



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 08:08 AM EDT

PDB ID : 1KPH
Title : Crystal Structure of mycolic acid cyclopropane synthase CmaA1 complexed with SAH and DDDMAB
Authors : Huang, C.-C.; Smith, C.V.; Jacobs Jr., W.R.; Glickman, M.S.; Sacchettini, J.C.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2001-12-30
Resolution : 2.00 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 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:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
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)	:	2.36.2

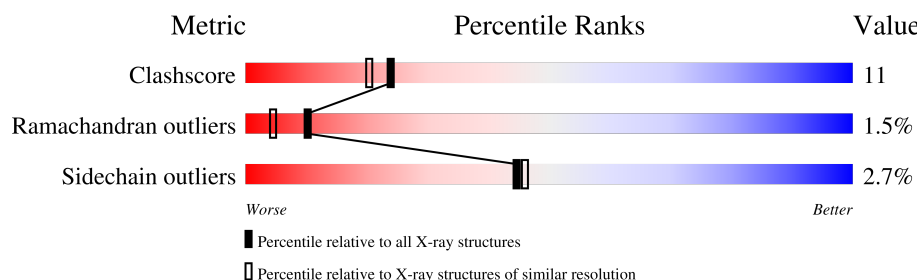
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	287	 71% 25% ..
1	B	287	 80% 18% ..
1	C	287	 78% 21% .
1	D	287	 79% 18% ..

2 Entry composition [i](#)

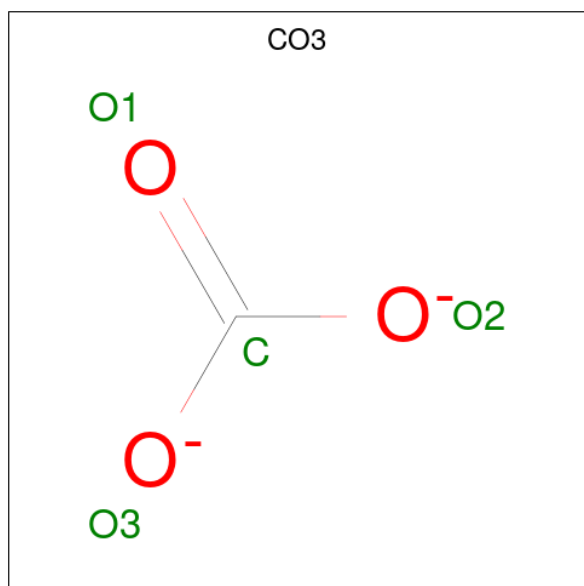
There are 5 unique types of molecules in this entry. The entry contains 10001 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CYCLOPROPANE-FATTY-ACYL-PHOSPHOLIPID SYNTHASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2252	1443	386	409	14			
1	B	285	Total	C	N	O	S	0	0	0
			2269	1452	388	415	14			
1	C	285	Total	C	N	O	S	0	0	0
			2269	1452	388	415	14			
1	D	285	Total	C	N	O	S	0	0	0
			2269	1452	388	415	14			

- Molecule 2 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).



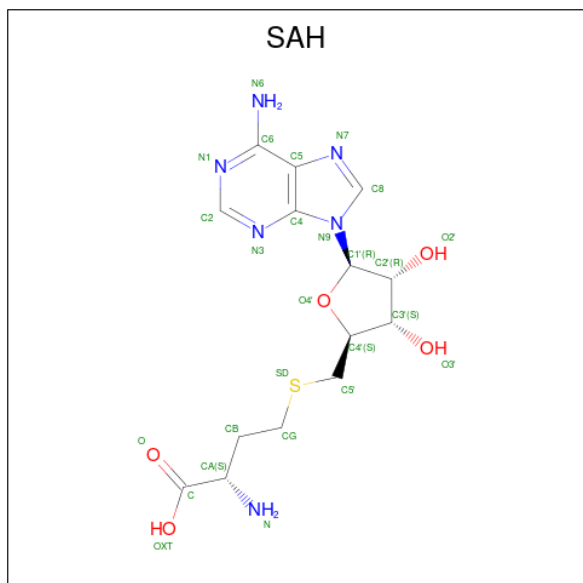
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	1	3		
2	B	1	Total	C	O	0	0
			4	1	3		

Continued on next page...

Continued from previous page...

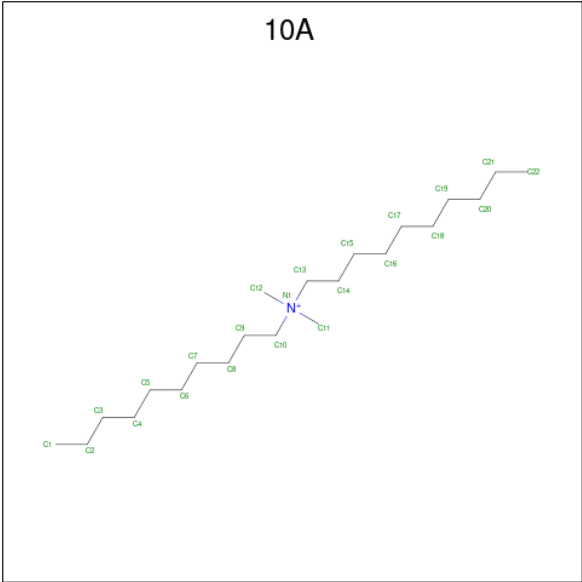
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			4	1	3		
2	D	1	Total	C	O	0	0
			4	1	3		

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O		0	0
			24	14	6	4			
3	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 4 is DIDECYL-DIMETHYL-AMMONIUM (three-letter code: 10A) (formula: $C_{22}H_{48}N$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			23	22	1		
4	B	1	Total	C	N	0	0
			23	22	1		
4	C	1	Total	C	N	0	0
			23	22	1		
4	D	1	Total	C	N	0	0
			23	22	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	156	Total	O	0	0
			156	156		
5	B	185	Total	O	0	0
			185	185		
5	C	210	Total	O	0	0
			210	210		
5	D	181	Total	O	0	0
			181	181		

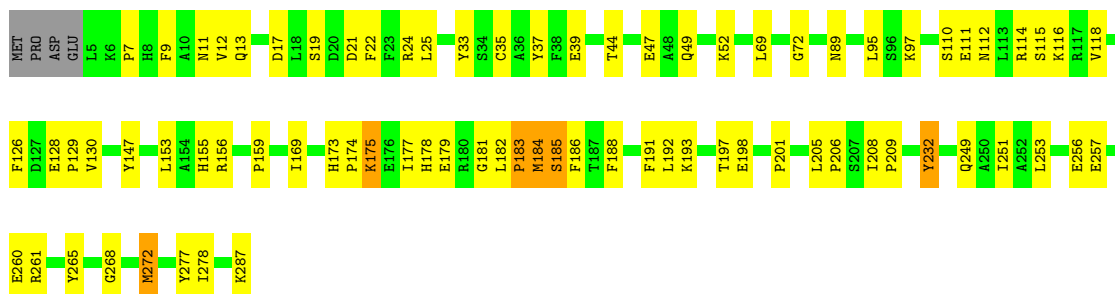
3 Residue-property plots

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.


Note EDS was not executed.

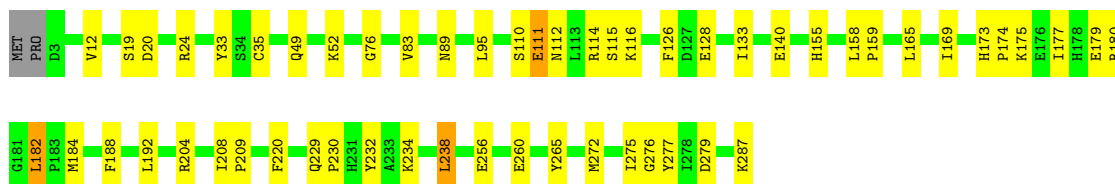
• Molecule 1: CYCLOPROPANE-FATTY-ACYL-PHOSPHOLIPID SYNTHASE 1

Chain A: 




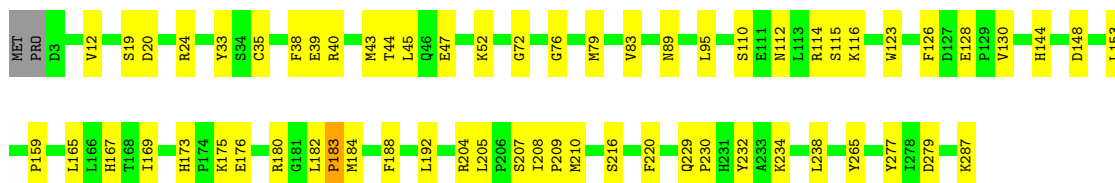
• Molecule 1: CYCLOPROPANE-FATTY-ACYL-PHOSPHOLIPID SYNTHASE 1

Chain B: 




• Molecule 1: CYCLOPROPANE-FATTY-ACYL-PHOSPHOLIPID SYNTHASE 1

Chain C: 



• Molecule 1: CYCLOPROPANE-FATTY-ACYL-PHOSPHOLIPID SYNTHASE 1

Chain D: 

MET	PRO	D3	E4	L5	K6	P7	V12	S19	D20	R24	Y33	S34	C35	T44	E47	A48	Q49	K52	A77	T78	M79	V83	N89	L95	V103	V107	N112	L113	R114	S115	L119	F126	D127	E128	I136	L165	L166	H167	P174	K175
E176	I177	H178	E179	R180	G181	L182	P183	M184	S185	F186	T187	F188	L192	V196	L205	I208	P209	M210	Q229	P230	H231	Y232	L243	Q249	M263	K264	Y265	L266	T267	E271	Y277	K287								

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	77.62Å 77.62Å 174.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.83 – 2.00	Depositor
% Data completeness (in resolution range)	97.0 (29.83-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.03	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.194 , 0.240	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10001	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 10A, CO3, SAH

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	0.31	0/2306	0.56	0/3122
1	B	0.32	0/2323	0.59	1/3145 (0.0%)
1	C	0.34	0/2323	0.59	1/3145 (0.0%)
1	D	0.33	0/2323	0.58	0/3145
All	All	0.33	0/9275	0.58	2/12557 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	76	GLY	N-CA-C	5.46	126.76	113.10
1	B	76	GLY	N-CA-C	5.33	126.43	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2252	0	2216	67	0
1	B	2269	0	2226	45	0
1	C	2269	0	2226	43	0
1	D	2269	0	2226	49	0
2	A	4	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
3	A	24	0	15	2	0
3	B	26	0	19	0	0
3	C	26	0	19	1	0
3	D	26	0	19	0	0
4	A	23	0	48	4	0
4	B	23	0	48	6	0
4	C	23	0	48	3	0
4	D	23	0	48	1	0
5	A	156	0	0	1	0
5	B	185	0	0	1	0
5	C	210	0	0	2	0
5	D	181	0	0	5	0
All	All	10001	0	9158	205	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 (205) 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:B:89:ASN:HD22	1:B:115:SER:H	1.26	0.83
1:A:205:LEU:HG	4:A:1901:10A:H31	1.62	0.82
1:A:173:HIS:HB3	1:A:175:LYS:NZ	1.98	0.78
1:A:175:LYS:HZ3	1:A:175:LYS:HB2	1.49	0.78
1:C:234:LYS:O	1:C:238:LEU:HD13	1.86	0.76
1:D:175:LYS:O	1:D:175:LYS:HD3	1.87	0.74
1:A:173:HIS:HB3	1:A:175:LYS:HZ1	1.51	0.73
1:C:144:HIS:CE1	1:C:204:ARG:HG2	2.24	0.72
1:B:256:GLU:CD	1:B:256:GLU:H	1.93	0.72
1:C:83:VAL:HG11	1:C:116:LYS:HE3	1.72	0.71
1:A:175:LYS:NZ	1:A:175:LYS:HB2	2.05	0.70
1:A:21:ASP:O	1:A:25:LEU:HD22	1.91	0.70
1:A:205:LEU:HD11	4:A:1901:10A:H223	1.72	0.70
1:A:175:LYS:HD3	1:A:175:LYS:H	1.57	0.68
1:C:39:GLU:H	1:C:43:MET:HE1	1.59	0.68
1:B:180:ARG:HH21	1:B:182:LEU:HD21	1.59	0.68
1:A:198:GLU:HB3	1:A:261:ARG:HD2	1.76	0.67
1:A:89:ASN:HD22	1:A:115:SER:H	1.42	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:LEU:HG	4:B:2901:10A:H12	1.77	0.66
1:C:89:ASN:HD22	1:C:115:SER:H	1.44	0.65
1:A:175:LYS:HD3	1:A:175:LYS:N	2.11	0.65
1:A:126:PHE:CZ	1:A:128:GLU:HB3	2.31	0.64
1:B:177:ILE:HG23	1:B:182:LEU:HD23	1.80	0.64
1:B:159:PRO:O	1:B:287:LYS:HD3	1.98	0.64
1:C:112:ASN:ND2	1:C:114:ARG:H	1.95	0.64
1:D:112:ASN:ND2	1:D:114:ARG:H	1.95	0.64
1:D:182:LEU:HD13	1:D:277:TYR:CE2	2.33	0.63
1:B:89:ASN:ND2	1:B:115:SER:H	1.94	0.63
1:C:112:ASN:HD22	1:C:114:ARG:H	1.45	0.63
1:A:112:ASN:HD22	1:A:114:ARG:H	1.47	0.63
1:D:20:ASP:O	1:D:24:ARG:HG3	1.99	0.63
1:D:177:ILE:HD12	5:D:1352:HOH:O	1.99	0.62
1:A:22:PHE:HA	1:A:25:LEU:HD23	1.80	0.62
1:B:229:GLN:HB3	1:B:230:PRO:HD3	1.81	0.62
1:A:35:CYS:HB2	1:A:232:TYR:CD2	2.35	0.61
1:A:89:ASN:ND2	1:A:115:SER:H	1.98	0.61
1:C:38:PHE:HA	1:C:43:MET:CE	2.31	0.60
1:C:229:GLN:HB2	1:C:279:ASP:OD1	2.02	0.60
1:A:182:LEU:HB3	1:A:277:TYR:CE2	2.37	0.60
1:D:177:ILE:HG12	1:D:180:ARG:NH2	2.16	0.60
1:D:205:LEU:HG	4:D:4901:10A:H31	1.84	0.60
1:B:234:LYS:O	1:B:238:LEU:HD22	2.02	0.60
1:A:13:GLN:OE1	1:A:97:LYS:HE2	2.03	0.59
1:C:175:LYS:O	1:C:175:LYS:HD3	2.01	0.59
1:A:192:LEU:HD22	4:A:1901:10A:H221	1.85	0.59
1:C:183:PRO:HB3	5:C:1721:HOH:O	2.03	0.59
1:D:12:VAL:HG21	1:D:95:LEU:HD12	1.84	0.59
3:A:1900:SAH:CG	3:A:1900:SAH:C5'	2.81	0.59
1:A:155:HIS:CE1	1:A:287:LYS:HE3	2.38	0.58
1:B:272:MET:HE3	1:B:275:ILE:HD11	1.85	0.58
1:C:229:GLN:HB3	1:C:230:PRO:HD3	1.85	0.58
1:A:184:MET:O	1:A:186:PHE:N	2.37	0.57
1:A:182:LEU:HD22	1:A:277:TYR:HE2	1.69	0.57
1:B:192:LEU:CD1	4:B:2901:10A:H221	2.35	0.57
1:D:112:ASN:HD22	1:D:114:ARG:H	1.51	0.57
1:A:249:GLN:HE21	1:A:253:LEU:HD21	1.69	0.57
1:B:256:GLU:O	1:B:260:GLU:HG2	2.05	0.57
1:A:12:VAL:HG21	1:A:95:LEU:HD12	1.86	0.56
1:A:35:CYS:HB2	1:A:232:TYR:CE2	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:PHE:HA	1:A:25:LEU:CD2	2.35	0.56
1:D:182:LEU:HB3	1:D:277:TYR:HE2	1.70	0.56
1:D:182:LEU:HD13	1:D:277:TYR:CD2	2.41	0.56
1:A:188:PHE:CE1	1:A:192:LEU:HD21	2.41	0.56
1:B:111:GLU:CD	1:B:111:GLU:H	2.07	0.56
1:A:7:PRO:HB2	1:A:9:PHE:CE1	2.40	0.56
1:A:112:ASN:ND2	1:A:114:ARG:H	2.03	0.56
1:A:169:ILE:HD13	4:A:1901:10A:H182	1.88	0.56
1:B:169:ILE:HD13	4:B:2901:10A:H182	1.87	0.56
1:D:136:ILE:CD1	1:D:167:HIS:HB3	2.36	0.56
1:D:136:ILE:HD13	1:D:167:HIS:HB3	1.87	0.55
1:C:144:HIS:HE1	1:C:204:ARG:HG2	1.70	0.55
1:D:229:GLN:HB3	1:D:230:PRO:HD3	1.89	0.55
1:D:178:HIS:O	1:D:182:LEU:HD12	2.06	0.55
1:C:169:ILE:HD13	4:C:3901:10A:H182	1.90	0.54
1:B:89:ASN:HD22	1:B:115:SER:N	2.00	0.54
1:B:110:SER:OG	1:B:116:LYS:HE2	2.07	0.54
1:B:83:VAL:HG11	1:B:116:LYS:HE3	1.90	0.53
1:B:112:ASN:HD22	1:B:114:ARG:H	1.55	0.53
1:C:44:THR:OG1	1:C:47:GLU:HG3	2.08	0.53
1:B:173:HIS:C	1:B:175:LYS:H	2.12	0.52
1:C:89:ASN:ND2	1:C:115:SER:H	2.06	0.52
1:A:173:HIS:O	1:A:177:ILE:HG13	2.08	0.52
1:A:35:CYS:O	1:A:52:LYS:HG3	2.10	0.52
1:D:89:ASN:HD22	1:D:115:SER:H	1.57	0.52
1:D:192:LEU:O	1:D:196:VAL:HG23	2.10	0.52
1:A:249:GLN:O	1:A:253:LEU:HD23	2.10	0.52
1:B:182:LEU:HB3	1:B:277:TYR:OH	2.10	0.52
1:C:39:GLU:N	1:C:43:MET:HE1	2.26	0.51
1:B:12:VAL:HG21	1:B:95:LEU:HD12	1.92	0.51
1:A:49:GLN:HA	1:A:49:GLN:OE1	2.11	0.51
1:A:182:LEU:HD13	1:A:277:TYR:CD2	2.46	0.51
1:C:110:SER:OG	1:C:116:LYS:HE2	2.11	0.51
1:A:159:PRO:O	1:A:287:LYS:HD3	2.11	0.50
1:C:20:ASP:O	1:C:24:ARG:HG3	2.11	0.50
1:D:35:CYS:HB2	1:D:232:TYR:CD2	2.46	0.50
1:C:79:MET:HG3	5:C:1035:HOH:O	2.11	0.50
1:B:133:ILE:HG13	1:B:158:LEU:HD21	1.92	0.50
1:A:147:TYR:CE1	1:A:206:PRO:HB3	2.47	0.50
1:A:182:LEU:HB3	1:A:277:TYR:CZ	2.45	0.50
1:C:38:PHE:HA	1:C:43:MET:HE3	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:ASN:ND2	1:B:114:ARG:H	2.09	0.50
1:B:180:ARG:NH2	1:B:182:LEU:HD21	2.26	0.49
1:A:69:LEU:HB2	1:A:130:VAL:HG11	1.94	0.49
1:D:83:VAL:CG1	1:D:112:ASN:ND2	2.75	0.49
1:D:35:CYS:HB2	1:D:232:TYR:CE2	2.46	0.49
1:D:177:ILE:HG12	1:D:180:ARG:CZ	2.42	0.49
1:C:39:GLU:N	1:C:43:MET:CE	2.75	0.49
1:D:181:GLY:O	1:D:182:LEU:HG	2.12	0.49
1:A:9:PHE:HB3	1:A:13:GLN:NE2	2.27	0.49
1:A:72:GLY:HA2	3:A:1900:SAH:H1'	1.94	0.49
1:A:110:SER:OG	1:A:116:LYS:HE2	2.13	0.49
1:A:208:ILE:HB	1:A:209:PRO:HD3	1.94	0.49
1:D:126:PHE:CZ	1:D:128:GLU:HB2	2.47	0.49
1:B:180:ARG:HH22	1:B:276:GLY:C	2.15	0.48
1:A:256:GLU:O	1:A:260:GLU:HG2	2.13	0.48
1:B:35:CYS:O	1:B:52:LYS:HG3	2.12	0.48
1:C:40:ARG:HB2	1:C:43:MET:HG3	1.95	0.48
1:C:208:ILE:HB	1:C:209:PRO:HD3	1.95	0.48
1:A:174:PRO:HA	1:A:177:ILE:HD12	1.95	0.48
1:C:130:VAL:O	1:C:159:PRO:HD3	2.13	0.48
1:A:130:VAL:O	1:A:159:PRO:HD3	2.13	0.47
1:C:184:MET:HB2	1:C:277:TYR:HE1	1.78	0.47
1:D:89:ASN:ND2	1:D:115:SER:H	2.12	0.47
1:D:119:LEU:HD12	1:D:119:LEU:N	2.30	0.47
1:D:188:PHE:O	1:D:192:LEU:HD13	2.13	0.47
1:B:126:PHE:CZ	1:B:128:GLU:HB2	2.49	0.47
1:C:173:HIS:HB2	1:C:176:GLU:OE1	2.14	0.47
1:B:177:ILE:O	1:B:182:LEU:HB2	2.14	0.47
1:D:83:VAL:HG12	1:D:112:ASN:CG	2.34	0.47
1:B:192:LEU:HD11	4:B:2901:10A:H221	1.96	0.47
1:A:44:THR:OG1	1:A:47:GLU:HG3	2.14	0.47
1:C:126:PHE:CZ	1:C:128:GLU:HB2	2.50	0.47
1:A:272:MET:HB3	1:A:278:ILE:CD1	2.45	0.47
1:A:175:LYS:H	1:A:175:LYS:CD	2.27	0.47
1:C:123:TRP:HE3	1:C:153:LEU:HD13	1.80	0.47
1:D:177:ILE:O	1:D:180:ARG:HG2	2.15	0.47
1:A:191:PHE:CZ	1:A:268:GLY:HA3	2.51	0.46
1:D:44:THR:OG1	1:D:47:GLU:HG3	2.16	0.46
1:D:208:ILE:HB	1:D:209:PRO:HD3	1.98	0.46
1:C:184:MET:HB2	1:C:277:TYR:CE1	2.50	0.46
1:C:39:GLU:H	1:C:43:MET:CE	2.27	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:SER:OG	1:C:210:MET:HB2	2.16	0.46
1:B:165:LEU:HD13	1:B:165:LEU:C	2.36	0.45
1:B:229:GLN:HB2	1:B:279:ASP:OD1	2.16	0.45
1:C:35:CYS:O	1:C:52:LYS:HG3	2.16	0.45
1:C:192:LEU:CD2	4:C:3901:10A:H221	2.46	0.45
1:D:35:CYS:O	1:D:52:LYS:HG3	2.15	0.45
1:D:243:LEU:HD23	1:D:263:MET:SD	2.55	0.45
1:D:267:THR:O	1:D:271:GLU:HG2	2.16	0.45
1:B:208:ILE:HB	1:B:209:PRO:HD3	1.99	0.45
1:D:177:ILE:HA	1:D:180:ARG:HG2	1.98	0.45
1:A:24:ARG:HD2	5:A:1338:HOH:O	2.17	0.45
1:B:140:GLU:HB3	4:B:2901:10A:H71	1.99	0.45
1:D:187:THR:HG23	5:D:1510:HOH:O	2.16	0.45
1:D:178:HIS:NE2	1:D:185:SER:HB2	2.32	0.45
1:A:193:LYS:HE2	1:A:197:THR:HG21	1.99	0.45
1:A:251:ILE:HG12	1:A:256:GLU:HA	1.98	0.45
1:A:179:GLU:C	1:A:181:GLY:H	2.19	0.45
1:B:49:GLN:OE1	1:B:49:GLN:HA	2.16	0.45
1:B:256:GLU:HG2	5:B:1599:HOH:O	2.17	0.44
1:A:177:ILE:HG23	1:A:182:LEU:HD12	1.99	0.44
1:C:72:GLY:HA2	3:C:3900:SAH:H1'	1.98	0.44
1:D:188:PHE:CE1	1:D:192:LEU:HD11	2.51	0.44
1:A:183:PRO:O	1:A:185:SER:N	2.51	0.44
1:A:173:HIS:HB3	1:A:175:LYS:HZ2	1.79	0.43
1:B:192:LEU:HD12	4:B:2901:10A:H221	1.99	0.43
1:D:4:GLU:HB2	5:D:1406:HOH:O	2.18	0.43
1:A:118:VAL:HG13	1:A:118:VAL:O	2.18	0.43
1:D:6:LYS:HA	1:D:7:PRO:HD3	1.92	0.43
1:A:37:TYR:CE2	1:A:39:GLU:HG3	2.54	0.43
1:A:182:LEU:HD13	1:A:277:TYR:CE2	2.54	0.43
1:B:155:HIS:NE2	1:B:287:LYS:HG3	2.33	0.42
1:C:159:PRO:O	1:C:287:LYS:HD3	2.19	0.42
1:D:49:GLN:OE1	1:D:49:GLN:HA	2.19	0.42
1:D:167:HIS:C	1:D:167:HIS:CD2	2.92	0.42
1:A:11:ASN:HB3	1:A:201:PRO:O	2.20	0.42
1:A:153:LEU:HD13	1:A:156:ARG:HH21	1.83	0.42
1:B:188:PHE:CE1	1:B:192:LEU:HD13	2.54	0.42
1:A:128:GLU:HA	1:A:129:PRO:HD3	1.93	0.42
1:C:45:LEU:HB2	1:C:238:LEU:HD23	2.01	0.42
1:A:193:LYS:O	1:A:197:THR:HG23	2.19	0.42
1:C:12:VAL:HG21	1:C:95:LEU:HD12	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:MET:O	1:D:83:VAL:HG23	2.19	0.42
1:D:249:GLN:HA	1:D:249:GLN:OE1	2.20	0.42
1:D:103:VAL:O	1:D:107:VAL:HG23	2.19	0.42
1:B:275:ILE:HD12	1:B:277:TYR:CE2	2.55	0.42
1:D:208:ILE:N	1:D:209:PRO:CD	2.83	0.41
1:C:205:LEU:HD11	4:C:3901:10A:H223	2.01	0.41
1:D:165:LEU:C	1:D:165:LEU:HD13	2.40	0.41
1:B:208:ILE:N	1:B:209:PRO:CD	2.83	0.41
1:A:188:PHE:CZ	1:A:192:LEU:HD21	2.55	0.41
1:B:182:LEU:HG	1:B:277:TYR:CE2	2.56	0.41
1:B:20:ASP:O	1:B:24:ARG:HG3	2.19	0.41
1:D:176:GLU:HB3	5:D:1466:HOH:O	2.21	0.41
1:D:77:ALA:HB3	5:D:1247:HOH:O	2.20	0.41
1:C:188:PHE:O	1:C:192:LEU:HG	2.20	0.41
1:A:272:MET:HB3	1:A:278:ILE:HD11	2.02	0.41
1:B:180:ARG:C	1:B:182:LEU:HD13	2.42	0.41
1:C:38:PHE:CE1	1:C:234:LYS:HG2	2.56	0.41
1:C:216:SER:HA	1:C:220:PHE:O	2.21	0.41
1:C:165:LEU:C	1:C:165:LEU:HD13	2.42	0.40
1:A:13:GLN:HG2	1:A:17:ASP:OD2	2.21	0.40
1:B:155:HIS:HB2	1:B:220:PHE:CE1	2.57	0.40
1:B:188:PHE:CD1	1:B:272:MET:HE2	2.57	0.40
1:D:210:MET:HE2	1:D:210:MET:O	2.21	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	281/287 (98%)	269 (96%)	8 (3%)	4 (1%)	11 5
1	B	283/287 (99%)	273 (96%)	6 (2%)	4 (1%)	11 5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	283/287 (99%)	267 (94%)	12 (4%)	4 (1%)	11	5
1	D	283/287 (99%)	270 (95%)	8 (3%)	5 (2%)	8	3
All	All	1130/1148 (98%)	1079 (96%)	34 (3%)	17 (2%)	10	4

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	SER
1	A	185	SER
1	C	19	SER
1	C	180	ARG
1	C	182	LEU
1	C	183	PRO
1	D	19	SER
1	D	177	ILE
1	D	183	PRO
1	B	19	SER
1	B	184	MET
1	A	184	MET
1	D	174	PRO
1	D	181	GLY
1	A	183	PRO
1	B	179	GLU
1	B	174	PRO

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	239/243 (98%)	231 (97%)	8 (3%)	38	37
1	B	241/243 (99%)	234 (97%)	7 (3%)	42	43
1	C	241/243 (99%)	236 (98%)	5 (2%)	53	57
1	D	241/243 (99%)	235 (98%)	6 (2%)	47	49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	962/972 (99%)	936 (97%)	26 (3%)	44	46

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	TYR
1	A	111	GLU
1	A	175	LYS
1	A	178	HIS
1	A	232	TYR
1	A	257	GLU
1	A	265	TYR
1	A	272	MET
1	B	33	TYR
1	B	111	GLU
1	B	182	LEU
1	B	204	ARG
1	B	232	TYR
1	B	238	LEU
1	B	265	TYR
1	C	33	TYR
1	C	148	ASP
1	C	167	HIS
1	C	232	TYR
1	C	265	TYR
1	D	33	TYR
1	D	167	HIS
1	D	178	HIS
1	D	184	MET
1	D	232	TYR
1	D	265	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	31	GLN
1	A	89	ASN
1	A	101	ASN
1	A	112	ASN
1	A	246	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	249	GLN
1	B	13	GLN
1	B	31	GLN
1	B	89	ASN
1	B	101	ASN
1	B	112	ASN
1	B	246	ASN
1	C	13	GLN
1	C	31	GLN
1	C	89	ASN
1	C	101	ASN
1	C	112	ASN
1	C	244	GLN
1	C	246	ASN
1	D	13	GLN
1	D	31	GLN
1	D	89	ASN
1	D	101	ASN
1	D	112	ASN
1	D	246	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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
3	SAH	D	4900	-	23,28,28	1.45	5 (21%)	22,40,40	1.12	1 (4%)
2	CO3	B	2902	-	3,3,3	4.02	1 (33%)	2,3,3	0.13	0
2	CO3	A	1902	-	3,3,3	4.15	1 (33%)	2,3,3	0.14	0
4	10A	B	2901	-	22,22,22	0.59	0	24,24,24	1.25	2 (8%)
3	SAH	C	3900	-	23,28,28	1.38	5 (21%)	22,40,40	1.12	1 (4%)
3	SAH	A	1900	-	21,25,28	1.79	6 (28%)	17,35,40	1.29	1 (5%)
3	SAH	B	2900	-	23,28,28	1.43	5 (21%)	22,40,40	1.09	1 (4%)
2	CO3	D	4902	-	3,3,3	3.94	1 (33%)	2,3,3	0.10	0
4	10A	A	1901	-	22,22,22	0.58	0	24,24,24	1.35	2 (8%)
4	10A	D	4901	-	22,22,22	0.60	0	24,24,24	1.37	3 (12%)
4	10A	C	3901	-	22,22,22	0.61	0	24,24,24	1.22	2 (8%)
2	CO3	C	3902	-	3,3,3	4.04	1 (33%)	2,3,3	0.22	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
3	SAH	D	4900	-	-	0/11/31/31	0/3/3/3
4	10A	B	2901	-	-	0/22/22/22	-
3	SAH	C	3900	-	-	0/11/31/31	0/3/3/3
3	SAH	A	1900	-	-	0/4/24/31	0/3/3/3
3	SAH	B	2900	-	-	0/11/31/31	0/3/3/3
4	10A	A	1901	-	-	0/22/22/22	-
4	10A	D	4901	-	-	1/22/22/22	-
4	10A	C	3901	-	-	1/22/22/22	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1902	CO3	O1-C	7.18	1.50	1.25
2	C	3902	CO3	O1-C	6.98	1.49	1.25
2	B	2902	CO3	O1-C	6.93	1.49	1.25
2	D	4902	CO3	O1-C	6.82	1.49	1.25
3	A	1900	SAH	OXT-C	-4.19	1.24	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1900	SAH	O4'-C1'	3.41	1.45	1.40
3	A	1900	SAH	C6-C5	3.13	1.55	1.43
3	C	3900	SAH	C6-C5	3.07	1.54	1.43
3	B	2900	SAH	C6-C5	3.02	1.54	1.43
3	C	3900	SAH	O4'-C1'	2.98	1.44	1.40
3	B	2900	SAH	O4'-C1'	2.97	1.44	1.40
3	D	4900	SAH	C6-C5	2.96	1.54	1.43
3	B	2900	SAH	C2-N3	2.82	1.36	1.32
3	D	4900	SAH	O4'-C1'	2.70	1.44	1.40
3	D	4900	SAH	C2-N3	2.67	1.36	1.32
3	D	4900	SAH	C4-N3	2.64	1.39	1.35
3	A	1900	SAH	C4-N3	2.64	1.39	1.35
3	B	2900	SAH	C8-N7	-2.56	1.30	1.34
3	D	4900	SAH	C8-N7	-2.55	1.30	1.34
3	A	1900	SAH	C8-N7	-2.54	1.30	1.34
3	A	1900	SAH	C2-N3	2.52	1.36	1.32
3	C	3900	SAH	C2-N3	2.36	1.35	1.32
3	C	3900	SAH	C4-N3	2.29	1.38	1.35
3	C	3900	SAH	C8-N7	-2.29	1.30	1.34
3	B	2900	SAH	C4-N3	2.14	1.38	1.35

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1901	10A	C14-C13-N1	3.66	122.78	115.35
4	D	4901	10A	C9-C10-N1	3.62	122.71	115.35
4	C	3901	10A	C9-C10-N1	3.57	122.61	115.35
4	B	2901	10A	C9-C10-N1	3.55	122.56	115.35
4	A	1901	10A	C9-C10-N1	3.48	122.43	115.35
4	D	4901	10A	C14-C13-N1	3.34	122.15	115.35
4	B	2901	10A	C14-C13-N1	3.07	121.59	115.35
4	C	3901	10A	C14-C13-N1	2.82	121.08	115.35
3	A	1900	SAH	C5'-C4'-C3'	-2.51	113.06	115.70
3	D	4900	SAH	C4'-O4'-C1'	-2.31	107.81	109.92
3	C	3900	SAH	C4'-O4'-C1'	-2.29	107.83	109.92
3	B	2900	SAH	C4'-O4'-C1'	-2.13	107.97	109.92
4	D	4901	10A	C11-N1-C10	-2.08	103.83	109.49

There are no chirality outliers.

All (2) torsion outliers are listed below:

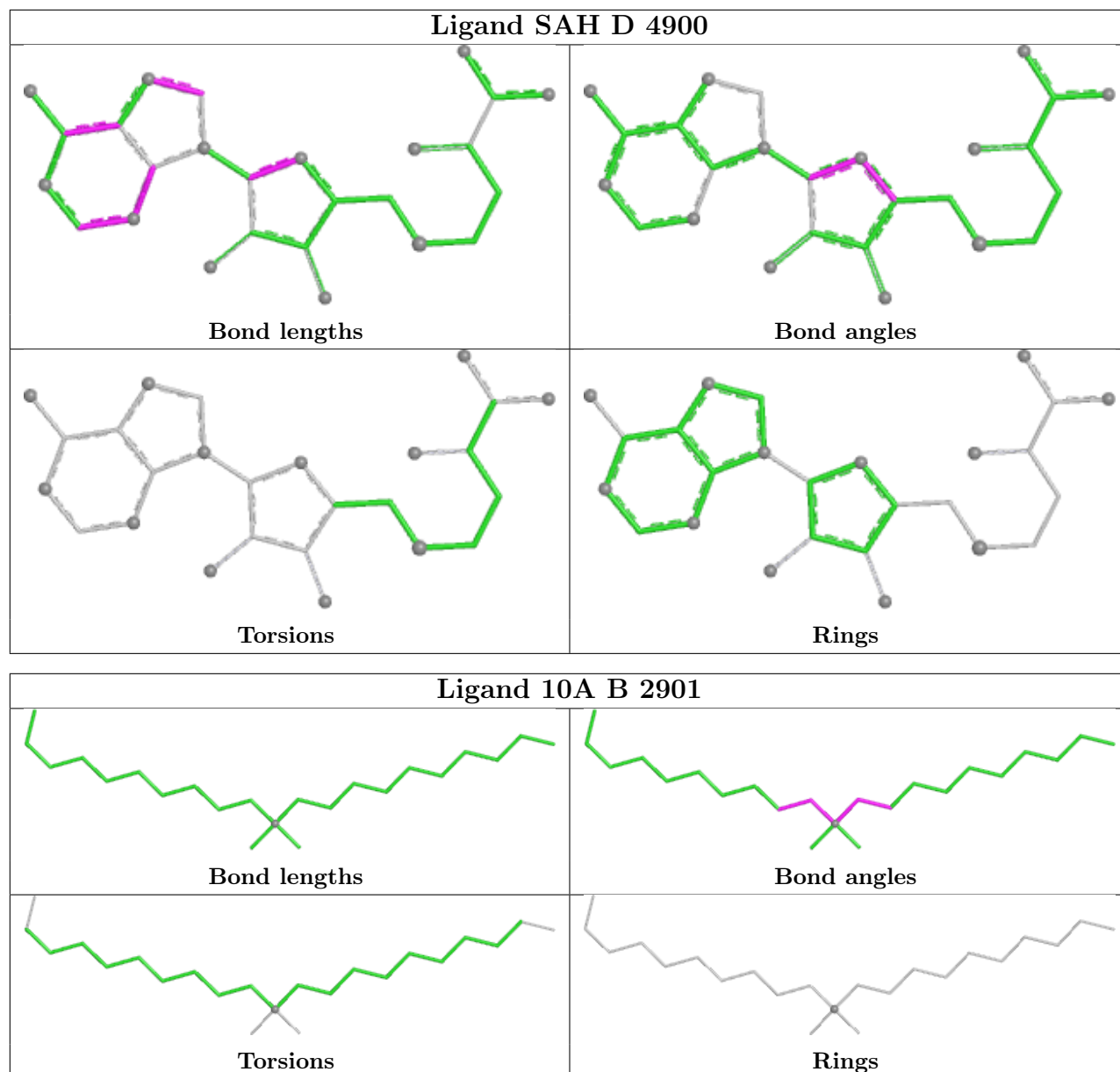
Mol	Chain	Res	Type	Atoms
4	D	4901	10A	C14-C15-C16-C17
4	C	3901	10A	C14-C15-C16-C17

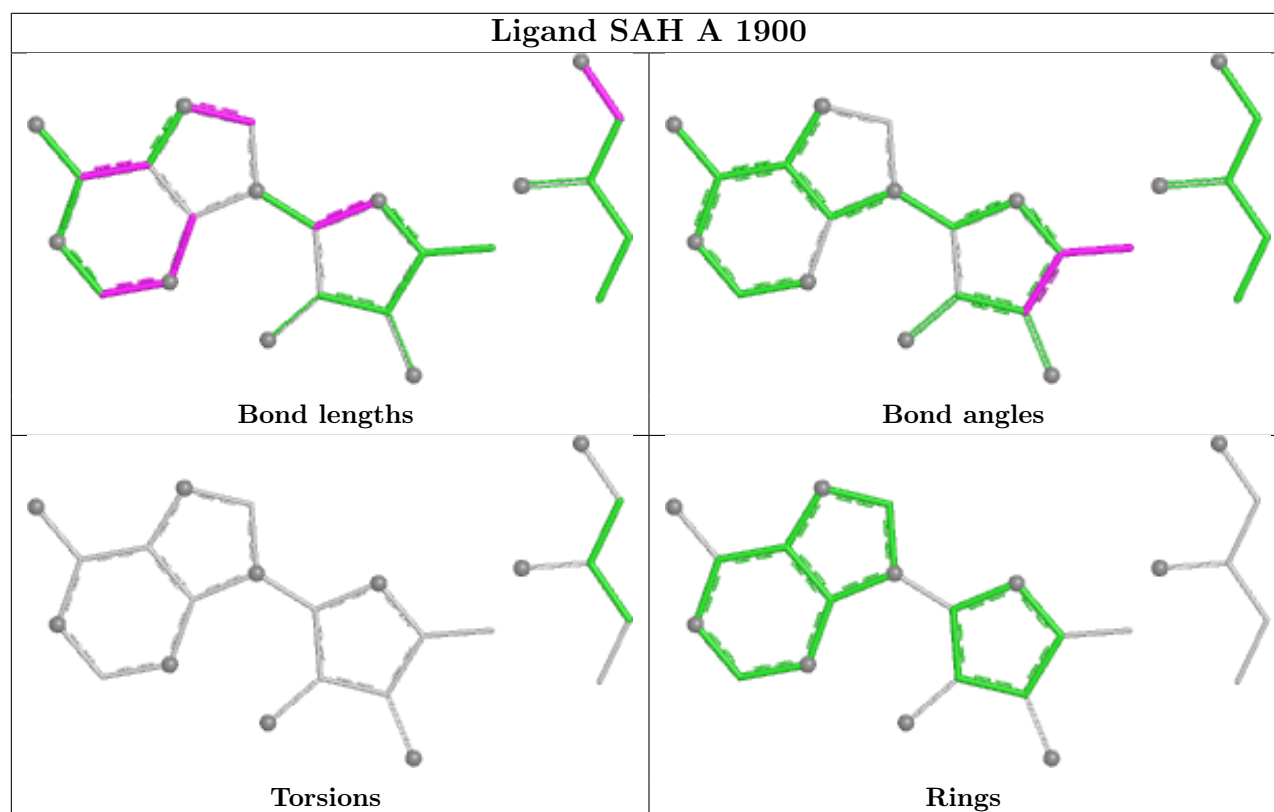
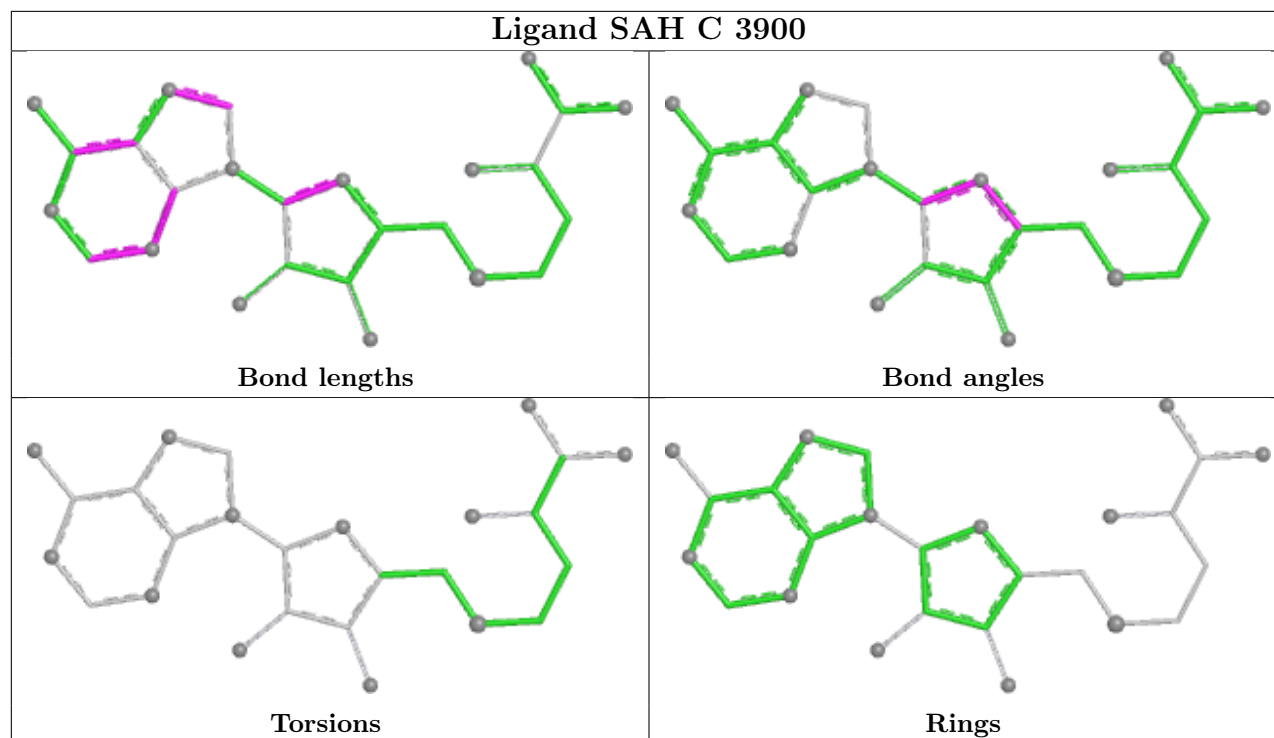
There are no ring outliers.

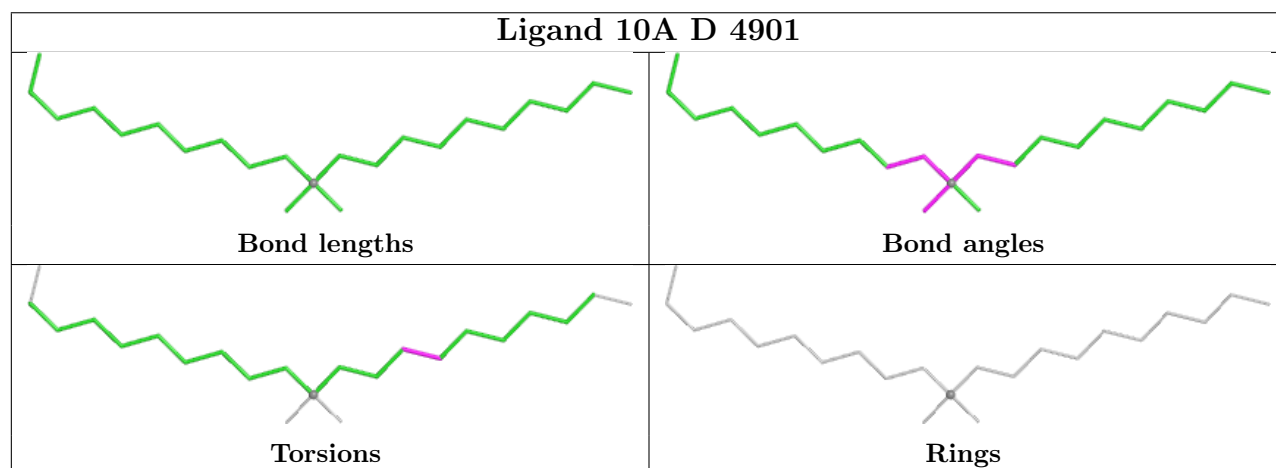
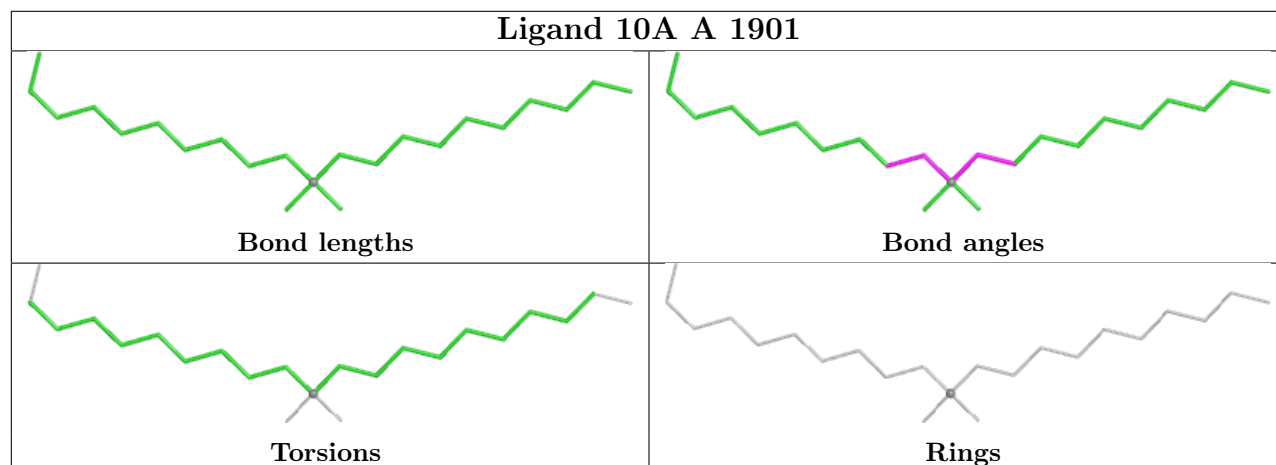
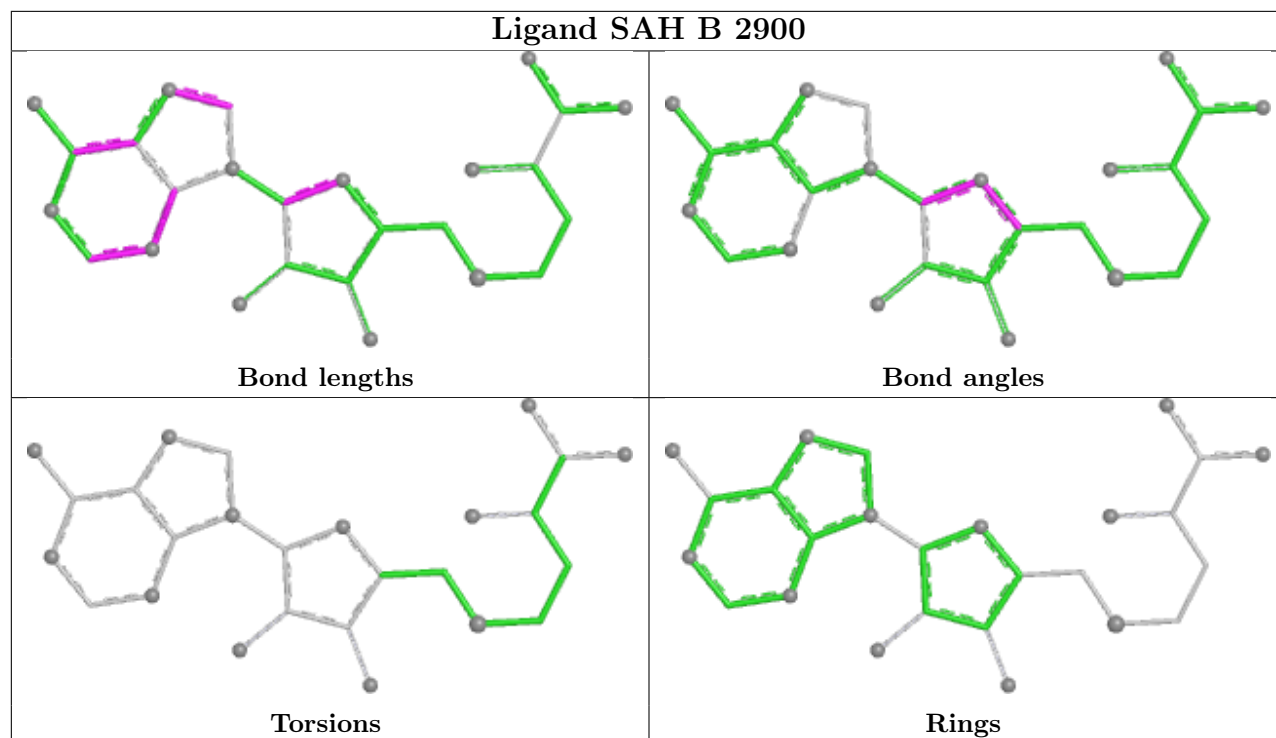
6 monomers are involved in 17 short contacts:

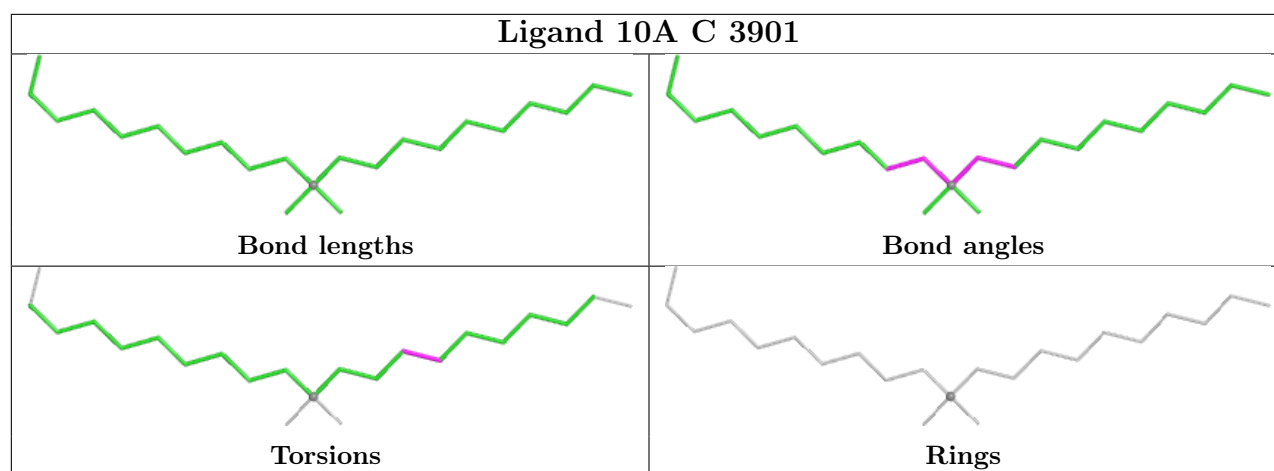
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2901	10A	6	0
3	C	3900	SAH	1	0
3	A	1900	SAH	2	0
4	A	1901	10A	4	0
4	D	4901	10A	1	0
4	C	3901	10A	3	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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.