WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jan 14, 2024 – 11:52 am GMT

PDB ID	:	6SLA
Title	:	Crystal structure of isomerase PaaG mutant - D136N with Oxepin-CoA
Authors	:	Saleem-Batcha, R.; Spieker, M.; Teufel, R.
Deposited on	:	2019-08-19
Resolution	:	2.55 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:

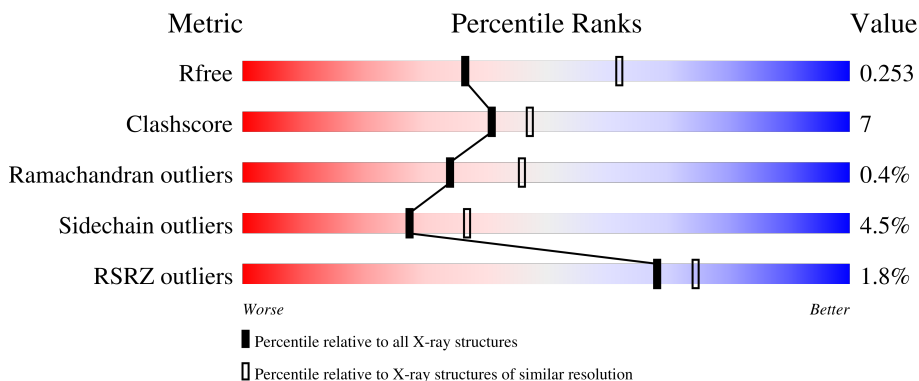|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.55 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	Percentile Ranks	Value
Rfree		0.253
Clashscore		7
Ramachandran outliers		0.4%
Sidechain outliers		4.5%
RSRZ outliers		1.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	254	% 78% 18% · ·
1	BBB	254	2% 81% 15% · ·
1	CCC	254	2% 81% 15% ·
1	DDD	254	2% 79% 16% · ·
1	EEE	254	2% 80% 15% · ·

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Mol	Chain	Length	Quality of chain
1	FFF	254	2% ▊▊▊▊▊ 78% ▊▊▊ 17% ··

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 11578 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 Enoyl-CoA hydratase/carnithine racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	245	Total	C	N	O	S	0	0	0
			1861	1180	336	342	3			
1	BBB	245	Total	C	N	O	S	0	0	0
			1861	1180	336	342	3			
1	CCC	245	Total	C	N	O	S	0	0	0
			1861	1180	336	342	3			
1	DDD	245	Total	C	N	O	S	0	0	0
			1861	1180	336	342	3			
1	EEE	245	Total	C	N	O	S	0	0	0
			1861	1180	336	342	3			
1	FFF	245	Total	C	N	O	S	0	0	0
			1861	1180	336	342	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	136	ASN	ASP	engineered mutation	UNP H9ZNW0
BBB	136	ASN	ASP	engineered mutation	UNP H9ZNW0
CCC	136	ASN	ASP	engineered mutation	UNP H9ZNW0
DDD	136	ASN	ASP	engineered mutation	UNP H9ZNW0
EEE	136	ASN	ASP	engineered mutation	UNP H9ZNW0
FFF	136	ASN	ASP	engineered mutation	UNP H9ZNW0

- Molecule 2 is {S}-[2-[3-[[(2 {R})-4-[[[(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-4-ox idanyl-3-phosphonooxy-oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl] oxy-3,3-dimethyl-2-oxidanyl-butanoyl]amino]propanoylamino]ethyl] 2-(2,5-dihydrooxepin-7- yl)ethanethioate (three-letter code: LHQ) (formula: $C_{29}H_{44}N_7O_{18}P_3S$) (labeled as "Ligand of Interest" by depositor).

LHQ
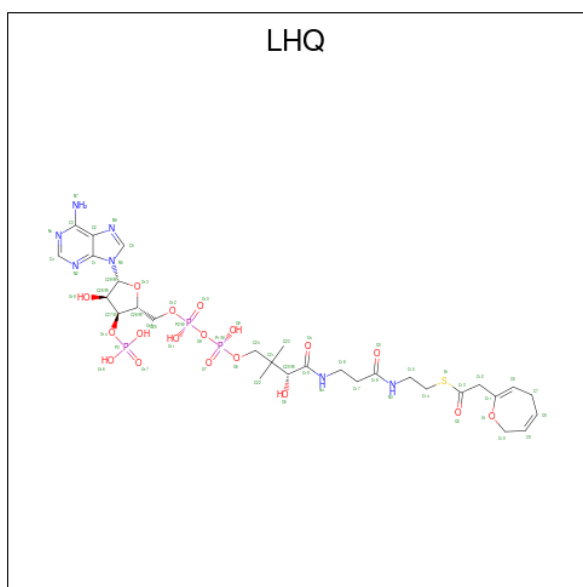
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	AAA	1	Total 58	C 29	N 7	O 18	P 3	S 1	0	0
2	BBB	1	Total 58	C 29	N 7	O 18	P 3	S 1	0	0
2	CCC	1	Total 58	C 29	N 7	O 18	P 3	S 1	0	0
2	DDD	1	Total 58	C 29	N 7	O 18	P 3	S 1	0	0
2	EEE	1	Total 58	C 29	N 7	O 18	P 3	S 1	0	0
2	FFF	1	Total 58	C 29	N 7	O 18	P 3	S 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	18	Total 18	O 18	0	0
3	BBB	12	Total 12	O 12	0	0
3	CCC	8	Total 8	O 8	0	0
3	DDD	10	Total 10	O 10	0	0
3	EEE	7	Total 7	O 7	0	0
3	FFF	9	Total 9	O 9	0	0

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Enoyl-CoA hydratase/carnithine racemase
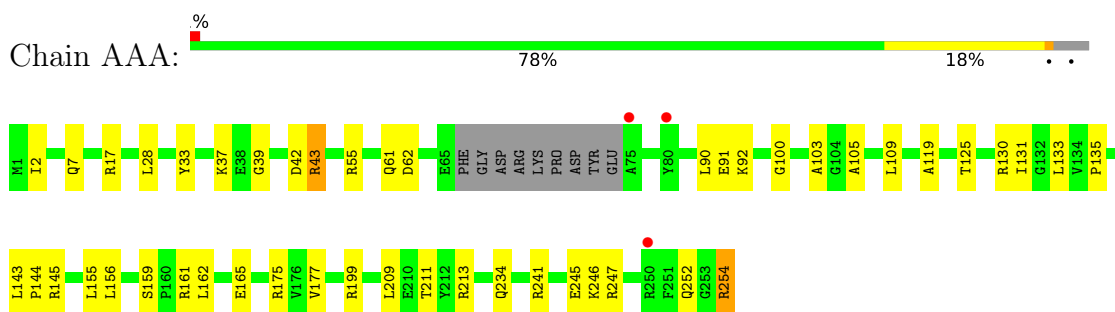
Chain AAA:

- Molecule 1: Enoyl-CoA hydratase/carnithine racemase

Chain BBB:

- Molecule 1: Enoyl-CoA hydratase/carnithine racemase

Chain CCC:

- Molecule 1: Enoyl-CoA hydratase/carnithine racemase

Chain DDD:
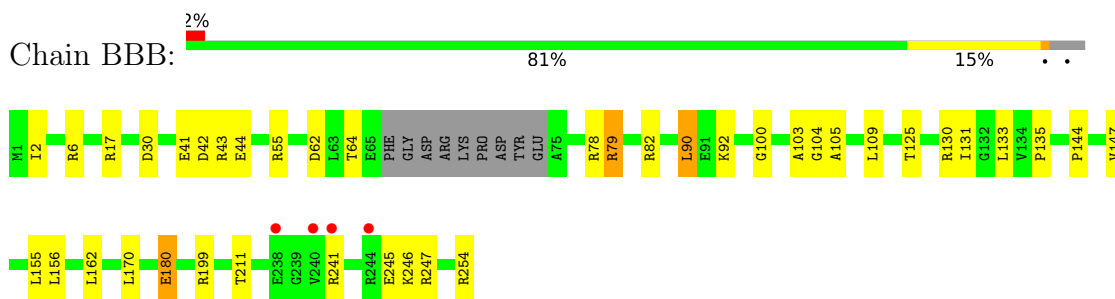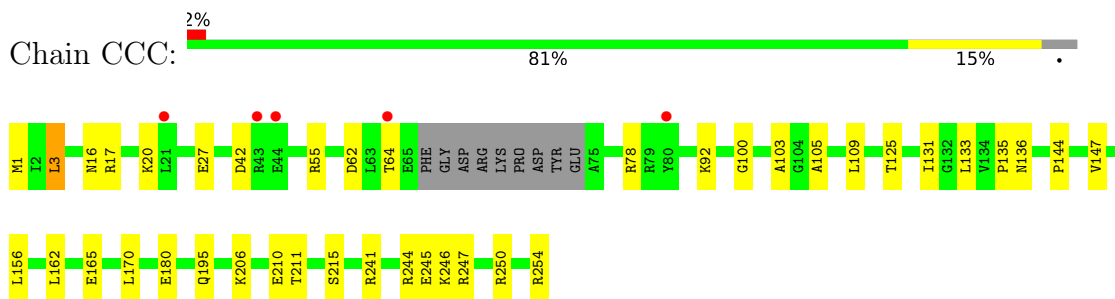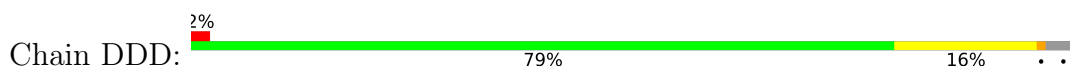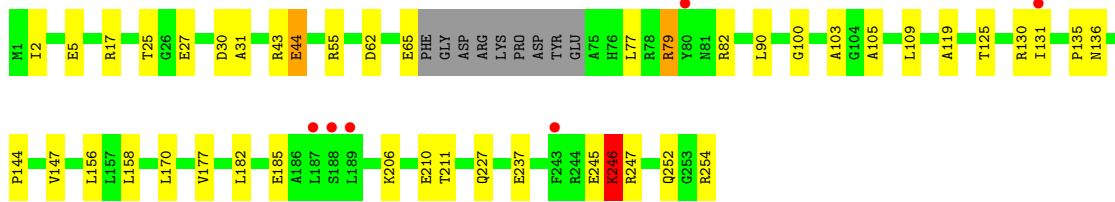
• Molecule 1: Enoyl-CoA hydratase/carnithine racemase

Chain EEE:

• Molecule 1: Enoyl-CoA hydratase/carnithine racemase

Chain FFF:
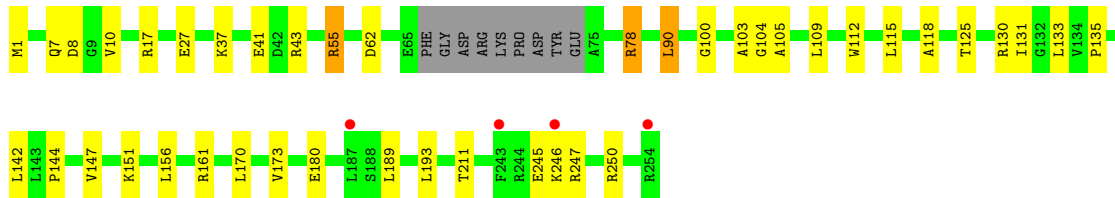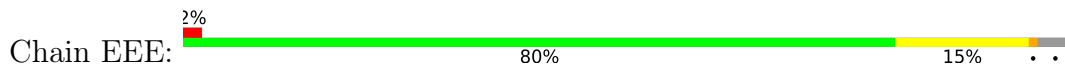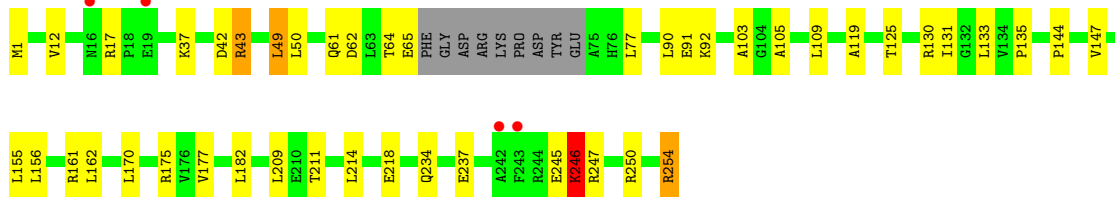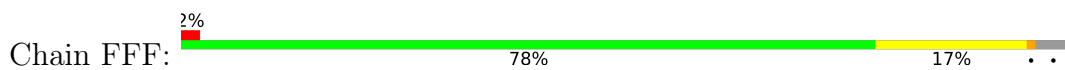
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.16Å 73.05Å 130.30Å 90.00° 92.48° 90.00°	Depositor
Resolution (Å)	48.65 – 2.55 48.60 – 2.55	Depositor EDS
% Data completeness (in resolution range)	96.8 (48.65-2.55) 96.9 (48.60-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.201 , 0.252 0.200 , 0.253	Depositor DCC
R_{free} test set	2301 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	51.7	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 39.7	EDS
L-test for twinning[2]	$< |L| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.007 for k,h,-l 0.018 for -k,-h,-l 0.032 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11578	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.12% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality (i)

5.1   Standard geometry (i)

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

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	AAA	0.47	0/1883	0.79	1/2544 (0.0%)
1	BBB	0.43	0/1883	0.75	0/2544
1	CCC	0.39	0/1883	0.73	2/2544 (0.1%)
1	DDD	0.41	0/1883	0.74	0/2544
1	EEE	0.41	0/1883	0.74	1/2544 (0.0%)
1	FFF	0.43	0/1883	0.75	0/2544
All	All	0.42	0/11298	0.75	4/15264 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	EEE	78	ARG	CB-CA-C	6.47	123.34	110.40
1	CCC	78	ARG	CB-CA-C	5.57	121.55	110.40
1	CCC	241	ARG	CG-CD-NE	-5.56	100.13	111.80
1	AAA	145	ARG	NE-CZ-NH2	5.54	123.07	120.30

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	AAA	1861	0	1954	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BBB	1861	0	1954	29	0
1	CCC	1861	0	1954	25	0
1	DDD	1861	0	1954	29	1
1	EEE	1861	0	1954	29	0
1	FFF	1861	0	1954	27	1
2	AAA	58	0	0	3	0
2	BBB	58	0	0	4	0
2	CCC	58	0	0	1	0
2	DDD	58	0	0	3	0
2	EEE	58	0	0	4	0
2	FFF	58	0	0	3	0
3	AAA	18	0	0	0	0
3	BBB	12	0	0	0	0
3	CCC	8	0	0	0	0
3	DDD	10	0	0	0	0
3	EEE	7	0	0	0	0
3	FFF	9	0	0	0	0
All	All	11578	0	11724	166	1

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 7.

All (166) 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)
2:FFF:301:LHQ:C10	2:FFF:301:LHQ:O1	1.64	1.44
2:DDD:301:LHQ:C10	2:DDD:301:LHQ:O1	1.65	1.43
1:EEE:7:GLN:O	1:EEE:10:VAL:HG22	1.58	1.04
1:AAA:234:GLN:HE21	1:AAA:252:GLN:NE2	1.76	0.84
1:AAA:234:GLN:HE21	1:AAA:252:GLN:HE22	1.31	0.79
1:BBB:42:ASP:OD1	1:BBB:44:GLU:HG2	1.89	0.72
1:EEE:37:LYS:HE2	1:EEE:41:GLU:OE2	1.91	0.70
1:BBB:79:ARG:HG2	1:BBB:82:ARG:NH2	2.08	0.69
1:CCC:195:GLN:OE1	1:CCC:250:ARG:NH1	2.26	0.69
1:DDD:2:ILE:HD13	1:DDD:31:ALA:HB3	1.75	0.69
1:BBB:131:ILE:HG22	1:BBB:131:ILE:O	1.94	0.67
1:CCC:3:LEU:HD11	1:CCC:16:ASN:HD22	1.59	0.67
1:EEE:131:ILE:O	1:EEE:131:ILE:HG22	1.94	0.67
2:DDD:301:LHQ:C10	2:DDD:301:LHQ:C11	2.73	0.66
1:DDD:206:LYS:O	1:DDD:210:GLU:HG2	1.95	0.66
1:BBB:155:LEU:HD21	1:BBB:162:LEU:HD11	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:133:LEU:HD13	2:AAA:301:LHQ:C10	2.26	0.66
1:DDD:131:ILE:HG22	1:DDD:131:ILE:O	1.94	0.65
1:CCC:3:LEU:HD22	1:CCC:16:ASN:HB2	1.77	0.65
1:DDD:252:GLN:NE2	1:DDD:254:ARG:NH2	2.45	0.65
1:AAA:133:LEU:CD1	2:AAA:301:LHQ:C10	2.75	0.65
1:CCC:245:GLU:O	1:CCC:247:ARG:N	2.31	0.64
1:AAA:130:ARG:NH1	1:AAA:159:SER:HB3	2.12	0.64
1:BBB:245:GLU:O	1:BBB:247:ARG:N	2.30	0.64
2:FFF:301:LHQ:C10	2:FFF:301:LHQ:C11	2.71	0.64
1:DDD:245:GLU:O	1:DDD:247:ARG:N	2.31	0.64
1:FFF:245:GLU:O	1:FFF:247:ARG:N	2.32	0.63
1:AAA:131:ILE:O	1:AAA:131:ILE:HG22	1.97	0.63
1:AAA:245:GLU:O	1:AAA:247:ARG:N	2.31	0.63
1:DDD:30:ASP:OD1	1:DDD:79:ARG:HD3	1.99	0.63
1:EEE:245:GLU:O	1:EEE:247:ARG:N	2.31	0.63
1:FFF:17:ARG:NH2	1:FFF:62:ASP:OD2	2.32	0.63
1:FFF:155:LEU:HD21	1:FFF:162:LEU:HD11	1.80	0.62
1:AAA:130:ARG:HH11	1:AAA:159:SER:HB3	1.63	0.61
1:AAA:17:ARG:NH2	1:AAA:62:ASP:OD2	2.32	0.61
1:DDD:2:ILE:HD13	1:DDD:31:ALA:CB	2.29	0.61
1:CCC:17:ARG:NH2	1:CCC:62:ASP:OD2	2.33	0.61
1:BBB:17:ARG:NH2	1:BBB:62:ASP:OD2	2.34	0.61
1:CCC:3:LEU:CD2	1:CCC:16:ASN:HB2	2.31	0.61
1:DDD:17:ARG:NH2	1:DDD:62:ASP:OD2	2.34	0.60
1:AAA:61:GLN:HB2	2:AAA:301:LHQ:C12	2.31	0.60
2:EEE:301:LHQ:S1	2:EEE:301:LHQ:O1	2.60	0.59
1:EEE:17:ARG:NH2	1:EEE:62:ASP:OD2	2.34	0.58
1:DDD:144:PRO:HG2	1:EEE:211:THR:HG21	1.86	0.57
1:EEE:115:LEU:HD12	1:EEE:193:LEU:HD11	1.85	0.57
1:BBB:133:LEU:CD1	2:BBB:301:LHQ:C10	2.82	0.57
1:DDD:131:ILE:HD11	2:DDD:301:LHQ:O3	2.05	0.57
1:DDD:25:THR:HA	1:DDD:65:GLU:OE2	2.03	0.56
1:DDD:44:GLU:HG2	1:DDD:44:GLU:O	2.05	0.56
1:BBB:135:PRO:HG3	1:BBB:156:LEU:HD22	1.87	0.55
1:DDD:135:PRO:HG3	1:DDD:156:LEU:HD22	1.87	0.55
1:EEE:135:PRO:HG3	1:EEE:156:LEU:HD22	1.88	0.55
1:BBB:105:ALA:O	1:BBB:109:LEU:HG	2.07	0.55
1:AAA:155:LEU:HD21	1:AAA:162:LEU:HD11	1.89	0.54
1:BBB:6:ARG:HD3	1:BBB:44:GLU:OE2	2.07	0.54
1:CCC:135:PRO:HG3	1:CCC:156:LEU:HD22	1.89	0.54
1:FFF:131:ILE:HD11	1:FFF:133:LEU:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:130:ARG:HH11	1:BBB:130:ARG:HG2	1.73	0.54
1:EEE:105:ALA:O	1:EEE:109:LEU:HG	2.08	0.54
1:FFF:135:PRO:HG3	1:FFF:156:LEU:HD22	1.90	0.53
1:DDD:105:ALA:O	1:DDD:109:LEU:HG	2.09	0.53
1:FFF:105:ALA:O	1:FFF:109:LEU:HG	2.09	0.52
1:FFF:214:LEU:HD22	1:FFF:218:GLU:OE2	2.09	0.52
1:BBB:211:THR:HG21	1:CCC:144:PRO:HG2	1.91	0.52
1:BBB:41:GLU:OE1	1:DDD:82:ARG:NE	2.42	0.51
1:CCC:105:ALA:O	1:CCC:109:LEU:HG	2.09	0.51
1:BBB:62:ASP:OD1	1:BBB:64:THR:HB	2.09	0.51
1:CCC:62:ASP:OD1	1:CCC:64:THR:HB	2.11	0.51
2:CCC:301:LHQ:O5	2:CCC:301:LHQ:C18	2.59	0.51
1:FFF:61:GLN:HB2	2:FFF:301:LHQ:C12	2.41	0.51
1:AAA:105:ALA:O	1:AAA:109:LEU:HG	2.10	0.51
1:EEE:144:PRO:HG2	1:FFF:211:THR:HG21	1.92	0.51
1:AAA:42:ASP:O	1:AAA:92:LYS:NZ	2.44	0.51
1:FFF:42:ASP:O	1:FFF:92:LYS:NZ	2.44	0.51
1:DDD:2:ILE:CD1	1:DDD:31:ALA:HB3	2.39	0.51
1:DDD:158:LEU:HD21	1:EEE:115:LEU:HD11	1.93	0.51
1:CCC:42:ASP:O	1:CCC:92:LYS:NZ	2.44	0.50
1:CCC:206:LYS:NZ	1:CCC:210:GLU:HG3	2.27	0.50
1:FFF:12:VAL:HG13	1:FFF:49:LEU:CD1	2.42	0.50
1:AAA:135:PRO:HG3	1:AAA:156:LEU:HD22	1.94	0.50
1:FFF:43:ARG:O	1:FFF:43:ARG:HD3	2.11	0.50
1:FFF:130:ARG:HH11	1:FFF:130:ARG:HG2	1.76	0.49
1:FFF:64:THR:O	1:FFF:65:GLU:C	2.51	0.49
1:EEE:1:MET:HE1	1:EEE:27:GLU:HB3	1.93	0.49
1:AAA:234:GLN:NE2	1:AAA:252:GLN:NE2	2.54	0.49
1:DDD:77:LEU:H	1:DDD:77:LEU:HD22	1.78	0.48
1:BBB:42:ASP:O	1:BBB:92:LYS:NZ	2.45	0.48
1:DDD:147:VAL:HG12	1:DDD:170:LEU:O	2.13	0.48
1:BBB:131:ILE:O	1:BBB:131:ILE:CG2	2.62	0.48
1:CCC:3:LEU:HD21	1:CCC:16:ASN:CG	2.34	0.48
1:AAA:211:THR:HG21	1:BBB:144:PRO:HG2	1.95	0.48
1:CCC:3:LEU:N	1:CCC:3:LEU:HD13	2.28	0.48
1:CCC:147:VAL:HG12	1:CCC:170:LEU:O	2.14	0.47
1:EEE:180:GLU:CD	1:EEE:180:GLU:H	2.18	0.47
1:CCC:1:MET:HE1	1:CCC:27:GLU:HB3	1.95	0.47
1:BBB:79:ARG:HG2	1:BBB:82:ARG:HH22	1.80	0.47
1:DDD:131:ILE:O	1:DDD:131:ILE:CG2	2.61	0.47
1:EEE:103:ALA:HA	1:EEE:125:THR:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:104:GLY:HA3	2:BBB:301:LHQ:O2	2.14	0.47
1:FFF:49:LEU:HD22	1:FFF:50:LEU:N	2.29	0.47
1:FFF:103:ALA:HA	1:FFF:125:THR:O	2.15	0.47
1:EEE:147:VAL:HG12	1:EEE:170:LEU:O	2.15	0.47
1:BBB:30:ASP:OD1	1:BBB:79:ARG:HD3	2.15	0.46
1:BBB:180:GLU:H	1:BBB:180:GLU:CD	2.18	0.46
1:EEE:55:ARG:NH1	2:EEE:301:LHQ:O7	2.48	0.46
1:EEE:131:ILE:O	1:EEE:131:ILE:CG2	2.60	0.46
1:DDD:252:GLN:HE22	1:DDD:254:ARG:NH2	2.13	0.46
1:CCC:131:ILE:HD11	1:CCC:133:LEU:HD12	1.98	0.46
1:AAA:33:TYR:OH	1:AAA:37:LYS:HE2	2.15	0.46
1:AAA:43:ARG:HD2	1:AAA:43:ARG:O	2.16	0.46
1:CCC:103:ALA:HA	1:CCC:125:THR:O	2.16	0.46
1:EEE:1:MET:HE1	1:EEE:27:GLU:CB	2.46	0.46
1:FFF:147:VAL:HG12	1:FFF:170:LEU:O	2.16	0.45
1:AAA:2:ILE:HD11	1:AAA:28:LEU:HG	1.96	0.45
1:DDD:211:THR:HG21	1:FFF:144:PRO:HG2	1.98	0.45
1:EEE:130:ARG:HH11	1:EEE:130:ARG:HG2	1.81	0.45
1:EEE:133:LEU:CD1	2:EEE:301:LHQ:C10	2.94	0.45
1:AAA:103:ALA:HA	1:AAA:125:THR:O	2.16	0.45
1:AAA:119:ALA:HA	1:AAA:177:VAL:O	2.16	0.45
1:BBB:133:LEU:HD13	2:BBB:301:LHQ:C10	2.45	0.45
1:BBB:103:ALA:HA	1:BBB:125:THR:O	2.17	0.45
1:BBB:147:VAL:HG12	1:BBB:170:LEU:O	2.16	0.45
1:DDD:103:ALA:HA	1:DDD:125:THR:O	2.17	0.45
1:FFF:246:LYS:H	1:FFF:246:LYS:HG2	1.43	0.45
1:AAA:39:GLY:O	1:AAA:92:LYS:NZ	2.46	0.44
1:FFF:119:ALA:HA	1:FFF:177:VAL:O	2.16	0.44
1:AAA:91:GLU:O	1:AAA:92:LYS:HG3	2.18	0.44
1:FFF:12:VAL:HG13	1:FFF:49:LEU:HD12	1.98	0.44
1:DDD:246:LYS:HE3	1:DDD:246:LYS:HB3	1.47	0.44
1:AAA:2:ILE:CD1	1:AAA:28:LEU:HG	2.48	0.43
1:DDD:227:GLN:HG2	1:FFF:77:LEU:HD21	1.99	0.43
1:FFF:234:GLN:HG3	1:FFF:254:ARG:NH2	2.33	0.43
1:BBB:90:LEU:HD12	1:BBB:90:LEU:HA	1.87	0.43
1:CCC:206:LYS:NZ	1:CCC:210:GLU:CG	2.81	0.43
1:BBB:133:LEU:HD11	2:BBB:301:LHQ:C10	2.49	0.43
1:EEE:245:GLU:HB2	1:EEE:247:ARG:HH11	1.84	0.43
1:EEE:115:LEU:HD13	1:EEE:189:LEU:HD21	2.00	0.42
1:AAA:213:ARG:CZ	1:CCC:215:SER:HB3	2.50	0.42
1:AAA:131:ILE:O	1:AAA:131:ILE:CG2	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:130:ARG:HG2	1:DDD:130:ARG:HH11	1.84	0.42
1:EEE:118:ALA:HB2	1:EEE:173:VAL:HG11	2.01	0.42
1:AAA:199:ARG:HA	1:AAA:199:ARG:HD2	1.87	0.42
1:CCC:162:LEU:HD21	1:CCC:170:LEU:HD11	2.02	0.42
1:FFF:91:GLU:O	1:FFF:92:LYS:HG3	2.19	0.42
1:BBB:55:ARG:O	1:BBB:100:GLY:HA3	2.20	0.42
1:BBB:155:LEU:CD2	1:BBB:162:LEU:HD11	2.49	0.42
1:EEE:104:GLY:HA3	2:EEE:301:LHQ:O2	2.20	0.42
1:FFF:177:VAL:HG21	1:FFF:182:LEU:HA	2.02	0.42
1:AAA:144:PRO:HG2	1:CCC:211:THR:HG21	2.00	0.42
1:BBB:199:ARG:HD2	1:BBB:199:ARG:HA	1.83	0.42
1:EEE:90:LEU:HD12	1:EEE:90:LEU:HA	1.87	0.42
1:FFF:155:LEU:CD2	1:FFF:162:LEU:HD11	2.47	0.42
1:CCC:3:LEU:HD21	1:CCC:16:ASN:ND2	2.34	0.41
1:DDD:55:ARG:O	1:DDD:100:GLY:HA3	2.21	0.41
1:AAA:55:ARG:O	1:AAA:100:GLY:HA3	2.20	0.41
1:DDD:177:VAL:HG21	1:DDD:182:LEU:HA	2.03	0.41
1:FFF:250:ARG:HG2	1:FFF:250:ARG:HH21	1.86	0.41
1:CCC:55:ARG:O	1:CCC:100:GLY:HA3	2.20	0.41
1:DDD:119:ALA:HA	1:DDD:177:VAL:O	2.21	0.41
1:EEE:151:LYS:HD3	1:EEE:151:LYS:HA	1.91	0.41
1:AAA:254:ARG:HB2	1:AAA:254:ARG:NH1	2.36	0.41
1:EEE:245:GLU:O	1:EEE:247:ARG:HG2	2.21	0.41
1:AAA:143:LEU:HB3	1:AAA:144:PRO:HD3	2.03	0.40
1:EEE:55:ARG:O	1:EEE:100:GLY:HA3	2.20	0.40
1:CCC:3:LEU:HD11	1:CCC:16:ASN:ND2	2.31	0.40
1:EEE:112:TRP:CD2	1:EEE:142:LEU:HD11	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:185:GLU:OE2	1:FFF:254:ARG:NH1[2_645]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	241/254 (95%)	230 (95%)	10 (4%)	1 (0%)	34	46
1	BBB	241/254 (95%)	230 (95%)	10 (4%)	1 (0%)	34	46
1	CCC	241/254 (95%)	232 (96%)	8 (3%)	1 (0%)	34	46
1	DDD	241/254 (95%)	232 (96%)	8 (3%)	1 (0%)	34	46
1	EEE	241/254 (95%)	233 (97%)	7 (3%)	1 (0%)	34	46
1	FFF	241/254 (95%)	231 (96%)	9 (4%)	1 (0%)	34	46
All	All	1446/1524 (95%)	1388 (96%)	52 (4%)	6 (0%)	34	46

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	246	LYS
1	BBB	246	LYS
1	CCC	246	LYS
1	DDD	246	LYS
1	EEE	246	LYS
1	FFF	246	LYS

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	AAA	189/197 (96%)	180 (95%)	9 (5%)	25	34
1	BBB	189/197 (96%)	181 (96%)	8 (4%)	30	40
1	CCC	189/197 (96%)	182 (96%)	7 (4%)	34	46
1	DDD	189/197 (96%)	180 (95%)	9 (5%)	25	34
1	EEE	189/197 (96%)	182 (96%)	7 (4%)	34	46
1	FFF	189/197 (96%)	178 (94%)	11 (6%)	20	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1134/1182 (96%)	1083 (96%)	51 (4%)	27	37

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	7	GLN
1	AAA	43	ARG
1	AAA	90	LEU
1	AAA	161	ARG
1	AAA	165	GLU
1	AAA	175	ARG
1	AAA	209	LEU
1	AAA	241	ARG
1	AAA	254	ARG
1	BBB	2	ILE
1	BBB	43	ARG
1	BBB	78	ARG
1	BBB	79	ARG
1	BBB	90	LEU
1	BBB	180	GLU
1	BBB	241	ARG
1	BBB	254	ARG
1	CCC	3	LEU
1	CCC	20	LYS
1	CCC	136	ASN
1	CCC	165	GLU
1	CCC	180	GLU
1	CCC	244	ARG
1	CCC	254	ARG
1	DDD	5	GLU
1	DDD	27	GLU
1	DDD	43	ARG
1	DDD	44	GLU
1	DDD	79	ARG
1	DDD	90	LEU
1	DDD	136	ASN
1	DDD	237	GLU
1	DDD	246	LYS
1	EEE	8	ASP
1	EEE	43	ARG
1	EEE	55	ARG
1	EEE	78	ARG

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Mol	Chain	Res	Type
1	EEE	90	LEU
1	EEE	161	ARG
1	EEE	250	ARG
1	FFF	1	MET
1	FFF	37	LYS
1	FFF	43	ARG
1	FFF	49	LEU
1	FFF	90	LEU
1	FFF	161	ARG
1	FFF	175	ARG
1	FFF	209	LEU
1	FFF	237	GLU
1	FFF	246	LYS
1	FFF	254	ARG

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

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 monosaccharides in this entry.

5.6　Ligand geometry ⓘ

6 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	LHQ	EEE	301	-	49,61,61	1.98	11 (22%)	59,89,89	2.26	16 (27%)
2	LHQ	BBB	301	-	49,61,61	2.55	15 (30%)	59,89,89	2.39	15 (25%)
2	LHQ	CCC	301	-	49,61,61	2.56	12 (24%)	59,89,89	2.11	10 (16%)
2	LHQ	DDD	301	-	49,61,61	2.77	9 (18%)	59,89,89	2.50	14 (23%)
2	LHQ	AAA	301	-	49,61,61	2.53	10 (20%)	59,89,89	2.40	15 (25%)
2	LHQ	FFF	301	-	49,61,61	2.60	12 (24%)	59,89,89	2.23	15 (25%)

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	LHQ	EEE	301	-	-	12/48/80/80	0/3/4/4
2	LHQ	BBB	301	-	-	11/48/80/80	0/3/4/4
2	LHQ	CCC	301	-	-	10/48/80/80	0/3/4/4
2	LHQ	DDD	301	-	-	8/48/80/80	0/3/4/4
2	LHQ	AAA	301	-	-	11/48/80/80	0/3/4/4
2	LHQ	FFF	301	-	-	15/48/80/80	0/3/4/4

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	DDD	301	LHQ	O1-C10	13.01	1.65	1.45
2	FFF	301	LHQ	O1-C10	12.82	1.64	1.45
2	AAA	301	LHQ	O1-C10	11.56	1.62	1.45
2	CCC	301	LHQ	O1-C10	11.03	1.62	1.45
2	BBB	301	LHQ	O1-C10	10.00	1.60	1.45
2	DDD	301	LHQ	C13-S1	7.11	1.93	1.76
2	BBB	301	LHQ	O13-C29	6.84	1.50	1.41
2	CCC	301	LHQ	O13-C29	6.23	1.49	1.41
2	EEE	301	LHQ	C12-C11	-6.22	1.39	1.49
2	BBB	301	LHQ	C12-C11	-6.13	1.39	1.49
2	AAA	301	LHQ	O13-C29	5.89	1.49	1.41
2	CCC	301	LHQ	C4-N2	5.66	1.41	1.32
2	BBB	301	LHQ	C4-N2	5.48	1.40	1.32
2	DDD	301	LHQ	O13-C29	5.46	1.48	1.41
2	FFF	301	LHQ	C12-C11	-5.15	1.40	1.49
2	CCC	301	LHQ	C12-C11	-4.98	1.41	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	DDD	301	LHQ	C4-N2	4.86	1.39	1.32
2	FFF	301	LHQ	C4-N2	4.81	1.39	1.32
2	EEE	301	LHQ	O1-C10	4.80	1.52	1.45
2	AAA	301	LHQ	C13-S1	4.67	1.87	1.76
2	FFF	301	LHQ	C13-S1	4.66	1.87	1.76
2	EEE	301	LHQ	C4-N2	4.65	1.39	1.32
2	AAA	301	LHQ	C12-C11	-4.47	1.41	1.49
2	DDD	301	LHQ	C12-C11	-4.36	1.42	1.49
2	AAA	301	LHQ	C10-C9	-4.35	1.38	1.49
2	FFF	301	LHQ	O13-C29	4.25	1.47	1.41
2	CCC	301	LHQ	C13-S1	4.20	1.86	1.76
2	AAA	301	LHQ	C4-N2	4.19	1.38	1.32
2	EEE	301	LHQ	C4-N1	4.08	1.41	1.33
2	FFF	301	LHQ	C10-C9	-4.01	1.39	1.49
2	BBB	301	LHQ	C10-C9	-3.92	1.39	1.49
2	DDD	301	LHQ	C10-C9	-3.91	1.39	1.49
2	EEE	301	LHQ	O13-C29	3.89	1.46	1.41
2	DDD	301	LHQ	C4-N1	3.89	1.41	1.33
2	CCC	301	LHQ	C4-N1	3.85	1.41	1.33
2	EEE	301	LHQ	C10-C9	-3.79	1.40	1.49
2	CCC	301	LHQ	C10-C9	-3.72	1.40	1.49
2	AAA	301	LHQ	C4-N1	3.63	1.40	1.33
2	BBB	301	LHQ	C4-N1	3.27	1.40	1.33
2	FFF	301	LHQ	C4-N1	2.95	1.39	1.33
2	BBB	301	LHQ	C13-S1	2.89	1.83	1.76
2	BBB	301	LHQ	O5-C20	2.48	1.46	1.42
2	CCC	301	LHQ	C3-C2	-2.45	1.34	1.43
2	EEE	301	LHQ	C3-C2	-2.39	1.34	1.43
2	BBB	301	LHQ	C17-C16	2.36	1.55	1.51
2	BBB	301	LHQ	C28-C29	-2.34	1.50	1.53
2	BBB	301	LHQ	C3-C2	-2.32	1.34	1.43
2	FFF	301	LHQ	O13-C26	2.31	1.50	1.45
2	FFF	301	LHQ	C3-C2	-2.30	1.34	1.43
2	CCC	301	LHQ	C2-C1	-2.28	1.34	1.40
2	EEE	301	LHQ	C17-C16	2.26	1.55	1.51
2	BBB	301	LHQ	C2-C1	-2.26	1.35	1.40
2	FFF	301	LHQ	C2-C1	-2.25	1.35	1.40
2	DDD	301	LHQ	P3-O14	2.24	1.63	1.59
2	DDD	301	LHQ	C3-C2	-2.24	1.35	1.43
2	BBB	301	LHQ	C23-C21	2.23	1.58	1.53
2	AAA	301	LHQ	C25-C26	2.19	1.58	1.51
2	CCC	301	LHQ	O13-C26	2.14	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	CCC	301	LHQ	O5-C20	2.13	1.46	1.42
2	EEE	301	LHQ	P3-O14	2.13	1.63	1.59
2	CCC	301	LHQ	P3-O15	-2.11	1.46	1.54
2	FFF	301	LHQ	C28-C29	2.10	1.56	1.53
2	BBB	301	LHQ	P3-O16	-2.09	1.46	1.54
2	BBB	301	LHQ	P3-O14	2.06	1.63	1.59
2	EEE	301	LHQ	O18-C28	-2.05	1.38	1.43
2	AAA	301	LHQ	C3-C2	-2.03	1.35	1.43
2	FFF	301	LHQ	O2-C13	2.02	1.24	1.21
2	AAA	301	LHQ	C17-C16	2.01	1.55	1.51
2	EEE	301	LHQ	O5-C20	2.01	1.46	1.42

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	301	LHQ	O1-C10-C9	8.98	130.13	113.50
2	BBB	301	LHQ	O1-C10-C9	8.89	129.96	113.50
2	DDD	301	LHQ	O1-C10-C9	8.79	129.79	113.50
2	FFF	301	LHQ	O1-C10-C9	8.12	128.54	113.50
2	CCC	301	LHQ	O1-C10-C9	8.10	128.51	113.50
2	DDD	301	LHQ	C12-C13-S1	7.81	123.42	113.69
2	EEE	301	LHQ	O1-C10-C9	7.49	127.37	113.50
2	CCC	301	LHQ	C12-C13-S1	7.37	122.88	113.69
2	BBB	301	LHQ	N2-C4-N1	-7.31	117.25	128.68
2	FFF	301	LHQ	N2-C4-N1	-7.15	117.50	128.68
2	AAA	301	LHQ	C12-C13-S1	6.76	122.12	113.69
2	EEE	301	LHQ	N2-C4-N1	-6.70	118.21	128.68
2	DDD	301	LHQ	N2-C4-N1	-6.66	118.26	128.68
2	DDD	301	LHQ	C18-N4-C19	6.65	134.44	122.59
2	CCC	301	LHQ	N2-C4-N1	-6.58	118.39	128.68
2	AAA	301	LHQ	C18-N4-C19	5.76	132.86	122.59
2	AAA	301	LHQ	N2-C4-N1	-5.72	119.73	128.68
2	EEE	301	LHQ	C18-N4-C19	5.61	132.59	122.59
2	BBB	301	LHQ	C18-N4-C19	5.48	132.36	122.59
2	BBB	301	LHQ	C12-C13-S1	5.41	120.43	113.69
2	EEE	301	LHQ	C17-C18-N4	-5.37	101.05	111.90
2	FFF	301	LHQ	C12-C13-S1	5.36	120.37	113.69
2	AAA	301	LHQ	C17-C18-N4	-4.91	101.99	111.90
2	EEE	301	LHQ	C20-C19-N4	4.68	125.89	116.58
2	DDD	301	LHQ	P2-O9-P1	-4.44	117.59	132.83
2	EEE	301	LHQ	C12-C13-S1	4.25	118.99	113.69
2	DDD	301	LHQ	O2-C13-C12	-4.22	116.04	123.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	301	LHQ	P2-O9-P1	-4.17	118.53	132.83
2	FFF	301	LHQ	C23-C21-C24	4.07	114.86	108.23
2	DDD	301	LHQ	C17-C18-N4	-3.77	104.28	111.90
2	AAA	301	LHQ	C20-C19-N4	3.77	124.09	116.58
2	BBB	301	LHQ	C20-C19-N4	3.61	123.76	116.58
2	BBB	301	LHQ	C15-N3-C16	-3.59	116.17	122.84
2	DDD	301	LHQ	C20-C19-N4	3.56	123.67	116.58
2	AAA	301	LHQ	O2-C13-C12	-3.55	117.20	123.35
2	BBB	301	LHQ	O2-C13-C12	-3.45	117.37	123.35
2	AAA	301	LHQ	O13-C26-C25	3.41	120.59	109.37
2	FFF	301	LHQ	C17-C18-N4	-3.30	105.24	111.90
2	CCC	301	LHQ	O2-C13-C12	-3.28	117.67	123.35
2	FFF	301	LHQ	O2-C13-C12	-3.22	117.77	123.35
2	AAA	301	LHQ	P2-O9-P1	-3.13	122.08	132.83
2	FFF	301	LHQ	C22-C21-C20	3.13	114.24	108.82
2	EEE	301	LHQ	O4-C19-N4	-3.06	116.43	122.99
2	BBB	301	LHQ	C18-C17-C16	2.99	117.34	112.36
2	EEE	301	LHQ	O2-C13-C12	-2.98	118.19	123.35
2	BBB	301	LHQ	C17-C18-N4	-2.93	105.99	111.90
2	EEE	301	LHQ	C14-C15-N3	-2.91	106.30	112.42
2	CCC	301	LHQ	C2-C3-N7	-2.91	115.93	120.35
2	AAA	301	LHQ	C22-C21-C20	2.89	113.84	108.82
2	EEE	301	LHQ	O13-C29-C28	-2.88	102.71	106.93
2	FFF	301	LHQ	C20-C19-N4	2.86	122.27	116.58
2	CCC	301	LHQ	O13-C26-C25	2.84	118.71	109.37
2	DDD	301	LHQ	C18-C17-C16	2.74	116.92	112.36
2	DDD	301	LHQ	O13-C29-C28	-2.72	102.95	106.93
2	BBB	301	LHQ	C23-C21-C20	2.64	113.40	108.82
2	AAA	301	LHQ	C1-C2-N6	-2.63	106.65	109.40
2	EEE	301	LHQ	O16-P3-O15	2.63	117.67	107.64
2	FFF	301	LHQ	C18-N4-C19	2.62	127.26	122.59
2	FFF	301	LHQ	C14-C15-N3	-2.56	107.05	112.42
2	FFF	301	LHQ	O13-C29-C28	-2.51	103.26	106.93
2	AAA	301	LHQ	O16-P3-O15	2.45	117.00	107.64
2	CCC	301	LHQ	O2-C13-S1	-2.44	119.45	122.61
2	DDD	301	LHQ	C2-C3-N7	-2.41	116.69	120.35
2	CCC	301	LHQ	O16-P3-O15	2.40	116.82	107.64
2	FFF	301	LHQ	O16-P3-O15	2.40	116.81	107.64
2	EEE	301	LHQ	C2-C3-N7	-2.39	116.72	120.35
2	FFF	301	LHQ	C22-C21-C24	-2.34	104.42	108.23
2	BBB	301	LHQ	C2-C3-N7	-2.30	116.85	120.35
2	CCC	301	LHQ	C18-N4-C19	2.30	126.69	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	EEE	301	LHQ	O14-P3-O17	-2.25	100.69	109.39
2	EEE	301	LHQ	C17-C16-N3	-2.23	112.67	116.42
2	AAA	301	LHQ	O6-C24-C21	-2.19	107.03	110.55
2	CCC	301	LHQ	C14-C15-N3	-2.13	107.94	112.42
2	EEE	301	LHQ	P2-O9-P1	-2.13	125.52	132.83
2	AAA	301	LHQ	C17-C16-N3	-2.11	112.87	116.42
2	EEE	301	LHQ	C28-C27-C26	-2.09	99.52	103.22
2	BBB	301	LHQ	O16-P3-O15	2.09	115.62	107.64
2	DDD	301	LHQ	C23-C21-C24	2.08	111.63	108.23
2	DDD	301	LHQ	O14-P3-O17	-2.06	101.44	109.39
2	AAA	301	LHQ	O4-C19-N4	-2.05	118.58	122.99
2	FFF	301	LHQ	C2-C3-N7	-2.05	117.24	120.35
2	BBB	301	LHQ	C1-C2-N6	-2.04	107.28	109.40
2	DDD	301	LHQ	O4-C19-N4	-2.02	118.65	122.99
2	BBB	301	LHQ	O13-C26-C25	2.02	116.02	109.37
2	FFF	301	LHQ	O15-P3-O14	-2.01	96.99	105.99

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	301	LHQ	C11-C12-C13-O2
2	AAA	301	LHQ	C16-C17-C18-N4
2	AAA	301	LHQ	C20-C19-N4-C18
2	BBB	301	LHQ	C11-C12-C13-O2
2	BBB	301	LHQ	C12-C13-S1-C14
2	BBB	301	LHQ	O2-C13-S1-C14
2	BBB	301	LHQ	C20-C19-N4-C18
2	BBB	301	LHQ	C25-O12-P2-O9
2	BBB	301	LHQ	C25-O12-P2-O10
2	BBB	301	LHQ	C25-O12-P2-O11
2	CCC	301	LHQ	C11-C12-C13-O2
2	CCC	301	LHQ	C20-C19-N4-C18
2	CCC	301	LHQ	C20-C21-C24-O6
2	DDD	301	LHQ	C11-C12-C13-O2
2	DDD	301	LHQ	C20-C19-N4-C18
2	DDD	301	LHQ	N4-C19-C20-O5
2	EEE	301	LHQ	C11-C12-C13-O2
2	EEE	301	LHQ	C16-C17-C18-N4
2	EEE	301	LHQ	C20-C19-N4-C18
2	EEE	301	LHQ	N4-C19-C20-O5
2	EEE	301	LHQ	C25-O12-P2-O9

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Mol	Chain	Res	Type	Atoms
2	EEE	301	LHQ	C25-O12-P2-O10
2	EEE	301	LHQ	C25-O12-P2-O11
2	FFF	301	LHQ	C11-C12-C13-O2
2	FFF	301	LHQ	C16-C17-C18-N4
2	FFF	301	LHQ	C20-C19-N4-C18
2	FFF	301	LHQ	N4-C19-C20-O5
2	FFF	301	LHQ	C20-C21-C24-O6
2	FFF	301	LHQ	C22-C21-C24-O6
2	FFF	301	LHQ	C23-C21-C24-O6
2	BBB	301	LHQ	O4-C19-N4-C18
2	CCC	301	LHQ	O4-C19-N4-C18
2	DDD	301	LHQ	O4-C19-N4-C18
2	FFF	301	LHQ	O4-C19-N4-C18
2	BBB	301	LHQ	O12-C25-C26-C27
2	AAA	301	LHQ	O4-C19-N4-C18
2	EEE	301	LHQ	O4-C19-N4-C18
2	BBB	301	LHQ	O12-C25-C26-O13
2	EEE	301	LHQ	O12-C25-C26-O13
2	EEE	301	LHQ	O12-C25-C26-C27
2	CCC	301	LHQ	C23-C21-C24-O6
2	DDD	301	LHQ	C16-C17-C18-N4
2	DDD	301	LHQ	O4-C19-C20-O5
2	EEE	301	LHQ	O4-C19-C20-O5
2	FFF	301	LHQ	O4-C19-C20-O5
2	CCC	301	LHQ	C22-C21-C24-O6
2	FFF	301	LHQ	P2-O9-P1-O7
2	AAA	301	LHQ	O2-C13-S1-C14
2	CCC	301	LHQ	O2-C13-S1-C14
2	FFF	301	LHQ	O2-C13-S1-C14
2	CCC	301	LHQ	C12-C13-S1-C14
2	AAA	301	LHQ	C24-O6-P1-O9
2	FFF	301	LHQ	C24-O6-P1-O9
2	FFF	301	LHQ	P2-O9-P1-O8
2	AAA	301	LHQ	C23-C21-C24-O6
2	BBB	301	LHQ	C23-C21-C24-O6
2	CCC	301	LHQ	C15-C14-S1-C13
2	DDD	301	LHQ	O2-C13-S1-C14
2	AAA	301	LHQ	O4-C19-C20-O5
2	AAA	301	LHQ	C22-C21-C24-O6
2	AAA	301	LHQ	C27-O14-P3-O16
2	CCC	301	LHQ	C27-O14-P3-O15
2	DDD	301	LHQ	C27-O14-P3-O16

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Mol	Chain	Res	Type	Atoms
2	FFF	301	LHQ	C21-C24-O6-P1
2	AAA	301	LHQ	C24-O6-P1-O7
2	EEE	301	LHQ	C24-O6-P1-O7
2	FFF	301	LHQ	C24-O6-P1-O7

There are no ring outliers.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	EEE	301	LHQ	4	0
2	BBB	301	LHQ	4	0
2	CCC	301	LHQ	1	0
2	DDD	301	LHQ	3	0
2	AAA	301	LHQ	3	0
2	FFF	301	LHQ	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 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 LHQ EEE 301

Bond lengths

Bond angles

Torsions

Rings

Ligand LHQ BBB 301

Bond lengths

Bond angles

Torsions

Rings

Ligand LHQ CCC 301

Bond lengths

Bond angles

Torsions

Rings

Ligand LHQ DDD 301

Bond lengths

Bond angles

Torsions

Rings

Ligand LHQ AAA 301

Bond lengths

Bond angles

Torsions

Rings

Ligand LHQ FFF 301

Bond lengths

Bond angles

Torsions

Rings
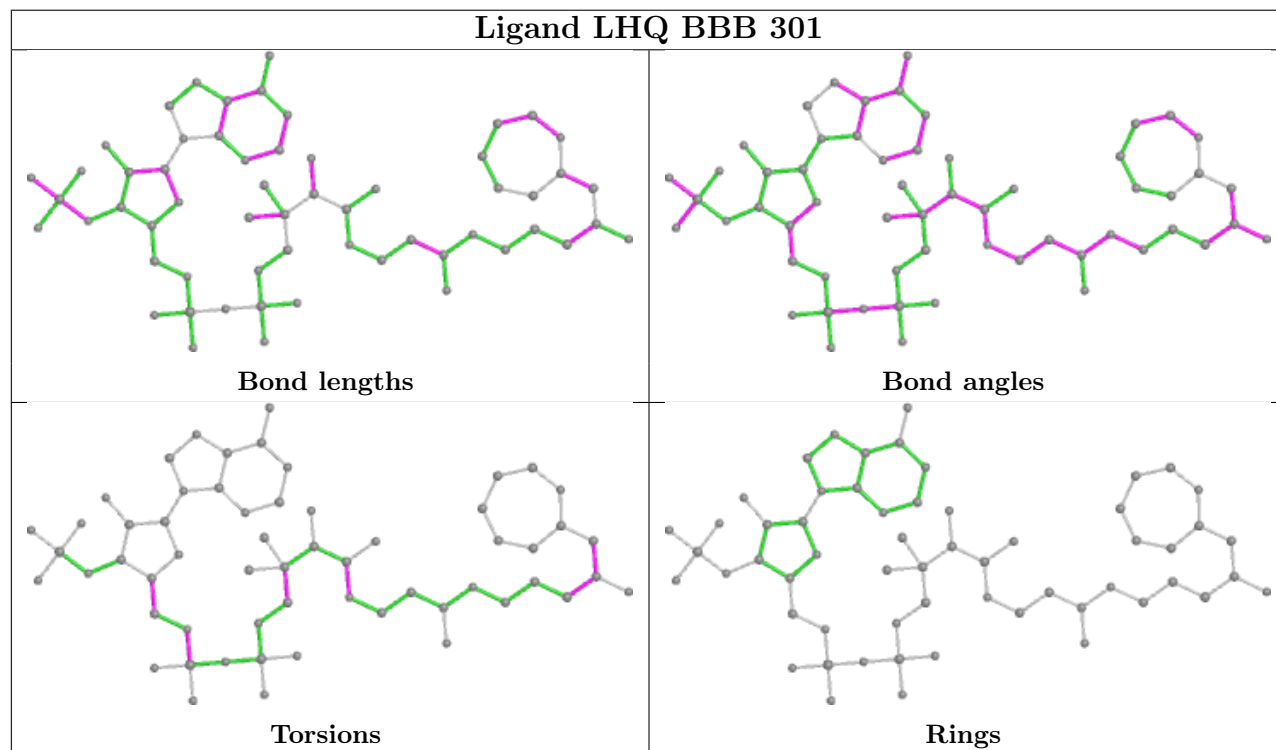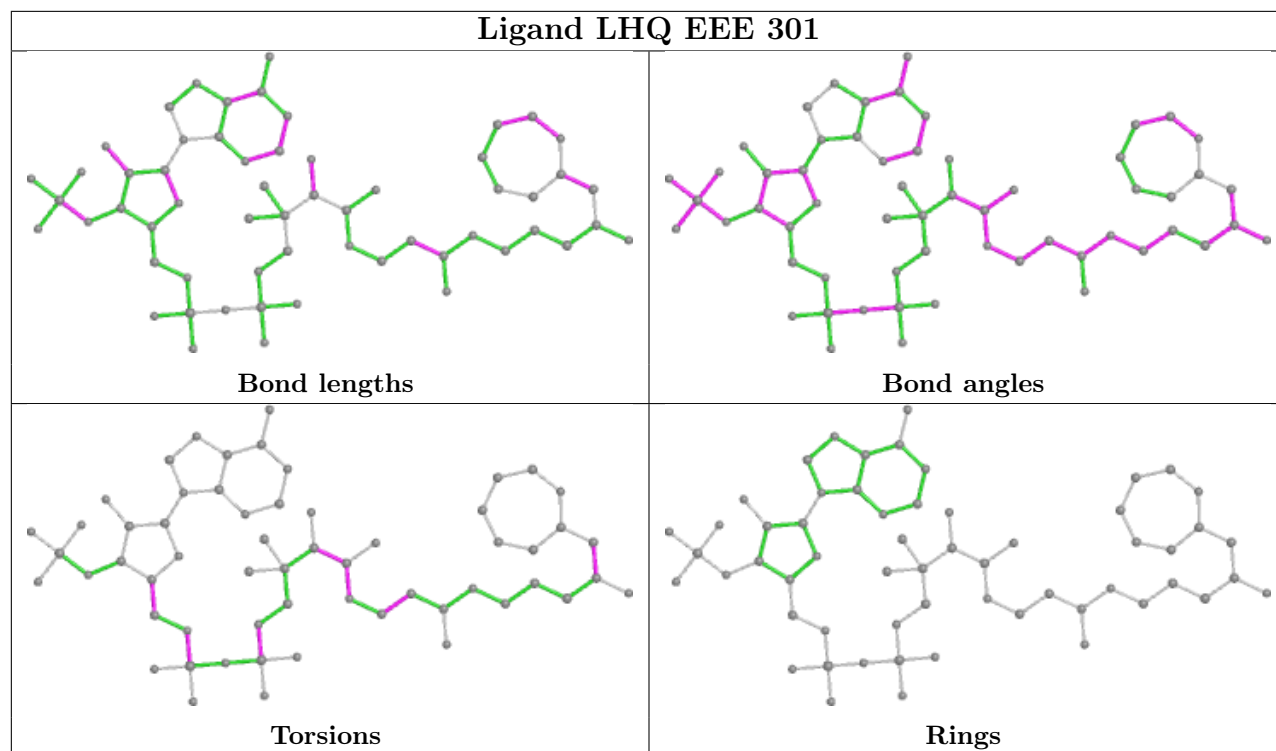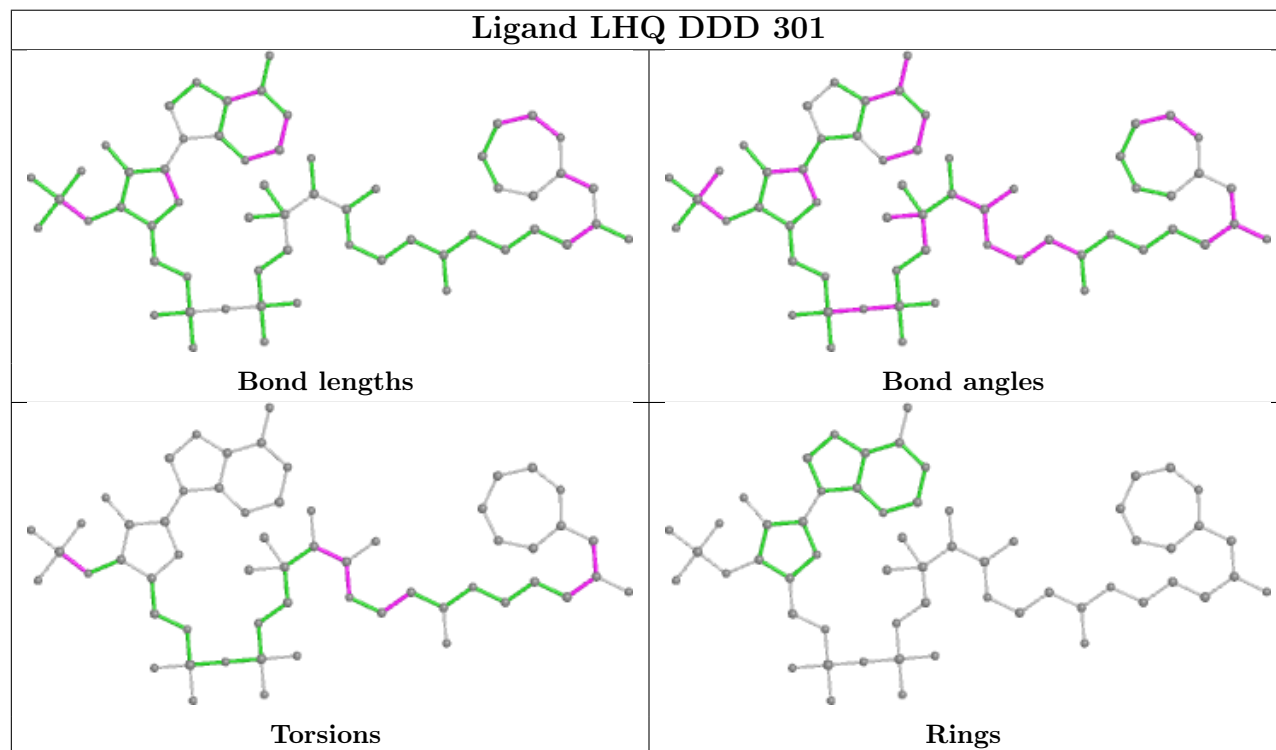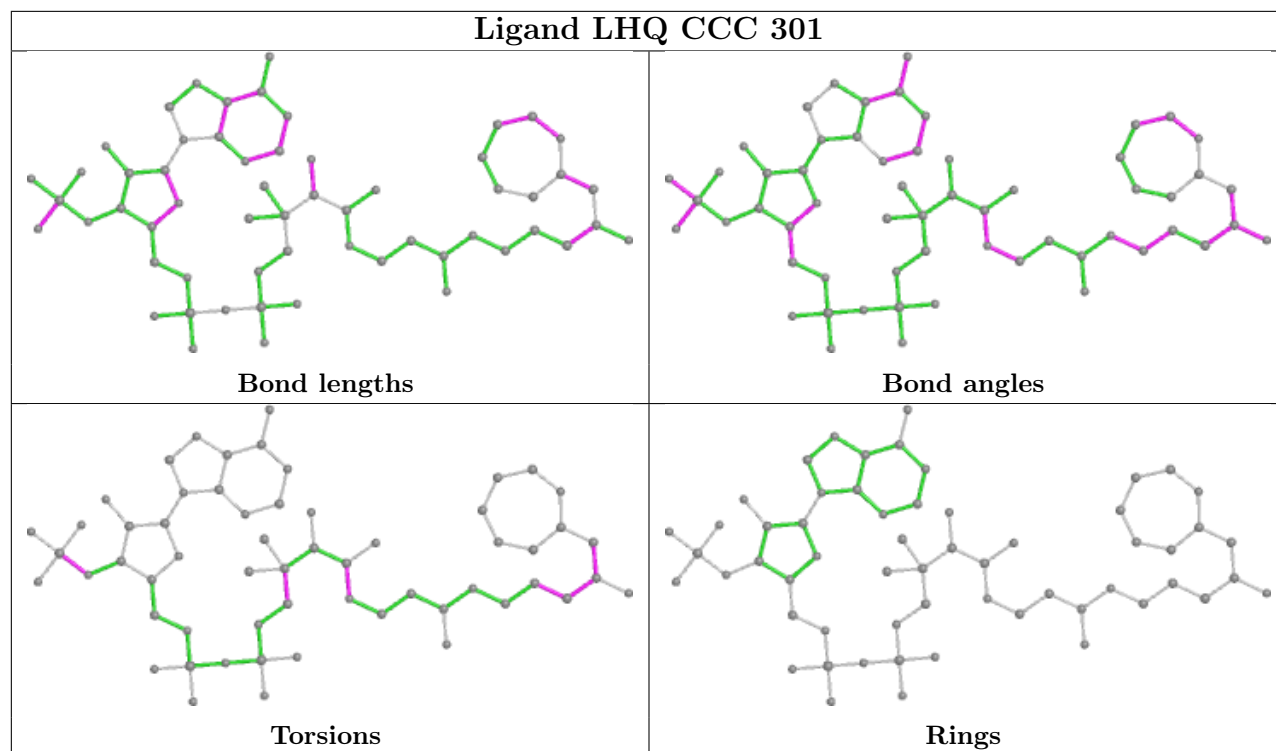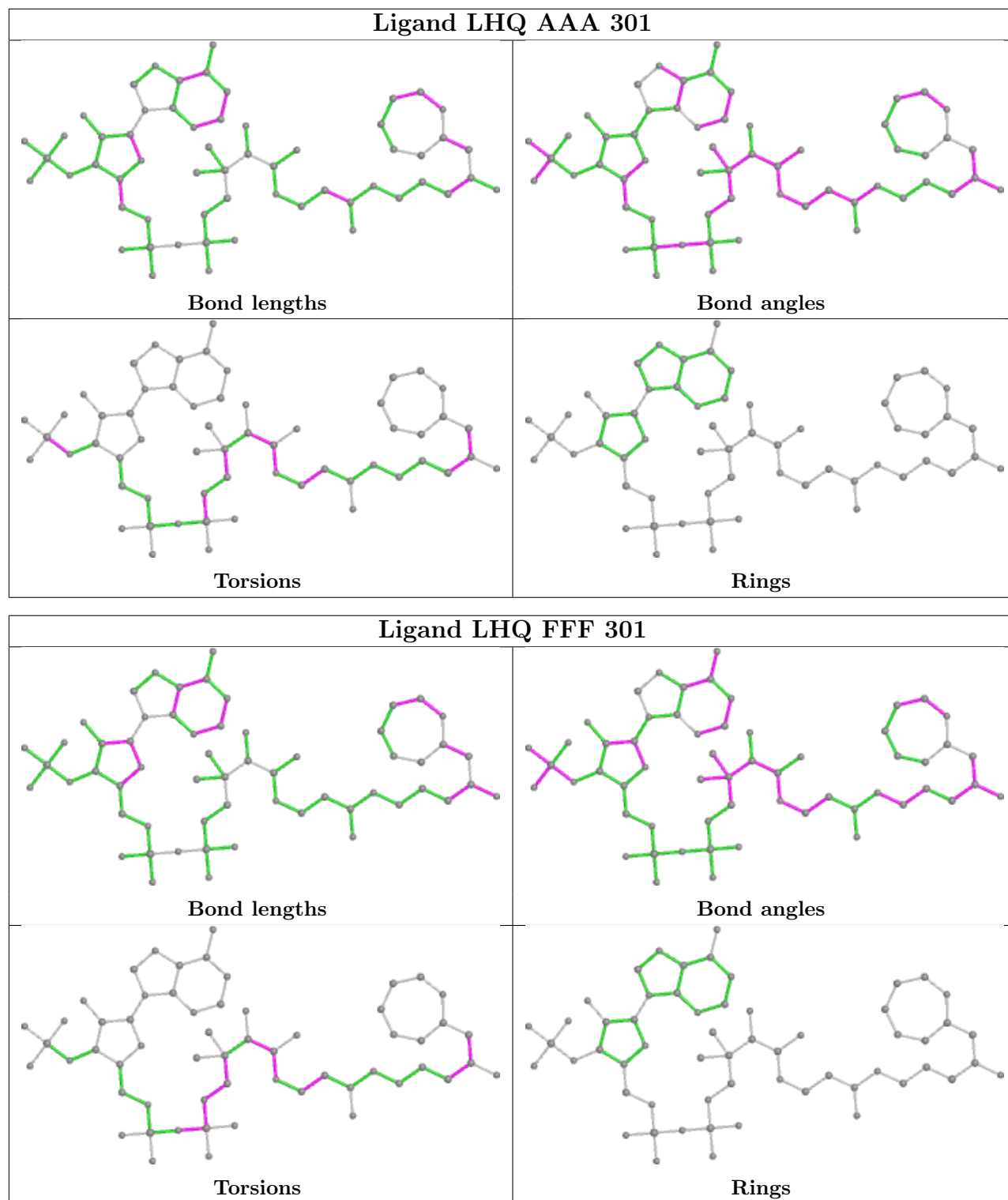
5.7 Other polymers ⓘ

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 ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AAA	245/254 (96%)	-0.08	3 (1%)	79	84	28, 41, 71, 87	0
1	BBB	245/254 (96%)	-0.02	4 (1%)	72	78	29, 47, 75, 94	0
1	CCC	245/254 (96%)	0.09	5 (2%)	65	72	30, 54, 83, 106	0
1	DDD	245/254 (96%)	0.07	6 (2%)	59	65	34, 53, 76, 110	0
1	EEE	245/254 (96%)	-0.02	4 (1%)	72	78	33, 52, 87, 112	0
1	FFF	245/254 (96%)	0.03	4 (1%)	72	78	34, 46, 73, 94	0
All	All	1470/1524 (96%)	0.01	26 (1%)	68	74	28, 49, 78, 112	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	240	VAL	4.3
1	BBB	244	ARG	3.9
1	FFF	19	GLU	3.6
1	BBB	241	ARG	3.0
1	CCC	80	TYR	3.0
1	DDD	187	LEU	2.9
1	DDD	189	LEU	2.9
1	AAA	250	ARG	2.9
1	AAA	80	TYR	2.9
1	FFF	242	ALA	2.8
1	EEE	187	LEU	2.8
1	CCC	43	ARG	2.7
1	DDD	243	PHE	2.6
1	DDD	188	SER	2.6
1	CCC	21	LEU	2.5
1	EEE	243	PHE	2.5
1	FFF	243	PHE	2.4
1	CCC	64	THR	2.4
1	AAA	75	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	EEE	254	ARG	2.3
1	DDD	80	TYR	2.2
1	BBB	238	GLU	2.1
1	DDD	131	ILE	2.1
1	FFF	16	ASN	2.1
1	EEE	246	LYS	2.0
1	CCC	44	GLU	2.0

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

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

6.3   Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4   Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LHQ	FFF	301	58/58	0.85	0.28	64,93,117,122	0
2	LHQ	CCC	301	58/58	0.87	0.38	72,112,133,146	0
2	LHQ	DDD	301	58/58	0.88	0.28	55,95,112,119	0
2	LHQ	AAA	301	58/58	0.91	0.26	49,78,104,112	0
2	LHQ	BBB	301	58/58	0.92	0.20	48,78,107,118	0
2	LHQ	EEE	301	58/58	0.94	0.16	47,68,84,101	0

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

Electron density around LHQ FFF 301:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
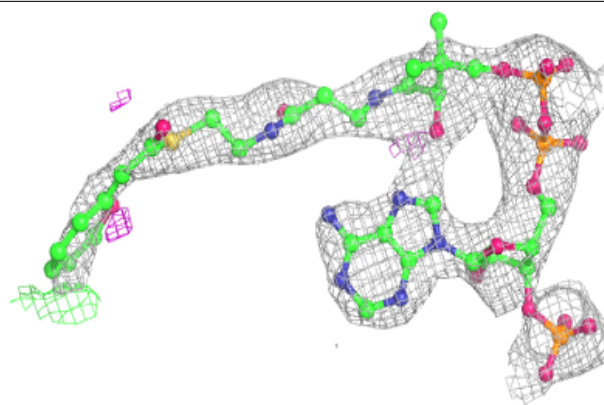and green (positive)
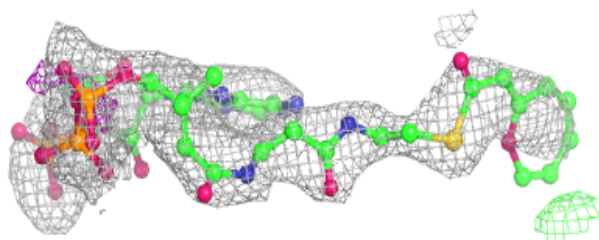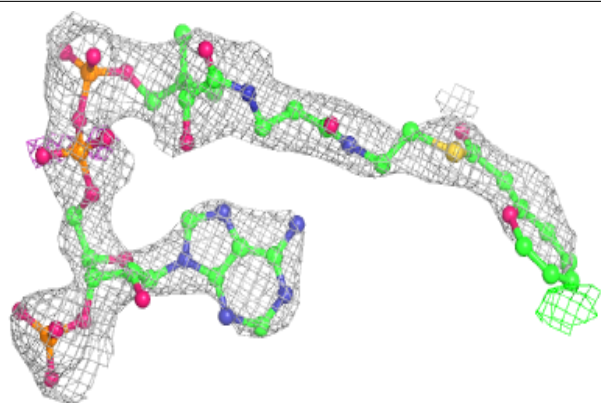
Electron density around LHQ CCC 301:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
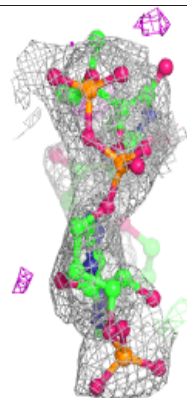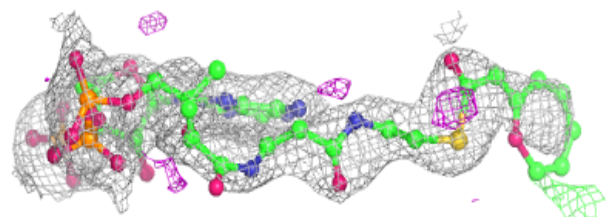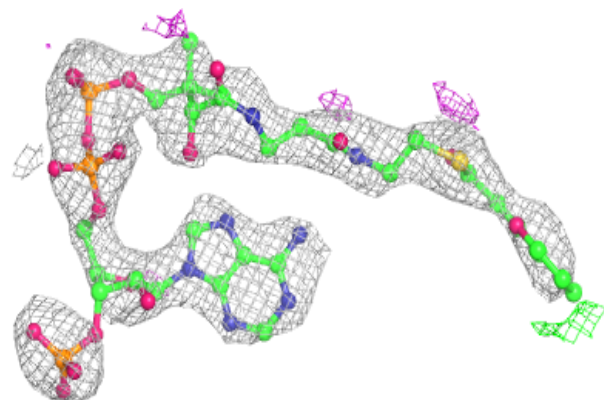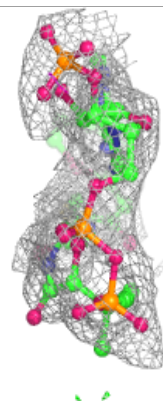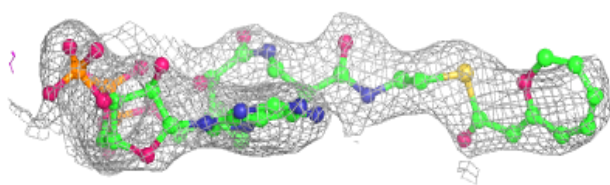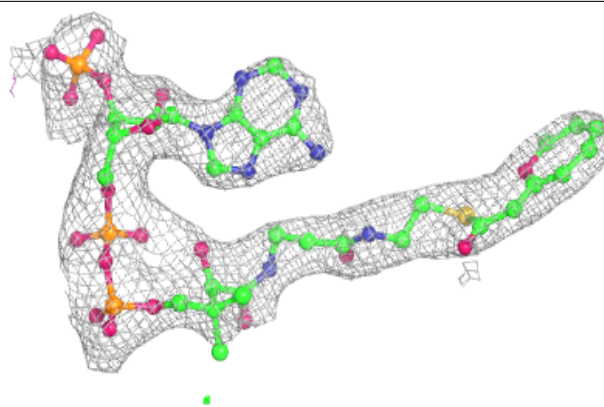mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
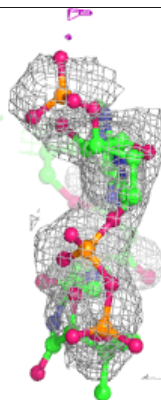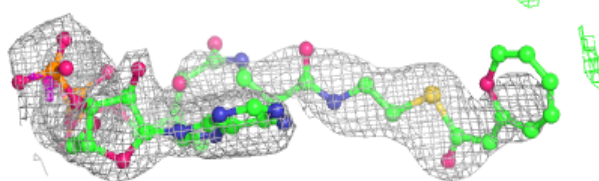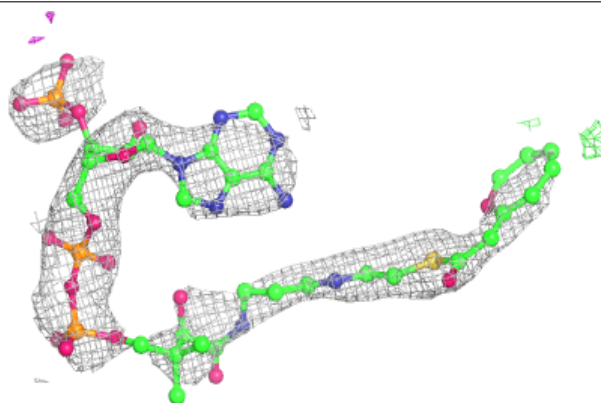
Electron density around LHQ DDD 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
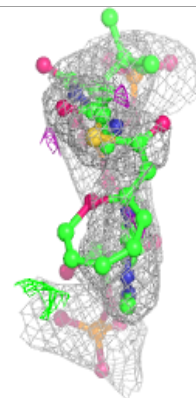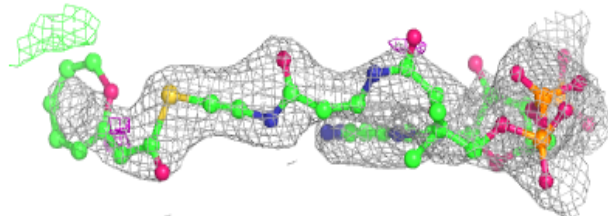
Electron density around LHQ AAA 301:

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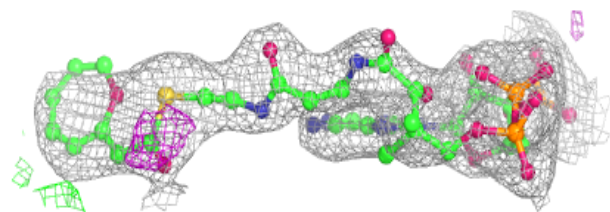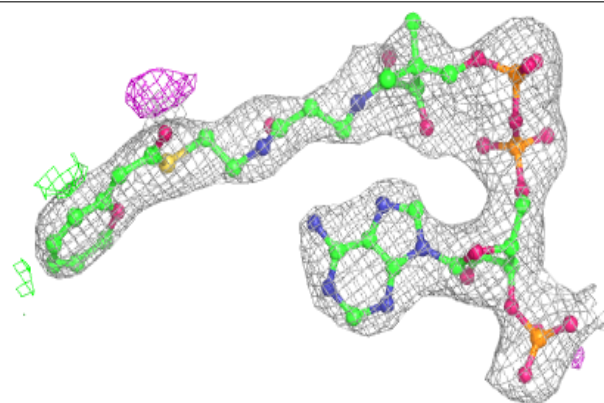mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around LHQ BBB 301:

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

Electron density around LHQ EEE 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
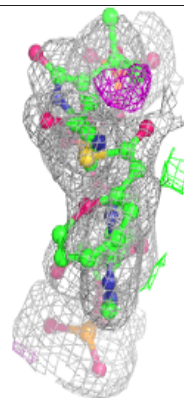
6.5 Other polymers (i)

There are no such residues in this entry.