

wwPDB X-ray Structure Validation Summary Report (i)

Aug 20, 2020 – 09:31 AM BST

PDB ID : 6TZV

Title: Crystal Structure of the carboxyltransferase subunit of ACC (AccD6) in com-

plex with inhibitor Phenyl-Cyclodiaone from Mycobacterium tuberculosis

Authors: Reddy, M.C.M.; Zhou, N.; Sacchettini, J.; TB Structural Genomics Consor-

tium (TBSGC)

 $Deposited \ on \quad : \quad 2019\text{-}08\text{-}13$

Resolution : 2.39 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 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 : 2.13

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)

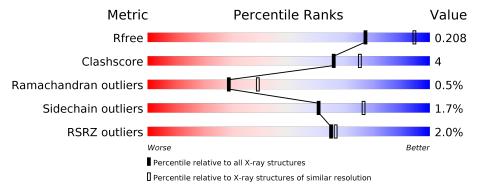
Validation Pipeline (wwPDB-VP) : 2.13

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.

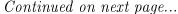
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\bf Similar \ resolution} \\ (\#{\bf Entries, \ resolution \ range(\AA)}) \end{array}$
R_{free}	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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 on 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	473	% • 84%	5% • 10%
1	В	473	82%	8% 10%
1	С	473	77%	9% • 13%
1	D	473	2% 	5% 10%
1	Е	473	% 	7% 10%
1	F	473	81%	8% 10%





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Mol	Chain	Length	Quality of chain						
1	G	473	78%	6 •	14%				
1	Н	473	84%	6%	10%				



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 26029 atoms, of which 0 are hydrogens and 0 are deuteriums.

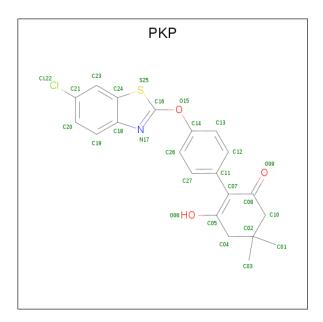
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called Probable propionyl-CoA carboxylase beta chain 6.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	A	426	Total	С	N	О	S	0	1	0
1	A	420	3147	1969	572	592	14	0	1	
1	В	424	Total	С	N	О	S	0	1	0
1	Ъ	424	3123	1958	569	582	14	0	1	
1	С	410	Total	С	N	О	S	0	1	0
1		410	2983	1869	539	561	14	0	1	
1	D	428	Total	С	N	О	S	0	0	0
1	ש	420	3093	1940	558	581	14	0		
1	Е	426	Total	С	N	О	S	0	1	0
1	12	420	3147	1969	572	592	14	0	l I	0
1	F	424	Total	С	N	О	S	0	1	0
1	I.	424	3123	1958	569	582	14	0	1	
1	G	409	Total	С	N	О	S	0	1	0
1	G	409	2977	1865	538	560	14	0	1	
1	Н	428	Total	С	N	О	S	0	0	0
1	11	420	3093	1940	558	581	14	U	U	U

• Molecule 2 is 4'-[(6-chloro-1,3-benzothiazol-2-yl)oxy]-6-hydroxy-4,4-dimethyl-4,5-dihydr o[1,1'-biphenyl]-2(3H)-one (three-letter code: PKP) (formula: $C_{21}H_{18}ClNO_3S$) (labeled as "Ligand of Interest" by author).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf				
2	A	1	Total C Cl N O S	0	0				
	A	1	27 21 1 1 3 1	0	U				
2	В	1	Total C Cl N O S	0	0				
	Б	1	27 21 1 1 3 1	0	U				
2	С	1	Total C Cl N O S	0	0				
		1	27 21 1 1 3 1	0	U				
2	D	1	Total C Cl N O S	0	0				
	ט					1	27 21 1 1 3 1	0	U
2	Е	1	Total C Cl N O S	0	0				
	ינו	1	27 21 1 1 3 1	0	U				
2	F	1	Total C Cl N O S	0	0				
	1'	1	27 21 1 1 3 1	0	U				
2	G	1	Total C Cl N O S	0	0				
	<u> </u>	1	27 21 1 1 3 1		U				
2	Н	1	Total C Cl N O S	0	0				
	11	1	27 21 1 1 3 1		U				

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	166	Total O 166 166	0	0
3	В	124	Total O 124 124	0	0
3	С	134	Total O 134 134	0	0
3	D	148	Total O 148 148	0	0

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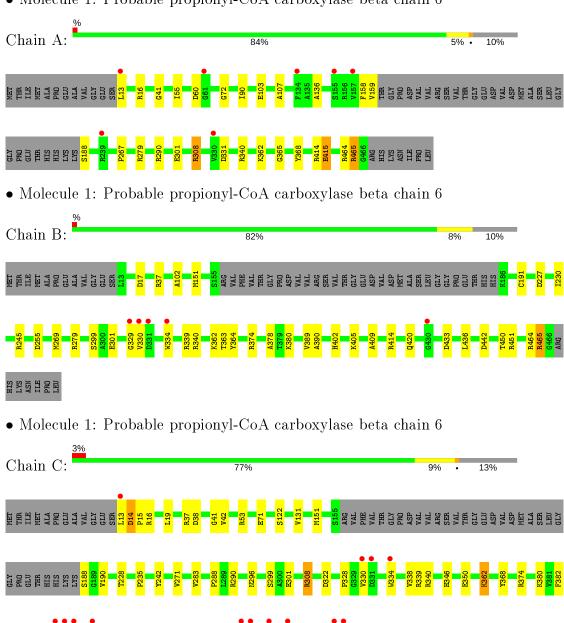
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	170	Total O 170 170	0	0
3	F	124	Total O 124 124	0	0
3	G	135	Total O 135 135	0	0
3	Н	126	Total O 126 126	0	0



3 Residue-property plots (i)

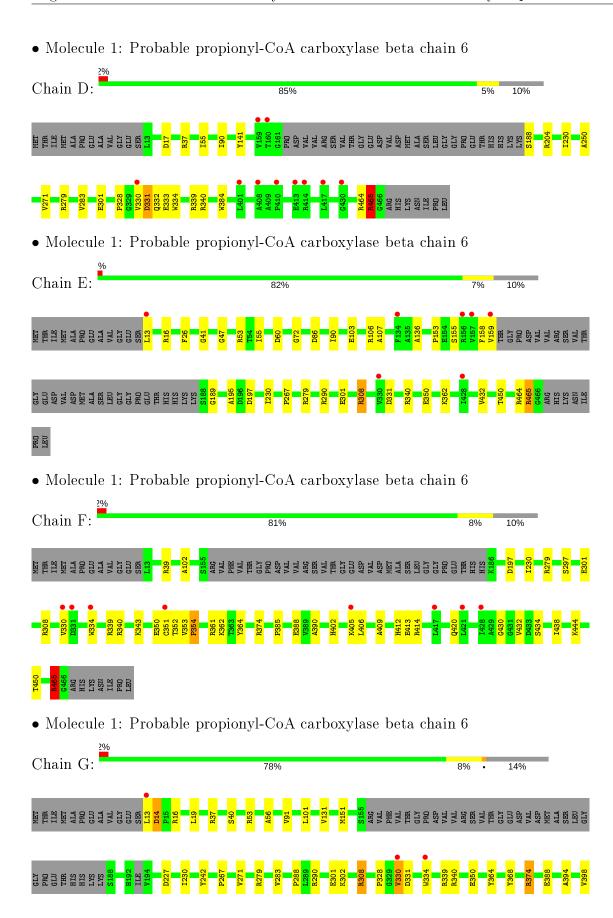
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Probable propionyl-CoA carboxylase beta chain 6

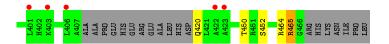


ALA
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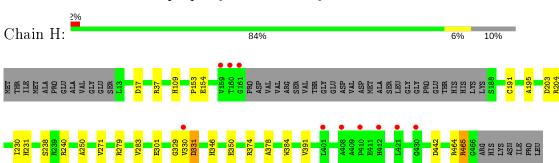








• Molecule 1: Probable propionyl-CoA carboxylase beta chain 6





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	102.34Å 153.07Å 150.18Å	Domositon
a, b, c, α , β , γ	90.00° 90.08° 90.00°	Depositor
Resolution (Å)	35.76 - 2.39	Depositor
resolution (A)	35.76 - 2.39	EDS
% Data completeness	98.7 (35.76-2.39)	Depositor
(in resolution range)	98.7 (35.76-2.39)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.09 \; ({ m at} \; 2.39 { m \AA})$	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.166 , 0.204	Depositor
Π , Π free	0.171 , 0.208	DCC
R_{free} test set	9047 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	$0.33 \;, 26.2$	EDS
L-test for twinning ²	$< L > = 0.50, < L^2> = 0.33$	Xtriage
	0.010 for -h,-l,-k	
Estimated twinning fraction	0.008 for -h,l,k	Xtriage
	0.468 for h,-k,-l	
F_o, F_c correlation	0.96	EDS
Total number of atoms	26029	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.29% 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: PKP

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	
MIOI	Chain	RMSZ	# Z >5	RMSZ	# Z > 5
1	A	0.42	0/3209	0.58	0/4365
1	В	0.41	0/3185	0.56	0/4330
1	С	0.46	0/3040	0.61	0/4137
1	D	0.48	0/3151	0.58	0/4294
1	E	0.42	0/3209	0.56	0/4365
1	F	0.43	0/3185	0.57	0/4330
1	G	0.49	0/3033	0.61	0/4126
1	Н	0.47	0/3151	0.58	0/4294
All	All	0.45	0/25163	0.58	0/34241

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Α	3147	0	3090	16	0
1	В	3123	0	3075	23	0
1	С	2983	0	2906	37	0
1	D	3093	0	3000	24	0
1	Ε	3147	0	3090	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3123	0	3075	36	0
1	G	2977	0	2901	33	0
1	Н	3093	0	3000	20	0
2	A	27	0	0	0	0
2	В	27	0	0	1	0
2	С	27	0	0	0	0
2	D	27	0	0	1	0
2	E	27	0	0	0	0
2	F	27	0	0	0	0
2	G	27	0	0	0	0
2	Н	27	0	0	0	0
3	A	166	0	0	2	0
3	В	124	0	0	0	0
3	С	134	0	0	3	0
3	D	148	0	0	1	0
3	Ε	170	0	0	3	0
3	F	124	0	0	2	0
3	G	135	0	0	1	0
3	Н	126	0	0	2	0
All	All	26029	0	24137	194	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.

The worst 5 of 194 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap} & (ext{Å}) \end{aligned}$
1:C:464:ARG:O	1:C:465:ARG:HB2	1.43	1.05
1:C:464:ARG:O	1:C:465:ARG:CB	2.12	0.97
1:G:330:VAL:HG12	1:G:331:ASP:N	1.83	0.92
1:D:464:ARG:O	1:D:465:ARG:HB2	1.67	0.91
1:C:346:HIS:HE1	1:C:350:GLU:OE2	1.56	0.88

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	Favoured Allowed		Perce	centiles	
1	A	423/473 (89%)	408 (96%)	13 (3%)	2 (0%)	29	39	
1	В	421/473 (89%)	410 (97%)	9 (2%)	2 (0%)	29	39	
1	С	405/473~(86%)	391 (96%)	12 (3%)	2 (0%)	29	39	
1	D	424/473 (90%)	408 (96%)	13 (3%)	3 (1%)	22	30	
1	Е	423/473 (89%)	412 (97%)	10 (2%)	1 (0%)	47	61	
1	F	421/473 (89%)	407 (97%)	11 (3%)	3 (1%)	22	30	
1	G	402/473 (85%)	389 (97%)	11 (3%)	2 (0%)	29	39	
1	Н	424/473 (90%)	407 (96%)	14 (3%)	3 (1%)	22	30	
All	All	3343/3784 (88%)	3232 (97%)	93 (3%)	18 (0%)	29	39	

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	465	ARG
1	В	465	ARG
1	С	330	VAL
1	С	465	ARG
1	D	332	GLN

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	${f Analysed}$	Rotameric	Outliers	Percentiles	
1	A	316/362~(87%)	311 (98%)	5 (2%)	62 78	

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	В	311/362 (86%)	306 (98%)	5 (2%)	62	78	
1	С	294/362~(81%)	285 (97%)	9 (3%)	40	57	
1	D	302/362~(83%)	300 (99%)	2 (1%)	84	92	
1	E	316/362~(87%)	310 (98%)	6 (2%)	57	73	
1	F	311/362~(86%)	306 (98%)	5 (2%)	62	78	
1	G	294/362~(81%)	286 (97%)	8 (3%)	44	62	
1	Н	302/362~(83%)	296 (98%)	6 (2%)	55	72	
All	All	2446/2896 (84%)	2400 (98%)	46 (2%)	60	73	

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	465	ARG
1	E	308[B]	ARG
1	Н	203	ASP
1	E	155	SER
1	E	279	ARG

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

Mol	Chain	${ m Res}$	\mathbf{Type}
1	A	109	HIS
1	С	346	HIS
1	F	460	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)

8 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	Tuna	Chain	Res	Link	В	ond leng	gths	Bond angles		
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	PKP	D	501	-	27,30,30	2.00	8 (29%)	37,45,45	1.93	11 (29%)
2	PKP	F	501	-	27,30,30	2.09	7 (25%)	37,45,45	1.88	9 (24%)
2	PKP	В	501	-	27,30,30	2.09	6 (22%)	37,45,45	1.94	10 (27%)
2	PKP	Н	501	-	27,30,30	1.85	6 (22%)	37,45,45	2.10	12 (32%)
2	PKP	G	501	-	27,30,30	2.08	8 (29%)	37,45,45	1.92	10 (27%)
2	PKP	Е	501	-	27,30,30	2.26	10 (37%)	37,45,45	1.71	9 (24%)
2	PKP	С	501	-	27,30,30	2.03	8 (29%)	37,45,45	2.00	11 (29%)
2	PKP	A	501	-	27,30,30	2.27	9 (33%)	37,45,45	1.82	8 (21%)

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	PKP	D	501	-	-	0/6/26/26	0/4/4/4
2	PKP	F	501	_	-	0/6/26/26	0/4/4/4
2	PKP	В	501	-	-	0/6/26/26	0/4/4/4
2	PKP	Н	501	-	-	0/6/26/26	0/4/4/4
2	PKP	G	501	-	-	0/6/26/26	0/4/4/4
2	PKP	E	501	-	-	0/6/26/26	0/4/4/4
2	PKP	С	501	-	-	0/6/26/26	0/4/4/4
2	PKP	A	501	_	-	0/6/26/26	0/4/4/4

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	${ m Observed}(m \AA)$	Ideal(Å)
2	A	501	PKP	O15-C16	6.34	1.44	1.36
2	Е	501	PKP	O15-C16	6.32	1.44	1.36

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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	${ m Observed}({ m \AA})$	$\operatorname{Ideal}(ext{\AA})$
2	В	501	PKP	O15-C16	6.17	1.43	1.36
2	F	501	PKP	O15-C16	5.65	1.43	1.36
2	С	501	PKP	O15-C16	4.96	1.42	1.36

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	F	501	PKP	C23-C24-S25	4.86	134.83	125.10
2	В	501	PKP	C23-C24-S25	4.71	134.52	125.10
2	A	501	PKP	C23-C24-S25	4.68	134.46	125.10
2	F	501	PKP	C18-C24-S25	-4.49	105.90	111.85
2	Н	501	PKP	C04-C02-C10	4.46	115.50	108.12

There are no chirality outliers.

There are no torsion outliers.

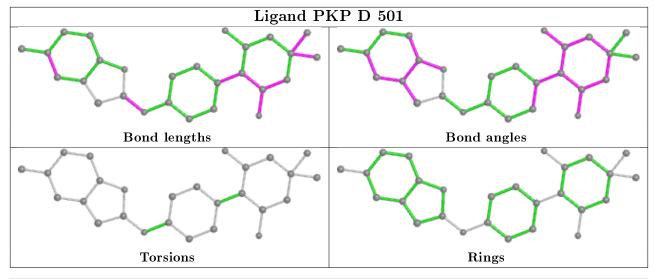
There are no ring outliers.

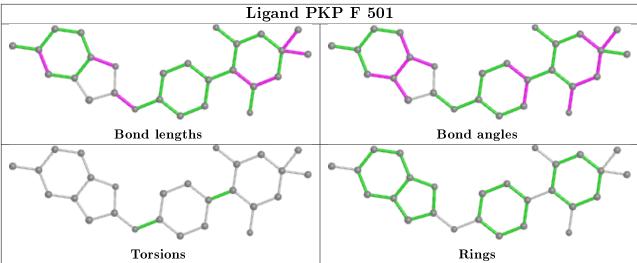
2 monomers are involved in 2 short contacts:

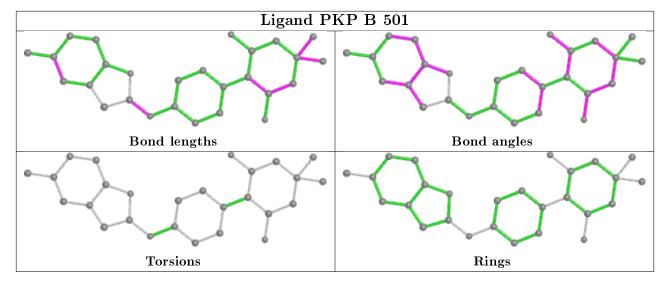
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	PKP	1	0
2	В	501	PKP	1	0

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.

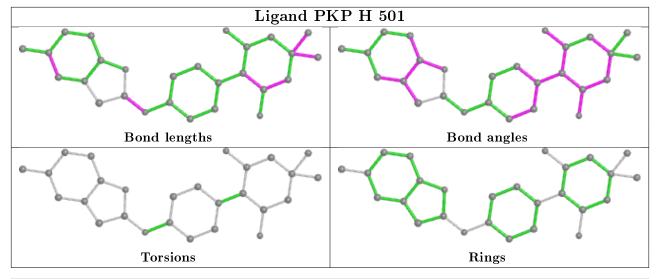


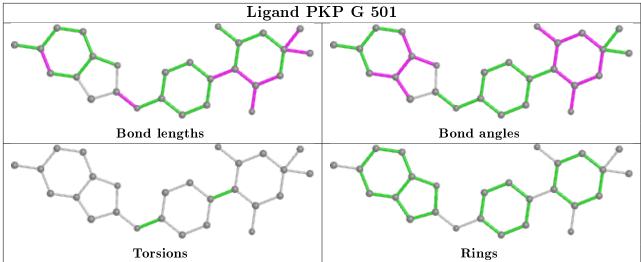


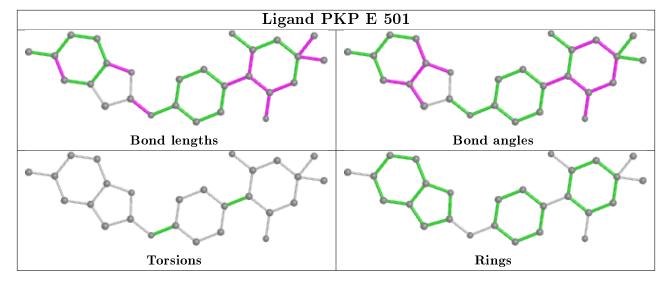




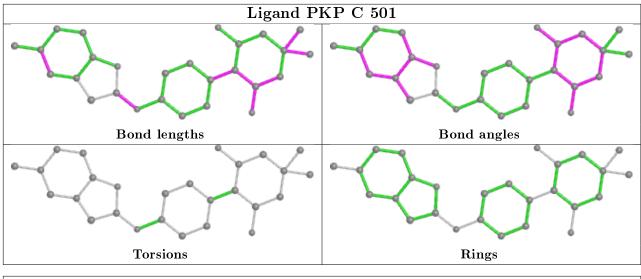


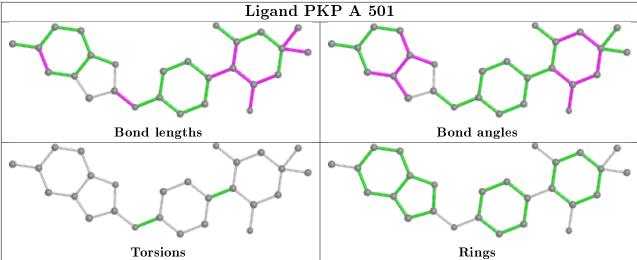












5.7 Other polymers (i)

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	$\langle { m RSRZ} \rangle$	$\#\mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	$426/473 \ (90\%)$	-0.08	7 (1%) 72 73	24, 37, 61, 73	0
1	В	424/473 (89%)	0.04	5 (1%) 79 80	25, 39, 67, 89	0
1	С	410/473 (86%)	0.05	14 (3%) 45 48	25, 36, 82, 110	0
1	D	428/473 (90%)	-0.06	10 (2%) 60 62	26, 38, 71, 88	0
1	Е	426/473 (90%)	-0.08	7 (1%) 72 73	24, 37, 59, 74	0
1	F	424/473 (89%)	0.01	8 (1%) 66 68	24, 38, 66, 95	0
1	G	409/473~(86%)	0.07	8 (1%) 65 66	26, 37, 79, 105	0
1	Н	428/473 (90%)	-0.04	10 (2%) 60 62	26, 39, 72, 92	0
All	All	3375/3784 (89%)	-0.01	69 (2%) 65 66	24, 38, 68, 110	0

The worst 5 of 69 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	330	VAL	7.2
1	G	330	VAL	7.1
1	С	13	LEU	5.9
1	E	13	LEU	5.5
1	G	13	LEU	5.3

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.

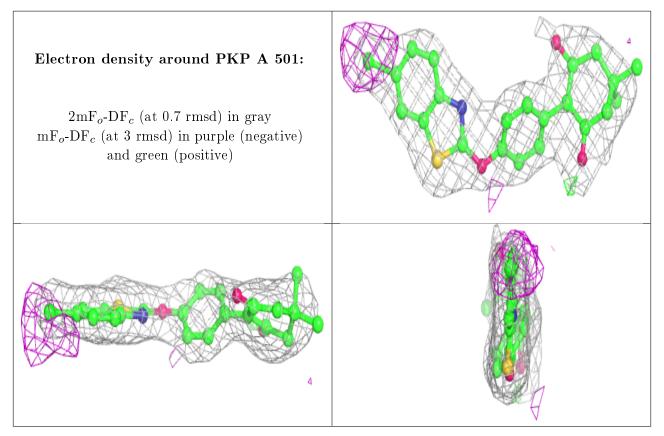


6.4 Ligands (i)

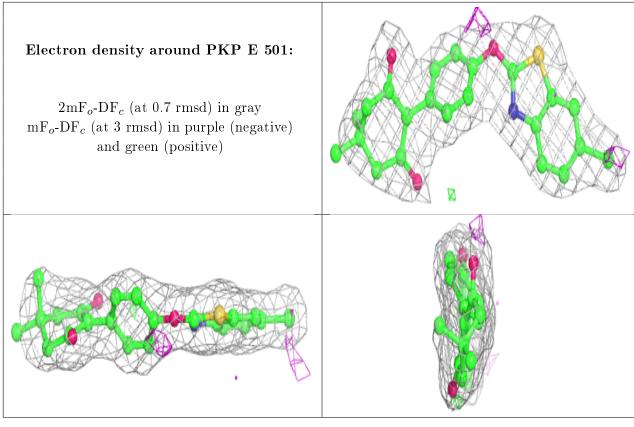
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	PKP	A	501	27/27	0.94	0.15	33,40,52,61	0
2	PKP	Е	501	27/27	0.95	0.15	33,42,53,62	0
2	PKP	Н	501	27/27	0.95	0.16	32,40,54,55	0
2	PKP	G	501	27/27	0.96	0.14	30,38,48,56	0
2	PKP	F	501	27/27	0.96	0.17	21,31,49,52	0
2	PKP	С	501	27/27	0.96	0.15	30,38,47,57	0
2	PKP	D	501	27/27	0.96	0.15	32,39,56,57	0
2	PKP	В	501	27/27	0.97	0.15	24,32,48,51	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.





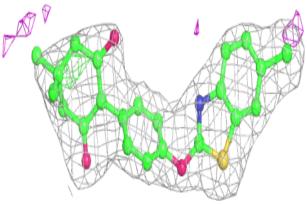


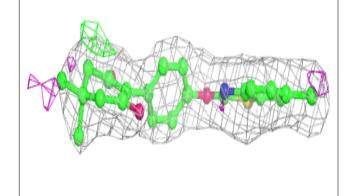
Electron density around PKP H 501: 2mF_o-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

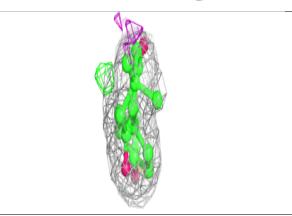


Electron density around PKP G 501:

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

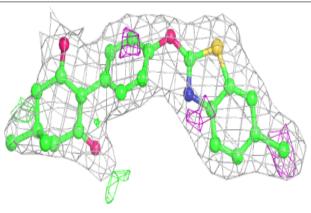


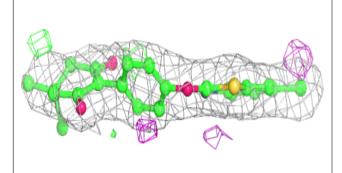


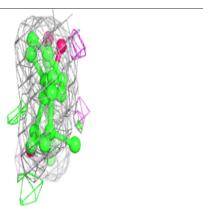


Electron density around PKP F 501:

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



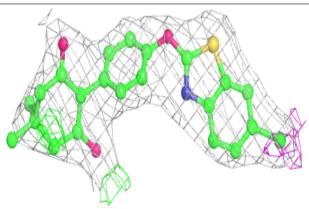


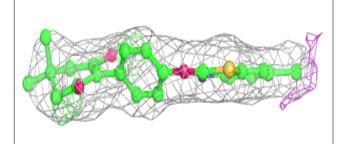


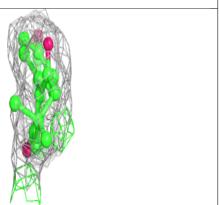


Electron density around PKP C 501: 2mF_o-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive) Electron density around PKP D 501:

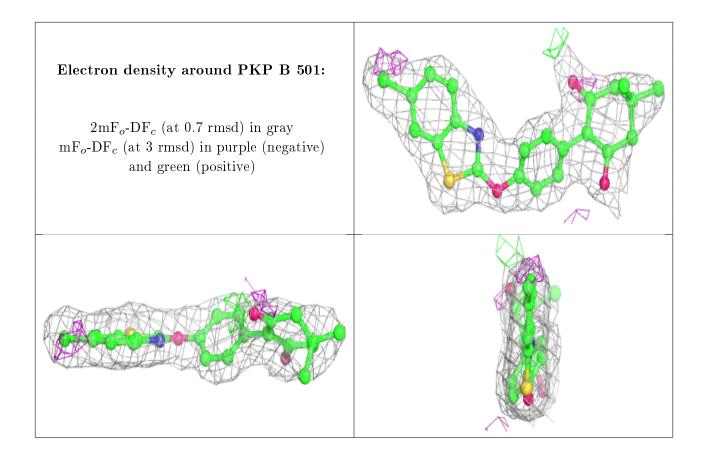
 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)











6.5 Other polymers (i)

There are no such residues in this entry.

