Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:06 am BST

PDB ID	:	1HAK
Title	:	CRYSTAL STRUCTURE OF RECOMBINANT HUMAN PLACENTAL ANNEXIN V COMPLEXED WITH K-201 AS A CALCIUM CHANNEL ACTIVITY INHIBITOR
Authors	:	Ago, H.; Inagaki, E.; Miyano, M.
Deposited on	:	1997-12-10
Resolution	:	3.00 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 ⓘ symbol.

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

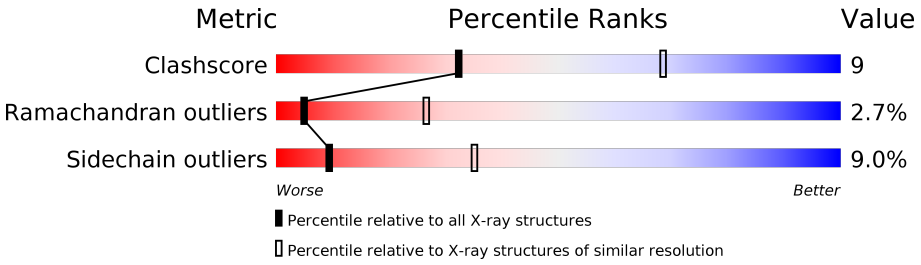
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.00 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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	320	66% 28% 5% •
1	B	320	71% 25% • •

2 Entry composition

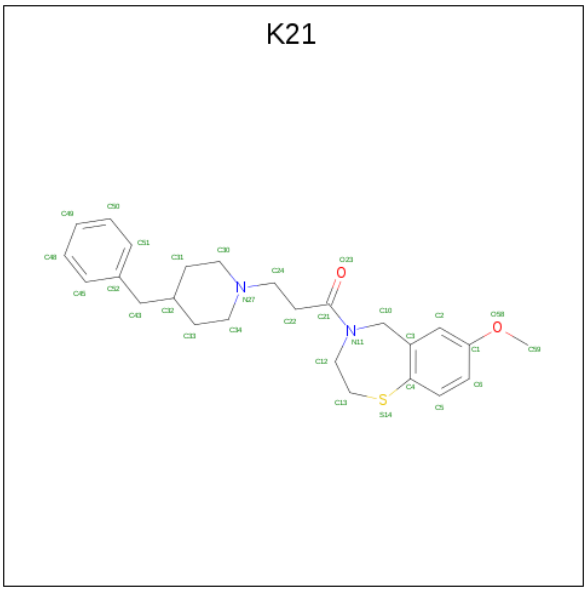
There are 3 unique types of molecules in this entry. The entry contains 5195 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ANNEXIN V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	318	Total	C	N	O	S	0	0	0
			2513	1582	422	501	8			
1	A	318	Total	C	N	O	S	0	0	0
			2513	1582	422	501	8			

- Molecule 2 is 4-[3-{1-(4-BENZYL)PIPERODINYL}PROPIONYL]-7-METHOXY-2,3,4,5-TERTRAHYDRO-1,4-BENZOTHIAZEPINE (three-letter code: K21) (formula: $C_{25}H_{32}N_2O_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			30	25	2	2	1		
2	A	1	Total	C	N	O	S	0	0
			30	25	2	2	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	59	Total O 59 59	0	0
3	A	50	Total O 50 50	0	0

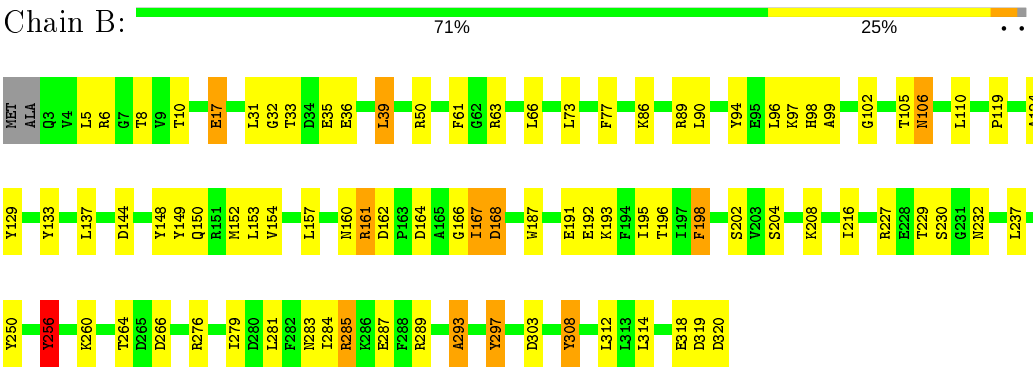
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

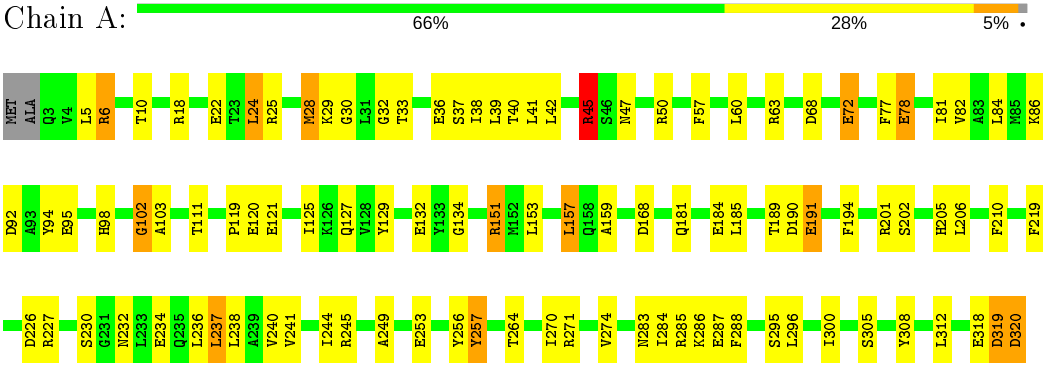
- Molecule 1: ANNEXIN V

Chain B:



- Molecule 1: ANNEXIN V

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	99.30Å 99.30Å 130.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	97.4 (20.00-3.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.206 , 0.331	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5195	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K21

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	0.88	1/2547 (0.0%)	1.53	9/3427 (0.3%)
1	B	0.91	0/2547	1.51	15/3427 (0.4%)
All	All	0.89	1/5094 (0.0%)	1.52	24/6854 (0.4%)

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	8
1	B	0	10
All	All	0	18

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	320	ASP	C-OXT	6.21	1.35	1.23

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	133	TYR	CB-CG-CD1	-7.51	116.49	121.00
1	A	308	TYR	CB-CG-CD2	-7.20	116.68	121.00
1	A	91	TYR	CB-CG-CD2	-6.55	117.07	121.00
1	A	50	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	B	227	ARG	CA-CB-CG	6.22	127.08	113.40
1	A	320	ASP	N-CA-C	6.21	127.78	111.00
1	B	106	ASN	CA-CB-CG	-6.04	100.12	113.40
1	B	230	SER	N-CA-C	5.96	127.09	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	28	MET	CG-SD-CE	-5.86	90.83	100.20
1	A	151	ARG	CD-NE-CZ	-5.77	115.52	123.60
1	B	250	TYR	CB-CG-CD2	-5.59	117.65	121.00
1	A	285	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	102	GLY	N-CA-C	5.51	126.88	113.10
1	B	106	ASN	N-CA-C	5.49	125.83	111.00
1	B	297	TYR	CB-CG-CD2	-5.44	117.74	121.00
1	A	318	GLU	N-CA-C	5.41	125.62	111.00
1	B	129	TYR	CB-CG-CD2	-5.30	117.82	121.00
1	B	227	ARG	N-CA-C	5.26	125.21	111.00
1	B	308	TYR	N-CA-CB	-5.20	101.23	110.60
1	B	293	ALA	N-CA-C	5.18	124.99	111.00
1	B	308	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	B	89	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	B	285	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	B	256	TYR	CB-CG-CD2	-5.08	117.95	121.00

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	ARG	Sidechain
1	A	245	ARG	Sidechain
1	A	256	TYR	Sidechain
1	A	257	TYR	Sidechain
1	A	30	GLY	Peptide
1	A	319	ASP	Peptide
1	A	45	ARG	Sidechain
1	A	94	TYR	Sidechain
1	B	105	THR	Peptide
1	B	148	TYR	Sidechain
1	B	161	ARG	Sidechain
1	B	191	GLU	Peptide
1	B	198	PHE	Sidechain
1	B	204	SER	Peptide
1	B	276	ARG	Sidechain
1	B	293	ALA	Peptide
1	B	297	TYR	Sidechain
1	B	50	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2513	0	2514	52	0
1	B	2513	0	2514	34	0
2	A	30	0	32	1	0
2	B	30	0	32	9	0
3	A	50	0	0	0	0
3	B	59	0	0	1	0
All	All	5195	0	5092	90	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 9.

All (90) 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:57:PHE:HE1	1:A:63:ARG:HB2	1.49	0.77
1:A:191:GLU:HA	1:A:194:PHE:CE2	2.23	0.73
1:A:6:ARG:H	1:A:283:ASN:HD21	1.40	0.68
1:A:41:LEU:HG	1:A:45:ARG:HH11	1.63	0.63
1:A:253:GLU:HG3	1:A:257:TYR:HE1	1.64	0.62
1:A:90:LEU:HD21	1:A:132:GLU:HG3	1.81	0.62
1:B:198:PHE:HB3	1:B:240:VAL:HG11	1.82	0.61
1:B:164:ASP:HB3	1:A:6:ARG:HG2	1.83	0.61
1:A:253:GLU:HG3	1:A:257:TYR:CE1	2.35	0.61
1:B:161:ARG:HD3	2:B:901:K21:H6	1.84	0.60
1:B:126:LYS:HG2	1:B:137:LEU:HD23	1.85	0.58
1:B:86:LYS:NZ	1:B:90:LEU:HB3	2.20	0.57
1:A:253:GLU:O	1:A:257:TYR:HD1	1.89	0.56
1:A:296:LEU:HG	1:A:300:ILE:HD11	1.89	0.55
1:A:153:LEU:O	1:A:157:LEU:HB2	2.05	0.55
1:A:98:HIS:O	1:A:103:ALA:HB2	2.06	0.55
1:B:119:PRO:HD3	2:B:901:K21:C5	2.37	0.55
1:A:201:ARG:HB3	1:A:205:HIS:HD2	1.72	0.55
1:A:249:ALA:HB2	1:A:287:GLU:HG2	1.89	0.55
1:B:61:PHE:HB3	1:B:63:ARG:HG3	1.89	0.55
1:B:96:LEU:HD22	1:B:110:LEU:HD23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:MET:HE3	1:B:195:ILE:HA	1.89	0.54
1:A:284:ILE:O	1:A:288:PHE:HB2	2.08	0.54
1:B:86:LYS:HE3	1:B:94:TYR:CD1	2.42	0.54
1:A:230:SER:OG	1:A:234:GLU:HB2	2.07	0.54
1:A:39:LEU:HD23	1:A:40:THR:HG23	1.90	0.53
1:B:97:LYS:HE3	1:B:98:HIS:CD2	2.43	0.53
1:A:18:ARG:HB2	1:A:60:LEU:HD21	1.91	0.53
1:A:57:PHE:CE1	1:A:63:ARG:HB2	2.39	0.52
1:A:191:GLU:HA	1:A:194:PHE:CZ	2.45	0.52
1:B:149:TYR:CZ	1:B:153:LEU:HD11	2.43	0.52
1:A:39:LEU:HD12	1:A:77:PHE:CE1	2.45	0.51
1:A:6:ARG:H	1:A:283:ASN:ND2	2.06	0.51
1:A:202:SER:O	1:A:205:HIS:HB3	2.10	0.51
1:B:153:LEU:O	1:B:157:LEU:HB2	2.11	0.51
1:B:285:ARG:NH2	1:B:319:ASP:HB2	2.26	0.50
1:B:35:GLU:O	1:B:39:LEU:HB2	2.11	0.50
1:B:279:ILE:HG21	2:B:901:K21:C49	2.40	0.50
1:A:181:GLN:O	1:A:185:LEU:HD13	2.12	0.50
1:A:78:GLU:O	1:A:82:VAL:HG23	2.12	0.50
2:B:901:K21:C24	2:B:901:K21:H101	2.42	0.49
1:A:25:ARG:NH2	1:A:29:LYS:HD3	2.27	0.49
1:B:162:ASP:O	1:B:202:SER:HB3	2.12	0.49
2:B:901:K21:H341	2:B:901:K21:H101	1.95	0.49
1:B:167:ILE:HD13	1:B:208:LYS:HG3	1.95	0.49
1:A:24:LEU:HD21	1:A:41:LEU:HD22	1.95	0.49
1:B:73:LEU:HD22	1:B:77:PHE:HE2	1.77	0.49
1:B:150:GLN:O	1:B:154:VAL:HG23	2.13	0.48
1:A:121:GLU:O	1:A:125:ILE:HG13	2.13	0.48
1:B:99:ALA:HB1	1:B:106:ASN:HB3	1.95	0.48
1:A:111:THR:HG23	1:A:236:LEU:HA	1.96	0.47
1:A:91:TYR:OH	1:A:271:ARG:HA	2.13	0.47
1:A:210:PHE:CZ	1:A:241:VAL:HG13	2.49	0.47
2:B:901:K21:C34	2:B:901:K21:H101	2.44	0.47
1:A:81:ILE:HA	1:A:84:LEU:HD12	1.95	0.47
2:B:901:K21:C34	2:B:901:K21:C10	2.93	0.47
1:A:95:GLU:HG2	1:A:271:ARG:HD3	1.97	0.47
1:A:25:ARG:HH22	1:A:63:ARG:HH11	1.62	0.46
1:A:28:MET:HB2	1:A:72:GLU:HG3	1.97	0.46
1:B:256:TYR:HE1	1:B:260:LYS:HD2	1.79	0.46
1:A:119:PRO:HD3	2:A:901:K21:C5	2.45	0.46
1:B:283:ASN:O	1:B:287:GLU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:HD12	1:A:81:ILE:HG13	1.99	0.45
1:B:266:ASP:HB3	1:B:308:TYR:OH	2.17	0.44
1:B:73:LEU:HD22	1:B:77:PHE:CE2	2.53	0.44
1:A:86:LYS:HA	1:A:87:PRO:HD3	1.74	0.44
1:A:240:VAL:O	1:A:244:ILE:HG12	2.18	0.44
1:B:8:THR:OG1	1:B:281:LEU:HD23	2.18	0.44
1:A:286:LYS:HB3	1:A:286:LYS:HE2	1.83	0.44
1:B:289:ARG:HD2	1:B:320:ASP:C	2.38	0.43
1:A:32:GLY:O	1:A:72:GLU:HB3	2.18	0.43
1:A:201:ARG:HB3	1:A:205:HIS:CD2	2.52	0.43
1:A:270:ILE:O	1:A:274:VAL:HG23	2.18	0.43
1:A:25:ARG:CZ	1:A:29:LYS:HD3	2.49	0.43
1:A:234:GLU:O	1:A:238:LEU:HB2	2.19	0.42
1:B:248:PRO:HA	1:B:284:ILE:HG12	2.00	0.42
1:B:6:ARG:H	1:B:283:ASN:ND2	2.16	0.42
2:B:901:K21:H342	2:B:901:K21:C10	2.50	0.42
1:A:157:LEU:HD12	1:A:157:LEU:HA	1.82	0.42
1:A:222:GLU:H	1:A:222:GLU:HG3	1.67	0.42
1:A:237:LEU:O	1:A:241:VAL:HG23	2.20	0.42
1:A:18:ARG:O	1:A:22:GLU:HG2	2.20	0.41
1:B:161:ARG:HD3	2:B:901:K21:C6	2.48	0.41
1:B:124:ALA:O	1:B:128:VAL:HG23	2.21	0.41
1:B:289:ARG:HH11	1:B:320:ASP:HA	1.86	0.41
1:B:36:GLU:HB2	3:B:932:HOH:O	2.21	0.41
1:A:201:ARG:HB2	1:A:206:LEU:HG	2.02	0.41
1:B:66:LEU:HA	1:B:66:LEU:HD12	1.90	0.41
1:A:129:TYR:C	1:A:129:TYR:CD1	2.94	0.40
1:A:219:PHE:HB2	1:A:223:GLU:HG3	2.03	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	316/320 (99%)	268 (85%)	40 (13%)	8 (2%)	5 28
1	B	316/320 (99%)	271 (86%)	36 (11%)	9 (3%)	5 25
All	All	632/640 (99%)	539 (85%)	76 (12%)	17 (3%)	5 26

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	168	ASP
1	B	192	GLU
1	B	232	ASN
1	B	318	GLU
1	A	191	GLU
1	A	232	ASN
1	B	32	GLY
1	B	166	GLY
1	B	187	TRP
1	A	102	GLY
1	A	159	ALA
1	B	102	GLY
1	A	134	GLY
1	A	227	ARG
1	B	17	GLU
1	A	47	ASN
1	A	38	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	271/272 (100%)	242 (89%)	29 (11%)	6 26
1	B	271/272 (100%)	251 (93%)	20 (7%)	13 44
All	All	542/544 (100%)	493 (91%)	49 (9%)	9 35

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	5	LEU
1	B	10	THR
1	B	17	GLU
1	B	31	LEU
1	B	33	THR
1	B	39	LEU
1	B	144	ASP
1	B	160	ASN
1	B	167	ILE
1	B	168	ASP
1	B	193	LYS
1	B	196	THR
1	B	216	ILE
1	B	229	THR
1	B	237	LEU
1	B	256	TYR
1	B	264	THR
1	B	303	ASP
1	B	312	LEU
1	B	314	LEU
1	A	5	LEU
1	A	6	ARG
1	A	10	THR
1	A	24	LEU
1	A	33	THR
1	A	36	GLU
1	A	37	SER
1	A	45	ARG
1	A	68	ASP
1	A	72	GLU
1	A	78	GLU
1	A	92	ASP
1	A	120	GLU
1	A	127	GLN
1	A	157	LEU
1	A	168	ASP
1	A	184	GLU
1	A	189	THR
1	A	190	ASP
1	A	221	ILE
1	A	223	GLU
1	A	226	ASP
1	A	237	LEU

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Mol	Chain	Res	Type
1	A	264	THR
1	A	295	SER
1	A	305	SER
1	A	312	LEU
1	A	319	ASP
1	A	320	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	160	ASN
1	B	177	GLN
1	B	181	GLN
1	B	283	ASN
1	A	51	GLN
1	A	127	GLN
1	A	283	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	K21	B	901	-	32,33,33	1.23	3 (9%)	40,44,44	2.38	10 (25%)
2	K21	A	901	-	32,33,33	1.25	3 (9%)	40,44,44	1.64	7 (17%)

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	K21	B	901	-	-	6/13/35/35	1/3/4/4
2	K21	A	901	-	-	5/13/35/35	0/3/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	K21	C4-S14	4.21	1.81	1.77
2	A	901	K21	C4-S14	3.50	1.81	1.77
2	A	901	K21	C22-C21	3.22	1.58	1.51
2	A	901	K21	C21-N11	2.96	1.41	1.35
2	B	901	K21	C22-C21	2.32	1.56	1.51
2	B	901	K21	C24-C22	2.08	1.56	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	901	K21	C13-S14-C4	-7.70	91.81	102.71
2	B	901	K21	C24-C22-C21	7.44	121.98	111.22
2	B	901	K21	C10-N11-C12	6.41	121.33	113.91
2	A	901	K21	C13-S14-C4	-5.37	95.11	102.71
2	A	901	K21	C24-N27-C30	3.45	120.05	111.23
2	B	901	K21	C33-C34-N27	3.35	116.31	111.11
2	A	901	K21	C24-C22-C21	3.33	116.04	111.22
2	A	901	K21	C24-N27-C34	3.31	119.69	111.23
2	B	901	K21	C3-C10-N11	3.19	119.61	113.26
2	B	901	K21	C2-C3-C4	2.87	120.98	118.10
2	A	901	K21	C12-C13-S14	2.50	117.36	114.22
2	B	901	K21	C5-C4-S14	2.45	123.47	117.23
2	A	901	K21	C10-N11-C12	2.42	116.71	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	901	K21	C52-C43-C32	-2.31	110.17	114.50
2	A	901	K21	C33-C34-N27	-2.16	107.76	111.11
2	B	901	K21	C10-C3-C4	-2.15	118.24	123.52
2	B	901	K21	C22-C24-N27	2.13	122.12	113.07

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	901	K21	C21-C22-C24-N27
2	B	901	K21	C31-C32-C43-C52
2	B	901	K21	C33-C32-C43-C52
2	A	901	K21	C21-C22-C24-N27
2	A	901	K21	C22-C24-N27-C30
2	A	901	K21	C22-C24-N27-C34
2	B	901	K21	O23-C21-C22-C24
2	B	901	K21	O23-C21-N11-C10
2	A	901	K21	O23-C21-C22-C24
2	B	901	K21	N11-C21-C22-C24
2	A	901	K21	N11-C21-C22-C24

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	901	K21	C30-C31-C32-C33-C34-N27

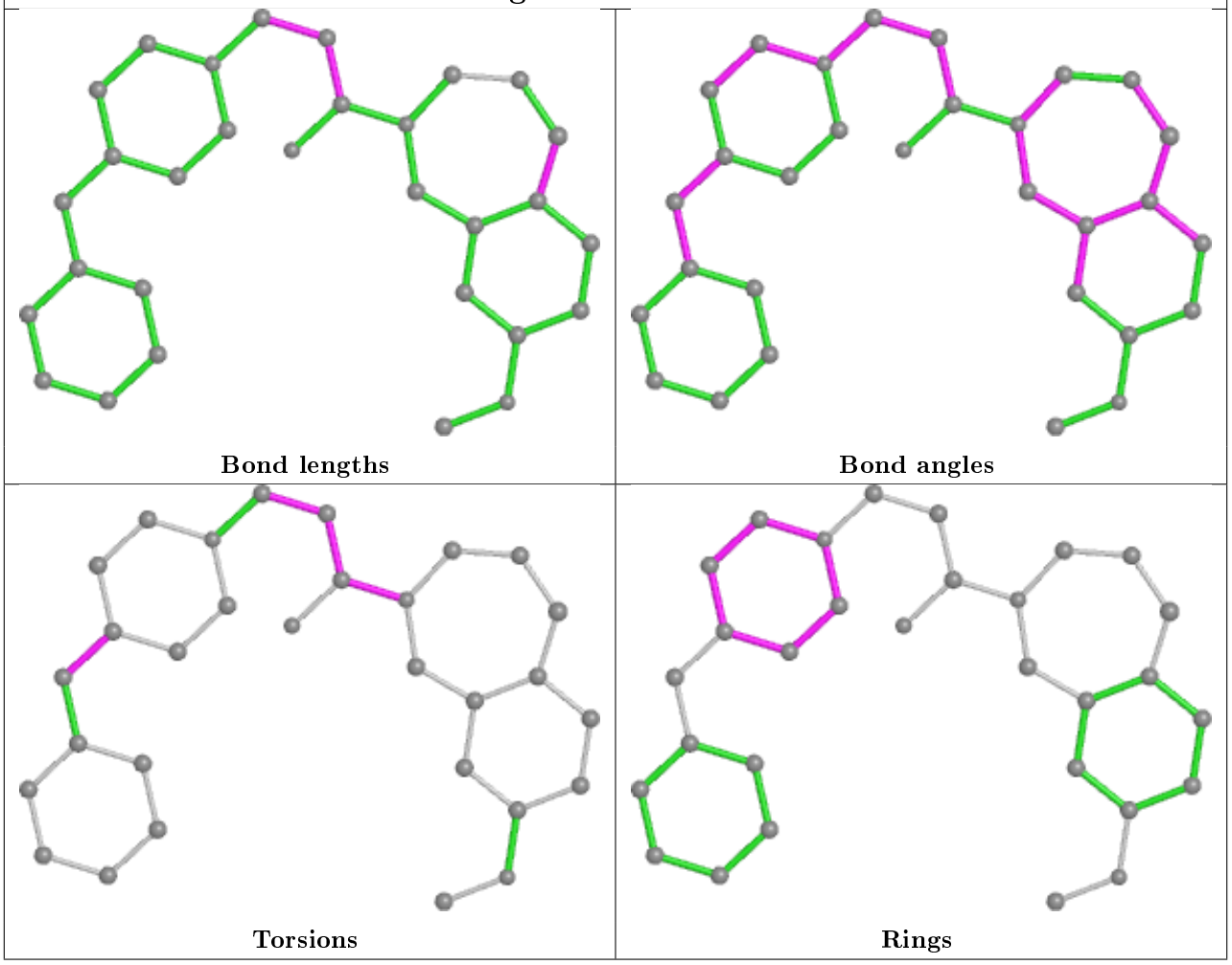
2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	K21	9	0
2	A	901	K21	1	0

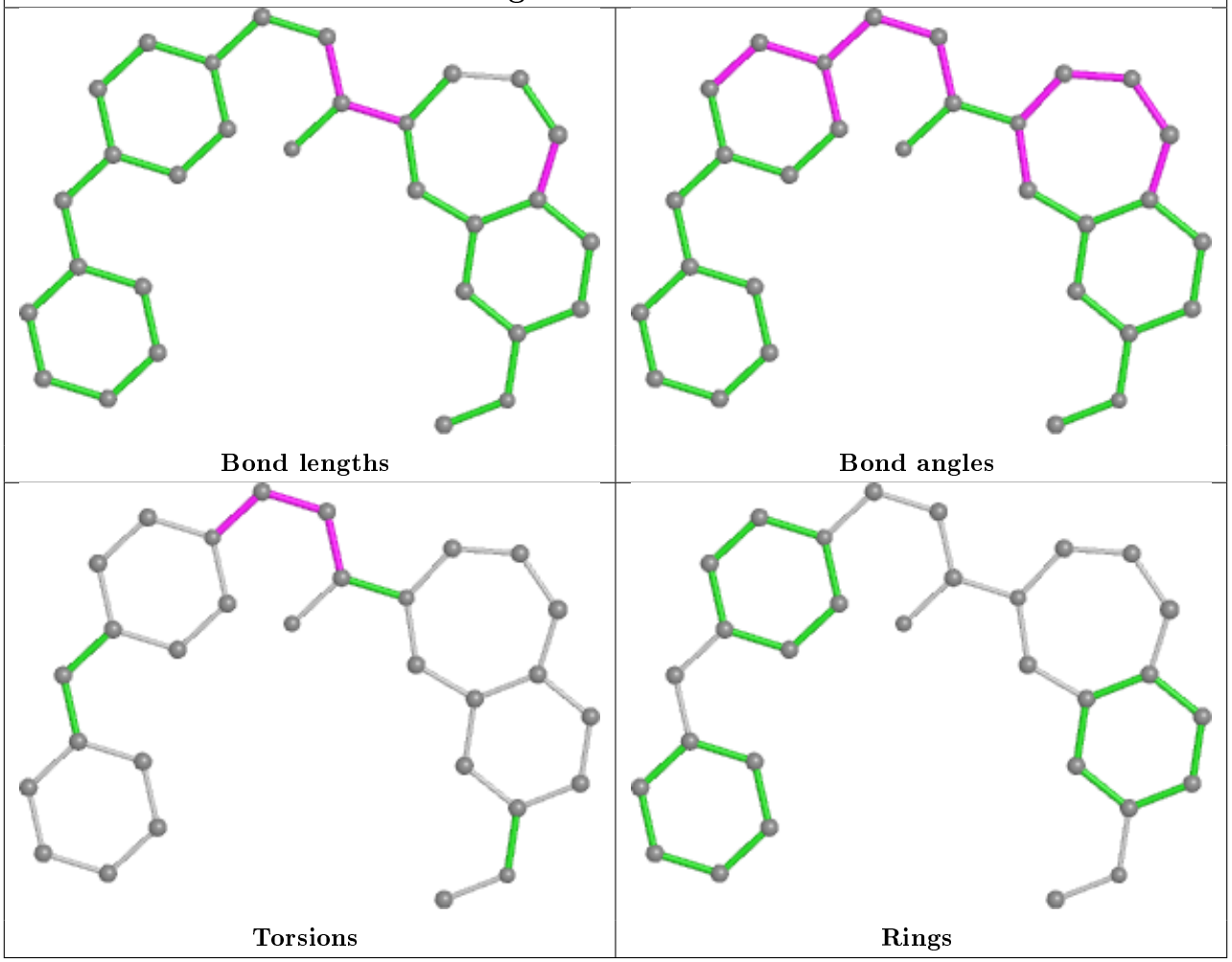
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand K21 B 901



Ligand K21 A 901



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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.