Full wwPDB X-ray Structure Validation Report (i)

May 14, 2020 – 12:19 pm BST

PDB ID	:	2I7N
Title	:	Crystal structure of human PANK1 alpha: the catalytic core domain in complex with AcCoA
Authors	:	Hong, B.S.; Wang, L.; Tempel, W.; Loppnau, P.; Allali-Hassani, A.; Arrowsmith, C.H.; Edwards, A.M.; Sundstrom, M.; Weigelt, J.; Bochkarev, A.; Park, H.W.
Deposited on	:	2006-08-31
Resolution	:	1.90 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:

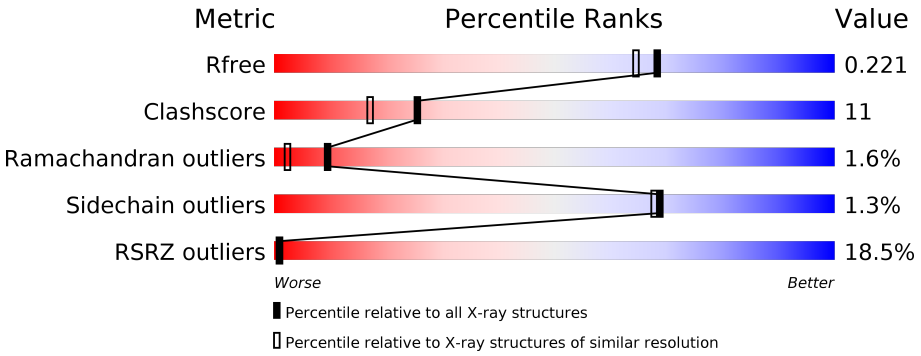
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.90 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	360	21% 68% 21% • 10%
1	B	360	13% 71% 20% • 8%

2 Entry composition

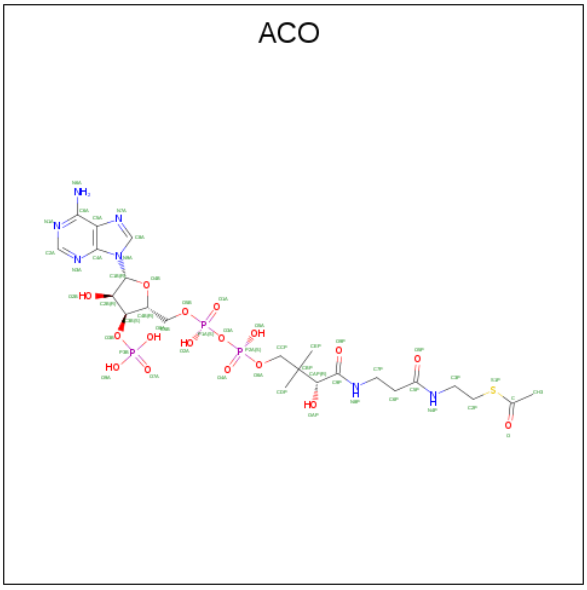
There are 3 unique types of molecules in this entry. The entry contains 5453 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Pantothenate kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	0	0
			2538	1628	419	468	23			
1	B	333	Total	C	N	O	S	0	0	0
			2605	1671	431	479	24			

- Molecule 2 is ACETYL COENZYME *A (three-letter code: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			29	13	2	11	2	1		
2	B	1	Total	C	N	O	P	S	0	0
			29	13	2	11	2	1		

- Molecule 3 is water.

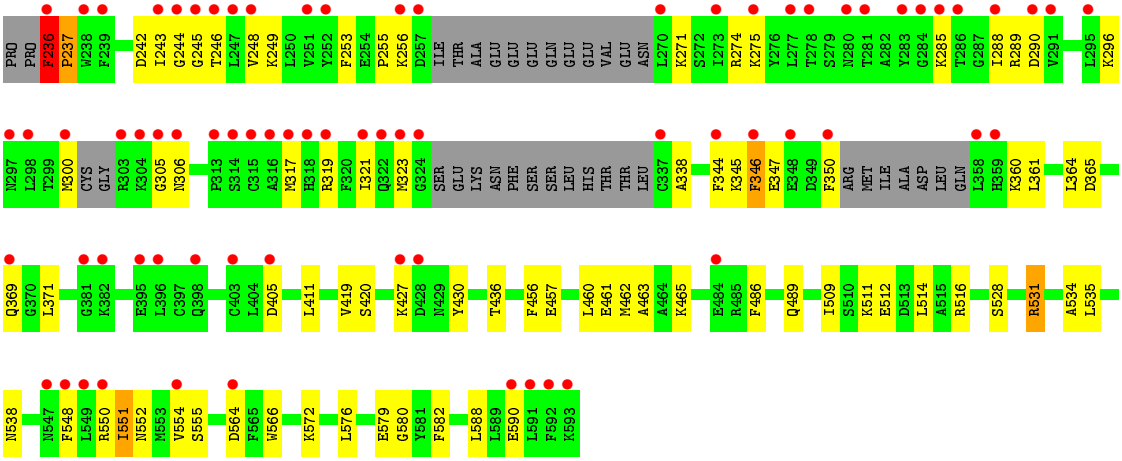
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	92	Total O 92 92	0	0
3	B	160	Total O 160 160	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

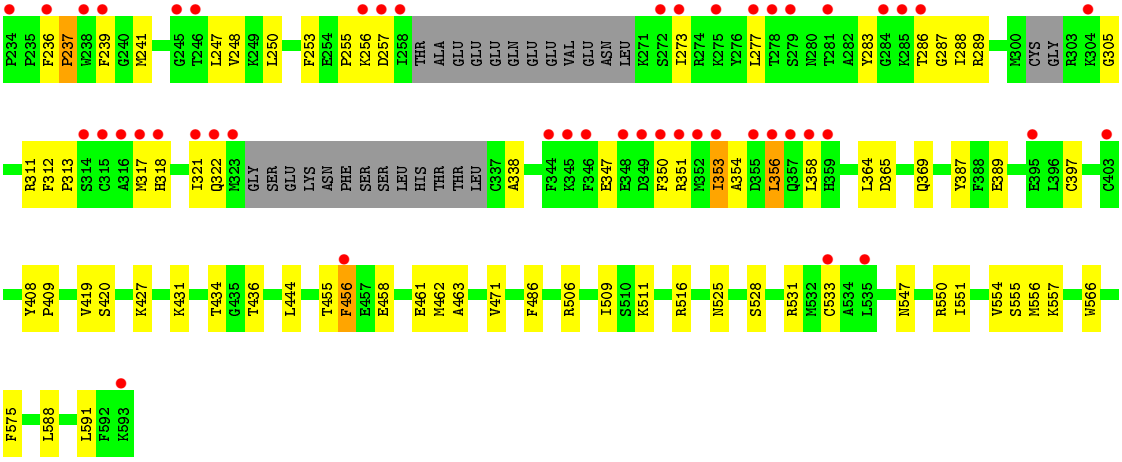
- Molecule 1: Pantothenate kinase 1

Chain A:



- Molecule 1: Pantothenate kinase 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	92.99Å 92.99Å 197.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.46 – 1.90 39.46 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.7 (39.46-1.90) 96.8 (39.46-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	7.93 (at 1.89Å)	Xtriage
Refinement program	CNS 1.1, REFMAC 5.2.0005	Depositor
R, R_{free}	0.222 , 0.243 0.219 , 0.221	Depositor DCC
R_{free} test set	3699 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	24.5	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 36.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.108 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5453	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACO

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	0.36	0/2586	0.58	2/3471 (0.1%)
1	B	0.39	0/2656	0.71	3/3568 (0.1%)
All	All	0.37	0/5242	0.65	5/7039 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	236	PHE	C-N-CD	-20.45	75.60	120.60
1	B	236	PHE	C-N-CA	13.64	179.29	122.00
1	A	236	PHE	C-N-CD	-11.72	94.82	120.60
1	A	551	ILE	N-CA-C	5.43	125.67	111.00
1	B	237	PRO	CA-N-CD	-5.33	104.04	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2538	0	2528	60	0
1	B	2605	0	2602	52	0
2	A	29	0	23	0	0
2	B	29	0	23	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	92	0	0	3	0
3	B	160	0	0	6	0
All	All	5453	0	5176	110	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 11.

All (110) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:ARG:HG3	1:A:551:ILE:HG13	1.54	0.89
1:A:457:GLU:O	1:A:461:GLU:HG2	1.74	0.86
1:A:552:ASN:OD1	1:A:554:VAL:HG12	1.83	0.78
1:B:239:PHE:HD2	1:B:250:LEU:HD11	1.55	0.69
1:A:344:PHE:HA	1:A:347:GLU:HB2	1.75	0.69
1:B:256:LYS:HG3	1:B:305:GLY:HA2	1.74	0.69
1:A:296:LYS:HG2	1:A:306:ASN:ND2	2.08	0.68
1:B:351:ARG:HB2	1:B:356:LEU:HB2	1.76	0.68
1:A:285:LYS:HD3	1:A:319:ARG:HH12	1.61	0.66
1:B:551:ILE:N	1:B:551:ILE:HD12	2.10	0.65
1:B:462:MET:HE1	1:B:511:LYS:HB3	1.80	0.63
1:B:365:ASP:O	1:B:369:GLN:HG2	1.99	0.62
1:B:431:LYS:HG2	3:B:994:HOH:O	2.00	0.60
1:B:353:ILE:HD12	1:B:353:ILE:N	2.17	0.60
1:B:286:THR:HG22	1:B:313:PRO:HD2	1.83	0.60
1:A:456:PHE:CE2	1:A:460:LEU:HD11	2.37	0.60
1:A:457:GLU:HG3	1:A:551:ILE:HD13	1.84	0.60
1:B:273:ILE:HD12	1:B:273:ILE:N	2.16	0.60
1:B:347:GLU:HG3	1:B:356:LEU:HD11	1.85	0.59
1:A:285:LYS:HD3	1:A:319:ARG:NH1	2.17	0.58
1:B:321:ILE:HD11	1:B:350:PHE:CE1	2.38	0.58
1:A:317:MET:O	1:A:321:ILE:HG12	2.04	0.57
1:B:247:LEU:HD23	1:B:248:VAL:N	2.18	0.57
1:B:273:ILE:HD12	1:B:273:ILE:H	1.68	0.57
1:B:463:ALA:O	1:B:516:ARG:HD3	2.05	0.56
1:B:356:LEU:HG	1:B:358:LEU:H	1.70	0.55
1:A:344:PHE:HD1	1:A:347:GLU:HG3	1.73	0.54
1:A:554:VAL:HG13	1:A:555:SER:N	2.22	0.54
1:A:531:ARG:NH1	1:A:535:LEU:HG	2.22	0.54
1:A:243:ILE:HD12	1:A:317:MET:HE1	1.89	0.54
1:A:365:ASP:OD1	1:A:430:TYR:OH	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:VAL:HB	1:A:436:THR:CG2	2.39	0.53
1:A:564:ASP:OD1	1:A:572:LYS:HD3	2.08	0.53
1:B:338:ALA:HB3	1:B:358:LEU:HD11	1.91	0.53
1:A:509:ILE:HD12	1:A:514:LEU:HD21	1.90	0.53
1:A:538:ASN:ND2	3:A:870:HOH:O	2.41	0.52
1:B:287:GLY:HA2	1:B:312:PHE:HB3	1.90	0.52
1:A:419:VAL:HB	1:A:436:THR:HG22	1.91	0.52
1:B:317:MET:O	1:B:321:ILE:HG12	2.10	0.52
1:B:528:SER:HB2	1:B:566:TRP:CE2	2.44	0.51
1:A:528:SER:HB2	1:A:566:TRP:CE2	2.46	0.50
1:A:364:LEU:HD22	1:B:486:PHE:HZ	1.77	0.50
1:B:462:MET:CE	1:B:511:LYS:HB3	2.42	0.50
1:A:456:PHE:HE2	1:A:460:LEU:HD11	1.76	0.49
1:A:288:ILE:HG22	1:A:289:ARG:N	2.28	0.48
1:A:243:ILE:HD12	1:A:317:MET:CE	2.44	0.48
1:B:347:GLU:O	1:B:356:LEU:HD13	2.13	0.48
1:A:465:LYS:HE2	1:A:512:GLU:OE2	2.14	0.48
1:A:456:PHE:HZ	1:A:548:PHE:HD1	1.62	0.48
1:B:387:TYR:CE1	1:B:389:GLU:HG2	2.49	0.48
1:B:427:LYS:HE2	3:B:965:HOH:O	2.12	0.47
1:B:247:LEU:HD21	1:B:311:ARG:HB2	1.95	0.47
1:B:444:LEU:HD22	1:B:456:PHE:CD1	2.49	0.47
1:A:296:LYS:HG2	1:A:306:ASN:HD21	1.78	0.47
1:A:253:PHE:O	1:A:255:PRO:HD3	2.15	0.47
1:A:344:PHE:CD1	1:A:347:GLU:HG3	2.50	0.47
1:A:256:LYS:HG2	1:A:305:GLY:HA2	1.97	0.47
1:B:588:LEU:HD12	1:B:591:LEU:HD12	1.95	0.46
1:A:319:ARG:O	1:A:323:MET:HG3	2.16	0.46
1:A:345:LYS:C	1:A:347:GLU:H	2.19	0.46
1:A:344:PHE:CE2	1:A:360:LYS:HD3	2.51	0.46
1:B:318:HIS:O	1:B:322:GLN:HG3	2.16	0.46
1:A:249:LYS:HD3	1:A:249:LYS:N	2.31	0.46
1:A:579:GLU:HA	1:A:582:PHE:CE2	2.51	0.46
1:A:271:LYS:O	1:A:275:LYS:HG3	2.16	0.45
1:B:397:CYS:SG	1:B:557:LYS:HE2	2.56	0.45
1:B:531:ARG:NH1	3:B:956:HOH:O	2.49	0.45
1:A:236:PHE:N	1:A:236:PHE:CD1	2.85	0.45
1:A:236:PHE:HA	1:A:237:PRO:HD2	1.52	0.45
1:B:554:VAL:HG13	1:B:555:SER:N	2.31	0.45
1:A:486:PHE:HZ	1:B:364:LEU:HD22	1.81	0.44
1:A:338:ALA:O	1:A:360:LYS:HA	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:ARG:CB	1:B:356:LEU:HB2	2.46	0.44
1:A:248:VAL:HG11	1:A:317:MET:HE1	1.99	0.44
1:A:371:LEU:HG	1:A:576:LEU:CD1	2.46	0.44
1:B:277:LEU:HA	1:B:283:TYR:HE2	1.82	0.44
1:B:506:ARG:O	1:B:509:ILE:HG12	2.17	0.44
1:A:242:ASP:HB3	1:A:249:LYS:HE2	2.00	0.44
1:B:283:TYR:HE1	1:B:289:ARG:HB2	1.82	0.44
1:B:419:VAL:HB	1:B:436:THR:HG22	1.99	0.44
1:A:462:MET:CE	1:A:511:LYS:HB3	2.48	0.44
1:B:556:MET:HG2	1:B:575:PHE:CE2	2.53	0.43
1:B:591:LEU:HD21	3:B:985:HOH:O	2.16	0.43
1:B:547:ASN:HA	1:B:550:ARG:CD	2.49	0.43
1:A:249:LYS:HG2	1:A:580:GLY:O	2.18	0.43
1:A:411:LEU:HD11	1:A:534:ALA:HA	2.01	0.43
1:B:461:GLU:HG3	3:B:971:HOH:O	2.17	0.43
1:B:551:ILE:CD1	1:B:551:ILE:N	2.80	0.43
1:B:241:MET:HG2	1:B:250:LEU:HD13	1.99	0.43
1:B:547:ASN:HA	1:B:550:ARG:HD2	2.00	0.43
1:A:300:MET:HE1	1:A:588:LEU:HD21	2.01	0.43
1:B:353:ILE:H	1:B:353:ILE:HD12	1.83	0.43
1:B:288:ILE:HD12	1:B:311:ARG:HH12	1.83	0.43
1:A:489:GLN:HG2	3:A:856:HOH:O	2.18	0.42
1:A:253:PHE:HB2	1:A:300:MET:HE1	2.01	0.42
1:A:427:LYS:HG2	3:A:862:HOH:O	2.18	0.42
1:B:525:ASN:HB3	3:B:916:HOH:O	2.19	0.42
1:A:345:LYS:HD3	1:A:346:PHE:CE1	2.54	0.42
1:B:434:THR:HG21	1:B:533:CYS:SG	2.60	0.42
1:A:248:VAL:C	1:A:249:LYS:HD3	2.40	0.42
1:A:361:LEU:HD21	1:A:590:GLU:HG2	2.01	0.42
1:A:365:ASP:O	1:A:369:GLN:HG3	2.21	0.41
1:A:461:GLU:O	1:A:465:LYS:HD3	2.21	0.41
1:A:244:GLY:O	1:A:246:THR:N	2.54	0.41
1:A:463:ALA:O	1:A:516:ARG:HD3	2.20	0.41
1:B:408:TYR:HA	1:B:409:PRO:HA	1.85	0.41
1:B:455:THR:OG1	1:B:458:GLU:HG3	2.21	0.41
1:B:253:PHE:O	1:B:255:PRO:HD3	2.22	0.40
1:A:248:VAL:HG21	1:A:317:MET:HE2	2.02	0.40
1:A:274:ARG:HG2	1:A:274:ARG:HH11	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	315/360 (88%)	298 (95%)	12 (4%)	5 (2%)	9 2
1	B	325/360 (90%)	310 (95%)	10 (3%)	5 (2%)	10 3
All	All	640/720 (89%)	608 (95%)	22 (3%)	10 (2%)	9 2

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	PRO
1	B	237	PRO
1	B	356	LEU
1	A	245	GLY
1	A	290	ASP
1	A	405	ASP
1	A	346	PHE
1	B	257	ASP
1	B	354	ALA
1	B	353	ILE

5.3.2 Protein sidechains

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	273/305 (90%)	269 (98%)	4 (2%)	65 62
1	B	281/305 (92%)	278 (99%)	3 (1%)	73 73
All	All	554/610 (91%)	547 (99%)	7 (1%)	69 68

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	236	PHE
1	A	350	PHE
1	A	420	SER
1	A	531	ARG
1	B	420	SER
1	B	456	PHE
1	B	471	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	429	ASN
1	A	538	ASN
1	B	292	HIS
1	B	499	ASN
1	B	538	ASN

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 carbohydrates 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ACO	B	896	-	23,28,53	1.58	4 (17%)	34,40,79	1.81	5 (14%)
2	ACO	A	796	-	23,28,53	1.60	4 (17%)	34,40,79	1.81	5 (14%)

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	ACO	B	896	-	-	2/36/36/67	-
2	ACO	A	796	-	-	2/36/36/67	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	896	ACO	CH3-C	3.86	1.66	1.50
2	B	896	ACO	C-S1P	-3.79	1.52	1.75
2	A	796	ACO	CH3-C	3.78	1.65	1.50
2	A	796	ACO	C-S1P	-3.46	1.54	1.75
2	A	796	ACO	O-C	2.73	1.34	1.20
2	B	896	ACO	O-C	2.42	1.32	1.20
2	A	796	ACO	O5P-C5P	2.07	1.27	1.23
2	B	896	ACO	C9P-N8P	2.03	1.38	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	896	ACO	C3P-N4P-C5P	5.80	133.60	122.84
2	A	796	ACO	C3P-N4P-C5P	5.46	132.97	122.84
2	A	796	ACO	O-C-CH3	-5.27	101.46	123.07
2	B	896	ACO	O-C-CH3	-4.97	102.69	123.07
2	B	896	ACO	O2A-P1A-O3A	3.51	116.41	104.64
2	A	796	ACO	O2A-P1A-O3A	3.30	115.69	104.64
2	A	796	ACO	C2P-C3P-N4P	-2.90	106.31	112.42
2	B	896	ACO	C2P-C3P-N4P	-2.41	107.36	112.42
2	A	796	ACO	CH3-C-S1P	2.02	128.15	114.20
2	B	896	ACO	CH3-C-S1P	2.01	128.11	114.20

There are no chirality outliers.

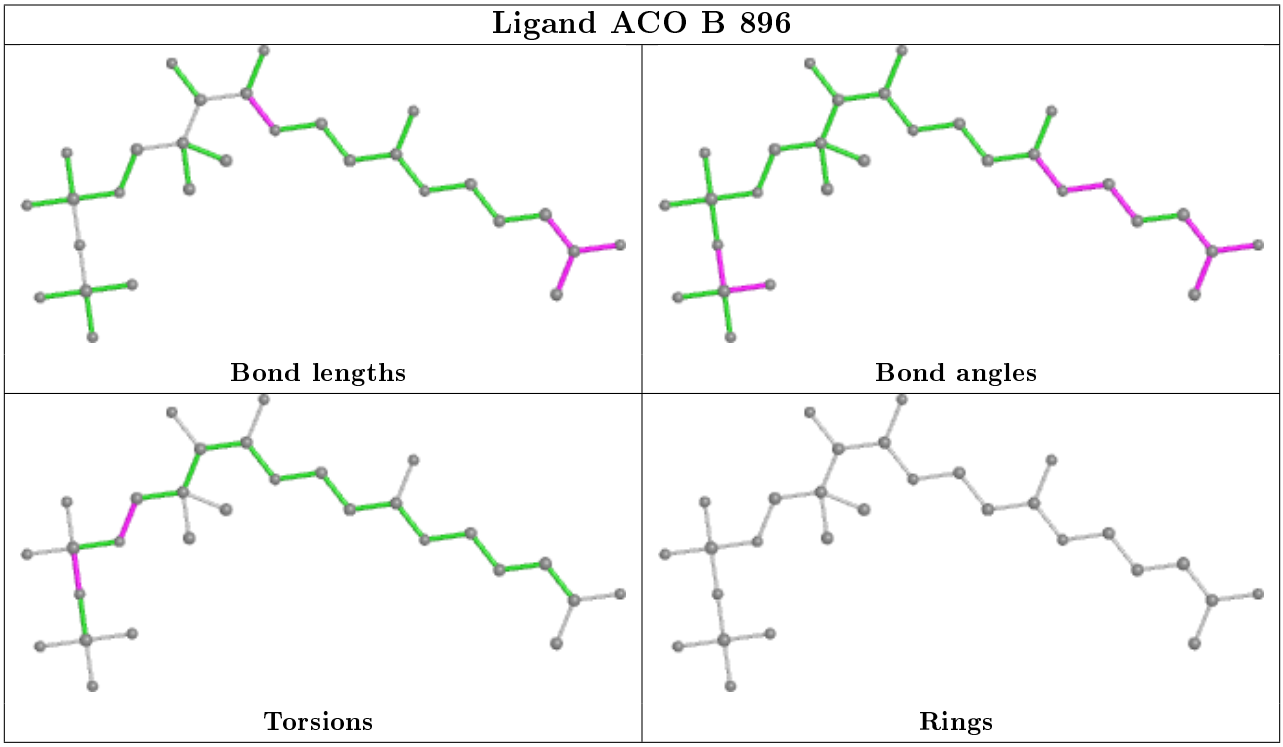
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	896	ACO	P1A-O3A-P2A-O5A
2	A	796	ACO	P1A-O3A-P2A-O5A
2	B	896	ACO	CBP-CCP-O6A-P2A
2	A	796	ACO	CBP-CCP-O6A-P2A

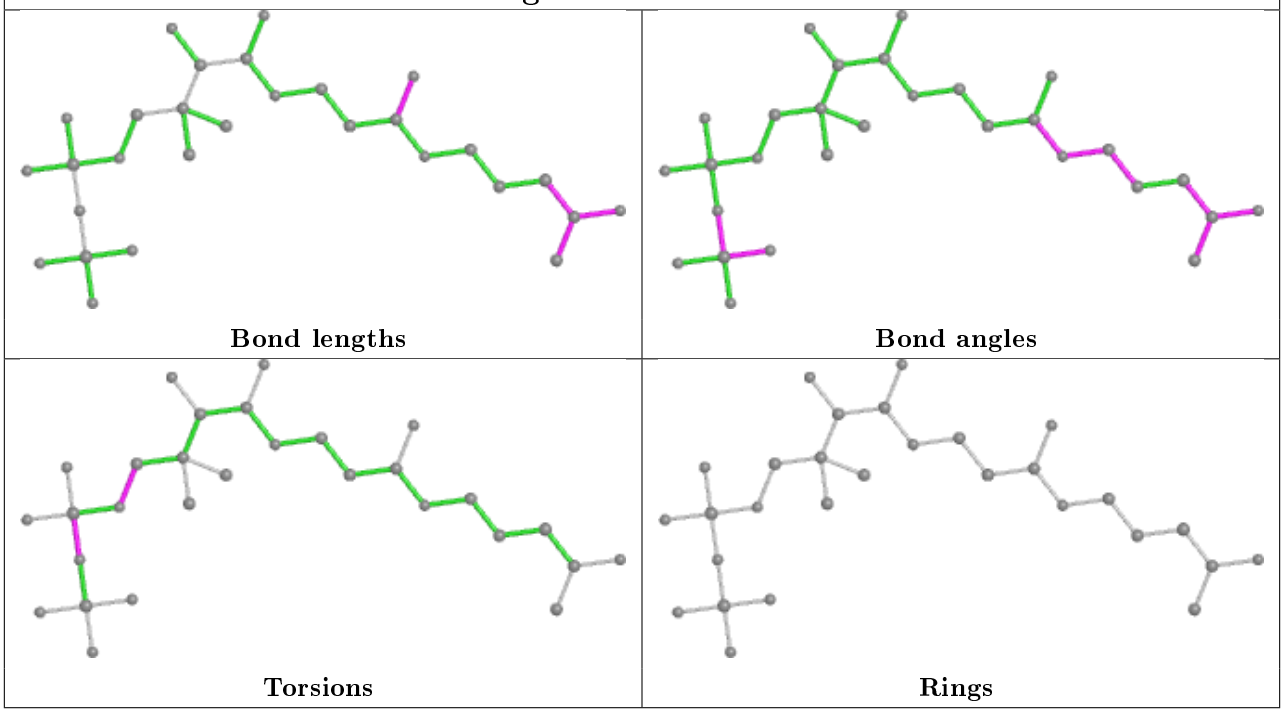
There are no ring outliers.

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.



Ligand ACO A 796



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	325/360 (90%)	1.25	74 (22%)	0	0	14, 38, 75, 83	0
1	B	333/360 (92%)	0.94	48 (14%)	2	2	12, 28, 72, 82	0
All	All	658/720 (91%)	1.09	122 (18%)	1	1	12, 33, 74, 83	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	350	PHE	16.4
1	B	318	HIS	9.8
1	A	321	ILE	8.7
1	B	356	LEU	8.7
1	B	352	MET	8.7
1	A	238	TRP	7.5
1	B	285	LYS	7.4
1	A	286	THR	7.2
1	B	258	ILE	6.8
1	A	236	PHE	6.4
1	B	353	ILE	6.3
1	A	246	THR	6.0
1	B	351	ARG	5.6
1	A	281	THR	5.6
1	B	321	ILE	5.5
1	A	318	HIS	5.5
1	B	236	PHE	5.4
1	B	286	THR	5.4
1	A	247	LEU	5.3
1	B	355	ASP	5.2
1	B	357	GLN	5.1
1	A	315	CYS	5.1
1	A	319	ARG	5.0
1	A	398	GLN	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	322	GLN	4.9
1	B	346	PHE	4.8
1	B	273	ILE	4.8
1	A	244	GLY	4.7
1	A	593	LYS	4.7
1	A	358	LEU	4.6
1	A	273	ILE	4.5
1	B	257	ASP	4.4
1	A	403	CYS	4.3
1	B	317	MET	4.3
1	A	592	PHE	4.3
1	A	248	VAL	4.2
1	A	297	ASN	4.1
1	A	288	ILE	4.1
1	B	278	THR	4.0
1	B	348	GLU	4.0
1	A	550	ARG	4.0
1	A	239	PHE	3.9
1	A	303	ARG	3.9
1	A	314	SER	3.8
1	B	350	PHE	3.7
1	B	239	PHE	3.7
1	A	280	ASN	3.6
1	A	291	VAL	3.6
1	B	395	GLU	3.6
1	A	245	GLY	3.6
1	B	284	GLY	3.5
1	A	270	LEU	3.5
1	A	405	ASP	3.5
1	A	344	PHE	3.5
1	B	323	MET	3.4
1	B	304	LYS	3.4
1	B	593	LYS	3.4
1	B	359	HIS	3.4
1	A	317	MET	3.4
1	A	277	LEU	3.3
1	B	344	PHE	3.3
1	A	359	HIS	3.2
1	B	234	PRO	3.2
1	A	256	LYS	3.2
1	A	285	LYS	3.1
1	A	298	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	358	LEU	3.1
1	A	547	ASN	3.1
1	A	300	MET	3.1
1	A	382	LYS	3.1
1	B	272	SER	3.1
1	B	315	CYS	3.0
1	B	314	SER	3.0
1	A	275	LYS	3.0
1	A	395	GLU	3.0
1	A	252	TYR	3.0
1	B	345	LYS	2.9
1	B	246	THR	2.8
1	A	427	LYS	2.8
1	A	324	GLY	2.8
1	A	313	PRO	2.8
1	B	322	GLN	2.8
1	A	283	TYR	2.8
1	B	403	CYS	2.8
1	A	348	GLU	2.7
1	A	278	THR	2.7
1	A	323	MET	2.7
1	B	245	GLY	2.7
1	B	238	TRP	2.7
1	B	316	ALA	2.7
1	B	279	SER	2.6
1	A	590	GLU	2.6
1	A	381	GLY	2.6
1	B	349	ASP	2.5
1	A	290	ASP	2.5
1	A	257	ASP	2.5
1	B	277	LEU	2.5
1	B	533	CYS	2.5
1	A	305	GLY	2.4
1	A	346	PHE	2.4
1	A	548	PHE	2.4
1	A	591	LEU	2.4
1	B	275	LYS	2.4
1	A	396	LEU	2.4
1	A	284	GLY	2.4
1	A	337	CYS	2.4
1	B	256	LYS	2.3
1	A	243	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	316	ALA	2.2
1	B	281	THR	2.2
1	B	535	LEU	2.2
1	A	484	GLU	2.2
1	A	251	VAL	2.2
1	A	369	GLN	2.1
1	A	428	ASP	2.1
1	A	564	ASP	2.1
1	B	456	PHE	2.1
1	A	306	ASN	2.1
1	A	554	VAL	2.0
1	A	295	LEU	2.0
1	A	549	LEU	2.0
1	A	304	LYS	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 carbohydrates in this entry.

6.4 Ligands (i)

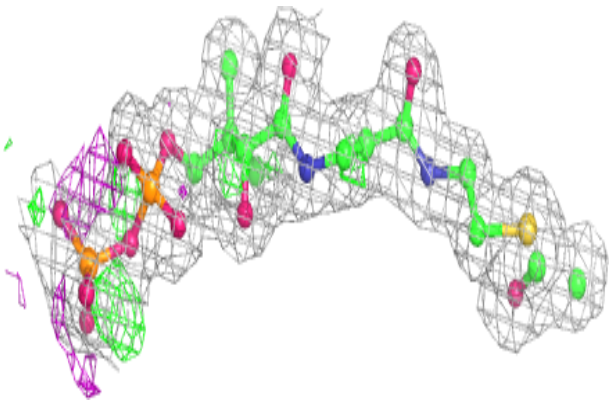
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

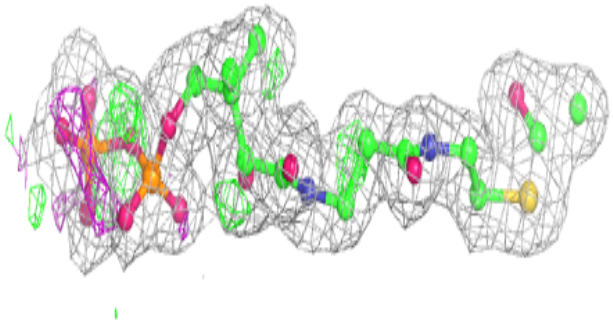
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ACO	B	896	29/51	0.92	0.14	16,20,37,39	0
2	ACO	A	796	29/51	0.93	0.14	15,20,43,45	0

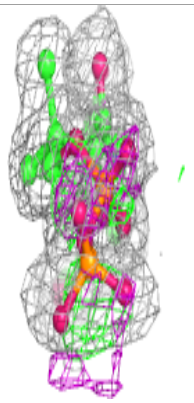
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACO B 896:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

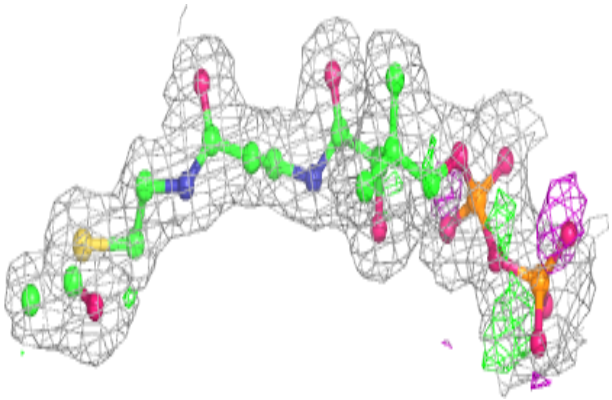


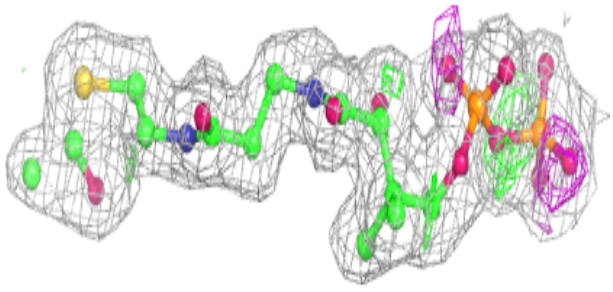


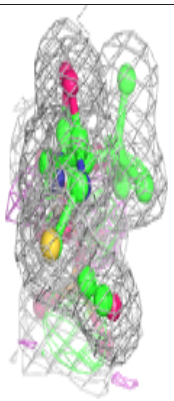


Electron density around ACO A 796:

$2mF_o$-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.