

Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2021 – 03:19 AM EDT

PDB ID : 2D52

Title: Pentaketide chromone synthase (M207G mutant complexed with Coa)

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Deposited on : 2005-10-27

Resolution : 1.60 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.orgA user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp

with specific help available everywhere you see the (i) symbol.

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)

 $Xtriage\ (Phenix) \quad : \quad 1.13$

EDS: 2.23.2

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)

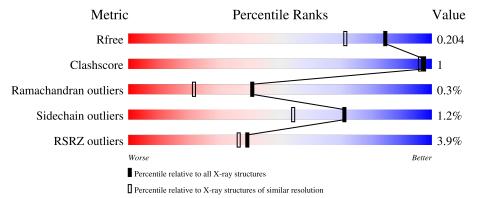
Validation Pipeline (wwPDB-VP) : 2.23.2

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 1.60 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{\rm A})}) \end{array}$
R_{free}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	406	96%				
1	В	406	93%	•	-		



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6887 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 pentaketide chromone synthase.

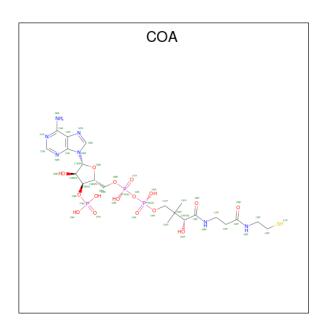
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	405	Total 3167	C 2014	N 535	O 593	S 25	0	6	0
1	В	395	Total 3079	C 1964	N 520	O 571	S 24	0	2	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP Q58VP7
A	2	PRO	-	cloning artifact	UNP Q58VP7
A	3	GLY	-	cloning artifact	UNP Q58VP7
A	177	CSD	CYS	modified residue	UNP Q58VP7
A	210	GLY	MET	engineered mutation	UNP Q58VP7
В	1	GLY	-	cloning artifact	UNP Q58VP7
В	2	PRO	-	cloning artifact	UNP Q58VP7
В	3	GLY	-	cloning artifact	UNP Q58VP7
В	177	CSD	CYS	modified residue	UNP Q58VP7
В	210	GLY	MET	engineered mutation	UNP Q58VP7

• Molecule 2 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
9	Λ	1	Total	С	N	О	Р	S	0	0
2	2 A	1	48	21	7	16	3	1	U	U
9	D	1	Total	С	N	О	Р	S	0	0
2	Б	1	48	21	7	16	3	1	0	U

• Molecule 3 is water.

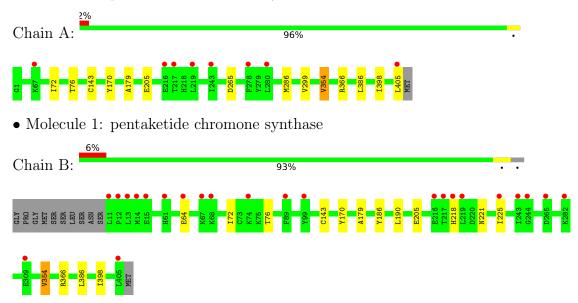
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	304	Total O 304 304	0	0
3	В	241	Total O 241 241	0	0



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: pentaketide chromone synthase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	74.07Å 89.17Å 70.77Å	Depositor
a, b, c, α , β , γ	90.00° 95.72° 90.00°	Depositor
Resolution (Å)	30.00 - 1.60	Depositor
resolution (A)	29.61 - 1.60	EDS
% Data completeness	(Not available) $(30.00-1.60)$	Depositor
(in resolution range)	100.0 (29.61-1.60)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.40 (at 1.60Å)	Xtriage
Refinement program	CNS 1.1	Depositor
D.D.	0.193 , 0.208	Depositor
R, R_{free}	0.188 , 0.204	DCC
R_{free} test set	6090 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	12.8	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.37 , 37.8	EDS
L-test for twinning ²	$< L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6887	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.90% 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: COA, CSD

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	0.59	0/3230	0.70	0/4379	
1	В	0.59	0/3141	0.70	0/4259	
All	All	0.59	0/6371	0.70	0/8638	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	В	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	170	TYR	Sidechain
1	В	170	TYR	Sidechain

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	3167	0	3162	4	0
1	В	3079	0	3080	6	0
2	A	48	0	31	0	0
2	В	48	0	31	0	0
3	A	304	0	0	0	0
3	В	241	0	0	0	0
All	All	6887	0	6304	10	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 1.

All (10) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:B:205:GLU:HG3	1:B:354:VAL:HB	1.85	0.57
1:B:143:CYS:SG	1:B:179:ALA:HB1	2.46	0.55
1:A:143:CYS:SG	1:A:179:ALA:HB1	2.49	0.53
1:A:205:GLU:HG3	1:A:354:VAL:HB	1.93	0.50
1:B:72:ILE:O	1:B:76:THR:HG23	2.18	0.43
1:A:386:LEU:HB3	1:A:398:ILE:HB	2.01	0.43
1:A:72:ILE:O	1:A:76:THR:HG23	2.18	0.43
1:B:386:LEU:HB3	1:B:398:ILE:HB	2.01	0.42
1:B:186:TYR:O	1:B:190:LEU:HG	2.18	0.42
1:B:221:ASN:O	1:B:225:ILE:HG12	2.20	0.42

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	408/406 (100%)	398 (98%)	9 (2%)	1 (0%)	47 26	
1	В	394/406 (97%)	387 (98%)	6 (2%)	1 (0%)	41 21	



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Mol	Chain	Analysed	Favoured Allowed		Outliers	Percentiles	
All	All	802/812 (99%)	785 (98%)	15 (2%)	2 (0%)	41	26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	354	VAL
1	В	354	VAL

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	343/338 (102%)	338 (98%)	5 (2%)	65 44		
1	В	331/338 (98%)	328 (99%)	3 (1%)	78 65		
All	All	674/676 (100%)	666 (99%)	8 (1%)	71 54		

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

Mol	Chain	Res	Type
1	A	265	ASP
1	A	286	MET
1	A	299	VAL
1	A	366	ARG
1	A	405	LEU
1	В	64	GLU
1	В	218	HIS
1	В	366	ARG

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

Mol	Chain	Res	Type
1	A	164	HIS
1	A	221	ASN
1	В	328	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)

2 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 Typ	Type	Chain	Res	Link	Bond lengths			В	ond ang	gles
IVIOI	Туре	Chain	nes	Lilik	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
1	CSD	В	177	1	3,7,8	0.76	0	1,8,10	0.89	0
1	CSD	A	177	1	3,7,8	0.69	0	1,8,10	0.38	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	CSD	В	177	1	-	1/2/6/8	-
1	CSD	A	177	1	-	1/2/6/8	ı

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	177	CSD	CA-CB-SG-OD1
1	В	177	CSD	CA-CB-SG-OD1

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)

2 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	Trunc	Chain	Res	Link	Bond lengths				Bond angles		
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
2	COA	В	501	-	41,50,50	2.95	18 (43%)	52,75,75	2.81	23 (44%)	
2	COA	A	500	-	41,50,50	2.97	18 (43%)	52,75,75	2.83	24 (46%)	

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	COA	В	501	-	-	7/44/64/64	0/3/3/3
2	COA	A	500	-	-	7/44/64/64	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
2	A	500	COA	O5P-C5P	-10.00	1.02	1.23
2	В	501	COA	O5P-C5P	-10.00	1.03	1.23
2	A	500	COA	C4A-N3A	6.09	1.44	1.35
2	В	501	COA	C4A-N3A	5.92	1.43	1.35
2	A	500	COA	P1A-O5B	-5.76	1.36	1.59
2	В	501	COA	P1A-O5B	-5.73	1.36	1.59
2	A	500	COA	C2B-C1B	-5.64	1.45	1.53
2	В	501	COA	C2B-C1B	-5.43	1.45	1.53
2	В	501	COA	O4B-C1B	4.83	1.47	1.41
2	A	500	COA	C2A-N1A	4.66	1.42	1.33



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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	$\operatorname{Ideal}(\text{\AA})$
2	A	500	COA	O4B-C1B	4.63	1.47	1.41
2	В	501	COA	C2A-N1A	4.55	1.42	1.33
2	В	501	COA	C7P-N8P	4.31	1.56	1.46
2	A	500	COA	C7P-N8P	4.10	1.55	1.46
2	A	500	COA	C3P-N4P	3.68	1.54	1.46
2	В	501	COA	C2A-N3A	3.61	1.37	1.32
2	A	500	COA	C2A-N3A	3.51	1.37	1.32
2	В	501	COA	O4B-C4B	3.39	1.52	1.45
2	A	500	COA	O4B-C4B	3.39	1.52	1.45
2	В	501	COA	P3B-O7A	3.20	1.60	1.50
2	A	500	COA	P3B-O7A	3.17	1.60	1.50
2	В	501	COA	C3P-N4P	3.08	1.53	1.46
2	В	501	COA	C5B-C4B	2.58	1.59	1.51
2	A	500	COA	C5B-C4B	2.46	1.59	1.51
2	A	500	COA	O2B-C2B	-2.40	1.37	1.43
2	В	501	COA	C3B-C4B	2.39	1.59	1.52
2	В	501	COA	O2B-C2B	-2.39	1.37	1.43
2	A	500	COA	C3B-C4B	2.33	1.59	1.52
2	В	501	COA	O9P-C9P	2.31	1.28	1.23
2	A	500	COA	O9P-C9P	2.19	1.27	1.23
2	В	501	COA	OAP-CAP	2.10	1.46	1.42
2	В	501	COA	O5B-C5B	2.09	1.52	1.44
2	A	500	COA	O5B-C5B	2.08	1.52	1.44
2	В	501	COA	O3B-C3B	2.08	1.51	1.44
2	A	500	COA	OAP-CAP	2.08	1.46	1.42
2	A	500	COA	O3B-C3B	2.01	1.51	1.44

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}(^{o})$
2	A	500	COA	O5P-C5P-C6P	-8.58	106.32	122.02
2	В	501	COA	O5P-C5P-C6P	-8.34	106.77	122.02
2	В	501	COA	C2B-C3B-C4B	6.76	115.20	103.22
2	A	500	COA	C2B-C3B-C4B	6.76	115.20	103.22
2	A	500	COA	O2B-C2B-C3B	5.77	127.55	111.17
2	В	501	COA	O5P-C5P-N4P	5.74	133.84	123.01
2	В	501	COA	O2B-C2B-C3B	5.73	127.45	111.17
2	A	500	COA	O5P-C5P-N4P	5.46	133.32	123.01
2	В	501	COA	O4B-C1B-C2B	5.00	114.23	106.93
2	A	500	COA	O4B-C1B-C2B	4.95	114.15	106.93
2	В	501	COA	C6P-C7P-N8P	-4.34	103.14	111.90
2	A	500	COA	N3A-C2A-N1A	-4.13	122.22	128.68



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\mathrm{Ideal}(^{o})$
2	В	501	COA	N3A-C2A-N1A	-4.08	122.30	128.68
2	A	500	COA	C6P-C7P-N8P	-3.99	103.84	111.90
2	В	501	COA	O4B-C4B-C3B	-3.80	96.72	104.87
2	A	500	COA	O4B-C4B-C3B	-3.76	96.80	104.87
2	A	500	COA	C7P-N8P-C9P	-3.62	116.14	122.59
2	A	500	COA	O2B-C2B-C1B	-3.55	97.75	110.85
2	В	501	COA	O2B-C2B-C1B	-3.48	98.00	110.85
2	В	501	COA	P1A-O5B-C5B	3.48	142.06	121.68
2	A	500	COA	C3P-N4P-C5P	-3.45	116.43	122.84
2	В	501	COA	C7P-N8P-C9P	-3.41	116.50	122.59
2	A	500	COA	P1A-O5B-C5B	3.40	141.59	121.68
2	A	500	COA	C2A-N1A-C6A	3.39	124.55	118.75
2	В	501	COA	C2A-N1A-C6A	3.35	124.49	118.75
2	В	501	COA	C3P-N4P-C5P	-3.31	116.69	122.84
2	A	500	COA	C4A-C5A-N7A	3.00	112.53	109.40
2	В	501	COA	CDP-CBP-CAP	2.96	113.96	108.82
2	В	501	COA	C4A-C5A-N7A	2.94	112.47	109.40
2	A	500	COA	CDP-CBP-CAP	2.83	113.73	108.82
2	В	501	COA	O3B-P3B-O7A	-2.76	98.75	109.39
2	A	500	COA	O3B-P3B-O7A	-2.64	99.20	109.39
2	A	500	COA	C2P-C3P-N4P	2.52	118.07	112.31
2	A	500	COA	C6P-C5P-N4P	2.34	120.36	116.42
2	В	501	COA	C5A-C6A-N1A	-2.24	115.28	120.35
2	В	501	COA	C3B-C2B-C1B	-2.23	94.95	99.89
2	A	500	COA	C5A-C6A-N1A	-2.23	115.30	120.35
2	В	501	COA	O9P-C9P-CAP	-2.23	114.27	121.06
2	A	500	COA	O9P-C9P-CAP	-2.22	114.29	121.06
2	A	500	COA	C3B-C2B-C1B	-2.22	94.98	99.89
2	В	501	COA	O6A-CCP-CBP	-2.19	107.03	110.55
2	A	500	COA	N6A-C6A-N1A	2.08	122.90	118.57
2	В	501	COA	O3B-C3B-C4B	-2.05	102.66	110.08
2	В	501	COA	N6A-C6A-N1A	2.03	122.79	118.57
2	В	501	COA	O6A-P2A-O4A	-2.03	101.13	109.07
2	A	500	COA	O6A-P2A-O4A	-2.01	101.20	109.07
2	A	500	COA	O6A-CCP-CBP	-2.00	107.33	110.55

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	COA	S1P-C2P-C3P-N4P
2	В	501	COA	C3B-O3B-P3B-O8A



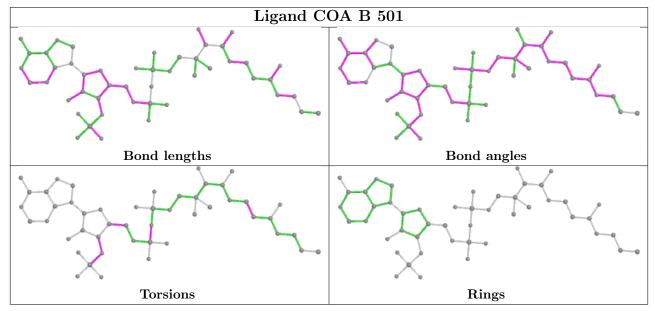
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Mol	Chain	Res	Type	Atoms
2	A	500	COA	C3B-C4B-C5B-O5B
2	В	501	COA	C3B-C4B-C5B-O5B
2	A	500	COA	C2B-C3B-O3B-P3B
2	В	501	COA	C2B-C3B-O3B-P3B
2	A	500	COA	O4B-C4B-C5B-O5B
2	В	501	COA	O4B-C4B-C5B-O5B
2	В	501	COA	P2A-O3A-P1A-O1A
2	A	500	COA	P2A-O3A-P1A-O1A
2	В	501	COA	P2A-O3A-P1A-O2A
2	В	501	COA	C5P-C6P-C7P-N8P
2	A	500	COA	P2A-O3A-P1A-O2A
2	A	500	COA	C4B-C3B-O3B-P3B

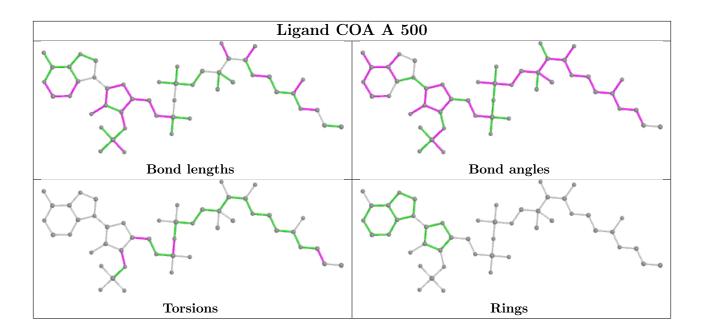
There are no ring outliers.

No monomer is involved in short contacts.

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	$\langle { m RSRZ} \rangle$	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q < 0.9
1	A	404/406 (99%)	0.09	8 (1%) 65 64	7, 12, 24, 34	0
1	В	394/406 (97%)	0.11	23 (5%) 23 20	6, 11, 27, 39	0
All	All	798/812 (98%)	0.10	31 (3%) 39 36	6, 12, 26, 39	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	217	THR	4.6
1	В	405	LEU	4.1
1	В	217	THR	3.9
1	В	11	LEU	3.7
1	В	13	LEU	3.6
1	В	15	GLU	3.5
1	В	14	MET	3.1
1	В	216	GLU	3.1
1	A	243	ILE	3.0
1	В	219	LEU	3.0
1	В	67	LYS	2.8
1	В	225	ILE	2.7
1	A	216	GLU	2.7
1	В	64	GLU	2.6
1	A	405	LEU	2.5
1	В	265	ASP	2.5
1	A	219	LEU	2.5
1	В	12	PRO	2.4
1	В	282	LYS	2.4
1	В	243	ILE	2.3
1	A	67	LYS	2.3
1	В	89	PHE	2.3
1	В	74	LYS	2.2
1	В	61	HIS	2.2



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Mol	Chain	Res	Type	RSRZ
1	A	278	PHE	2.1
1	В	244	GLY	2.1
1	В	309	GLU	2.1
1	В	99	TYR	2.1
1	A	280	LEU	2.1
1	В	68	LYS	2.0
1	В	218	HIS	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	CSD	A	177	8/9	0.96	0.12	9,10,13,16	0
1	CSD	В	177	8/9	0.97	0.09	9,10,12,16	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
2	COA	В	501	48/48	0.83	0.15	18,24,39,41	0
2	COA	A	500	48/48	0.87	0.13	17,22,34,35	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 COA B 501: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${ m mF}_o{ m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive) Electron density around COA A 500: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (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.

