

Full wwPDB X-ray Structure Validation Report (i)

Jul 6, 2022 – 04:19 am BST

PDB ID : 7PJM

Title: Crystal Structure of Ivosidenib-resistant IDH1 variant R132C S280F in com-

plex with NADPH and Ca2+/2-Oxoglutarate

Authors: Reinbold, R.; Rabe, P.; Abboud, M.I.; Schofield, C.J.

Deposited on : 2021-08-24

Resolution : 2.10 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 : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.29

buster-report : 1.1.7 (2018)

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

Refmac : 5.8.0267

CCP4 : 7.1.010 (Gargrove)

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

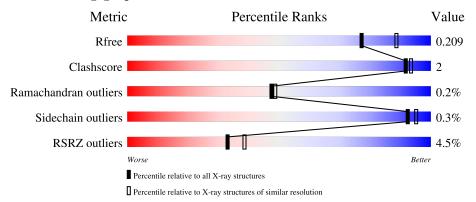
Validation Pipeline (wwPDB-VP) : 2.29

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	422	96%	
1	В	422	92%	6% •
1	С	422	95%	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	502	-	-	-	X



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 19700 atoms, of which 9425 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 Isocitrate dehydrogenase [NADP] cytoplasmic.

Mol	Chain	Residues		Atoms					ZeroOcc	AltConf	Trace
1	Λ	415	Total	С	Н	N	О	S	0	8	0
1	A	410	6433	2096	3145	544	626	22	U		
1	D	412	Total	С	Н	N	О	S	0	2	1
1	Ъ		6245	2036	3052	532	605	20			
1	1 C	C 414	Total	С	Н	N	О	S	0	5	0
1			6345	2073	3096	535	620	21	0		U

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	132	CYS	ARG	engineered mutation	UNP O75874
A	280	PHE	SER	engineered mutation	UNP O75874
A	415	LEU	-	expression tag	UNP O75874
A	416	GLU	-	expression tag	UNP O75874
A	417	HIS	-	expression tag	UNP O75874
A	418	HIS	-	expression tag	UNP O75874
A	419	HIS	-	expression tag	UNP O75874
A	420	HIS	-	expression tag	UNP O75874
A	421	HIS	-	expression tag	UNP O75874
A	422	HIS	-	expression tag	UNP O75874
В	132	CYS	ARG	engineered mutation	UNP O75874
В	280	PHE	SER	engineered mutation	UNP O75874
В	415	LEU	-	expression tag	UNP O75874
В	416	GLU	-	expression tag	UNP O75874
В	417	HIS	-	expression tag	UNP O75874
В	418	HIS	-	expression tag	UNP O75874
В	419	HIS	-	expression tag	UNP O75874
В	420	HIS	-	expression tag	UNP O75874
В	421	HIS	-	expression tag	UNP O75874
В	422	HIS	-	expression tag	UNP O75874
С	132	CYS	ARG	engineered mutation	UNP O75874
С	280	PHE	SER	engineered mutation	UNP O75874
С	415	LEU	-	expression tag	UNP O75874

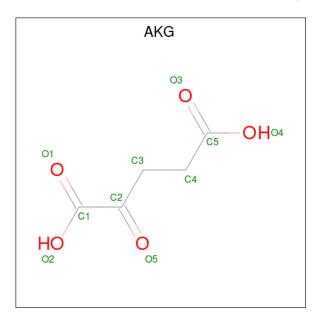
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Chain	Residue	Modelled	Actual Comment		Reference
С	416	GLU	-	expression tag	UNP O75874
С	417	HIS	-	expression tag	UNP O75874
С	418	HIS	-	expression tag	UNP O75874
С	419	HIS	-	expression tag	UNP 075874
С	420	HIS	-	expression tag	UNP 075874
С	421	HIS	-	expression tag	UNP 075874
С	422	HIS	-	expression tag	UNP O75874

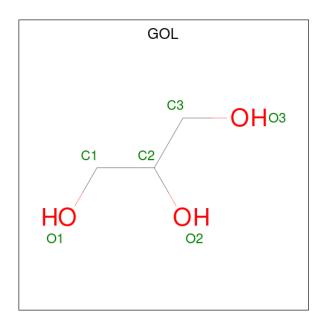
• Molecule 2 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H O 14 5 4 5	0	0
2	В	1	Total C H O 14 5 4 5	0	0
2	С	1	Total C H O 14 5 4 5	0	0

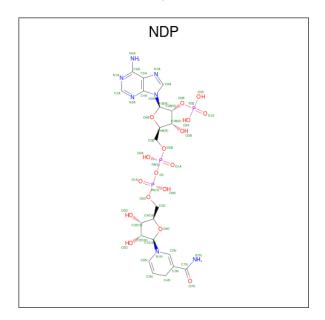
• Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 13 3 7 3	0	0
3	Α	1	Total C H O	0	0
		1	14 3 8 3 Total C H O	0	
3	С	1	13 3 7 3	0	0
3	С	1	Total C H O	0	0
			14 3 8 3		

• Molecule 4 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
4	Λ	1	Total	С	Н	N	О	Р	0	0
4	4 A	1	78	21	30	7	17	3	U	0
1	D	1	Total	С	Н	N	О	Р	0	0
4	Ъ	1	78	21	30	7	17	3	0	U
1	С	1	Total	С	Н	N	О	Р	0	0
4	C	1	78	21	30	7	17	3	0	0

• Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0
5	В	1	Total Ca 1 1	0	0
5	С	1	Total Ca 1 1	0	0

• Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	1
6	В	1	Total Cl 1 1	0	1
6	С	1	Total Cl 1 1	0	1

• Molecule 7 is water.

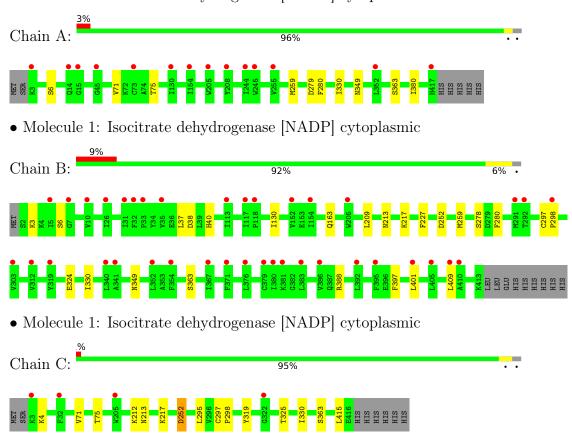
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	130	Total O 130 130	0	0
7	В	81	Total O 81 81	0	0
7	С	130	Total O 130 130	0	2



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: Isocitrate dehydrogenase [NADP] cytoplasmic





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	96.58Å 273.01Å 117.42Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.01 - 2.10	Depositor
resolution (A)	59.01 - 2.10	EDS
% Data completeness	100.0 (59.01-2.10)	Depositor
(in resolution range)	100.0 (59.01-2.10)	EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.18 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
P.P.	0.180 , 0.210	Depositor
R, R_{free}	0.180 , 0.209	DCC
R_{free} test set	4466 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	47.6	Xtriage
Anisotropy	0.324	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	0.96	EDS
Total number of atoms	19700	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.92% 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: NDP, CA, GOL, CL, AKG

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	0.27	0/3357	0.45	0/4543	
1	В	0.26	0/3262	0.44	0/4416	
1	С	0.26	0/3318	0.45	0/4495	
All	All	0.26	0/9937	0.45	0/13454	

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	A	3288	3145	3136	7	0
1	В	3193	3052	3048	14	0
1	С	3249	3096	3086	10	0
2	A	10	4	4	0	0
2	В	10	4	4	0	0
2	С	10	4	4	0	0
3	A	12	15	16	2	0
3	С	12	15	16	0	0
4	A	48	30	26	1	0
4	В	48	30	26	1	0

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Mol	Chain	Non-H	H(model)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
4	С	48	30	26	2	0
5	A	1	0	0	0	0
5	В	1	0	0	0	0
5	С	1	0	0	0	0
6	A	1	0	0	0	0
6	В	1	0	0	0	0
6	С	1	0	0	0	0
7	A	130	0	0	0	0
7	В	81	0	0	0	0
7	С	130	0	0	1	0
All	All	10275	9425	9392	31	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 2.

All (31) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
1:B:163:GLN:NE2	1:C:4:LYS:O	<u>distance (Å)</u> 2.26	overlap (Å) 0.68
1:C:212:LYS:NZ	1:C:252:ASP:OD1	2.26	0.67
1:C:330:ILE:HD12	1:C:363:SER:HB3	1.91	0.52
1:B:38:ASP:OD2	1:B:40:HIS:NE2	2.43	0.51
1:B:252:ASP:OD1	1:B:252:ASP:N	2.43	0.51
1:C:295:LEU:HD23	1:C:295:LEU:C	2.31	0.51
1:B:6:SER:O	1:B:349:ASN:ND2	2.43	0.50
1:B:324:GLU:OE2	1:B:388:ARG:NE	2.44	0.50
1:A:280:PHE:O	1:B:259:MET:HE3	2.11	0.49
4:B:503:NDP:O2X	4:B:503:NDP:O3B	2.28	0.49
1:A:279:ASP:OD2	1:B:252:ASP:HB2	2.13	0.48
1:B:330:ILE:HD12	1:B:363:SER:HB3	1.95	0.48
4:C:1205:NDP:O3X	7:C:1301:HOH:O	2.20	0.47
1:B:130:ILE:HD12	1:B:278:SER:HA	1.97	0.46
1:A:259:MET:HE1	1:B:280:PHE:O	2.17	0.45
1:B:209:LEU:HD22	1:B:227:PHE:CG	2.53	0.44
1:C:75:THR:O	4:C:1205:NDP:H2N	2.18	0.44
1:C:297[B]:CYS:SG	1:C:298:PRO:HD2	2.59	0.43
1:B:213:ASN:O	1:B:217:LYS:HA	2.19	0.43
1:C:319:TYR:HB2	1:C:325:THR:HG21	2.01	0.43
3:A:502:GOL:HO3	3:A:502:GOL:HO1	1.63	0.43
1:C:213:ASN:O	1:C:217:LYS:HA	2.19	0.42
1:C:415:LEU:N	1:C:415:LEU:HD22	2.33	0.42

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COHABABACA		DIEUIUU	DUIUE
0 0 1000100000			

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	$\operatorname{distance}\ (ext{Å})$	$overlap (\AA)$
1:A:71:VAL:O	1:A:71:VAL:HG23	2.20	0.42
1:C:71:VAL:HG23	1:C:71:VAL:O	2.21	0.41
3:A:502:GOL:O1	3:A:502:GOL:O3	2.24	0.41
1:A:75:THR:O	4:A:504:NDP:H2N	2.21	0.41
1:A:330:ILE:HD12	1:A:363:SER:HB3	2.03	0.40
1:B:297[B]:CYS:SG	1:B:298:PRO:HD2	2.61	0.40
1:A:6:SER:O	1:A:349:ASN:ND2	2.54	0.40
1:B:397:PHE:CE2	1:B:401:LEU:HD11	2.57	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	421/422 (100%)	404 (96%)	16 (4%)	1 (0%)	47 49	
1	В	412/422 (98%)	395 (96%)	16 (4%)	1 (0%)	47 49	
1	С	417/422 (99%)	403 (97%)	14 (3%)	0	100 100	
All	All	1250/1266 (99%)	1202 (96%)	46 (4%)	2 (0%)	47 49	

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	3	LYS
1	A	380	ILE

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	333/358~(93%)	333 (100%)	0		100	100
1	В	325/358 (91%)	323 (99%)	2 (1%)		86	90
1	С	327/358 (91%)	326 (100%)	1 (0%)		92	95
All	All	985/1074 (92%)	982 (100%)	3 (0%)		92	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	37	LEU
1	В	409	LEU
1	С	252	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the



expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Во	Bond lengths			Bond lengths Bond angles			les
MIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2		
2	AKG	A	501	5	9,9,9	1.35	0	11,11,11	1.54	3 (27%)		
2	AKG	В	502	5	9,9,9	1.37	1 (11%)	11,11,11	1.55	2 (18%)		
4	NDP	A	504	-	45,52,52	0.50	1 (2%)	53,80,80	0.58	1 (1%)		
4	NDP	В	503	-	45,52,52	0.52	0	53,80,80	0.56	1 (1%)		
4	NDP	С	1205	-	45,52,52	0.64	0	53,80,80	0.68	1 (1%)		
3	GOL	С	1204	-	5,5,5	0.88	0	5,5,5	0.91	0		
3	GOL	A	503	-	5,5,5	0.92	0	5,5,5	0.93	0		
3	GOL	A	502	-	5,5,5	0.89	0	5,5,5	0.94	0		
3	GOL	С	1201	-	5,5,5	0.88	0	5,5,5	0.92	0		
2	AKG	С	1203	5	9,9,9	1.41	1 (11%)	11,11,11	1.40	1 (9%)		

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	AKG	A	501	5	-	0/9/9/9	-
2	AKG	В	502	5	-	1/9/9/9	-
4	NDP	A	504	-	-	8/30/77/77	0/5/5/5
4	NDP	В	503	-	-	8/30/77/77	0/5/5/5
4	NDP	С	1205	-	-	8/30/77/77	0/5/5/5
3	GOL	С	1204	-	-	0/4/4/4	-
3	GOL	A	503	-	-	0/4/4/4	-
3	GOL	A	502	-	-	0/4/4/4	-
3	GOL	С	1201	-	-	0/4/4/4	-
2	AKG	С	1203	5	-	0/9/9/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\mathring{\mathbf{A}})$	$\operatorname{Ideal}(\text{\AA})$
2	С	1203	AKG	C3-C2	2.10	1.53	1.51
4	A	504	NDP	C8A-N7A	-2.09	1.31	1.34
2	В	502	AKG	C3-C2	2.06	1.53	1.51

All (9) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
4	В	503	NDP	C5A-C6A-N6A	2.37	123.95	120.35
2	A	501	AKG	C3-C2-C1	2.27	120.18	115.97
2	В	502	AKG	O2-C1-C2	2.26	120.16	113.97
4	A	504	NDP	C5A-C6A-N6A	2.26	123.78	120.35
4	С	1205	NDP	C5A-C6A-N6A	2.24	123.75	120.35
2	В	502	AKG	C3-C2-C1	2.17	120.00	115.97
2	A	501	AKG	O2-C1-C2	2.07	119.64	113.97
2	A	501	AKG	C3-C4-C5	-2.05	109.19	113.60
2	С	1203	AKG	O4-C5-C4	2.03	120.55	114.03

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	504	NDP	C5B-O5B-PA-O1A
4	A	504	NDP	C5D-O5D-PN-O1N
4	В	503	NDP	C5D-O5D-PN-O1N
4	В	503	NDP	C5D-O5D-PN-O2N
4	С	1205	NDP	C5B-O5B-PA-O1A
4	С	1205	NDP	C5D-O5D-PN-O2N
4	A	504	NDP	C5D-O5D-PN-O3
4	В	503	NDP	C5D-O5D-PN-O3
4	С	1205	NDP	C5B-O5B-PA-O3
4	A	504	NDP	C5D-O5D-PN-O2N
4	С	1205	NDP	C5D-O5D-PN-O1N
4	A	504	NDP	O4D-C1D-N1N-C2N
2	В	502	AKG	O2-C1-C2-O5
4	В	503	NDP	O4D-C1D-N1N-C2N
4	С	1205	NDP	O4D-C1D-N1N-C2N
4	A	504	NDP	C2D-C1D-N1N-C2N
4	В	503	NDP	C2D-C1D-N1N-C2N
4	С	1205	NDP	C2D-C1D-N1N-C2N
4	A	504	NDP	O4D-C1D-N1N-C6N
4	С	1205	NDP	C5D-O5D-PN-O3
4	В	503	NDP	O4D-C1D-N1N-C6N
4	В	503	NDP	C5B-O5B-PA-O1A
4	С	1205	NDP	O4D-C1D-N1N-C6N
4	A	504	NDP	C2D-C1D-N1N-C6N
4	В	503	NDP	C2D-C1D-N1N-C6N

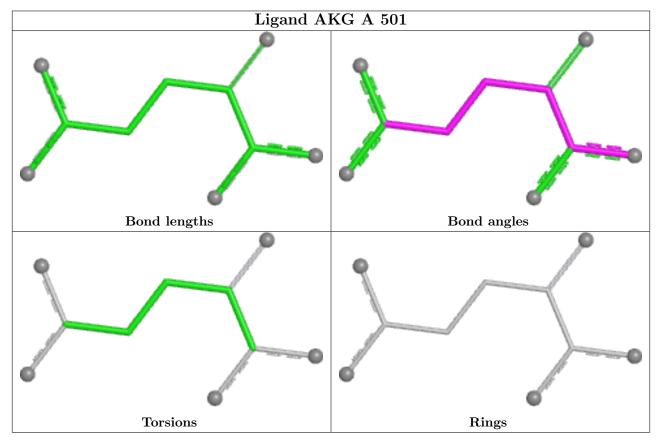
There are no ring outliers.

4 monomers are involved in 6 short contacts:

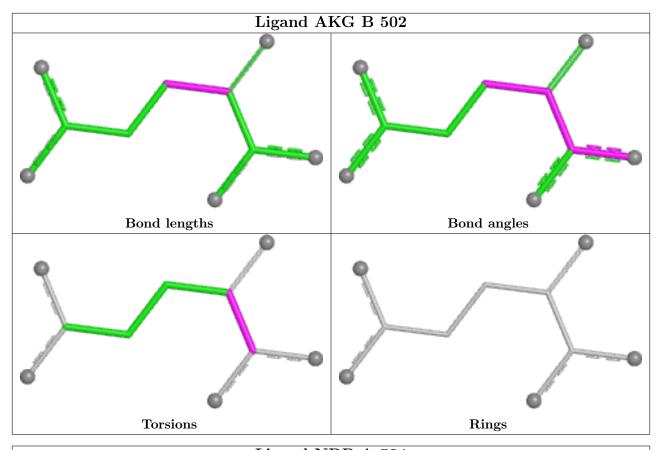


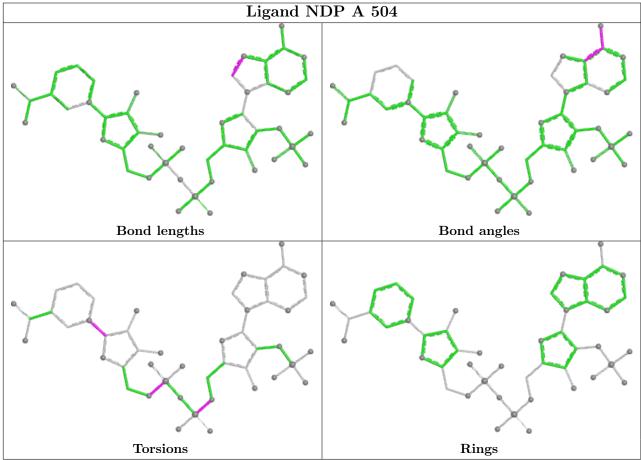
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	504	NDP	1	0
4	В	503	NDP	1	0
4	С	1205	NDP	2	0
3	A	502	GOL	2	0

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.

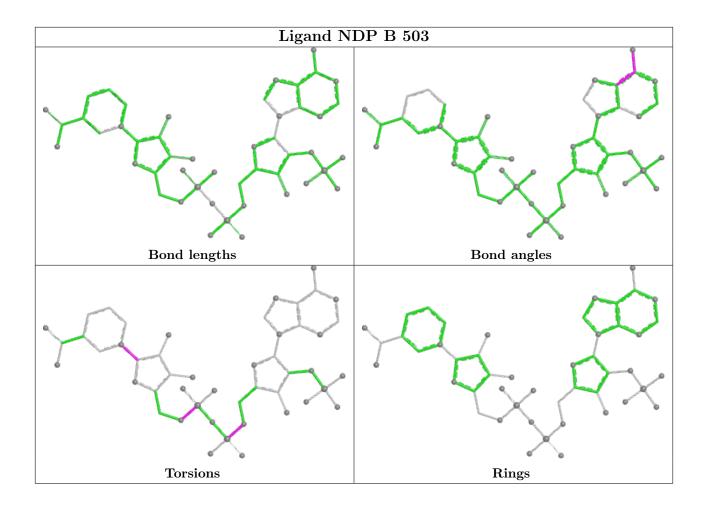




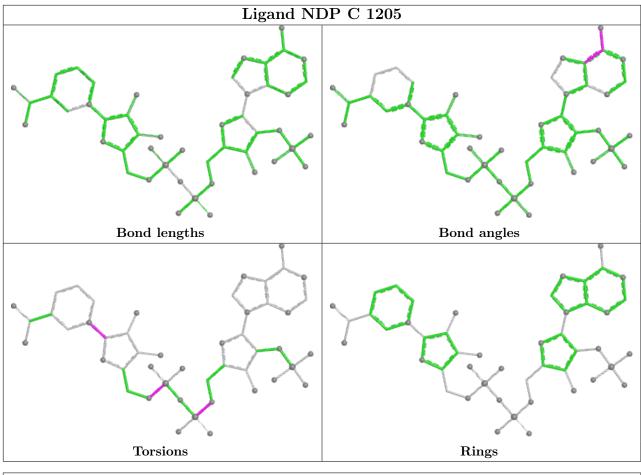


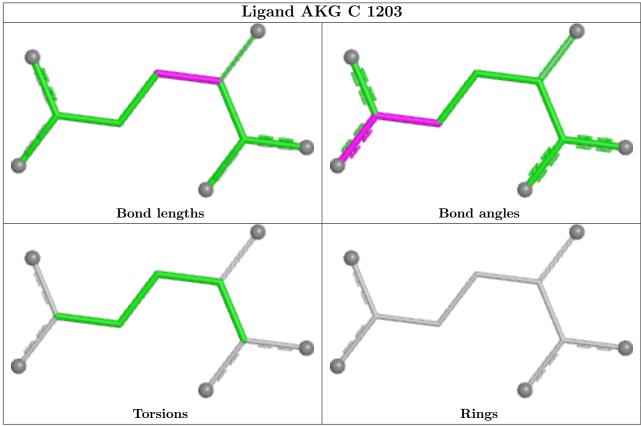














5.7 Other polymers (i)

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>	# RSRZ > 2	$OWAB(A^2)$	Q<0.9
1	A	415/422 (98%)	0.49	14 (3%) 45 51	39, 53, 79, 134	0
1	В	412/422 (97%)	0.72	38 (9%) 9 11	41, 67, 99, 138	0
1	С	414/422 (98%)	0.27	4 (0%) 82 85	38, 54, 81, 121	0
All	All	1241/1266 (98%)	0.49	56 (4%) 33 38	38, 57, 90, 138	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	409	LEU	5.6
1	В	31	ILE	4.4
1	В	32	PHE	3.9
1	В	405	LEU	3.8
1	В	386	VAL	3.8
1	В	10	VAL	3.6
1	В	380	ILE	3.6
1	С	205	TRP	3.5
1	В	312	VAL	3.5
1	A	244	ILE	3.5
1	A	205	TRP	3.4
1	В	352	LEU	3.4
1	В	319	TYR	3.3
1	В	113	ILE	3.2
1	В	205	TRP	3.2
1	В	395	PHE	3.1
1	В	5	ILE	3.1
1	В	371	PHE	3.0
1	В	354	PHE	2.9
1	A	14[A]	GLN	2.9
1	A	73	CYS	2.9
1	В	381	LYS	2.8
1	В	401	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	В	340	LEU	2.7
1	В	35	VAL	2.7
1	A	154	ILE	2.7
1	A	352	LEU	2.7
1	В	367	ILE	2.6
1	В	118	PRO	2.6
1	В	379	CYS	2.6
1	В	376	LEU	2.5
1	В	7	GLY	2.5
1	A	208	TYR	2.5
1	В	117	ILE	2.5
1	С	322	GLY	2.5
1	A	3	LYS	2.5
1	В	292	THR	2.4
1	В	298	PRO	2.4
1	В	341	ALA	2.4
1	С	3	LYS	2.3
1	В	303	VAL	2.3
1	В	26	ILE	2.3
1	A	255	VAL	2.2
1	A	245	TRP	2.2
1	В	392	LEU	2.2
1	A	417	HIS	2.2
1	В	33	PRO	2.1
1	A	45	GLY	2.1
1	С	32	PHE	2.1
1	В	154	ILE	2.1
1	В	291	MET	2.1
1	В	152	VAL	2.1
1	A	130	ILE	2.0
1	В	383	LEU	2.0
1	В	410	ALA	2.0
1	A	15	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.



6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

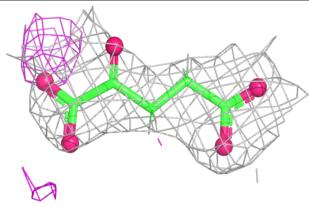
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
3	GOL	С	1204	6/6	0.10	0.28	70,99,119,127	0
3	GOL	С	1201	6/6	0.60	0.27	76,92,111,115	0
3	GOL	A	502	6/6	0.68	0.63	115,129,152,155	0
6	CL	В	504[A]	1/1	0.75	0.11	97,97,97,97	0
3	GOL	A	503	6/6	0.83	0.17	101,121,136,143	0
2	AKG	В	502	10/10	0.83	0.23	57,73,88,88	0
6	CL	С	1206[A]	1/1	0.83	0.10	88,88,88,88	0
2	AKG	A	501	10/10	0.89	0.15	42,48,55,55	0
4	NDP	В	503	48/48	0.89	0.20	63,90,138,166	0
2	AKG	С	1203	10/10	0.91	0.14	44,46,55,55	0
5	CA	В	501	1/1	0.92	0.07	60,60,60,60	0
6	CL	A	506[B]	1/1	0.92	0.22	86,86,86,86	0
4	NDP	A	504	48/48	0.96	0.17	38,46,54,60	0
4	NDP	С	1205	48/48	0.96	0.15	38,48,59,69	0
5	CA	A	505	1/1	0.97	0.14	46,46,46,46	0
5	CA	С	1202	1/1	0.98	0.09	46,46,46,46	0

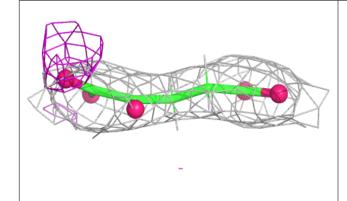
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

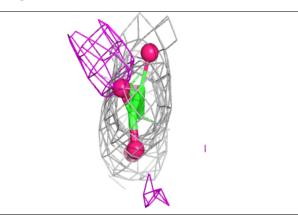


Electron density around AKG B 502:

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

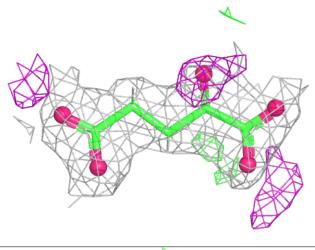


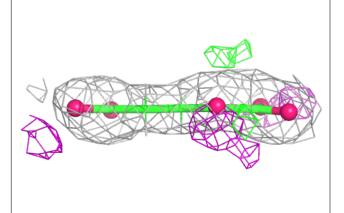


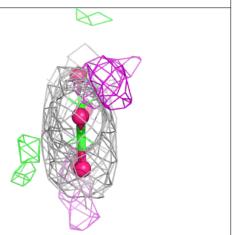


Electron density around AKG A 501:

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



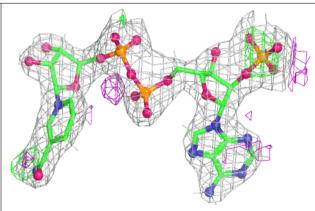


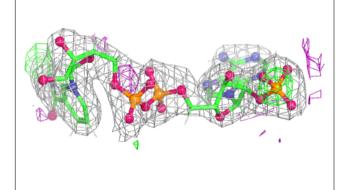


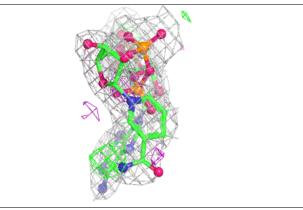


Electron density around NDP B 503:

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

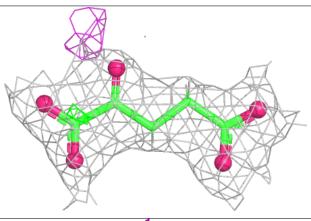


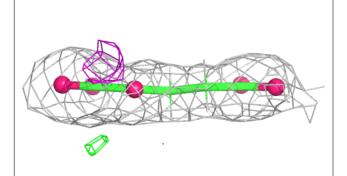


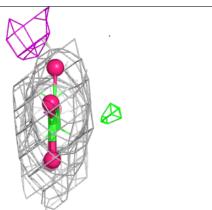


Electron density around AKG C 1203:

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







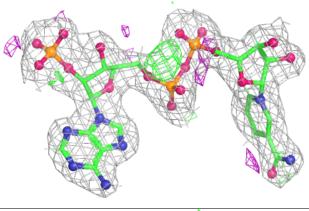


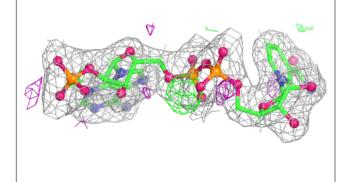
Electron density around CA B 501: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

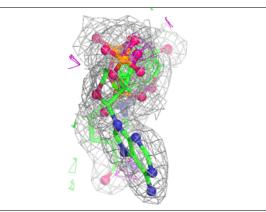


Electron density around NDP A 504:

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

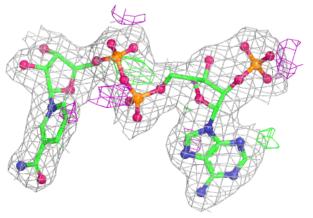


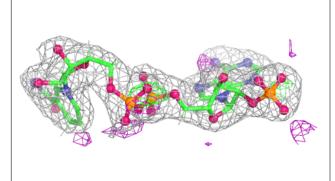


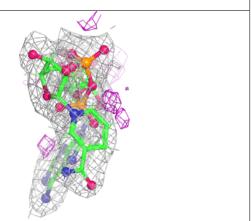


Electron density around NDP C 1205:

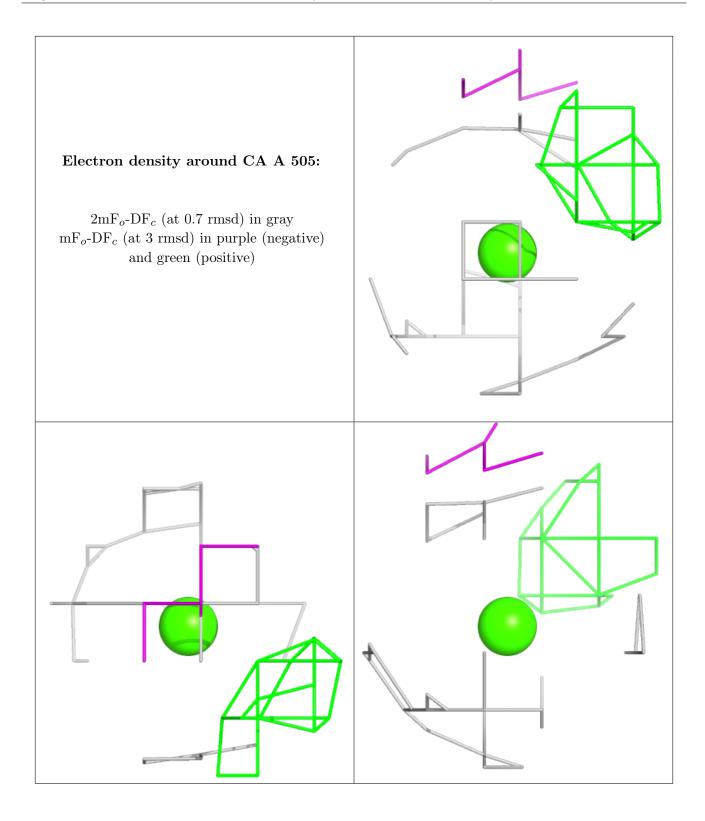
 $2 \mathrm{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



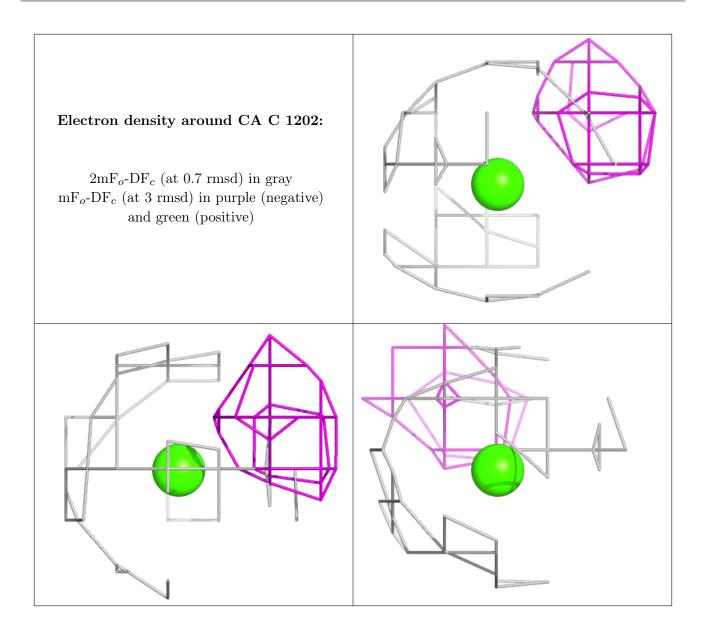












6.5 Other polymers (i)

There are no such residues in this entry.

