Full wwPDB EM Validation Report ⓘ

Apr 2, 2025 – 01:50 am BST

PDB ID	:	6Z1F / pdb_00006z1f
EMDB ID	:	EMD-11028
Title	:	CryoEM structure of Rubisco Activase with its substrate Rubisco from Nostoc sp. (strain PCC7120)
Authors	:	Wang, H.; Bracher, A.; Flecken, M.; Popilka, L.; Hartl, F.U.; Hayer-Hartl, M.
Deposited on	:	2020-05-13
Resolution	:	2.86 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

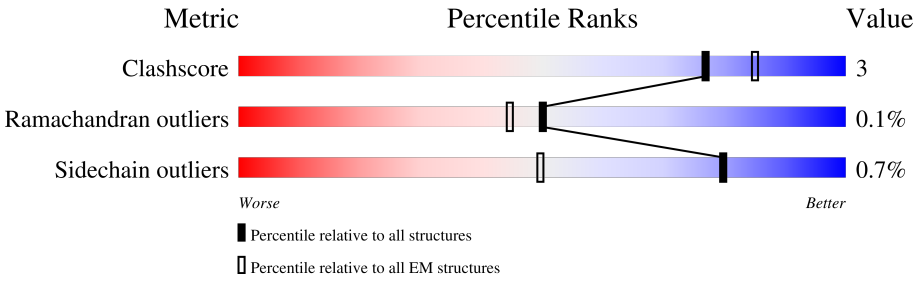
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.86 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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%

Mol	Chain	Length	Quality of chain
1	1	290	79% 17% .
1	2	290	89% 8% .
1	3	290	92% 6% .
1	4	290	89% 8% .
1	5	290	88% 9% .
1	6	290	89% 7% 5%
2	A	476	92% 5% .
2	B	476	90% 6% .
2	C	476	86% 12% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	476	85% 12%
2	E	476	92% 5%
2	F	476	93%
2	G	476	94%
2	H	476	93%
3	I	109	94% 6%
3	J	109	88% 11%
3	K	109	93% 6%
3	L	109	91% 8%
3	M	109	92% 7%
3	N	109	93% 6%
3	O	109	88% 11%
3	P	109	91% 8%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 49815 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Ribulose bisphosphate carboxylase/oxygenase activase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	280	Total	C	N	O	S	0	0
			2184	1392	380	405	7		
1	2	281	Total	C	N	O	S	0	0
			2215	1411	388	409	7		
1	3	284	Total	C	N	O	S	0	0
			2241	1423	391	420	7		
1	4	281	Total	C	N	O	S	0	0
			2222	1414	389	412	7		
1	5	280	Total	C	N	O	S	0	0
			2206	1405	386	408	7		
1	6	276	Total	C	N	O	S	0	0
			2174	1385	381	401	7		

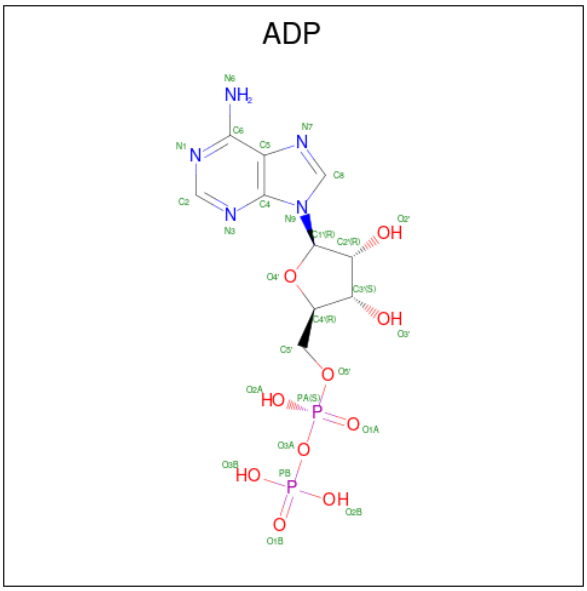
- Molecule 2 is a protein called Ribulose bisphosphate carboxylase large chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	466	Total	C	N	O	S	0	0
			3665	2329	640	682	14		
2	B	459	Total	C	N	O	S	0	0
			3601	2295	634	659	13		
2	C	464	Total	C	N	O	S	0	0
			3649	2322	639	674	14		
2	D	464	Total	C	N	O	S	0	0
			3649	2322	639	674	14		
2	E	464	Total	C	N	O	S	0	0
			3649	2322	639	674	14		
2	F	464	Total	C	N	O	S	0	0
			3649	2322	639	674	14		
2	G	464	Total	C	N	O	S	0	0
			3649	2322	639	674	14		
2	H	464	Total	C	N	O	S	0	0
			3649	2322	639	674	14		

- Molecule 3 is a protein called Ribulose bisphosphate carboxylase small chain.

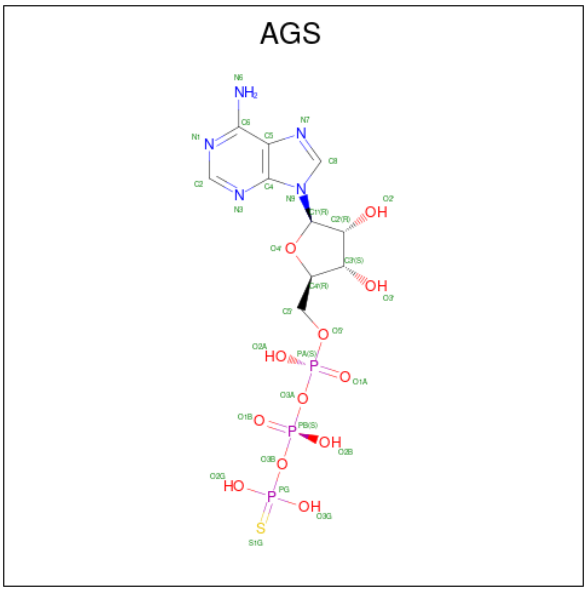
Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	108	Total	C	N	O	S	0	0
			884	574	145	162	3		
3	J	108	Total	C	N	O	S	0	0
			884	574	145	162	3		
3	K	108	Total	C	N	O	S	0	0
			884	574	145	162	3		
3	L	108	Total	C	N	O	S	0	0
			884	574	145	162	3		
3	M	108	Total	C	N	O	S	0	0
			884	574	145	162	3		
3	N	108	Total	C	N	O	S	0	0
			884	574	145	162	3		
3	O	108	Total	C	N	O	S	0	0
			884	574	145	162	3		
3	P	108	Total	C	N	O	S	0	0
			884	574	145	162	3		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
4	1	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 5 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



Mol	Chain	Residues	Atoms						AltConf
5	2	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
5	3	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
5	4	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
5	5	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
5	6	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

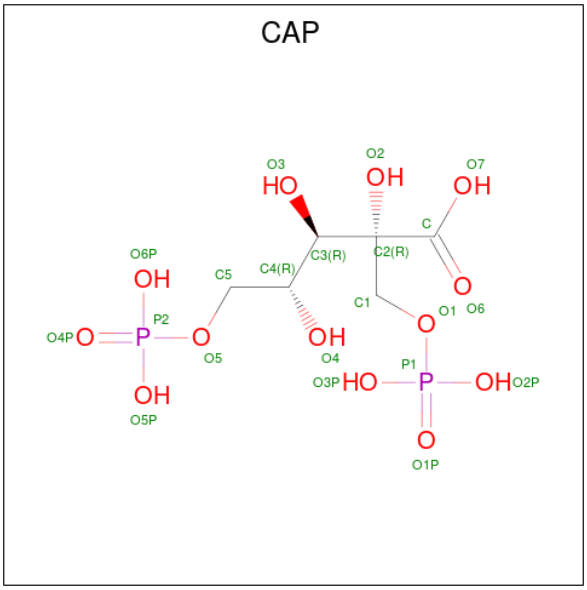
Mol	Chain	Residues	Atoms		AltConf
6	2	1	Total	Mg	0
			1	1	
6	3	1	Total	Mg	0
			1	1	
6	4	1	Total	Mg	0
			1	1	
6	5	1	Total	Mg	0
			1	1	
6	A	1	Total	Mg	0
			1	1	
6	B	1	Total	Mg	0
			1	1	
6	C	1	Total	Mg	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
6	D	1	Total Mg 1 1	0
6	E	1	Total Mg 1 1	0
6	F	1	Total Mg 1 1	0
6	G	1	Total Mg 1 1	0
6	H	1	Total Mg 1 1	0

- Molecule 7 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (CCD ID: CAP) (formula: $C_6H_{14}O_{13}P_2$).



Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total C O P 21 6 13 2	0
7	C	1	Total C O P 21 6 13 2	0
7	D	1	Total C O P 21 6 13 2	0
7	E	1	Total C O P 21 6 13 2	0
7	F	1	Total C O P 21 6 13 2	0
7	G	1	Total C O P 21 6 13 2	0

Continued on next page...

Continued from previous page...

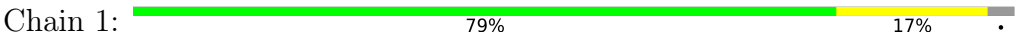
Mol	Chain	Residues	Atoms				AltConf
7	H	1	Total	C	O	P	0
			21	6	13	2	

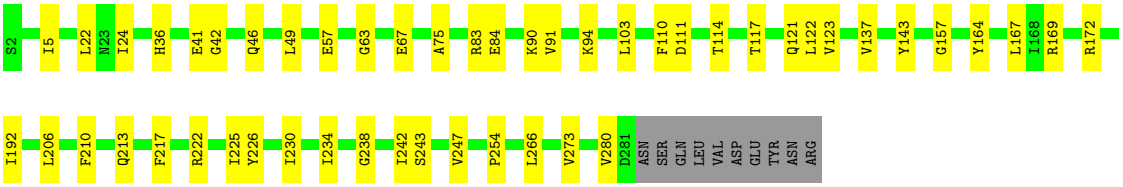
3 Residue-property plots (i)

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. 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.

• Molecule 1: Ribulose bisphosphate carboxylase/oxygenase activase

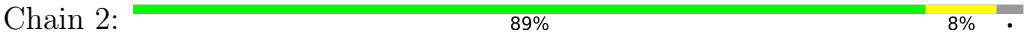
Chain 1:





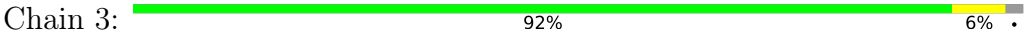
• Molecule 1: Ribulose bisphosphate carboxylase/oxygenase activase

Chain 2:



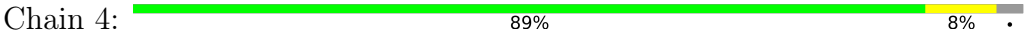
• Molecule 1: Ribulose bisphosphate carboxylase/oxygenase activase

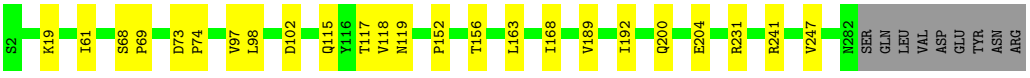
Chain 3:



• Molecule 1: Ribulose bisphosphate carboxylase/oxygenase activase

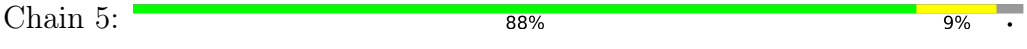
Chain 4:





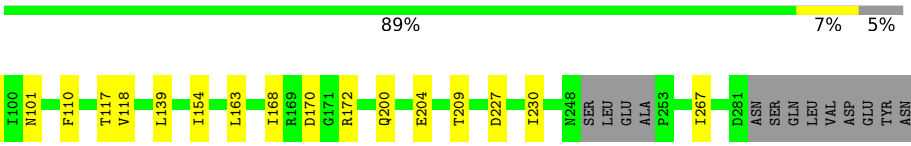
• Molecule 1: Ribulose bisphosphate carboxylase/oxygenase activase

Chain 5:



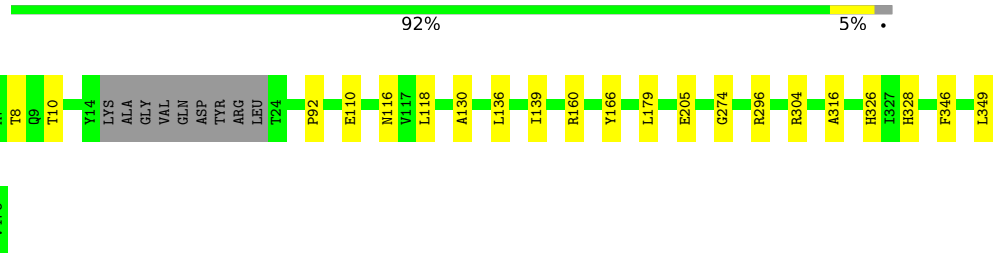
• Molecule 1: Ribulose bisphosphate carboxylase/oxygenase activase

Chain 6:



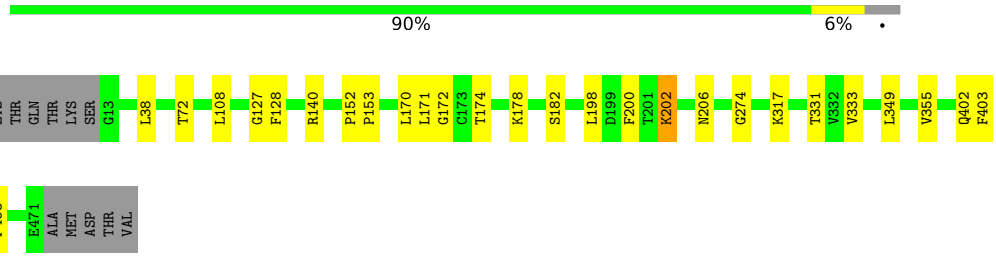
• Molecule 2: Ribulose bisphosphate carboxylase large chain

Chain A:



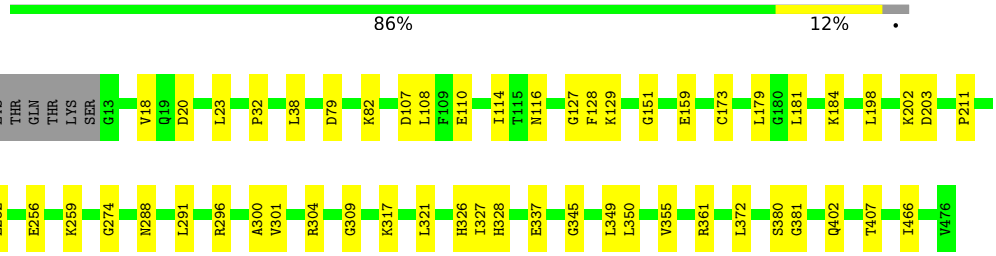
• Molecule 2: Ribulose bisphosphate carboxylase large chain

Chain B:



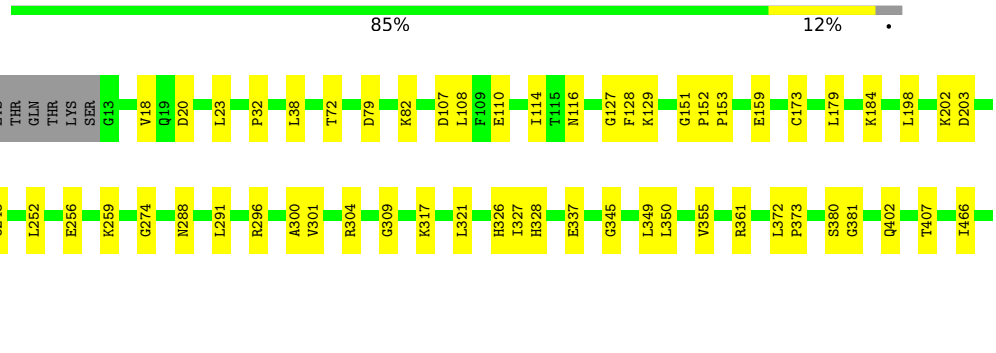
• Molecule 2: Ribulose bisphosphate carboxylase large chain

Chain C:



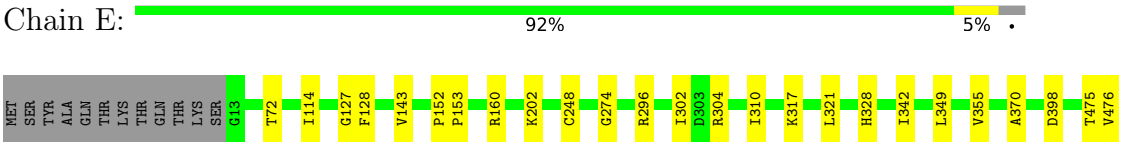
• Molecule 2: Ribulose bisphosphate carboxylase large chain

Chain D:



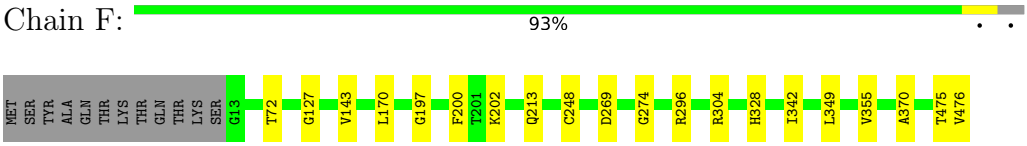
• Molecule 2: Ribulose bisphosphate carboxylase large chain

Chain E:



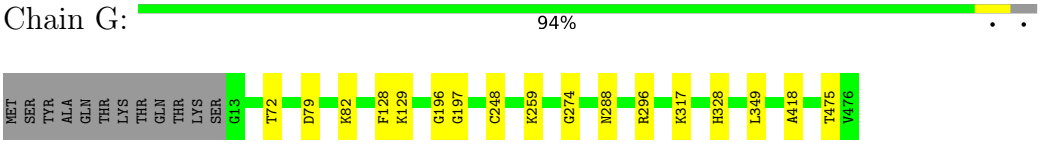
• Molecule 2: Ribulose bisphosphate carboxylase large chain

Chain F:



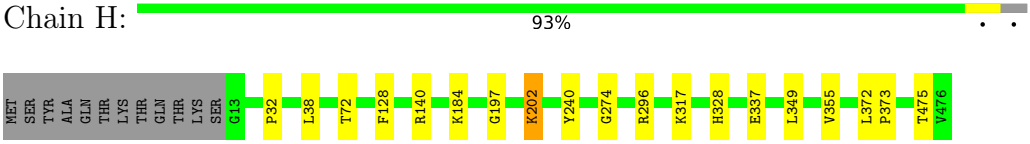
• Molecule 2: Ribulose bisphosphate carboxylase large chain

Chain G:



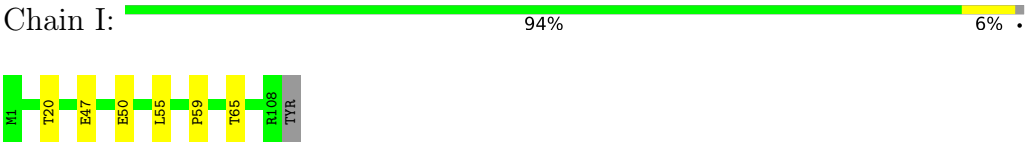
• Molecule 2: Ribulose bisphosphate carboxylase large chain

Chain H:



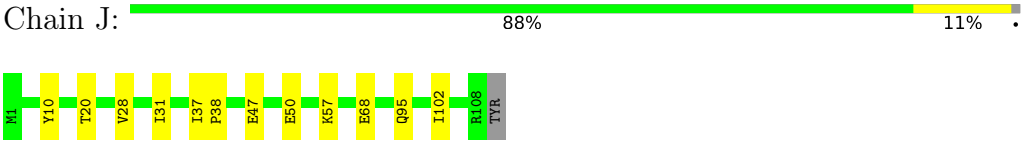
• Molecule 3: Ribulose bisphosphate carboxylase small chain

Chain I:



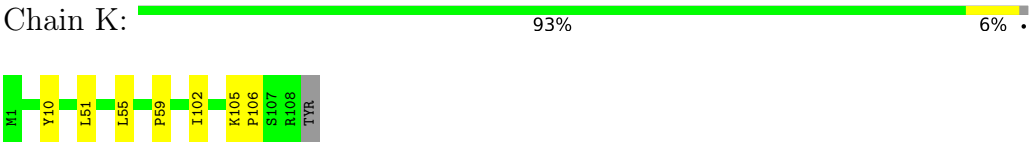
• Molecule 3: Ribulose bisphosphate carboxylase small chain

Chain J:



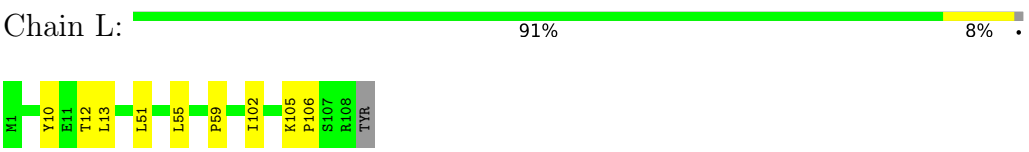
• Molecule 3: Ribulose bisphosphate carboxylase small chain

Chain K:



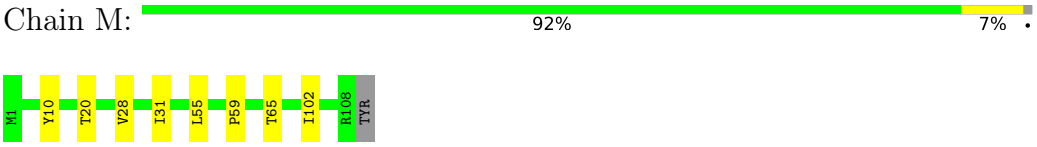
• Molecule 3: Ribulose bisphosphate carboxylase small chain

Chain L:



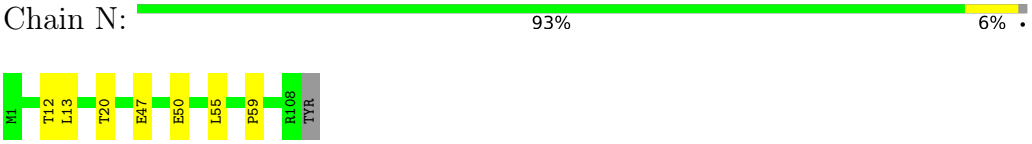
• Molecule 3: Ribulose bisphosphate carboxylase small chain

Chain M:



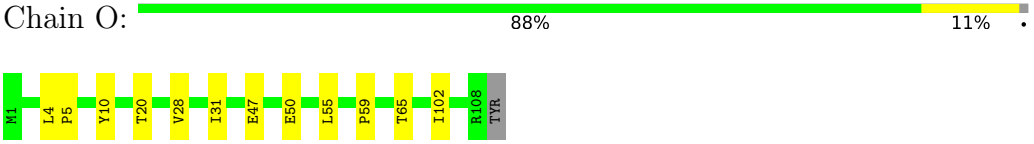
• Molecule 3: Ribulose bisphosphate carboxylase small chain

Chain N:



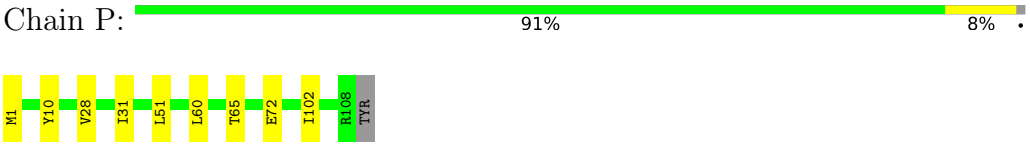
• Molecule 3: Ribulose bisphosphate carboxylase small chain

Chain O:



• Molecule 3: Ribulose bisphosphate carboxylase small chain

Chain P:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	21149	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AGS, KCX, ADP, CAP

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	1	0.26	0/2227	0.57	0/3018
1	2	0.26	0/2258	0.57	0/3054
1	3	0.27	0/2284	0.58	0/3090
1	4	0.26	0/2265	0.58	0/3063
1	5	0.26	0/2249	0.57	0/3043
1	6	0.26	0/2216	0.58	0/2997
2	A	0.40	0/3740	0.58	0/5074
2	B	0.41	0/3677	0.57	0/4992
2	C	0.40	0/3725	0.59	0/5055
2	D	0.40	0/3725	0.59	0/5055
2	E	0.41	0/3725	0.57	0/5055
2	F	0.40	0/3725	0.57	0/5055
2	G	0.41	0/3725	0.57	0/5055
2	H	0.41	0/3725	0.57	0/5055
3	I	0.42	0/908	0.56	0/1237
3	J	0.42	0/908	0.56	0/1237
3	K	0.41	0/908	0.58	0/1237
3	L	0.41	0/908	0.58	0/1237
3	M	0.42	0/908	0.56	0/1237
3	N	0.42	0/908	0.55	0/1237
3	O	0.41	0/908	0.56	0/1237
3	P	0.42	0/908	0.56	0/1237
All	All	0.37	0/50530	0.57	0/68557

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	1	2184	0	2169	53	0
1	2	2215	0	2225	33	0
1	3	2241	0	2237	11	0
1	4	2222	0	2233	16	0
1	5	2206	0	2212	19	0
1	6	2174	0	2172	17	0
2	A	3665	0	3586	21	0
2	B	3601	0	3527	25	0
2	C	3649	0	3573	36	0
2	D	3649	0	3573	38	0
2	E	3649	0	3573	12	0
2	F	3649	0	3573	8	0
2	G	3649	0	3573	7	0
2	H	3649	0	3573	10	0
3	I	884	0	878	2	0
3	J	884	0	878	12	0
3	K	884	0	878	4	0
3	L	884	0	878	5	0
3	M	884	0	878	3	0
3	N	884	0	878	3	0
3	O	884	0	878	5	0
3	P	884	0	878	5	0
4	1	27	0	12	1	0
5	2	31	0	12	6	0
5	3	31	0	12	1	0
5	4	31	0	12	1	0
5	5	31	0	12	2	0
5	6	31	0	12	2	0
6	2	1	0	0	0	0
6	3	1	0	0	0	0
6	4	1	0	0	0	0
6	5	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
7	A	21	0	9	0	0
7	C	21	0	9	0	0
7	D	21	0	9	0	0
7	E	21	0	9	0	0
7	F	21	0	9	0	0
7	G	21	0	9	0	0
7	H	21	0	9	0	0
All	All	49815	0	48958	277	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 (277) 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)
5:2:301:AGS:PG	5:2:301:AGS:S1G	1.53	1.53
1:1:84:GLU:CD	2:B:464:LYS:HG3	1.64	1.17
1:1:247:VAL:HG21	1:2:95:MET:HG2	1.11	1.11
1:2:143:TYR:HB3	3:P:1:MET:HB2	1.36	1.03
1:1:247:VAL:CG2	1:2:95:MET:HG2	1.88	1.01
1:1:91:VAL:HG22	2:B:467:LYS:HB2	1.36	1.00
1:2:139:LEU:HD13	3:J:68:GLU:OE2	1.67	0.92
1:1:243:SER:HB2	1:2:95:MET:HG3	1.53	0.90
1:2:143:TYR:HB2	3:J:57:LYS:HE3	1.53	0.90
1:1:247:VAL:HG21	1:2:95:MET:CG	1.99	0.88
1:1:280:VAL:HG21	1:2:175:LYS:HD2	1.57	0.86
1:1:90:LYS:HB3	2:B:467:LYS:HE3	1.58	0.84
1:1:84:GLU:OE1	2:B:464:LYS:HG3	1.77	0.84
1:2:143:TYR:HB2	3:J:57:LYS:CE	2.08	0.84
1:2:168:ILE:HG23	1:2:175:LYS:HD3	1.63	0.80
1:1:84:GLU:CD	2:B:464:LYS:CG	2.47	0.79
1:1:91:VAL:CG2	2:B:467:LYS:HB2	2.13	0.77
1:1:5:ILE:HD11	1:1:49:LEU:HB3	1.67	0.77
1:6:117:THR:HG22	1:6:118:VAL:H	1.51	0.75
1:2:139:LEU:CD1	3:J:68:GLU:OE2	2.35	0.75
1:2:143:TYR:CB	3:J:57:LYS:HE3	2.16	0.75
5:2:301:AGS:S1G	5:2:301:AGS:O3B	2.46	0.73
5:6:301:AGS:H5'1	5:6:301:AGS:H8	1.73	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:168:ILE:CG2	1:2:175:LYS:HD3	2.19	0.71
5:2:301:AGS:S1G	5:2:301:AGS:O2G	2.49	0.71
1:1:210:PHE:HB3	1:1:213:GLN:HG3	1.73	0.70
1:1:90:LYS:HB3	2:B:467:LYS:CE	2.23	0.69
2:A:304:ARG:HD3	2:B:127:GLY:HA2	1.76	0.68
2:C:317:LYS:HE2	2:C:349:LEU:HD21	1.76	0.67
2:D:317:LYS:HE2	2:D:349:LEU:HD21	1.78	0.66
1:1:167:LEU:HD23	1:1:172:ARG:HH21	1.61	0.65
1:3:163:LEU:HD23	1:3:168:ILE:HD11	1.78	0.65
1:2:143:TYR:O	3:J:57:LYS:NZ	2.22	0.64
2:C:18:VAL:HG21	2:D:466:ILE:HG13	1.79	0.64
2:C:466:ILE:HG13	2:D:18:VAL:HG21	1.81	0.63
1:1:83:ARG:NH2	1:1:137:VAL:O	2.32	0.62
1:1:57:GLU:HG2	1:1:94:LYS:HD2	1.81	0.62
1:1:75:ALA:HB2	1:1:122:LEU:HD22	1.80	0.61
2:A:316:ALA:HB1	2:A:350:LEU:HD21	1.80	0.61
2:C:110:GLU:HB2	2:C:116:ASN:HD22	1.65	0.61
2:D:110:GLU:HB2	2:D:116:ASN:HD22	1.64	0.60
1:1:217:PHE:HE1	1:1:273:VAL:HB	1.67	0.60
1:1:210:PHE:HB3	1:1:213:GLN:CG	2.33	0.59
1:1:210:PHE:CB	1:1:213:GLN:HG3	2.32	0.59
2:B:182:SER:HB2	3:J:95:GLN:HG3	1.84	0.59
1:1:169:ARG:NH2	1:6:44:THR:OG1	2.36	0.59
1:1:169:ARG:NH1	1:6:101:ASN:HD21	2.00	0.58
5:6:301:AGS:H8	5:6:301:AGS:C5'	2.32	0.58
2:C:337:GLU:HA	2:D:129:LYS:HD3	1.86	0.57
2:A:179:LEU:HD22	2:B:108:LEU:HB2	1.86	0.57
1:1:243:SER:CB	1:2:95:MET:HG3	2.31	0.56
1:5:119:ASN:HD21	2:A:6:THR:HG21	1.70	0.56
1:6:117:THR:HG22	1:6:118:VAL:N	2.21	0.56
2:D:114:ILE:HD11	2:D:321:LEU:HB2	1.88	0.56
2:C:114:ILE:HD11	2:C:321:LEU:HB2	1.88	0.56
2:C:129:LYS:HD3	2:D:337:GLU:HA	1.87	0.55
2:D:20:ASP:HB3	2:D:23:LEU:HG	1.88	0.55
2:D:226:ILE:HD11	2:D:239:HIS:HB3	1.88	0.55
1:3:119:ASN:HD21	2:A:10:THR:HG21	1.70	0.55
2:C:226:ILE:HD11	2:C:239:HIS:HB3	1.88	0.55
3:K:55:LEU:HD21	3:K:59:PRO:HD3	1.89	0.55
2:C:20:ASP:HB3	2:C:23:LEU:HG	1.89	0.55
2:G:274:GLY:HA3	2:H:274:GLY:HA3	1.87	0.55
2:C:349:LEU:HA	2:C:355:VAL:HG21	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:163:LEU:HB3	1:4:168:ILE:HD11	1.90	0.54
3:I:55:LEU:HD21	3:I:59:PRO:HD3	1.88	0.54
2:H:38:LEU:HD12	2:H:140:ARG:HD3	1.90	0.54
1:5:200:GLN:O	1:5:204:GLU:HG2	2.07	0.54
2:D:198:LEU:HD11	2:D:407:THR:HG21	1.89	0.54
2:D:349:LEU:HA	2:D:355:VAL:HG21	1.90	0.54
1:5:92:ARG:HB3	1:5:94:LYS:HE3	1.90	0.54
2:C:198:LEU:HD11	2:C:407:THR:HG21	1.90	0.54
3:L:55:LEU:HD21	3:L:59:PRO:HD3	1.89	0.54
1:1:103:LEU:HD11	1:1:123:VAL:HG11	1.88	0.53
1:1:117:THR:O	1:1:121:GLN:HG2	2.08	0.53
2:H:296:ARG:HG2	2:H:328:HIS:HB2	1.89	0.53
1:1:254:PRO:HG2	1:2:22:LEU:CD2	2.38	0.53
2:G:296:ARG:HG2	2:G:328:HIS:HB2	1.90	0.53
1:3:79:ARG:HH22	1:3:129:ASN:HD22	1.56	0.53
1:4:247:VAL:CG2	1:5:95:MET:HG2	2.38	0.52
5:4:301:AGS:H5'1	5:4:301:AGS:H8	1.91	0.52
2:G:317:LYS:HE2	2:G:349:LEU:HD21	1.90	0.52
1:2:137:VAL:HB	1:2:148:ILE:HD11	1.90	0.52
2:D:203:ASP:OD1	2:D:239:HIS:NE2	2.41	0.52
1:4:231:ARG:HD2	1:5:11:ASP:OD2	2.10	0.52
2:C:327:ILE:HG21	2:C:350:LEU:HD13	1.92	0.52
3:O:55:LEU:HD21	3:O:59:PRO:HD3	1.92	0.52
1:3:230:ILE:HD13	1:4:19:LYS:HG3	1.91	0.52
1:1:22:LEU:HB3	1:1:24:ILE:HD12	1.90	0.51
3:P:10:TYR:HB3	3:P:102:ILE:HD12	1.90	0.51
1:1:84:GLU:OE2	2:B:464:LYS:CG	2.58	0.51
2:D:327:ILE:HG21	2:D:350:LEU:HD13	1.92	0.51
1:5:248:ASN:OD1	2:A:92:PRO:HA	2.10	0.51
1:6:83:ARG:HD3	1:6:139:LEU:HD13	1.91	0.51
1:2:241:ARG:NH1	1:2:241:ARG:HB2	2.26	0.51
3:K:10:TYR:HB3	3:K:102:ILE:HD12	1.93	0.51
1:2:241:ARG:HB2	1:2:241:ARG:HH11	1.76	0.51
1:1:164:TYR:HD1	1:1:167:LEU:HD12	1.76	0.50
2:C:301:VAL:HG13	2:D:309:GLY:HA2	1.93	0.50
2:C:274:GLY:HA3	2:D:274:GLY:HA3	1.93	0.50
5:2:301:AGS:H5'1	5:2:301:AGS:H8	1.94	0.50
5:5:301:AGS:H5'1	5:5:301:AGS:H8	1.93	0.50
2:F:296:ARG:HG2	2:F:328:HIS:HB2	1.93	0.50
2:F:349:LEU:HA	2:F:355:VAL:HG21	1.94	0.50
1:6:117:THR:HG21	2:A:4:ALA:HB3	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:129:LYS:HD3	2:H:337:GLU:HA	1.93	0.50
1:1:169:ARG:HH12	1:6:101:ASN:HD21	1.59	0.50
3:L:10:TYR:HB3	3:L:102:ILE:HD12	1.93	0.50
2:D:300:ALA:O	2:D:304:ARG:HB2	2.12	0.50
2:B:38:LEU:HD12	2:B:140:ARG:HD3	1.94	0.49
2:E:304:ARG:HD3	2:F:127:GLY:HA2	1.94	0.49
1:5:221:LEU:HD21	1:5:270:GLY:HA2	1.95	0.49
2:D:159:GLU:CD	2:D:326:HIS:HE2	2.15	0.49
3:P:60:LEU:HD21	3:P:72:GLU:HG3	1.95	0.49
1:2:139:LEU:HD13	3:J:68:GLU:CD	2.33	0.49
2:C:259:LYS:HD3	2:C:288:ASN:HB3	1.95	0.49
3:N:55:LEU:HD21	3:N:59:PRO:HD3	1.95	0.49
1:2:221:LEU:O	1:2:225:ILE:HG12	2.12	0.49
3:M:55:LEU:HD21	3:M:59:PRO:HD3	1.95	0.49
1:4:247:VAL:HG23	1:5:95:MET:HG2	1.94	0.49
1:4:200:GLN:O	1:4:204:GLU:HG2	2.12	0.48
2:C:173:CYS:HB2	2:C:198:LEU:HD13	1.95	0.48
2:C:300:ALA:O	2:C:304:ARG:HB2	2.13	0.48
2:D:79:ASP:HA	2:D:82:LYS:HE3	1.95	0.48
2:D:173:CYS:HB2	2:D:198:LEU:HD13	1.95	0.48
2:A:110:GLU:H	2:A:116:ASN:HD22	1.59	0.48
2:C:179:LEU:HD13	2:D:108:LEU:HD13	1.96	0.48
2:C:108:LEU:HD13	2:D:179:LEU:HD13	1.95	0.48
1:1:238:GLY:O	1:1:242:ILE:HG23	2.14	0.48
3:J:28:VAL:HA	3:J:31:ILE:HD12	1.94	0.48
1:1:254:PRO:HG2	1:2:22:LEU:HD22	1.96	0.48
2:C:79:ASP:HA	2:C:82:LYS:HE3	1.96	0.48
1:1:169:ARG:NH1	1:6:101:ASN:ND2	2.62	0.48
1:1:192:ILE:CG2	1:1:222:ARG:HD2	2.44	0.48
2:B:317:LYS:HE2	2:B:349:LEU:HD21	1.95	0.48
2:C:309:GLY:HA2	2:D:301:VAL:HG13	1.96	0.48
1:1:63:GLY:O	1:1:67:GLU:HG2	2.14	0.48
1:4:117:THR:HG21	2:A:8:THR:HG23	1.96	0.48
2:C:32:PRO:HB3	2:C:38:LEU:HD21	1.95	0.48
2:D:184:LYS:HE3	3:L:51:LEU:HD13	1.95	0.48
2:C:159:GLU:CD	2:C:326:HIS:HE2	2.16	0.48
2:D:32:PRO:HB3	2:D:38:LEU:HD21	1.95	0.47
2:D:259:LYS:HD3	2:D:288:ASN:HB3	1.95	0.47
2:H:349:LEU:HA	2:H:355:VAL:HG21	1.96	0.47
1:3:119:ASN:ND2	2:A:10:THR:HG21	2.30	0.47
1:6:200:GLN:O	1:6:204:GLU:HG2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:333:VAL:HA	2:B:468:PHE:HE1	1.79	0.47
1:3:107:ALA:O	1:3:163:LEU:HD12	2.15	0.47
1:6:117:THR:CG2	1:6:118:VAL:H	2.25	0.47
2:C:203:ASP:OD1	2:C:239:HIS:NE2	2.42	0.47
3:P:28:VAL:HA	3:P:31:ILE:HD12	1.97	0.47
1:2:245:ARG:O	1:2:245:ARG:NH1	2.44	0.46
1:3:200:GLN:O	1:3:204:GLU:HG2	2.15	0.46
1:5:277:GLN:NE2	1:6:170:ASP:OD2	2.48	0.46
3:J:10:TYR:HB3	3:J:102:ILE:HD12	1.97	0.46
2:C:107:ASP:O	2:D:211:PRO:HD2	2.16	0.46
1:6:99:MET:HG3	1:6:154:ILE:HB	1.98	0.46
2:E:274:GLY:HA3	2:F:274:GLY:HA3	1.97	0.46
2:C:184:LYS:HE3	3:K:51:LEU:HD13	1.96	0.46
2:C:211:PRO:HD2	2:D:107:ASP:O	2.14	0.46
5:3:301:AGS:H5'1	5:3:301:AGS:H8	1.96	0.46
2:E:296:ARG:HG2	2:E:328:HIS:HB2	1.97	0.46
1:1:143:TYR:CB	2:A:130:ALA:HB2	2.46	0.46
2:A:274:GLY:HA3	2:B:274:GLY:HA3	1.98	0.46
2:B:170:LEU:HD13	2:B:200:PHE:HE2	1.81	0.46
2:F:143:VAL:HG13	2:F:370:ALA:HB2	1.98	0.46
2:G:79:ASP:HA	2:G:82:LYS:HE3	1.98	0.46
2:E:160:ARG:HH21	2:E:398:ASP:HA	1.80	0.45
1:1:42:GLY:O	1:1:46:GLN:HG2	2.16	0.45
1:1:206:LEU:HD11	1:1:266:LEU:HD13	1.98	0.45
5:2:301:AGS:S1G	1:3:172:ARG:NH2	2.90	0.45
5:2:301:AGS:S1G	5:2:301:AGS:O3G	2.55	0.45
3:M:10:TYR:HB3	3:M:102:ILE:HD12	1.98	0.45
1:4:97:VAL:HG22	1:4:152:PRO:HG2	1.98	0.45
2:A:326:HIS:HD2	2:A:376:MET:HB2	1.81	0.45
1:4:117:THR:HG22	1:4:118:VAL:N	2.31	0.45
2:E:127:GLY:HA2	2:F:304:ARG:HD3	1.98	0.45
1:1:247:VAL:CG2	1:2:95:MET:CG	2.74	0.45
2:E:342:ILE:HD11	2:E:476:VAL:HG22	1.98	0.45
2:E:349:LEU:HA	2:E:355:VAL:HG21	1.99	0.45
1:1:84:GLU:CG	2:B:464:LYS:HG3	2.45	0.44
3:M:28:VAL:HA	3:M:31:ILE:HD12	1.99	0.44
2:D:345:GLY:HA2	2:D:361:ARG:HD3	1.99	0.44
2:E:143:VAL:HG13	2:E:370:ALA:HB2	1.99	0.44
2:A:346:PHE:HA	2:A:349:LEU:HB2	1.98	0.44
2:B:178:LYS:HD2	2:B:206:ASN:HD21	1.81	0.44
2:C:296:ARG:HG2	2:C:328:HIS:HB2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:234:ILE:HG23	1:1:242:ILE:HG21	1.98	0.44
2:D:151:GLY:HA3	2:D:372:LEU:HD11	1.99	0.44
3:O:28:VAL:HA	3:O:31:ILE:HD12	2.00	0.44
1:1:22:LEU:HB3	1:1:24:ILE:CD1	2.48	0.44
2:F:170:LEU:HD13	2:F:200:PHE:HE2	1.83	0.44
3:J:47:GLU:HB2	3:J:50:GLU:HG2	2.00	0.44
1:2:163:LEU:HD23	1:2:168:ILE:HD11	2.00	0.43
1:5:240:GLU:HG3	1:5:241:ARG:HG2	2.00	0.43
3:O:10:TYR:HB3	3:O:102:ILE:HD12	1.99	0.43
2:C:252:LEU:O	2:C:256:GLU:HG2	2.18	0.43
2:H:32:PRO:HB3	2:H:38:LEU:HD21	2.00	0.43
1:1:225:ILE:HG13	1:1:226:TYR:CD1	2.54	0.43
1:5:269:SER:O	1:5:273:VAL:HG23	2.18	0.43
2:D:296:ARG:HG2	2:D:328:HIS:HB2	1.99	0.43
1:1:143:TYR:HB3	2:A:130:ALA:HB2	2.00	0.43
1:4:189:VAL:HA	1:4:192:ILE:HD12	2.01	0.43
2:A:136:LEU:HD21	2:A:139:ILE:HD11	2.01	0.43
2:C:345:GLY:HA2	2:C:361:ARG:HD3	1.99	0.43
1:5:225:ILE:HG21	1:5:261:PHE:HE1	1.83	0.43
2:B:174:THR:HG23	2:B:202:KCX:HG3	2.01	0.43
2:C:151:GLY:HA3	2:C:372:LEU:HD11	1.99	0.43
2:E:317:LYS:HE2	2:E:349:LEU:HD21	2.00	0.43
1:1:36:HIS:HA	1:1:157:GLY:O	2.19	0.43
1:1:41:GLU:HA	1:1:41:GLU:OE1	2.18	0.43
1:4:68:SER:HB2	1:5:76:ARG:HH11	1.84	0.43
2:A:296:ARG:HG2	2:A:328:HIS:HB2	2.00	0.43
2:B:171:LEU:HD22	2:B:403:PHE:HE2	1.84	0.43
2:D:252:LEU:O	2:D:256:GLU:HG2	2.18	0.43
1:1:84:GLU:OE2	2:B:464:LYS:HG2	2.19	0.42
1:5:109:ARG:HA	1:5:116:TYR:OH	2.19	0.42
1:1:42:GLY:HA3	4:1:301:ADP:C8	2.53	0.42
2:A:160:ARG:HH21	2:A:398:ASP:HA	1.85	0.42
2:C:127:GLY:HA2	2:D:304:ARG:HD3	2.01	0.42
2:E:114:ILE:HD11	2:E:321:LEU:HB2	2.02	0.42
3:N:12:THR:HG22	3:N:13:LEU:HG	2.00	0.42
3:O:4:LEU:HA	3:O:5:PRO:HD3	1.94	0.42
3:O:47:GLU:HB2	3:O:50:GLU:HG2	2.01	0.42
1:2:72:GLY:HA2	1:2:122:LEU:HD13	2.01	0.42
1:5:277:GLN:HE21	1:6:170:ASP:CG	2.23	0.42
2:B:349:LEU:HA	2:B:355:VAL:HG21	2.01	0.42
2:E:302:ILE:HG22	2:E:310:ILE:H	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:342:ILE:HD11	2:F:476:VAL:HG22	2.02	0.42
1:4:119:ASN:ND2	2:A:8:THR:HG21	2.33	0.42
1:6:209:THR:HG21	1:6:267:ILE:HG12	2.01	0.42
2:G:259:LYS:HD3	2:G:288:ASN:HB3	2.02	0.42
1:1:230:ILE:O	1:1:234:ILE:HG12	2.19	0.42
1:2:165:ALA:HB3	1:2:166:PRO:HD3	2.01	0.42
1:4:61:ILE:HD11	1:4:98:LEU:HD11	2.01	0.42
1:1:110:PHE:HB3	1:2:109:ARG:HH21	1.84	0.42
1:5:119:ASN:ND2	2:A:6:THR:HG21	2.33	0.42
2:D:159:GLU:HG3	2:D:291:LEU:HD22	2.02	0.42
5:5:301:AGS:S1G	1:6:172:ARG:NH2	2.93	0.42
2:D:152:PRO:HA	2:D:153:PRO:HD3	1.97	0.42
1:6:227:ASP:HA	1:6:230:ILE:HG22	2.02	0.42
2:E:152:PRO:HA	2:E:153:PRO:HD3	1.95	0.42
2:G:196:GLY:HA3	2:G:418:ALA:HB3	2.00	0.42
1:2:218:PHE:O	1:2:221:LEU:HG	2.21	0.41
1:3:31:LEU:HD13	1:3:150:ARG:HE	1.85	0.41
1:4:102:ASP:H	1:4:156:THR:HB	1.84	0.41
2:H:317:LYS:HE2	2:H:349:LEU:HD21	2.02	0.41
1:2:258:LYS:HA	1:2:259:PRO:HD3	1.91	0.41
1:3:117:THR:HG22	1:3:118:VAL:N	2.36	0.41
2:D:380:SER:HB2	2:D:402:GLN:HB2	2.02	0.41
3:K:105:LYS:HB3	3:K:106:PRO:HD2	2.02	0.41
1:4:69:PRO:HB3	1:5:70:ASP:HB3	2.02	0.41
1:5:38:ARG:O	1:5:43:LYS:NZ	2.54	0.41
2:A:110:GLU:H	2:A:116:ASN:ND2	2.19	0.41
2:B:198:LEU:HD11	2:B:407:THR:HG21	2.02	0.41
3:N:47:GLU:HB2	3:N:50:GLU:HG2	2.03	0.41
3:L:105:LYS:HB3	3:L:106:PRO:HD2	2.02	0.41
1:2:280:VAL:HG22	1:3:36:HIS:CE1	2.56	0.41
1:2:200:GLN:O	1:2:204:GLU:HG2	2.21	0.41
2:B:172:GLY:HA3	2:B:402:GLN:HE21	1.86	0.41
2:C:304:ARG:HD3	2:D:127:GLY:HA2	2.03	0.41
3:J:37:ILE:HA	3:J:38:PRO:HD3	1.95	0.41
1:1:254:PRO:HG2	1:2:22:LEU:HD21	2.02	0.41
1:4:73:ASP:N	1:4:74:PRO:CD	2.84	0.41
1:5:97:VAL:HG22	1:5:152:PRO:HG2	2.03	0.41
1:6:163:LEU:HB3	1:6:168:ILE:HD11	2.02	0.41
2:H:184:LYS:HE3	3:P:51:LEU:HD13	2.02	0.41
1:1:111:ASP:HB3	1:1:114:THR:HB	2.03	0.41
2:B:152:PRO:HA	2:B:153:PRO:HD3	1.93	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:159:GLU:HG3	2:C:291:LEU:HD22	2.02	0.41
2:H:202:KCX:HB3	2:H:240:TYR:CD2	2.56	0.41
2:H:372:LEU:HA	2:H:373:PRO:HD3	1.93	0.41
2:C:181:LEU:HD21	2:D:72:THR:HG22	2.04	0.40
2:C:380:SER:HB2	2:C:402:GLN:HB2	2.03	0.40
2:D:372:LEU:HA	2:D:373:PRO:HD3	1.95	0.40
3:I:47:GLU:HB2	3:I:50:GLU:HG2	2.04	0.40
3:L:12:THR:HG22	3:L:13:LEU:HG	2.04	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 PDB entries followed by that with respect to all EM entries.

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	1	278/290 (96%)	269 (97%)	9 (3%)	0	100	100
1	2	279/290 (96%)	257 (92%)	21 (8%)	1 (0%)	30	49
1	3	282/290 (97%)	263 (93%)	19 (7%)	0	100	100
1	4	279/290 (96%)	269 (96%)	10 (4%)	0	100	100
1	5	278/290 (96%)	261 (94%)	17 (6%)	0	100	100
1	6	272/290 (94%)	264 (97%)	7 (3%)	1 (0%)	30	49
2	A	461/476 (97%)	437 (95%)	24 (5%)	0	100	100
2	B	456/476 (96%)	439 (96%)	17 (4%)	0	100	100
2	C	461/476 (97%)	449 (97%)	11 (2%)	1 (0%)	44	63
2	D	461/476 (97%)	449 (97%)	11 (2%)	1 (0%)	44	63
2	E	461/476 (97%)	447 (97%)	14 (3%)	0	100	100
2	F	461/476 (97%)	448 (97%)	12 (3%)	1 (0%)	44	63
2	G	461/476 (97%)	446 (97%)	14 (3%)	1 (0%)	44	63

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	H	461/476 (97%)	448 (97%)	12 (3%)	1 (0%)	44 63
3	I	106/109 (97%)	102 (96%)	4 (4%)	0	100 100
3	J	106/109 (97%)	102 (96%)	4 (4%)	0	100 100
3	K	106/109 (97%)	101 (95%)	5 (5%)	0	100 100
3	L	106/109 (97%)	101 (95%)	5 (5%)	0	100 100
3	M	106/109 (97%)	103 (97%)	3 (3%)	0	100 100
3	N	106/109 (97%)	102 (96%)	4 (4%)	0	100 100
3	O	106/109 (97%)	103 (97%)	3 (3%)	0	100 100
3	P	106/109 (97%)	102 (96%)	4 (4%)	0	100 100
All	All	6199/6420 (97%)	5962 (96%)	230 (4%)	7 (0%)	50 69

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	381	GLY
2	D	381	GLY
1	6	110	PHE
1	2	225	ILE
2	H	197	GLY
2	F	197	GLY
2	G	197	GLY

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 PDB entries followed by that with respect to all EM entries.

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	1	233/252 (92%)	233 (100%)	0	100 100
1	2	239/252 (95%)	239 (100%)	0	100 100
1	3	243/252 (96%)	242 (100%)	1 (0%)	89 95
1	4	241/252 (96%)	239 (99%)	2 (1%)	79 90
1	5	238/252 (94%)	238 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	6	234/252 (93%)	234 (100%)	0	100	100
2	A	377/385 (98%)	374 (99%)	3 (1%)	79	90
2	B	366/385 (95%)	363 (99%)	3 (1%)	79	90
2	C	373/385 (97%)	371 (100%)	2 (0%)	86	94
2	D	373/385 (97%)	371 (100%)	2 (0%)	86	94
2	E	373/385 (97%)	369 (99%)	4 (1%)	70	85
2	F	373/385 (97%)	368 (99%)	5 (1%)	65	83
2	G	373/385 (97%)	369 (99%)	4 (1%)	70	85
2	H	373/385 (97%)	370 (99%)	3 (1%)	79	90
3	I	99/102 (97%)	97 (98%)	2 (2%)	50	73
3	J	99/102 (97%)	98 (99%)	1 (1%)	73	87
3	K	99/102 (97%)	99 (100%)	0	100	100
3	L	99/102 (97%)	99 (100%)	0	100	100
3	M	99/102 (97%)	97 (98%)	2 (2%)	50	73
3	N	99/102 (97%)	98 (99%)	1 (1%)	73	87
3	O	99/102 (97%)	97 (98%)	2 (2%)	50	73
3	P	99/102 (97%)	98 (99%)	1 (1%)	73	87
All	All	5201/5408 (96%)	5163 (99%)	38 (1%)	80	91

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	3	245	ARG
1	4	115	GLN
1	4	241	ARG
2	A	118	LEU
2	A	166	TYR
2	A	205	GLU
2	B	72	THR
2	B	128	PHE
2	B	331	THR
2	C	128	PHE
2	C	248	CYS
2	D	128	PHE
2	D	248	CYS
2	E	72	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	128	PHE
2	E	248	CYS
2	E	475	THR
2	F	72	THR
2	F	213	GLN
2	F	248	CYS
2	F	269	ASP
2	F	475	THR
2	G	72	THR
2	G	128	PHE
2	G	248	CYS
2	G	475	THR
2	H	72	THR
2	H	128	PHE
2	H	475	THR
3	I	20	THR
3	I	65	THR
3	J	20	THR
3	M	20	THR
3	M	65	THR
3	N	20	THR
3	O	20	THR
3	O	65	THR
3	P	65	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	265	HIS
1	3	129	ASN
1	3	133	ASN
1	4	265	HIS
1	6	129	ASN
2	A	46	GLN
2	A	326	HIS
2	B	154	HIS
2	B	213	GLN
2	C	116	ASN
2	C	154	HIS
2	C	208	ASN
2	C	213	GLN
2	C	421	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	116	ASN
2	D	154	HIS
2	D	208	ASN
2	D	213	GLN
2	D	421	ASN
2	E	116	ASN
2	E	154	HIS
2	F	116	ASN
2	F	154	HIS
2	F	213	GLN
2	G	116	ASN
2	G	154	HIS
2	G	213	GLN
2	H	116	ASN
2	H	154	HIS
2	H	213	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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	KCX	D	202	6,2	9,11,12	2.18	1 (11%)	5,12,14	2.37	2 (40%)
2	KCX	E	202	6,2	9,11,12	0.54	0	5,12,14	1.09	1 (20%)
2	KCX	C	202	6,2	9,11,12	0.53	0	5,12,14	1.40	1 (20%)
2	KCX	H	202	6,2	9,11,12	2.19	1 (11%)	5,12,14	2.11	2 (40%)
2	KCX	B	202	6,2	9,11,12	2.18	1 (11%)	5,12,14	2.16	2 (40%)
2	KCX	A	202	6,2	9,11,12	0.51	0	5,12,14	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	KCX	G	202	6,2	9,11,12	0.54	0	5,12,14	0.98	0
2	KCX	F	202	6,2	9,11,12	2.21	1 (11%)	5,12,14	2.14	2 (40%)

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	KCX	D	202	6,2	-	4/9/10/12	-
2	KCX	E	202	6,2	-	5/9/10/12	-
2	KCX	C	202	6,2	-	4/9/10/12	-
2	KCX	H	202	6,2	-	3/9/10/12	-
2	KCX	B	202	6,2	-	3/9/10/12	-
2	KCX	A	202	6,2	-	2/9/10/12	-
2	KCX	G	202	6,2	-	4/9/10/12	-
2	KCX	F	202	6,2	-	4/9/10/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	202	KCX	OQ1-CX	6.45	1.33	1.21
2	H	202	KCX	OQ1-CX	6.40	1.33	1.21
2	B	202	KCX	OQ1-CX	6.39	1.33	1.21
2	D	202	KCX	OQ1-CX	6.37	1.33	1.21

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	202	KCX	OQ1-CX-NZ	-4.33	118.24	124.96
2	B	202	KCX	OQ1-CX-NZ	-4.18	118.48	124.96
2	F	202	KCX	OQ1-CX-NZ	-4.17	118.50	124.96
2	H	202	KCX	OQ1-CX-NZ	-4.04	118.69	124.96
2	C	202	KCX	CE-NZ-CX	2.51	125.91	121.89
2	D	202	KCX	CE-NZ-CX	2.47	125.84	121.89
2	B	202	KCX	CE-NZ-CX	2.13	125.31	121.89
2	E	202	KCX	CE-NZ-CX	2.11	125.27	121.89
2	F	202	KCX	CE-NZ-CX	2.05	125.17	121.89
2	H	202	KCX	CE-NZ-CX	2.02	125.13	121.89

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	202	KCX	C-CA-CB-CG
2	B	202	KCX	C-CA-CB-CG
2	C	202	KCX	N-CA-CB-CG
2	C	202	KCX	O-C-CA-CB
2	D	202	KCX	N-CA-CB-CG
2	D	202	KCX	O-C-CA-CB
2	E	202	KCX	N-CA-CB-CG
2	E	202	KCX	C-CA-CB-CG
2	F	202	KCX	N-CA-CB-CG
2	G	202	KCX	N-CA-CB-CG
2	H	202	KCX	N-CA-CB-CG
2	C	202	KCX	C-CA-CB-CG
2	D	202	KCX	C-CA-CB-CG
2	F	202	KCX	C-CA-CB-CG
2	G	202	KCX	C-CA-CB-CG
2	H	202	KCX	C-CA-CB-CG
2	H	202	KCX	CE-CD-CG-CB
2	C	202	KCX	CE-CD-CG-CB
2	B	202	KCX	CA-CB-CG-CD
2	D	202	KCX	CE-CD-CG-CB
2	F	202	KCX	CE-CD-CG-CB
2	E	202	KCX	CA-CB-CG-CD
2	B	202	KCX	N-CA-CB-CG
2	G	202	KCX	CE-CD-CG-CB
2	F	202	KCX	CA-CB-CG-CD
2	A	202	KCX	CE-CD-CG-CB
2	G	202	KCX	CA-CB-CG-CD
2	E	202	KCX	CG-CD-CE-NZ
2	E	202	KCX	CE-CD-CG-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	202	KCX	1	0
2	B	202	KCX	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 25 ligands modelled in this entry, 12 are monoatomic - leaving 13 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	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	CAP	E	502	6	17,20,20	0.76	0	22,31,31	1.09	1 (4%)
5	AGS	6	301	-	26,33,33	2.59	7 (26%)	26,52,52	1.76	5 (19%)
4	ADP	1	301	-	24,29,29	0.66	0	29,45,45	0.72	1 (3%)
7	CAP	C	502	6	17,20,20	0.75	0	22,31,31	1.04	0
7	CAP	F	502	6	17,20,20	0.74	0	22,31,31	1.03	0
5	AGS	5	301	6	26,33,33	2.84	7 (26%)	26,52,52	1.89	5 (19%)
5	AGS	4	301	6	26,33,33	2.50	7 (26%)	26,52,52	1.82	4 (15%)
7	CAP	A	502	6	17,20,20	0.74	0	22,31,31	1.10	1 (4%)
5	AGS	2	301	6	26,33,33	3.88	5 (19%)	26,52,52	1.67	4 (15%)
5	AGS	3	301	6	26,33,33	2.08	6 (23%)	26,52,52	1.82	4 (15%)
7	CAP	G	502	6	17,20,20	0.76	0	22,31,31	1.06	0
7	CAP	H	502	6	17,20,20	0.71	0	22,31,31	1.06	0
7	CAP	D	502	6	17,20,20	0.74	0	22,31,31	1.03	0

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
7	CAP	E	502	6	-	5/29/29/29	-
5	AGS	6	301	-	-	7/17/38/38	0/3/3/3
4	ADP	1	301	-	-	1/12/32/32	0/3/3/3
7	CAP	C	502	6	-	7/29/29/29	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CAP	F	502	6	-	8/29/29/29	-
5	AGS	5	301	6	-	2/17/38/38	0/3/3/3
5	AGS	4	301	6	-	4/17/38/38	0/3/3/3
7	CAP	A	502	6	-	5/29/29/29	-
5	AGS	2	301	6	-	5/17/38/38	0/3/3/3
5	AGS	3	301	6	-	5/17/38/38	0/3/3/3
7	CAP	G	502	6	-	8/29/29/29	-
7	CAP	H	502	6	-	6/29/29/29	-
7	CAP	D	502	6	-	7/29/29/29	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	2	301	AGS	PG-S1G	-16.93	1.53	1.90
5	5	301	AGS	PG-S1G	-10.57	1.67	1.90
5	6	301	AGS	PG-S1G	9.26	2.10	1.90
5	4	301	AGS	PG-S1G	8.33	2.08	1.90
5	3	301	AGS	C2-N3	6.00	1.41	1.32
5	2	301	AGS	C2-N3	5.81	1.41	1.32
5	4	301	AGS	C2-N3	5.60	1.41	1.32
5	6	301	AGS	C2-N3	5.48	1.40	1.32
5	2	301	AGS	O4'-C1'	5.25	1.48	1.41
5	5	301	AGS	C2-N3	5.20	1.40	1.32
5	3	301	AGS	O4'-C1'	4.97	1.48	1.41
5	5	301	AGS	O4'-C1'	4.22	1.47	1.41
5	3	301	AGS	C2-N1	3.95	1.41	1.33
5	6	301	AGS	C2-N1	3.91	1.41	1.33
5	2	301	AGS	C2-N1	3.74	1.40	1.33
5	4	301	AGS	C2-N1	3.72	1.40	1.33
5	5	301	AGS	C2-N1	3.72	1.40	1.33
5	4	301	AGS	O4'-C1'	3.43	1.45	1.41
5	6	301	AGS	O4'-C1'	3.22	1.45	1.41
5	5	301	AGS	PG-O2G	2.84	1.64	1.54
5	4	301	AGS	PG-O2G	2.71	1.63	1.54
5	3	301	AGS	PG-O2G	2.58	1.63	1.54
5	5	301	AGS	C6-C5	-2.54	1.33	1.43
5	5	301	AGS	C5-C4	-2.45	1.34	1.40
5	4	301	AGS	C6-C5	-2.40	1.34	1.43
5	6	301	AGS	C6-C5	-2.38	1.34	1.43
5	3	301	AGS	C5-C4	-2.35	1.34	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	3	301	AGS	C6-C5	-2.29	1.34	1.43
5	2	301	AGS	C5-C4	-2.26	1.34	1.40
5	4	301	AGS	C5-C4	-2.22	1.35	1.40
5	6	301	AGS	PG-O2G	2.08	1.61	1.54
5	6	301	AGS	C5-C4	-2.07	1.35	1.40

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	5	301	AGS	N3-C2-N1	-6.68	118.24	128.68
5	4	301	AGS	N3-C2-N1	-6.63	118.32	128.68
5	3	301	AGS	N3-C2-N1	-6.47	118.56	128.68
5	2	301	AGS	N3-C2-N1	-6.29	118.85	128.68
5	6	301	AGS	N3-C2-N1	-6.14	119.08	128.68
5	3	301	AGS	PA-O3A-PB	-4.31	118.03	132.83
5	4	301	AGS	PA-O3A-PB	-4.10	118.77	132.83
5	5	301	AGS	PA-O3A-PB	-3.82	119.71	132.83
5	6	301	AGS	PA-O3A-PB	-3.37	121.27	132.83
5	3	301	AGS	O3G-PG-O3B	2.77	113.90	104.64
5	2	301	AGS	PA-O3A-PB	-2.75	123.38	132.83
5	5	301	AGS	C3'-C2'-C1'	2.55	104.82	100.98
5	2	301	AGS	O3G-PG-O3B	2.53	113.09	104.64
5	4	301	AGS	O3G-PG-O3B	2.45	112.82	104.64
5	4	301	AGS	C5-C6-N6	-2.40	116.70	120.35
5	5	301	AGS	C5-C6-N6	-2.39	116.72	120.35
5	3	301	AGS	C5-C6-N6	-2.34	116.80	120.35
7	A	502	CAP	C2-C3-C4	2.33	118.74	114.00
5	5	301	AGS	O3G-PG-O3B	2.30	112.32	104.64
5	6	301	AGS	O3G-PG-O3B	2.29	112.30	104.64
7	E	502	CAP	C2-C3-C4	2.28	118.64	114.00
5	2	301	AGS	C4-C5-N7	-2.28	107.02	109.40
5	6	301	AGS	C5-C6-N6	-2.27	116.90	120.35
5	6	301	AGS	C3'-C2'-C1'	2.27	104.39	100.98
4	1	301	ADP	C5-C6-N6	2.06	123.48	120.35

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	2	301	AGS	C5'-O5'-PA-O1A
5	2	301	AGS	C5'-O5'-PA-O3A
5	2	301	AGS	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	3	301	AGS	C5'-O5'-PA-O3A
5	4	301	AGS	PB-O3B-PG-O3G
7	A	502	CAP	O6-C-C2-C1
7	A	502	CAP	O7-C-C2-C1
7	A	502	CAP	O6-C-C2-O2
7	A	502	CAP	O7-C-C2-O2
7	C	502	CAP	O6-C-C2-C1
7	C	502	CAP	O7-C-C2-C1
7	C	502	CAP	O6-C-C2-O2
7	C	502	CAP	O7-C-C2-O2
7	C	502	CAP	O3-C3-C4-O4
7	D	502	CAP	O6-C-C2-O2
7	D	502	CAP	O7-C-C2-O2
7	D	502	CAP	O3-C3-C4-O4
7	E	502	CAP	O6-C-C2-O2
7	E	502	CAP	O7-C-C2-O2
7	F	502	CAP	O6-C-C2-O2
7	F	502	CAP	O7-C-C2-O2
7	F	502	CAP	O3-C3-C4-O4
7	G	502	CAP	O6-C-C2-O2
7	G	502	CAP	O7-C-C2-O2
7	G	502	CAP	O3-C3-C4-O4
7	H	502	CAP	O6-C-C2-C3
7	H	502	CAP	C2-C3-C4-O4
7	H	502	CAP	O3-C3-C4-O4
5	3	301	AGS	O4'-C4'-C5'-O5'
7	D	502	CAP	O7-C-C2-C1
7	E	502	CAP	O6-C-C2-C1
7	E	502	CAP	O7-C-C2-C1
7	F	502	CAP	O7-C-C2-C1
7	G	502	CAP	O6-C-C2-C1
7	G	502	CAP	O7-C-C2-C1
5	6	301	AGS	O4'-C4'-C5'-O5'
5	6	301	AGS	C3'-C4'-C5'-O5'
7	A	502	CAP	O2-C2-C3-C4
7	C	502	CAP	O2-C2-C3-C4
7	D	502	CAP	O2-C2-C3-C4
7	E	502	CAP	O2-C2-C3-C4
7	F	502	CAP	O2-C2-C3-C4
7	G	502	CAP	O2-C2-C3-C4
7	H	502	CAP	O2-C2-C3-C4
7	D	502	CAP	O6-C-C2-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	6	301	AGS	PB-O3A-PA-O5'
7	F	502	CAP	O6-C-C2-C3
5	6	301	AGS	C5'-O5'-PA-O3A
5	2	301	AGS	PA-O3A-PB-O2B
5	2	301	AGS	C5'-O5'-PA-O2A
5	3	301	AGS	C5'-O5'-PA-O1A
5	3	301	AGS	C5'-O5'-PA-O2A
7	G	502	CAP	C2-C3-C4-O4
7	F	502	CAP	O7-C-C2-C3
7	G	502	CAP	O7-C-C2-C3
7	H	502	CAP	O7-C-C2-C3
7	F	502	CAP	O6-C-C2-C1
5	6	301	AGS	C4'-C5'-O5'-PA
5	4	301	AGS	PB-O3B-PG-O2G
5	3	301	AGS	PA-O3A-PB-O1B
5	6	301	AGS	PA-O3A-PB-O1B
7	H	502	CAP	O6-C-C2-O2
5	4	301	AGS	O4'-C4'-C5'-O5'
5	5	301	AGS	O4'-C4'-C5'-O5'
4	1	301	ADP	C5'-O5'-PA-O1A
5	4	301	AGS	C5'-O5'-PA-O1A
5	5	301	AGS	C5'-O5'-PA-O1A
5	6	301	AGS	C5'-O5'-PA-O2A
7	C	502	CAP	O4-C4-C5-O5
7	D	502	CAP	O4-C4-C5-O5

There are no ring outliers.

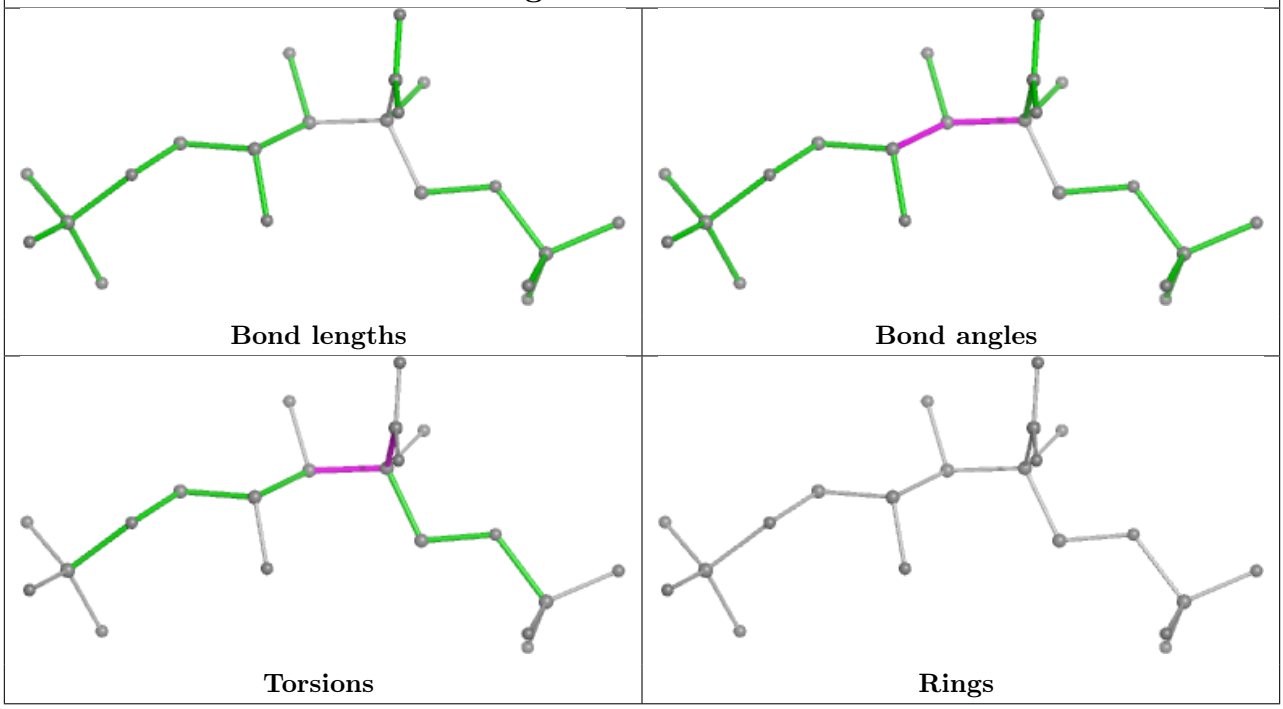
6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	6	301	AGS	2	0
4	1	301	ADP	1	0
5	5	301	AGS	2	0
5	4	301	AGS	1	0
5	2	301	AGS	6	0
5	3	301	AGS	1	0

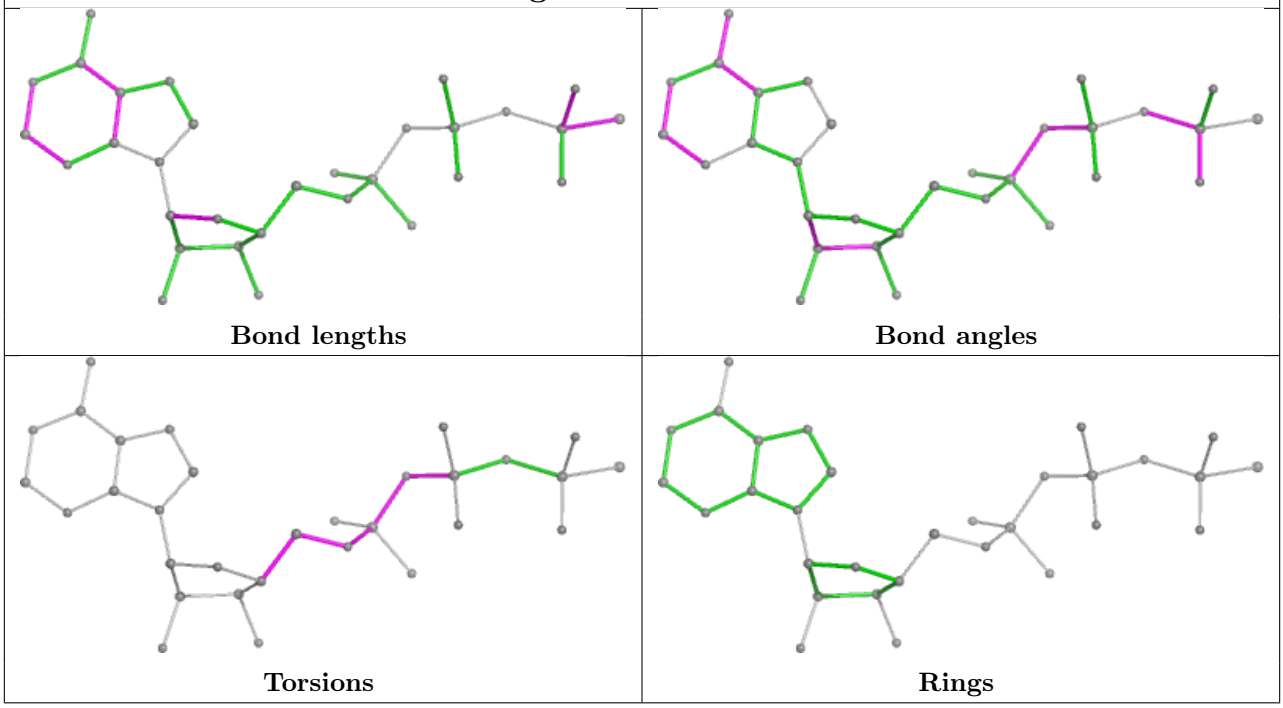
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

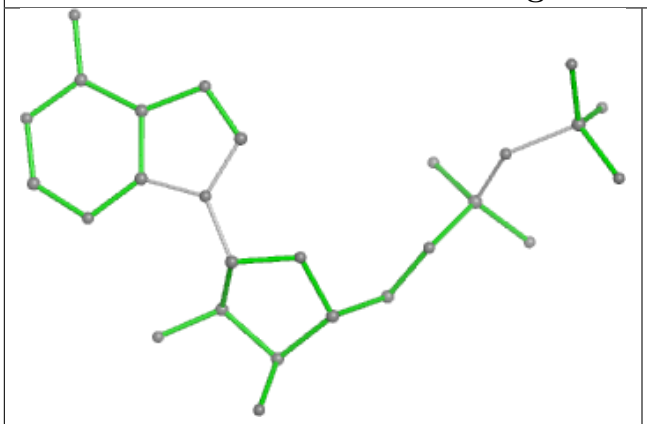
Ligand CAP E 502



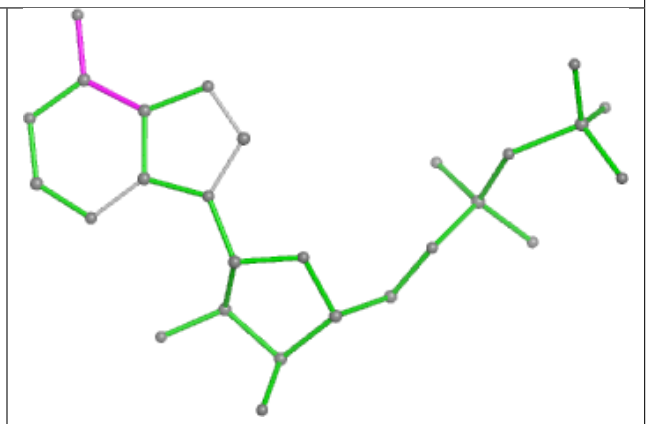
Ligand AGS 6 301



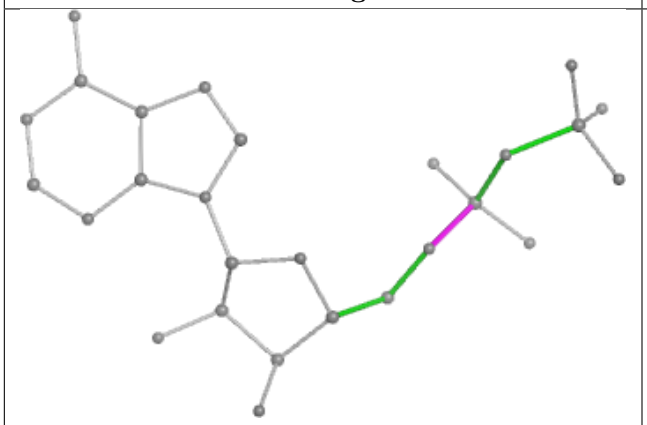
Ligand ADP 1 301



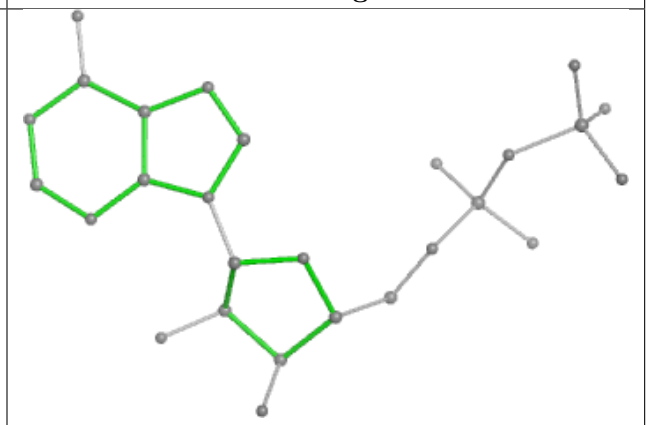
Bond lengths



Bond angles

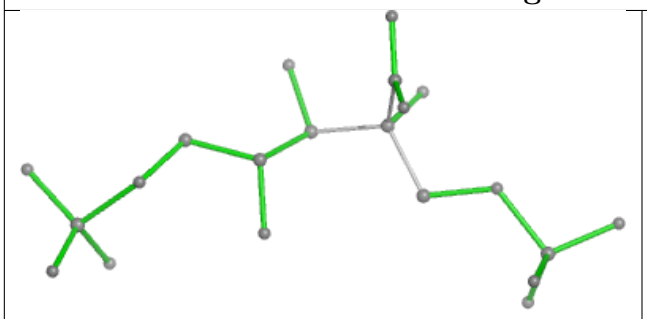


Torsions

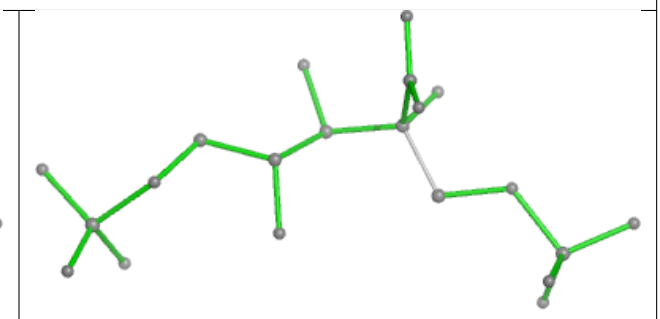


Rings

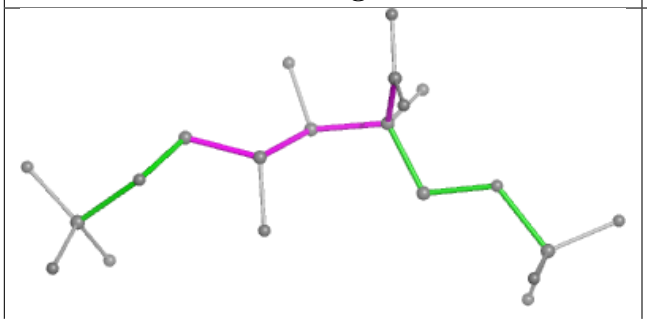
Ligand CAP C 502



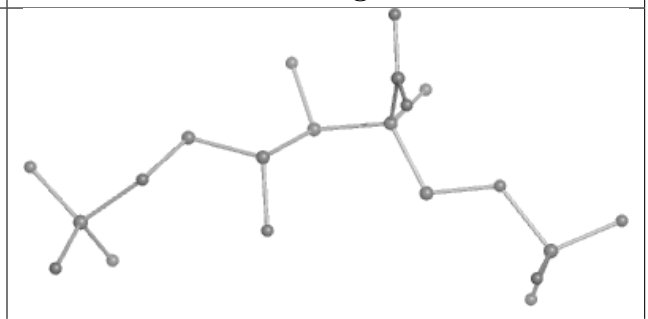
Bond lengths



Bond angles

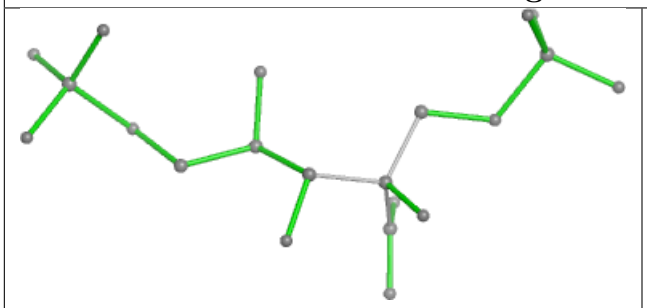


Torsions

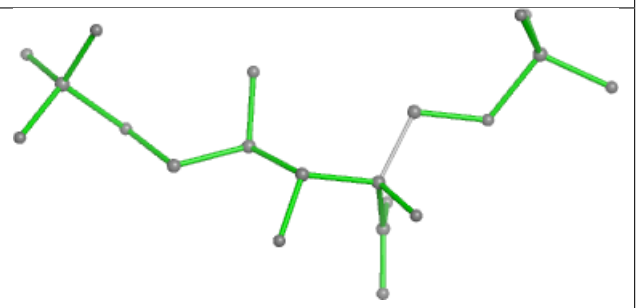


Rings

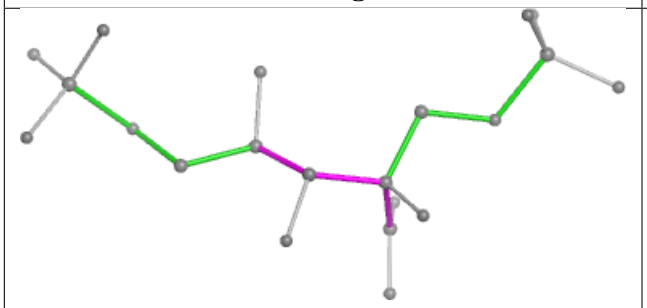
Ligand CAP F 502



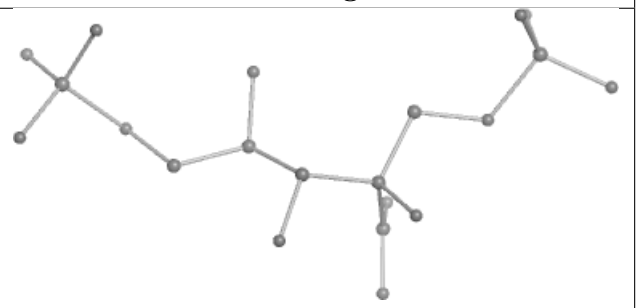
Bond lengths



Bond angles

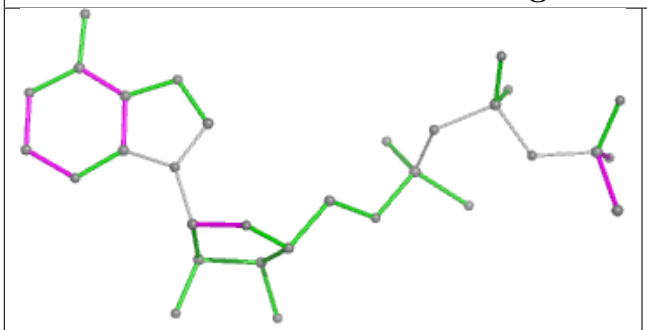


Torsions

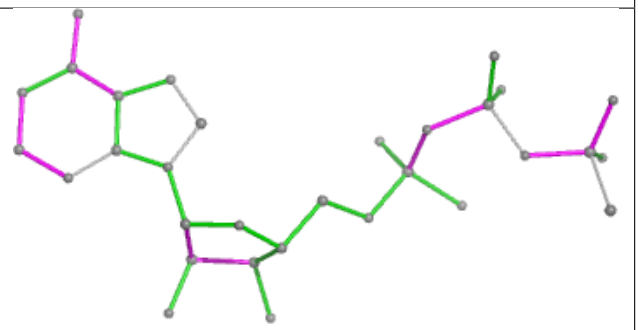


Rings

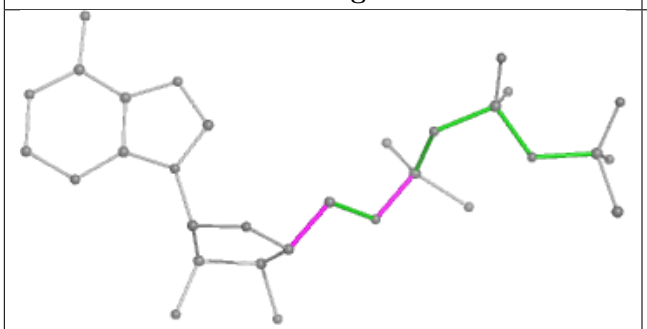
Ligand AGS 5 301



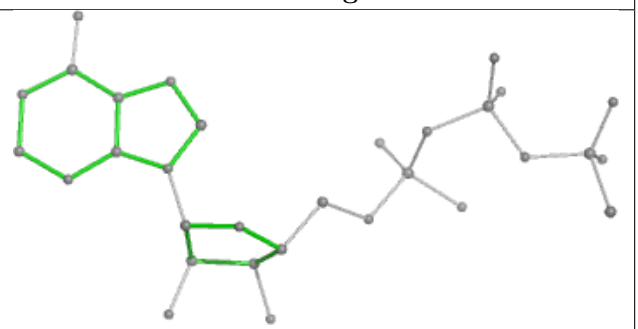
Bond lengths



Bond angles

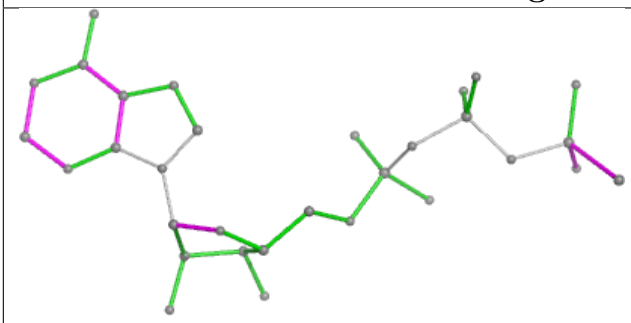


Torsions

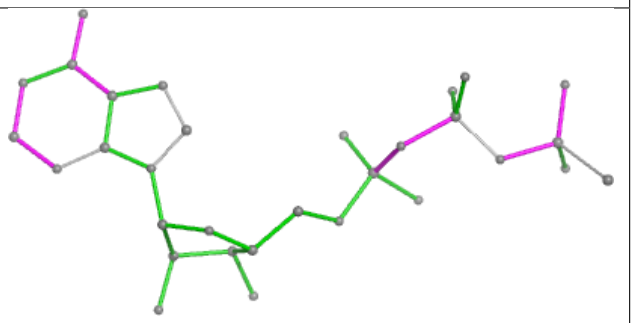


Rings

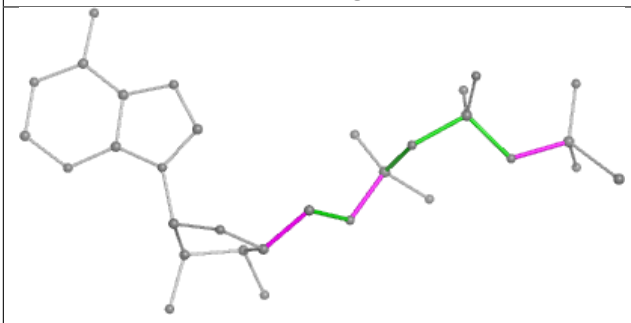
Ligand AGS 4 301



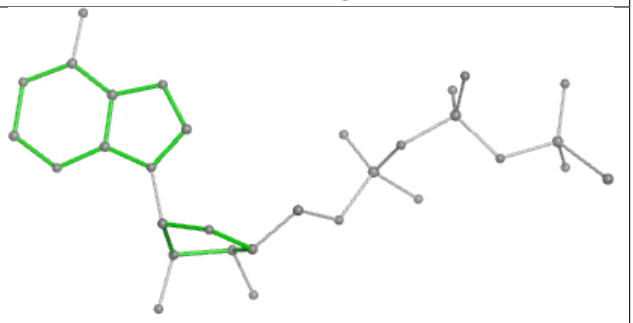
Bond lengths



Bond angles

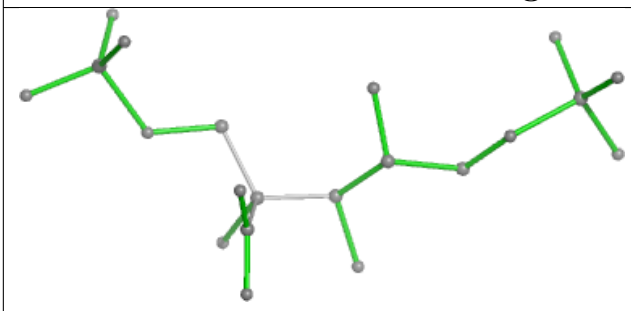


Torsions

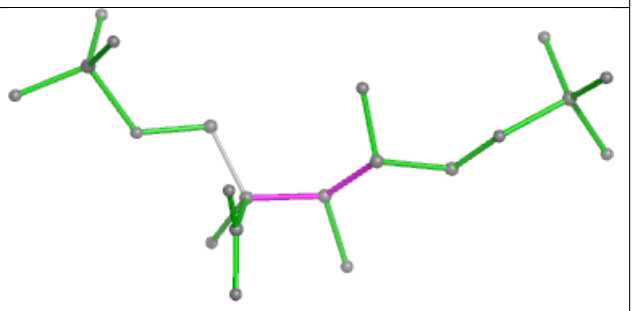


Rings

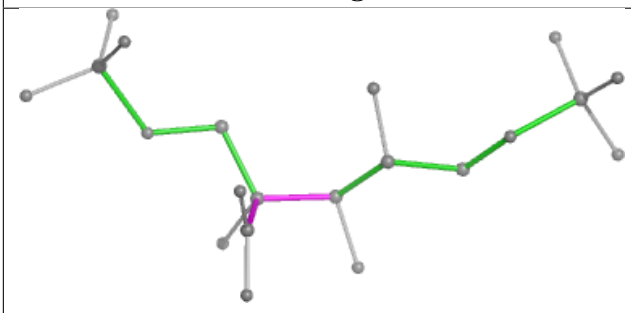
Ligand CAP A 502



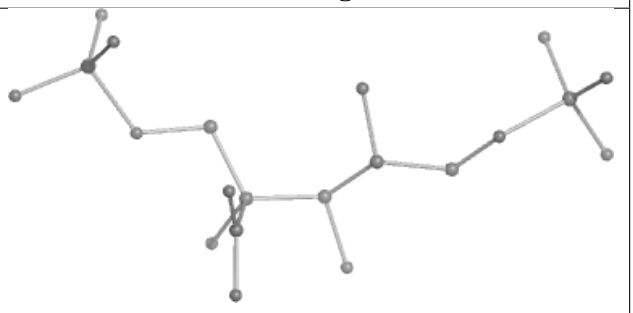
Bond lengths



Bond angles

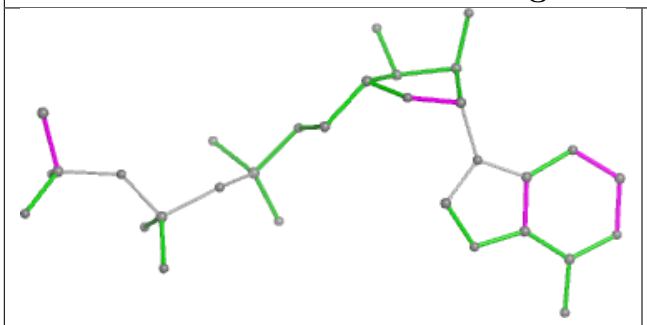


Torsions

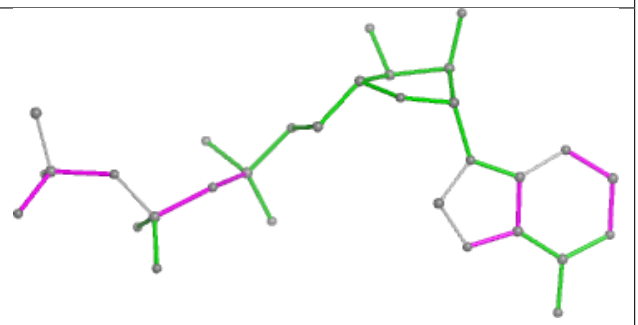


Rings

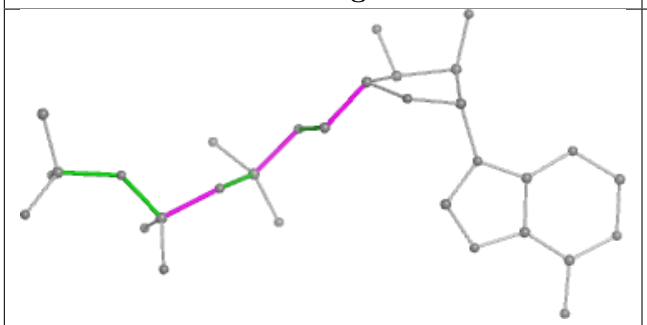
Ligand AGS 2 301



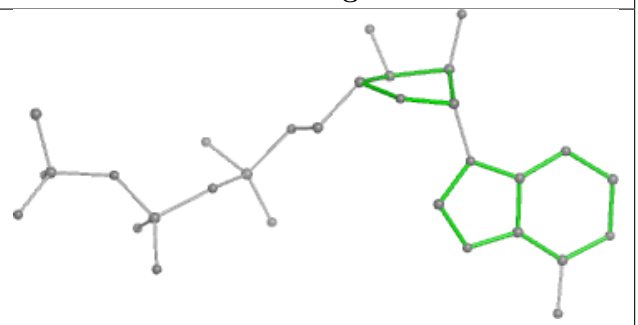
Bond lengths



Bond angles

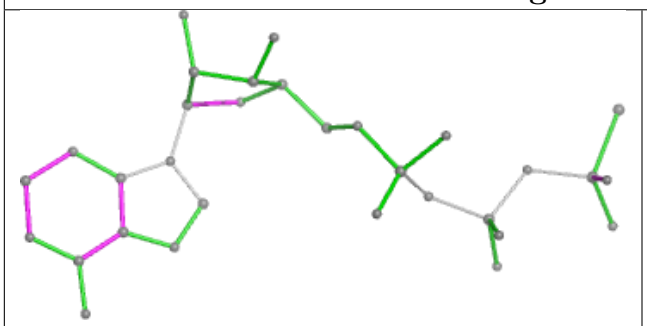


Torsions

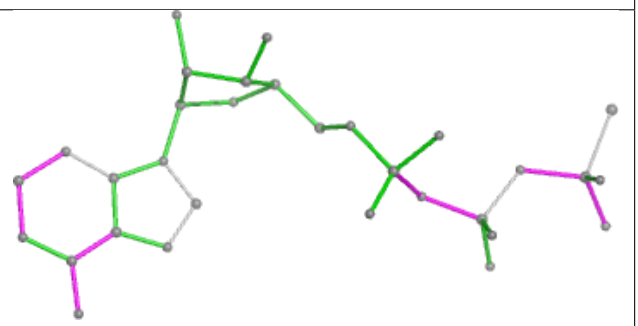


Rings

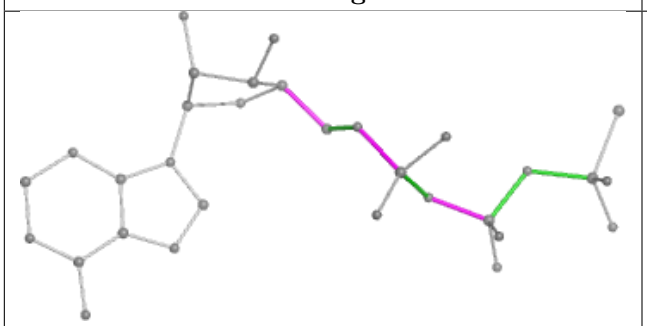
Ligand AGS 3 301



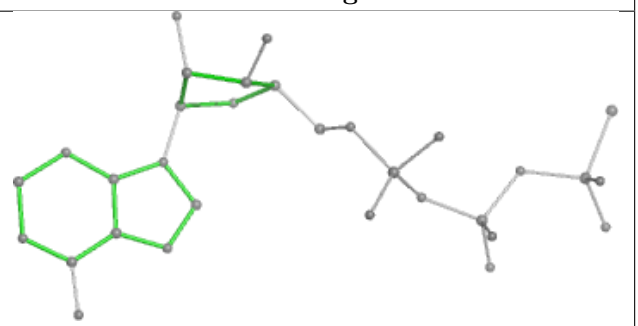
Bond lengths



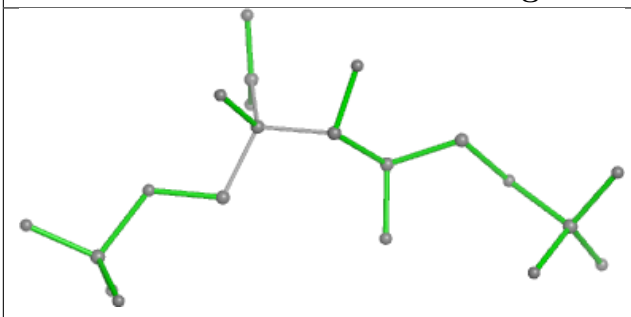
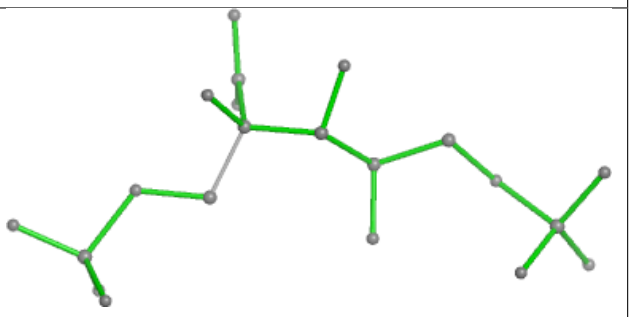
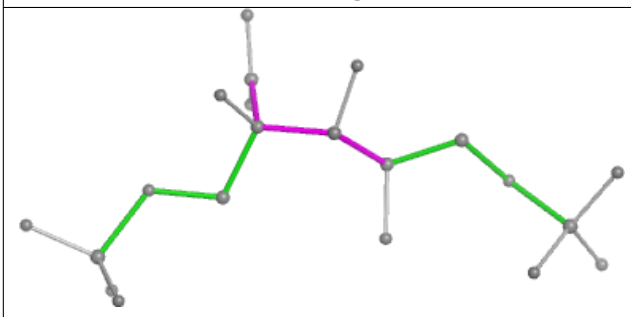
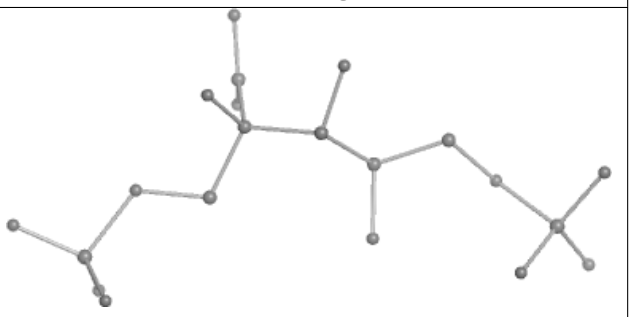
Bond angles

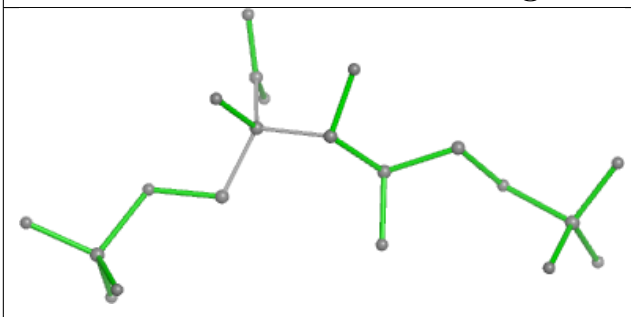
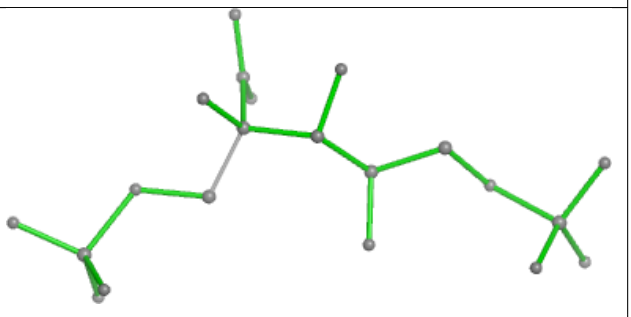
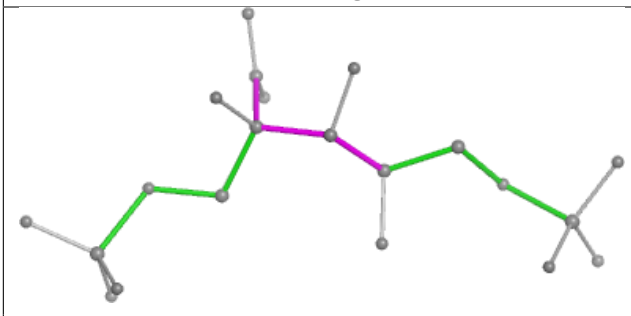
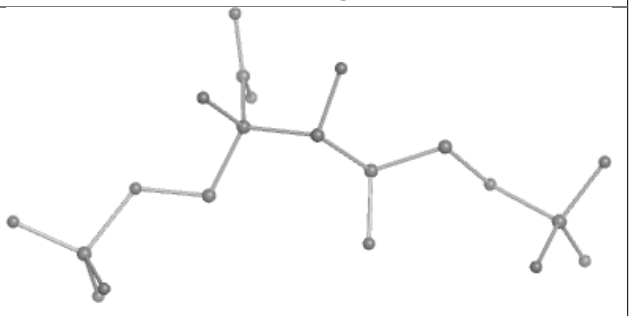


Torsions

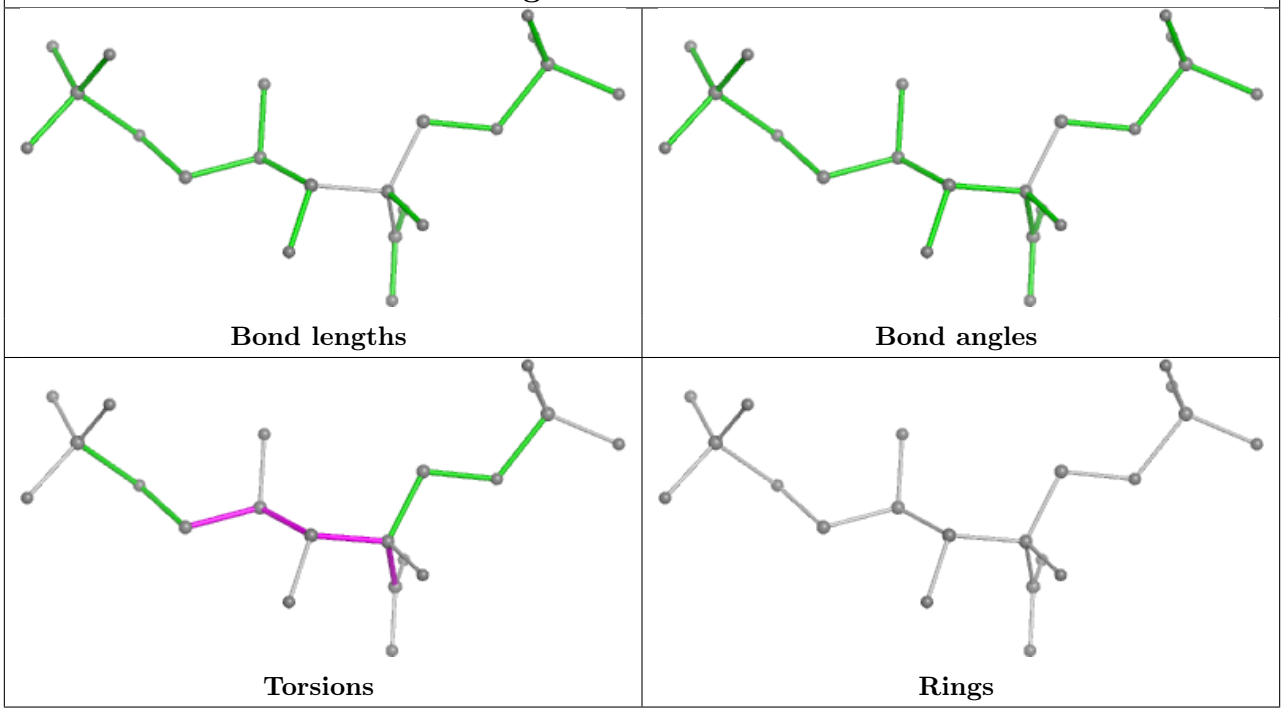


Rings

Ligand CAP G 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CAP H 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CAP D 502



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 Map visualisation

This section contains visualisations of the EMDB entry EMD-11028. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.