

Full wwPDB X-ray Structure Validation Report (i)

Jan 27, 2022 – 06:12 pm GMT

PDB ID : 7PT3

Title : Actinobacterial 2-hydroxyacyl-CoA lyase (AcHACL) mutant E493A structure

in complex with substrate 2-HIB-CoA and inactive cofactor 3-deaza-ThDP

Authors : Zahn, M.; Rohwerder, T.

Deposited on : 2021-09-25

Resolution : 1.62 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 following versions of software and data (see references (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul: 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.26

buster-report : 1.1.7 (2018)

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

 $Refmac \quad : \quad 5.8.0267$

CCP4 : 7.1.010 (Gargrove)

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

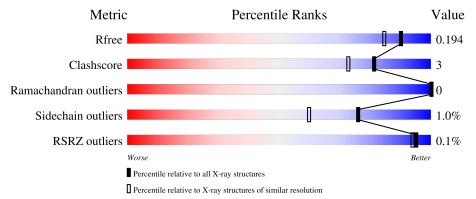
Validation Pipeline (wwPDB-VP) : 2.26

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 1.62 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 $(\# \mathrm{Entries})$	$egin{aligned} ext{Similar resolution} \ (\# ext{Entries, resolution range}(ext{Å})) \end{aligned}$		
R_{free}	130704	4693 (1.64-1.60)		
Clashscore	141614	5002 (1.64-1.60)		
Ramachandran outliers	138981	4888 (1.64-1.60)		
Sidechain outliers	138945	4887 (1.64-1.60)		
RSRZ outliers	127900	4609 (1.64-1.60)		

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	612	87%	7%	6%
1	В	612	85%	8%	7%



2 Entry composition (i)

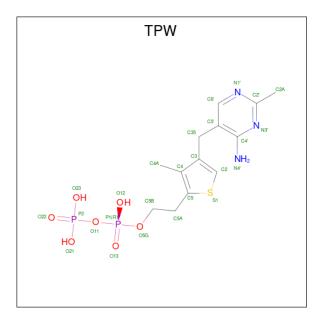
There are 5 unique types of molecules in this entry. The entry contains 18448 atoms, of which 8691 are hydrogens and 0 are deuteriums.

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 2-hydroxyacyl-CoA lyase.

Mol	Chain	Residues		Atoms					ZeroOcc	AltConf	Trace
1	Λ	574	Total	С	Н	N	О	S	101	4	0
1	A	314	8633	2687	4304	802	831	9	101	4	0
1	D	572	Total	С	Н	N	О	S	102	1	0
1	Б	312	8569	2667	4273	797	823	9	102	1	

• Molecule 2 is 2-{4-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-3-METHYL THIOPHEN-2-YL}ETHYL TRIHYDROGEN DIPHOSPHATE (three-letter code: TPW) (formula: C₁₃H₁₉N₃O₇P₂S) (labeled as "Ligand of Interest" by depositor).

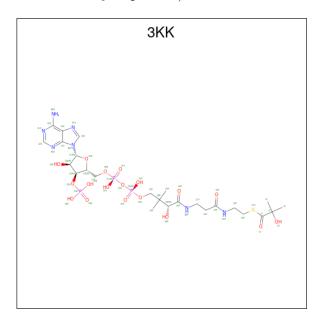


Mol	Chain	Residues		Atoms						ZeroOcc	AltConf	
2	Λ	1	Total	С	Н	N	О	Р	S	3	0	
	A	1	45	13	19	3	7	2	1			
2	D	1	Total	С	Н	N	О	Р	S	9	0	
	Б	1	45	13	19	3	7	2	1	3	0	

• Molecule 3 is $S-\{(3R,5R,9R)-1-[(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-4-hydroxy-3-(phosphonooxy)tetrahydrofuran-2-yl]-3,5,9-trihydroxy-8,8-dimethyl-3,5-dioxido-10,14-dioxo-2,4,$



6-trioxa-11,15-diaza-3lambda 5 ,5lambda 5 -diphosphaheptadecan-17-yl} 2-hydroxy-2-meth ylpropanethioate (three-letter code: 3KK) (formula: $C_{25}H_{42}N_7O_{18}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	
2	Λ	1	Total	С	Н	N	О	Р	S	2	0
3	3 A	1	92	25	38	7	18	3	1	3	
9	D	1	Total	С	Н	N	О	Р	S	3	0
3	D	1	92	25	38	7	18	3	1		

• Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mg 2 2	0	0
4	В	1	Total Mg 1 1	0	0

• Molecule 5 is water.

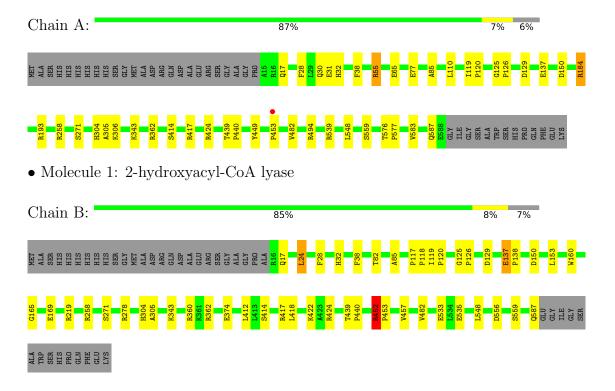
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	482	Total O 482 482	0	0
5	В	487	Total O 487 487	0	0



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: 2-hydroxyacyl-CoA lyase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	103.92Å 146.72Å 174.41Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.21 - 1.62	Depositor
Resolution (A)	87.21 - 1.62	EDS
% Data completeness	61.5 (87.21-1.62)	Depositor
(in resolution range)	57.1 (87.21-1.62)	EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.83 (at 1.63Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
D D.	0.154 , 0.186	Depositor
R, R_{free}	0.165 , 0.194	DCC
R_{free} test set	5146 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	18.3	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$ < L > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18448	wwPDB-VP
Average B, all atoms $(Å^2)$	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.38% 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: TPW, 3KK, 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	Bo	nd lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5	
1	A	0.82	$2/4423 \ (0.0\%)$	0.96	8/6029 (0.1%)	
1	В	0.83	3/4381 (0.1%)	0.96	8/5972 (0.1%)	
All	All	0.83	5/8804 (0.1%)	0.96	16/12001 (0.1%)	

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	Ideal(Å)
1	A	453	PRO	C-O	9.77	1.42	1.23
1	В	137	GLU	CD-OE1	7.50	1.33	1.25
1	A	77	GLU	CD-OE1	7.20	1.33	1.25
1	В	343	LYS	C-O	5.29	1.33	1.23
1	В	533	GLU	CD-OE1	5.02	1.31	1.25

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
1	В	417	ARG	NE-CZ-NH2	-11.05	114.78	120.30
1	A	417	ARG	NE-CZ-NH2	-10.21	115.20	120.30
1	В	150	ASP	CB-CA-C	-8.18	94.05	110.40
1	В	417	ARG	NE-CZ-NH1	8.05	124.32	120.30



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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	417	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	A	258	ARG	NE-CZ-NH2	7.80	124.20	120.30
1	В	258	ARG	NE-CZ-NH2	7.73	124.17	120.30
1	A	539[A]	ARG	NE-CZ-NH1	-7.37	116.61	120.30
1	A	539[B]	ARG	NE-CZ-NH1	-7.37	116.61	120.30
1	В	452	ARG	CB-CA-C	-6.59	97.23	110.40
1	В	219	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	55	ARG	CG-CD-NE	-5.78	99.67	111.80
1	В	278	ARG	NE-CZ-NH2	5.67	123.13	120.30
1	A	184	ARG	NE-CZ-NH2	5.49	123.05	120.30
1	A	184	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	В	360	ARG	NE-CZ-NH2	-5.27	117.67	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	305	ALA	Peptide
1	В	305	ALA	Peptide

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	4329	4304	4291	22	0
1	В	4296	4273	4257	24	0
2	A	26	19	16	0	0
2	В	26	19	16	1	0
3	A	54	38	38	0	0
3	В	54	38	38	0	0
4	A	2	0	0	0	0
4	В	1	0	0	0	0
5	A	482	0	0	8	0
5	В	487	0	0	6	0
All	All	9757	8691	8656	46	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 3.

All (46) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A + 1	A4 2	Interatomic	Clash
Atom-1	Atom-2	${\rm distance}({\rm \AA})$	$overlap (\AA)$
1:B:424:ARG:NH2	5:B:801:HOH:O	2.05	0.87
1:A:137[B]:GLU:OE1	5:A:801:HOH:O	2.12	0.67
1:A:193:ARG:NH1	5:A:804:HOH:O	2.24	0.67
1:B:453:PRO:O	5:B:802:HOH:O	2.14	0.66
1:A:271:SER:O	1:A:362:ARG:NH1	2.30	0.63
1:A:184:ARG:NH1	5:A:806:HOH:O	2.32	0.63
1:B:535:GLU:HG3	5:B:1161:HOH:O	2.03	0.59
1:B:126:PRO:HG2	1:B:129:ASP:HB2	1.86	0.58
1:A:126:PRO:HG2	1:A:129:ASP:HB2	1.88	0.56
1:A:449:TYR:OH	5:A:802:HOH:O	2.19	0.52
1:B:271:SER:O	1:B:362:ARG:NH1	2.45	0.50
1:B:38:PHE:O	1:B:85:ALA:HA	2.13	0.49
1:A:30:GLN:OE1	1:A:55:ARG:NH2	2.47	0.48
1:B:412:LEU:HD11	1:B:457:VAL:HG12	1.96	0.47
1:A:28:PHE:CE1	1:A:32:HIS:CE1	3.03	0.47
1:B:125:GLY:N	1:B:126:PRO:CD	2.78	0.47
1:B:28:PHE:CE2	1:B:32:HIS:CE1	3.04	0.46
1:A:38:PHE:O	1:A:85:ALA:HA	2.17	0.45
1:A:31:GLU:HG3	5:A:877:HOH:O	2.15	0.45
1:A:304:HIS:HD2	5:A:1254:HOH:O	2.00	0.45
1:A:306:LYS:NZ	5:A:824:HOH:O	2.50	0.44
1:B:374:GLU:HG2	5:B:1048:HOH:O	2.16	0.44
1:B:82:THR:HB	1:B:160:TRP:CZ2	2.53	0.43
1:B:452:ARG:HE	1:B:452:ARG:HB2	1.40	0.43
1:A:494:ARG:NH2	5:A:805:HOH:O	2.27	0.43
1:A:576:THR:HB	1:A:577:PRO:HD3	2.01	0.43
1:B:414:SER:HB3	1:B:559:SER:HB2	2.01	0.42
1:A:125:GLY:N	1:A:126:PRO:CD	2.82	0.42
1:B:439:THR:HB	1:B:440:PRO:HD3	2.01	0.42
1:B:304:HIS:HD2	5:B:1251:HOH:O	2.02	0.42
1:B:418:LEU:HD12	1:B:418:LEU:N	2.35	0.42
1:B:117:PRO:HA	1:B:118:PRO:HD3	1.93	0.42
1:B:482:VAL:O	1:B:548:LEU:HA	2.20	0.42
1:A:482:VAL:O	1:A:548:LEU:HA	2.19	0.42
1:B:24:LEU:HD12	1:B:24:LEU:HA	1.92	0.41
1:B:137:GLU:N	1:B:138:PRO:CD	2.84	0.41
1:B:119:ILE:N	1:B:120:PRO:CD	2.84	0.41
1:A:414:SER:HB3	1:A:559:SER:HB2	2.03	0.41



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COHABABACA		DIEUIUU	DUIUE
0 0 1000100000			

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	$\operatorname{distance}\ (ext{Å})$	overlap (Å)
1:A:65:GLU:OE2	2:B:701:TPW:N1'	2.53	0.41
1:A:439:THR:HB	1:A:440:PRO:HD3	2.02	0.41
1:A:119:ILE:N	1:A:120:PRO:CD	2.83	0.41
1:B:153:LEU:HD12	1:B:153:LEU:HA	1.93	0.41
1:A:583:VAL:O	1:A:587:GLN:HG3	2.21	0.40
1:B:556:ASP:HB3	5:B:1128:HOH:O	2.21	0.40
1:B:165:GLY:HA2	1:B:169:GLU:C	2.42	0.40
1:A:110:LEU:C	1:A:110:LEU:HD12	2.41	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	576/612 (94%)	561 (97%)	15 (3%)	0	100 100		
1	В	571/612 (93%)	555 (97%)	16 (3%)	0	100 100		
All	All	1147/1224 (94%)	1116 (97%)	31 (3%)	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	442/466 (95%)	438 (99%)	4 (1%)	78 64	



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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	В	438/466 (94%)	433 (99%)	5 (1%)	73 56		
All	All	880/932 (94%)	871 (99%)	9 (1%)	76 60		

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	150	ASP
1	A	343	LYS
1	A	424	ARG
1	В	17	GLN
1	В	24	LEU
1	В	422	LYS
1	В	452	ARG
1	В	587	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	304	HIS
1	В	371	HIS

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 7 ligands modelled in this entry, 3 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	Tuno	Chain Res	Res Link	Bond lengths			Bond angles			
	Type		nes	LILK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TPW	A	701	4	23,27,27	1.07	3 (13%)	30,40,40	0.82	0
3	3KK	В	702	-	47,56,56	0.76	2 (4%)	58,85,85	0.87	3 (5%)
3	3KK	A	702	-	47,56,56	0.79	0	58,85,85	1.05	5 (8%)
2	TPW	В	701	4	23,27,27	0.88	0	30,40,40	0.83	1 (3%)

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	TPW	A	701	4	-	2/16/17/17	0/2/2/2
3	3KK	В	702	-	-	3/52/73/73	0/3/3/3
3	3KK	A	702	-	-	4/52/73/73	0/3/3/3
2	TPW	В	701	4	-	1/16/17/17	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\mathring{A}})$	$Ideal(\AA)$
2	A	701	TPW	C5A-C5	2.57	1.52	1.50
2	A	701	TPW	C2-S1	2.47	1.74	1.70
3	В	702	3KK	P3B-O9A	-2.24	1.46	1.54
2	A	701	TPW	C2-C3	-2.13	1.35	1.37
3	В	702	3KK	C8A-N7A	-2.04	1.31	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
3	A	702	3KK	O7A-P3B-O3B	-2.79	93.48	105.99
3	A	702	3KK	O2A-P1A-O1A	2.61	125.13	112.24
2	В	701	TPW	P1-O11-P2	-2.55	124.07	132.83
3	A	702	3KK	OAP-CAP-CBP	-2.45	104.47	110.25
3	В	702	3KK	O3B-P3B-O8A	-2.45	99.95	109.39



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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
3	A	702	3KK	C7P-C6P-C5P	-2.16	108.76	112.36
3	В	702	3KK	O2A-P1A-O1A	2.12	122.72	112.24
3	В	702	3KK	O7A-P3B-O3B	2.06	115.23	105.99
3	A	702	3KK	O9A-P3B-O7A	2.00	115.29	107.64

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	TPW	P1-O11-P2-O21
3	A	702	3KK	C3P-C2P-S1P-C1
3	A	702	3KK	C5B-O5B-P1A-O2A
3	В	702	3KK	C3P-C2P-S1P-C1
3	В	702	3KK	CCP-O6A-P2A-O5A
2	A	701	TPW	P1-O11-P2-O22
2	В	701	TPW	P1-O11-P2-O23
3	A	702	3KK	C5B-O5B-P1A-O3A
3	В	702	3KK	C5B-O5B-P1A-O3A
3	A	702	3KK	C5B-O5B-P1A-O1A

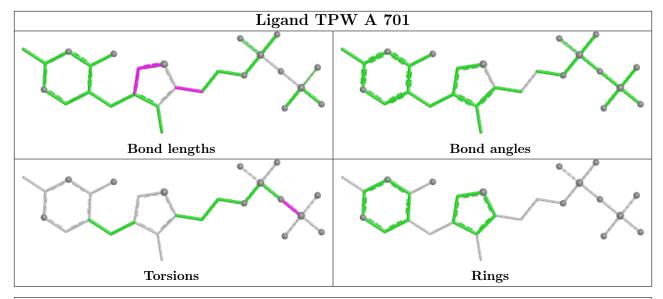
There are no ring outliers.

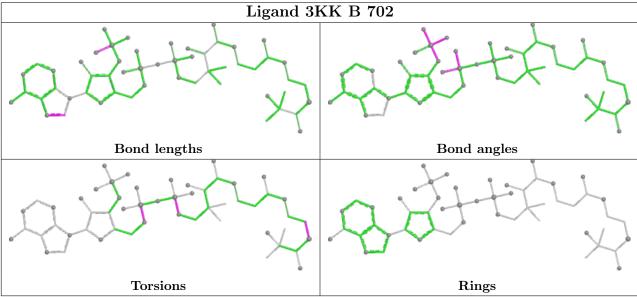
1 monomer is involved in 1 short contact:

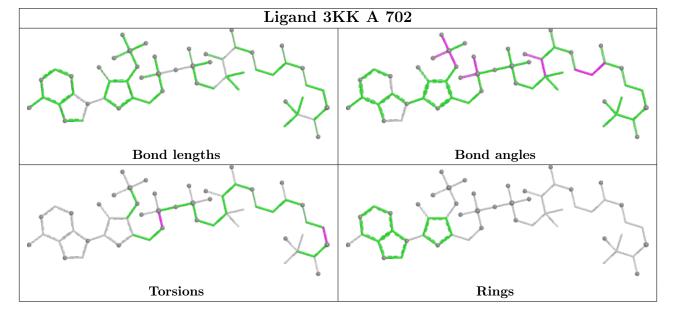
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	701	TPW	1	0

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.

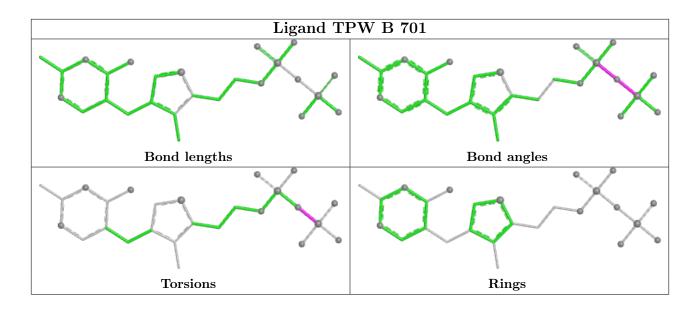












5.7 Other polymers (i)

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	$\langle { m RSRZ} \rangle$	# RSRZ > 2	$OWAB(Å^2)$	Q<0.9
1	A	574/612 (93%)	-0.56	1 (0%) 95 94	13, 21, 39, 74	0
1	В	572/612 (93%)	-0.60	0 100 100	13, 21, 35, 59	0
All	All	1146/1224 (93%)	-0.58	1 (0%) 95 94	13, 21, 37, 74	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	453	PRO	2.2

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.

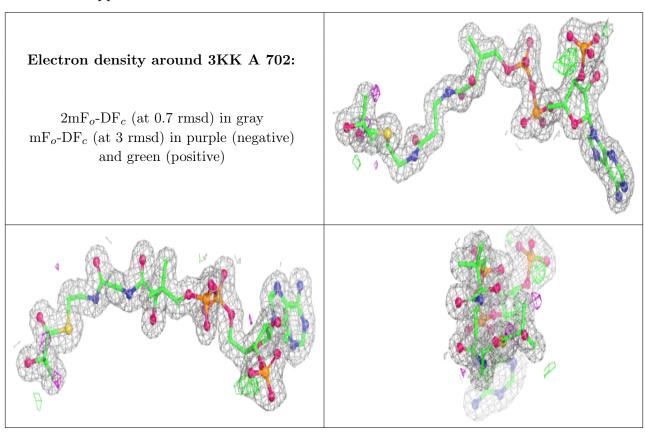
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
3	3KK	A	702	54/54	0.98	0.07	20,23,30,38	3
2	TPW	В	701	26/26	0.99	0.07	13,14,16,16	3
2	TPW	A	701	26/26	0.99	0.07	15,17,20,20	3
3	3KK	В	702	54/54	0.99	0.06	16,18,23,27	3



Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
4	MG	A	703	1/1	0.99	0.04	20,20,20,20	0
4	MG	A	704	1/1	1.00	0.06	21,21,21,21	0
4	MG	В	703	1/1	1.00	0.07	14,14,14,14	0

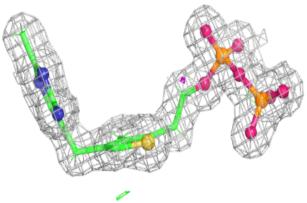
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

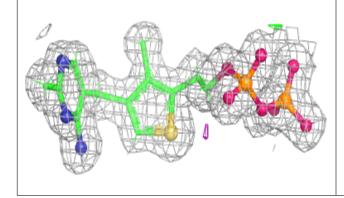


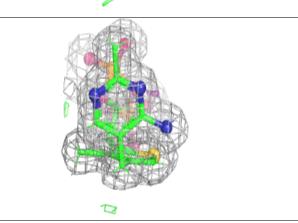


Electron density around TPW B 701:

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

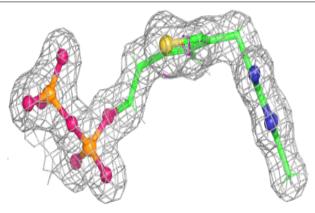


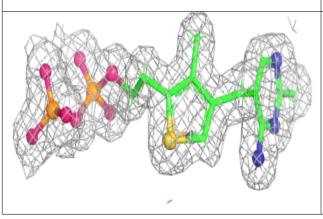


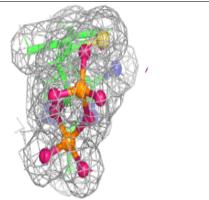


Electron density around TPW A 701:

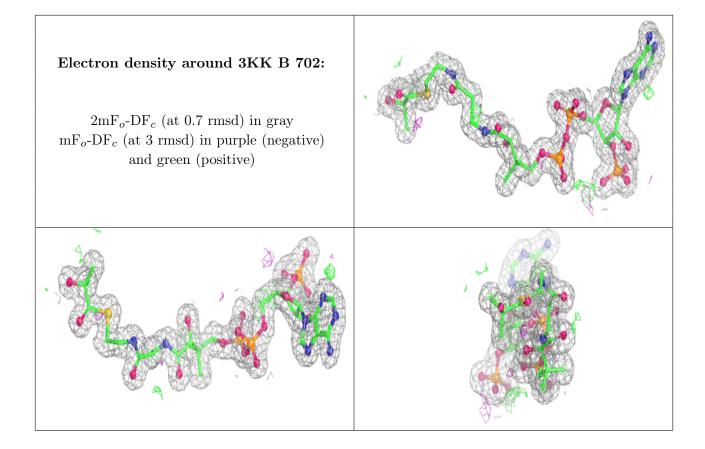
 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



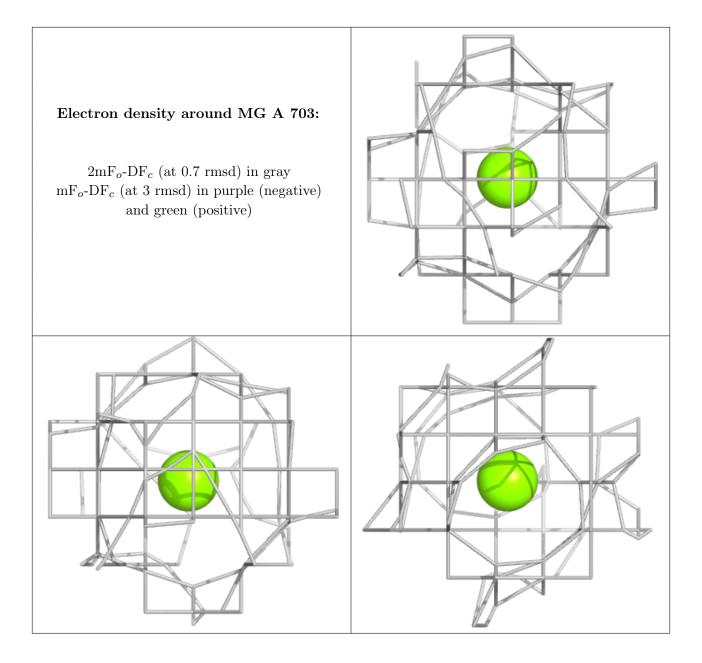








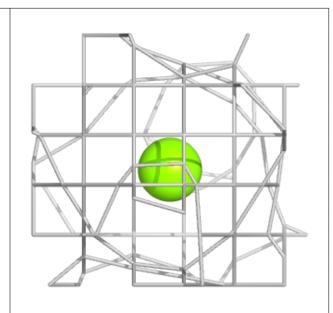


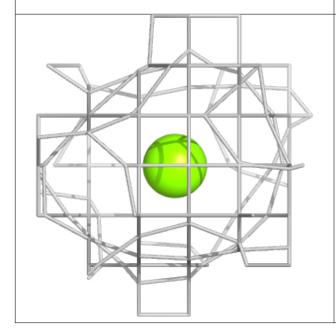


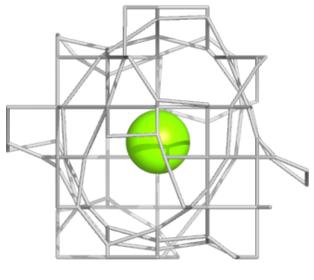


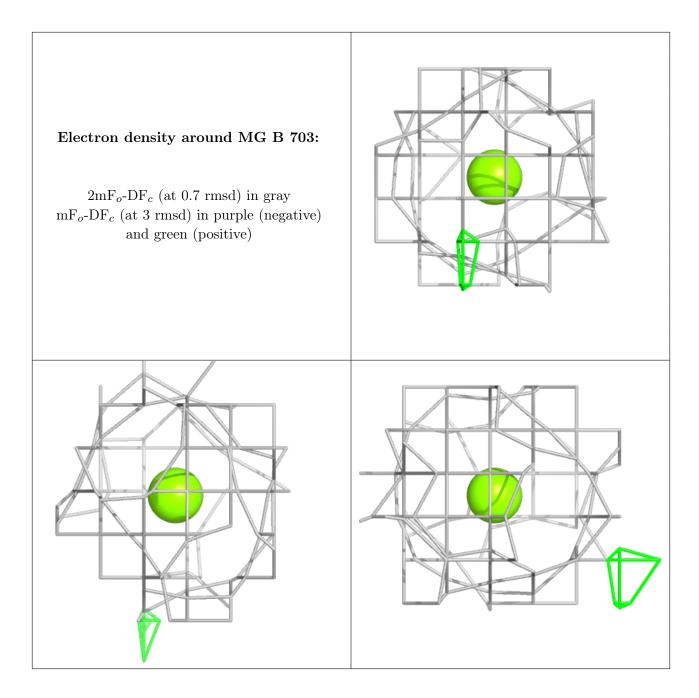
Electron density around MG A 704:

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









6.5 Other polymers (i)

There are no such residues in this entry.

