HIS:HB2	2.19	0.42	
1:B:638:TYR:CD1	1:B:671:THR:HG21	2.54	0.42	
1:C:497:SER:O	1:C:553:ARG:HD2	2.18	0.42	
1:C:548:PHE:O	1:C:553:ARG:NH2	2.48	0.42	
1:D:514:SER:OG	1:D:608:HIS:NE2	2.46	0.42	
1:D:492:TYR:CZ	1:D:496:ARG:HD2	2.54	0.42	
1:C:551:LEU:HD23	1:C:551:LEU:HA	1.90	0.41	
1:D:462:PHE:CE1	1:D:491:VAL:HG11	2.56	0.41	
1:D:635:LEU:HD12	1:D:635:LEU:HA	1.93	0.41	
1:C:638:TYR:CD1	1:C:671:THR:HG21	2.56	0.41	
1:C:727:LEU:HD23	1:C:759:LEU:HD11	2.02	0.41	
1:C:749:GLU:N	1:C:750:PRO:CD	2.84	0.41	
1:B:493:MET:SD	1:B:535:HIS:HA	2.60	0.41	
1:C:533:VAL:HG13	1:C:673:CYS:HB3	2.03	0.41	
1:C:727:LEU:HD23	1:C:759:LEU:CD1	2.51	0.41	
1:B:571:SER:O	1:B:575:LEU:HD23	2.20	0.41	
1:C:486:TRP:N	1:C:487:PRO:CD	2.84	0.41	
1:A:682:TRP:N	1:A:683:PRO:CD	2.84	0.40	
1:B:492:TYR:CZ	1:B:496:ARG:HD2	2.56	0.40	
1:C:477:PHE:HB3	1:C:535:HIS:CE1	2.56	0.40	
1:C:580:HIS:CG	1:C:581:PRO:HD2	2.55	0.40	
1:C:730:TYR:HA	1:C:734:ALA:HB3	2.03	0.40	
1:B:471:GLU:HA	1:B:474:LEU:HD12	2.03	0.40	
1:A:497:SER:O	1:A:553:ARG:HD2	2.22	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 r	number of	residues for	which	the	backbone	conformation	was
analysed, and the total number of	residues.						

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	A	310/343 (90%)	300 (97%)	10 (3%)	0	100	100
1	В	312/343 (91%)	298 (96%)	14 (4%)	0	100	100
1	\mathbf{C}	310/343 (90%)	298 (96%)	12 (4%)	0	100	100
1	D	307/343 (90%)	292 (95%)	15 (5%)	0	100	100
All	All	1239/1372 (90%)	1188 (96%)	51 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric Outliers		Percentiles		
1	A	281/305~(92%)	270 (96%)	11 (4%)	32 50		
1	В	281/305~(92%)	271 (96%)	10 (4%)	35 54		
1	С	281/305 (92%)	271 (96%)	10 (4%)	35 54		
1	D	279/305~(92%)	270 (97%)	9 (3%)	39 59		
All	All	1122/1220 (92%)	1082 (96%)	40 (4%)	35 54		

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	471	GLU
1	A	497	SER
1	A	504	GLU
1	A	573	SER
1	A	575	LEU
1	A	587	SER
1	A	605	LEU
1	A	617	SER
1	A	622	VAL
1	A	638	TYR



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Mol	Chain	Res	Type
1	A	760	SER
1	В	459	LEU
1	В	463	THR
1	В	502	CYS
1	В	547	LEU
1	В	575	LEU
1	В	576	GLN
1	В	597	SER
1	В	605	LEU
1	В	650	GLN
1	В	727	LEU
1	С	463	THR
1	С	471	GLU
1	С	496	ARG
1	C C C C C C C	517	LYS
1	С	568	ARG
1	С	597	SER
1	С	617	SER
1	С	623	LEU
1	С	727	LEU
1	С	760	SER
1	D	459	LEU
1	D	500	THR
1	D	504	GLU
1	D	573	SER
1	D	605	LEU
1	D	613	THR
1	D	617	SER
1	D	638	TYR
1	D	709	GLN

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such side chains are listed below:

Mol	Chain	Res	Type
1	A	461	GLN
1	A	484	ASN
1	A	604	GLN
1	A	644	GLN
1	A	743	GLN
1	В	604	GLN
1	В	731	ASN
1	В	743	GLN



Continued from previous page...

Mol	Chain	Res	Type
1	С	542	GLN
1	С	604	GLN
1	С	724	GLN
1	С	743	GLN
1	D	484	ASN
1	D	542	GLN
1	D	604	GLN
1	D	621	GLN
1	D	644	GLN
1	D	726	GLN
1	D	731	ASN
1	D	743	GLN
1	D	761	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)

4 non-standard protein/DNA/RNA residues 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 Trun		Clasia	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Dan	T 2 1-	Bond lengths			Bond angles		
Mol Type	Type	Res		Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2											
1	CME	В	509	1	8,9,10	0.41	0	5,9,11	0.48	0											
1	CME	A	509	1	8,9,10	0.33	0	5,9,11	0.50	0											
1	CME	С	509	1	8,9,10	0.54	0	5,9,11	0.63	0											
1	CME	D	509	1	8,9,10	0.44	0	5,9,11	0.18	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
1	CME	В	509	1	-	1/5/8/10	-
1	CME	A	509	1	-	1/5/8/10	-
1	CME	С	509	1	-	2/5/8/10	_
1	CME	D	509	1	-	1/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	С	509	CME	CE-SD-SG-CB
1	A	509	CME	CZ-CE-SD-SG
1	С	509	CME	CZ-CE-SD-SG
1	D	509	CME	CZ-CE-SD-SG
1	В	509	CME	CZ-CE-SD-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 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	Chain	Chain	Res	Link	Bo	ond leng	$ ag{ths}$	В	ond ang	les
1	VIOI	туре	Chain	rtes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
	4	IWG	D	803	-	15,19,19	0.68	0	19,26,26	1.33	4 (21%)	
	4	IWG	A	803	-	15,19,19	1.15	1 (6%)	19,26,26	2.10	6 (31%)	



Mol	Trunc	Chain	in Res	es Link	Bo	Bond lengths			Bond angles		
IVIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2	
4	IWG	С	803	-	15,19,19	0.64	0	19,26,26	1.51	4 (21%)	
4	IWG	В	803	-	15,19,19	0.78	0	19,26,26	1.97	5 (26%)	

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	IWG	D	803	-	-	0/2/4/4	0/3/3/3
4	IWG	A	803	-	-	0/2/4/4	0/3/3/3
4	IWG	С	803	-	-	0/2/4/4	0/3/3/3
4	IWG	В	803	-	-	0/2/4/4	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\textup{\AA})$	$\operatorname{Ideal}(ext{\AA})$
4	A	803	IWG	O8-C2	-3.22	1.32	1.36

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
4	A	803	IWG	C9-C10-CL13	-4.68	110.63	119.21
4	В	803	IWG	C9-C10-CL13	-4.64	110.71	119.21
4	A	803	IWG	C15-C9-C10	-3.58	118.68	125.06
4	A	803	IWG	C15-C9-C7	3.44	122.72	118.45
4	В	803	IWG	C15-C9-C10	-3.30	119.18	125.06
4	В	803	IWG	C15-C9-C7	3.12	122.32	118.45
4	A	803	IWG	C12-C10-CL13	3.07	126.07	118.57
4	С	803	IWG	C15-C9-C10	-2.97	119.78	125.06
4	В	803	IWG	C12-C10-CL13	2.96	125.81	118.57
4	D	803	IWG	C15-C9-C10	-2.70	120.25	125.06
4	С	803	IWG	C9-C10-CL13	-2.69	114.28	119.21
4	В	803	IWG	C11-C12-C10	-2.68	117.64	120.89
4	D	803	IWG	C9-C10-CL13	-2.67	114.33	119.21
4	A	803	IWG	C17-C16-C14	2.60	124.08	120.44
4	D	803	IWG	C10-C9-C7	2.55	119.64	117.66
4	D	803	IWG	C12-C10-CL13	2.34	124.29	118.57
4	A	803	IWG	C14-C7-C9	-2.19	115.73	118.45
4	С	803	IWG	C15-C9-C7	2.15	121.12	118.45
4	С	803	IWG	C17-C15-C9	-2.05	118.06	120.89



There are no chirality outliers.

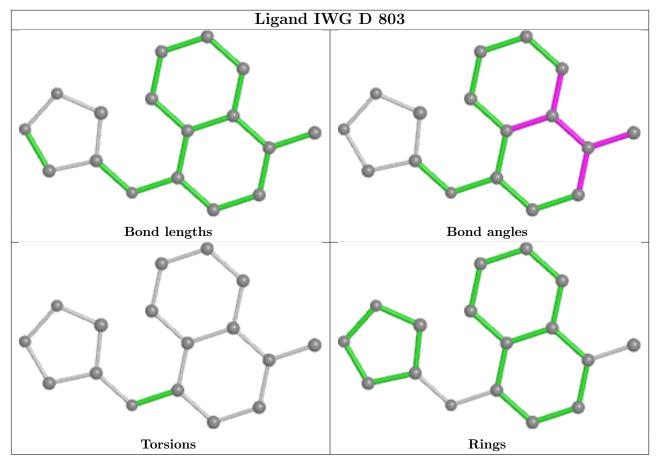
There are no torsion outliers.

There are no ring outliers.

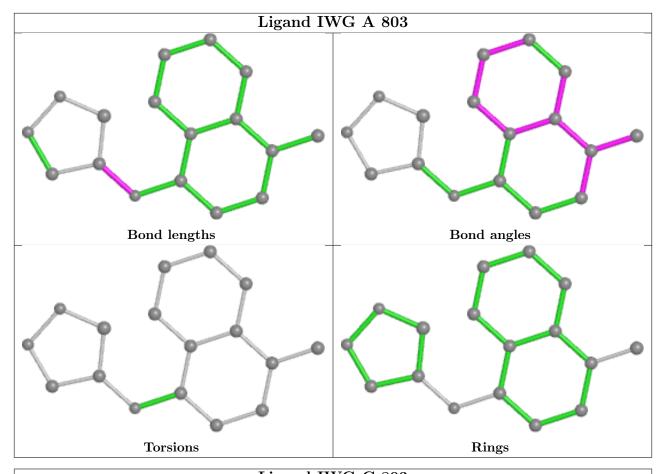
1 monomer is involved in 1 short contact:

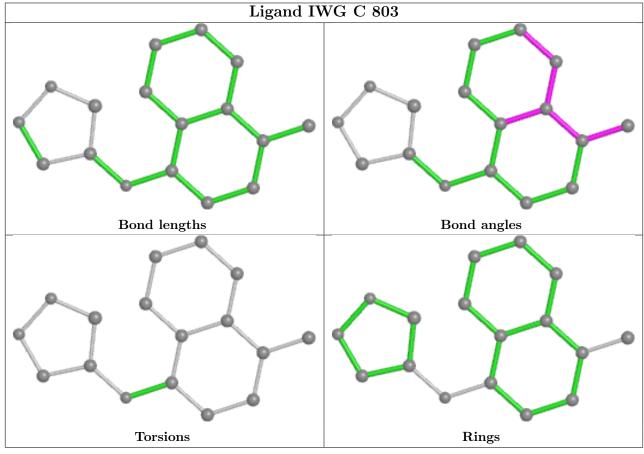
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	803	IWG	1	0

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 then 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.

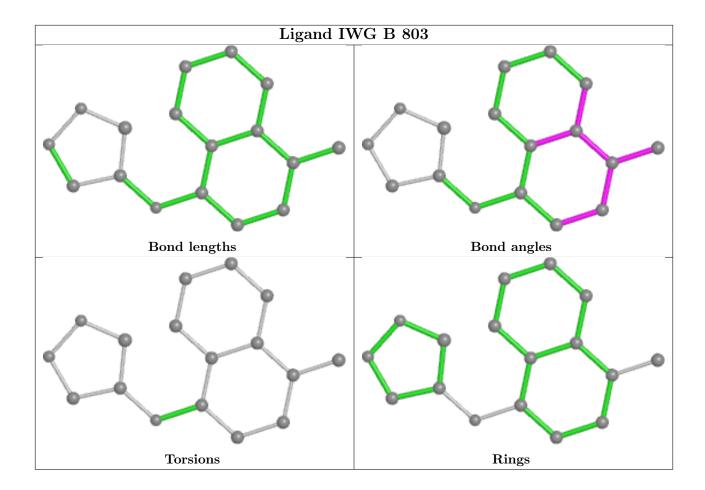












5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95^{th} 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	$OWAB(A^2)$	Q<0.9
1	A	312/343 (90%)	-0.14	3 (0%) 82 80	27, 42, 74, 103	0
1	В	314/343 (91%)	-0.02	3 (0%) 82 80	29, 42, 76, 116	0
1	С	312/343 (90%)	-0.28	0 100 100	28, 41, 68, 101	0
1	D	309/343 (90%)	0.15	18 (5%) 23 22	40, 58, 84, 104	0
All	All	1247/1372 (90%)	-0.07	24 (1%) 66 64	27, 46, 77, 116	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	765	VAL	4.2
1	A	458	GLY	3.9
1	D	657	ASN	3.9
1	В	769	GLU	3.8
1	В	768	GLY	3.4
1	D	603	LEU	3.3
1	D	720	ASP	3.2
1	В	770	GLU	3.0
1	D	767	ARG	2.9
1	D	609	ASN	2.9
1	D	764	LYS	2.8
1	D	768	GLY	2.6
1	D	605	LEU	2.5
1	D	505	LEU	2.4
1	D	550	ASP	2.4
1	A	770	GLU	2.3
1	D	654	LEU	2.3
1	D	712	PRO	2.2
1	D	722	VAL	2.1
1	D	649	TYR	2.1
1	D	766	ILE	2.1



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Mol	Chain	Res	Type	RSRZ
1	A	462	PHE	2.1
1	D	656	LEU	2.0
1	D	606	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	CME	D	509	10/11	0.93	0.20	59,77,105,105	0
1	CME	В	509	10/11	0.94	0.16	44,57,79,85	0
1	CME	С	509	10/11	0.94	0.14	45,53,100,101	0
1	CME	A	509	10/11	0.94	0.12	46,55,88,93	0

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, 95^{th} 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.

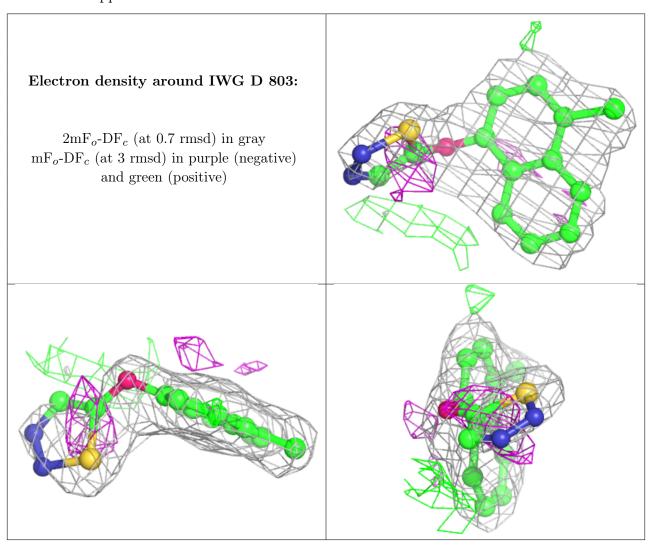
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
4	IWG	D	803	17/17	0.84	0.25	67,76,99,102	0
4	IWG	A	803	17/17	0.88	0.19	46,56,77,79	0
4	IWG	В	803	17/17	0.89	0.13	51,60,79,83	0
4	IWG	С	803	17/17	0.92	0.21	48,55,78,79	0
3	MG	В	802	1/1	0.96	0.15	24,24,24,24	0
3	MG	D	802	1/1	0.97	0.05	47,47,47,47	0
3	MG	С	802	1/1	0.98	0.08	27,27,27,27	0
2	ZN	D	801	1/1	0.99	0.07	46,46,46,46	0
3	MG	A	802	1/1	0.99	0.10	28,28,28,28	0
2	ZN	С	801	1/1	0.99	0.09	36,36,36,36	0
2	ZN	A	801	1/1	1.00	0.11	33,33,33,33	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	ZN	В	801	1/1	1.00	0.12	35,35,35,35	0

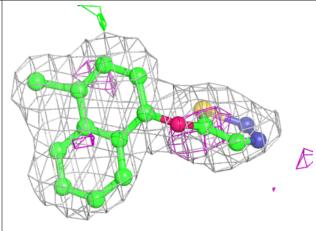
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

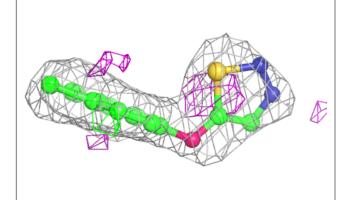


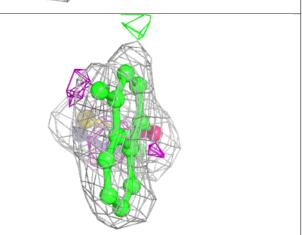


Electron density around IWG A 803:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

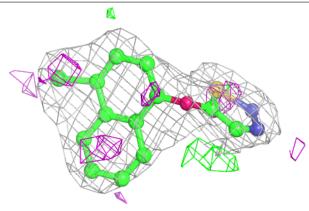


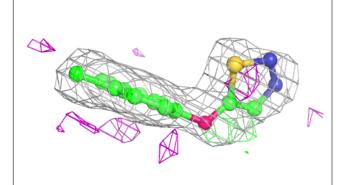


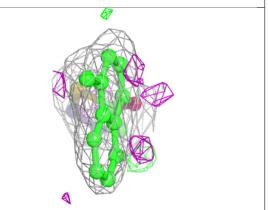


Electron density around IWG B 803:

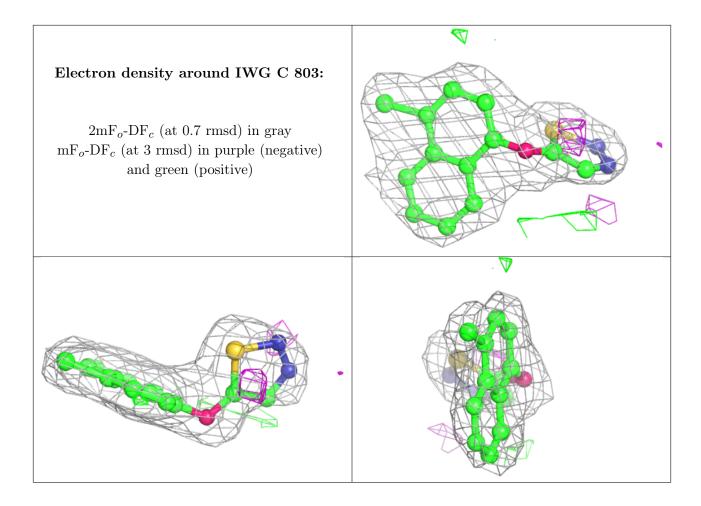
 $2 \text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray $\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)











6.5 Other polymers (i)

There are no such residues in this entry.

