WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB EM Validation Report ⓘ

Jul 14, 2024 – 12:08 AM JST

PDB ID	:	8XQR
EMDB ID	:	EMD-38586
Title	:	Structure 2 of human class T GPCR TAS2R14-miniGs/gust complex with Flufenamic acid.
Authors	:	Hu, X.L.; Wu, L.J.; Hua, T.; Liu, Z.J.
Deposited on	:	2024-01-05
Resolution	:	3.20 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.

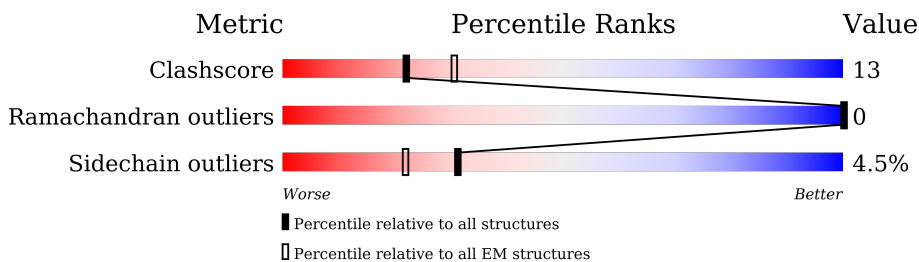The following versions of software and data (see references ⓘ) were used in the production of this report:

EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1　Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.20 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
Clashscore		13
Ramachandran outliers		0
Sidechain outliers		4.5%

Worse .... *Better*

■ Percentile relative to all structures
▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A	264	62%　　　27%　·　9%
2	B	366	62%　　　29%　·　7%
3	C	71	61%　　18%　·　20%
4	N	135	70%　　　24%　·　·
5	R	990	20%　8%　　72%

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2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 8273 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 Guanine nucleotide-binding protein G(t) subunit alpha-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	240	Total 1964	C 1242	N 348	O 368	S 6	0	0

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	341	Total 2616	C 1612	N 470	O 513	S 21	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	341	GLY	-	expression tag	UNP P62873
B	342	SER	-	expression tag	UNP P62873
B	343	SER	-	expression tag	UNP P62873
B	344	GLY	-	expression tag	UNP P62873
B	345	GLY	-	expression tag	UNP P62873
B	346	GLY	-	expression tag	UNP P62873
B	347	GLY	-	expression tag	UNP P62873
B	348	SER	-	expression tag	UNP P62873
B	349	GLY	-	expression tag	UNP P62873
B	350	GLY	-	expression tag	UNP P62873
B	351	GLY	-	expression tag	UNP P62873
B	352	GLY	-	expression tag	UNP P62873
B	353	SER	-	expression tag	UNP P62873
B	354	SER	-	expression tag	UNP P62873
B	355	GLY	-	expression tag	UNP P62873
B	356	VAL	-	expression tag	UNP P62873
B	357	SER	-	expression tag	UNP P62873
B	358	GLY	-	expression tag	UNP P62873
B	359	TRP	-	expression tag	UNP P62873
B	360	ARG	-	expression tag	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
B	361	LEU	-	expression tag	UNP P62873
B	362	PHE	-	expression tag	UNP P62873
B	363	LYS	-	expression tag	UNP P62873
B	364	LYS	-	expression tag	UNP P62873
B	365	ILE	-	expression tag	UNP P62873
B	366	SER	-	expression tag	UNP P62873

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	57	436	273	77	83	3	0	0

- Molecule 4 is a protein called Nanobody 35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	N	129	981	610	171	193	7	0	0

- Molecule 5 is a protein called Exo-alpha-sialidase,Taste receptor type 2 member 14,LgBiT.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	R	279	2256	1523	365	357	11	0	0

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-499	MET	-	initiating methionine	UNP A0A6M1VLG5
R	-498	LYS	-	expression tag	UNP A0A6M1VLG5
R	-497	THR	-	expression tag	UNP A0A6M1VLG5
R	-496	ILE	-	expression tag	UNP A0A6M1VLG5
R	-495	ILE	-	expression tag	UNP A0A6M1VLG5
R	-494	ALA	-	expression tag	UNP A0A6M1VLG5
R	-493	LEU	-	expression tag	UNP A0A6M1VLG5
R	-492	SER	-	expression tag	UNP A0A6M1VLG5
R	-491	TYR	-	expression tag	UNP A0A6M1VLG5
R	-490	ILE	-	expression tag	UNP A0A6M1VLG5
R	-489	PHE	-	expression tag	UNP A0A6M1VLG5
R	-488	CYS	-	expression tag	UNP A0A6M1VLG5
R	-487	LEU	-	expression tag	UNP A0A6M1VLG5

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-486	VAL	-	expression tag	UNP A0A6M1VLG5
R	-485	PHE	-	expression tag	UNP A0A6M1VLG5
R	-484	ALA	-	expression tag	UNP A0A6M1VLG5
R	-483	ASP	-	expression tag	UNP A0A6M1VLG5
R	-482	TYR	-	expression tag	UNP A0A6M1VLG5
R	-481	LYS	-	expression tag	UNP A0A6M1VLG5
R	-480	ASP	-	expression tag	UNP A0A6M1VLG5
R	-479	ASP	-	expression tag	UNP A0A6M1VLG5
R	-478	ASP	-	expression tag	UNP A0A6M1VLG5
R	-477	ASP	-	expression tag	UNP A0A6M1VLG5
R	-476	ALA	-	expression tag	UNP A0A6M1VLG5
R	-475	HIS	-	expression tag	UNP A0A6M1VLG5
R	-474	HIS	-	expression tag	UNP A0A6M1VLG5
R	-473	HIS	-	expression tag	UNP A0A6M1VLG5
R	-472	HIS	-	expression tag	UNP A0A6M1VLG5
R	-471	HIS	-	expression tag	UNP A0A6M1VLG5
R	-470	HIS	-	expression tag	UNP A0A6M1VLG5
R	-469	HIS	-	expression tag	UNP A0A6M1VLG5
R	-468	HIS	-	expression tag	UNP A0A6M1VLG5
R	-467	HIS	-	expression tag	UNP A0A6M1VLG5
R	-466	HIS	-	expression tag	UNP A0A6M1VLG5
R	-465	GLU	-	expression tag	UNP A0A6M1VLG5
R	-464	ASN	-	expression tag	UNP A0A6M1VLG5
R	-463	LEU	-	expression tag	UNP A0A6M1VLG5
R	-462	TYR	-	expression tag	UNP A0A6M1VLG5
R	-461	PHE	-	expression tag	UNP A0A6M1VLG5
R	-460	GLN	-	expression tag	UNP A0A6M1VLG5
R	-459	SER	-	expression tag	UNP A0A6M1VLG5
R	-458	GLY	-	expression tag	UNP A0A6M1VLG5
R	-457	ARG	-	expression tag	UNP A0A6M1VLG5
R	-456	ALA	-	expression tag	UNP A0A6M1VLG5
R	-305	SER	GLY	conflict	UNP A0A6M1VLG5
R	-3	GLY	-	linker	UNP A0A6M1VLG5
R	-2	SER	-	linker	UNP A0A6M1VLG5
R	-1	ALA	-	linker	UNP A0A6M1VLG5
R	0	GLY	-	linker	UNP A0A6M1VLG5
R	1	SER	-	linker	UNP A0A6M1VLG5

- Molecule 6 is 2-[[3-(TRIFLUOROMETHYL)PHENYL]AMINO] BENZOIC ACID (three-letter code: FLF) (formula: $C_{14}H_{10}F_3NO_2$) (labeled as "Ligand of Interest" by depositor).
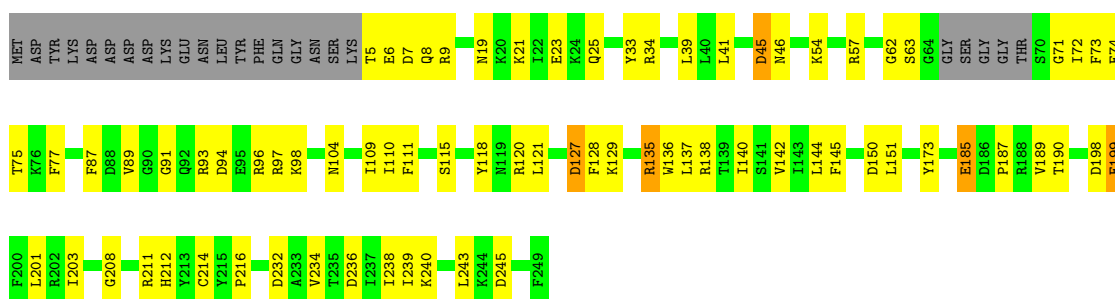
FLF
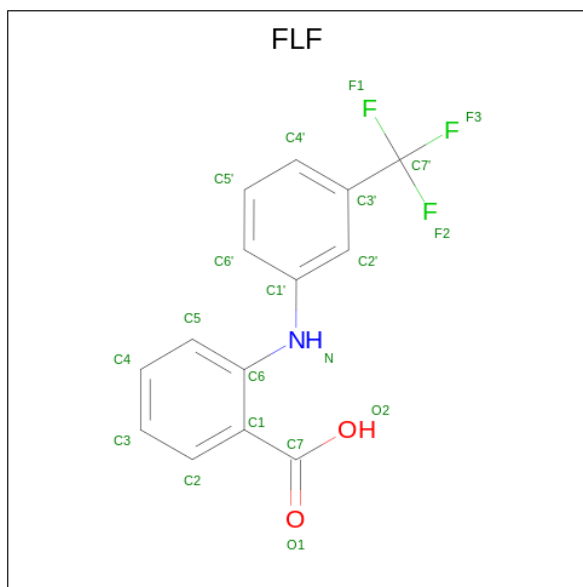
Mol	Chain	Residues	Atoms					AltConf
6	R	1	Total	C	F	N	O	0
			20	14	3	1	2	

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.
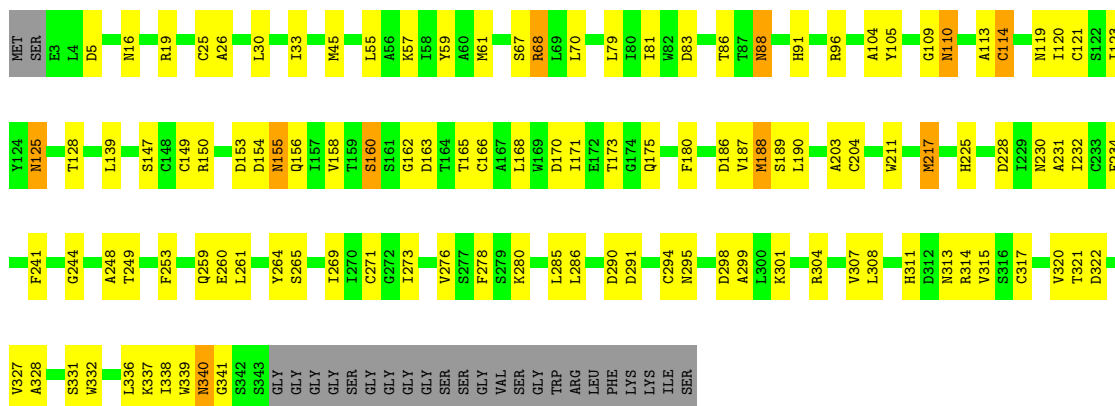
• Molecule 1: Guanine nucleotide-binding protein G(t) subunit alpha-3

Chain A:

• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B:

• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain C:

• Molecule 4: Nanobody 35

Chain N:

70%   24%

M1 S8 L19 S22 F30 Y33 K34 M35 N36 W37 Q40 K44 G45 L46 E47 W48 I52 S53 Q54 I59 T62 G63 S64 V65 R68 I71 S72 R73 L80 M84 L87 K88 Y95 R99 C100 R106 F109 T123 T126

V127 S128 S129 HIS HIS HIS HIS HIS HIS

• Molecule 5: Exo-alpha-sialidase,Taste receptor type 2 member 14,LgBiT

Chain R:

20%   8%   72%

MET LYS THR ILE ALA LEU SER TYR PHE CYS LEU VAL PHE ASP TYR LYS ASP ASP ASP ALA HIS HIS HIS HIS HIS HIS HIS HIS HIS GLU ASN LEU TYR PHE GLN GLY ARG ALA VAL GLU GLY ALA VAL LYS THR GLU PRO VAL ASP LEU

PHE LEU ASN SER ASN SER TYR ARG ILE PRO ALA LEU LYS THR LYS GLU GLY THR LEU ILE SER ILE ALA ARG HIS GLY ALA ASP PRO ASN ASN ASP ILE THR ALA VAL ARG ARG SER GLU ASP GLY GLY LYS THR TRP ASP GLU GLN ILE ILE MET

ASP TYR PRO LYS SER VAL ILE ASP THR THR LEU ILE ILE GLN ASP GLU GLU THR GLY ARG ILE PHE LEU LEU VAL THR HIS PHE PRO SER LYS TYR PHE TRP ASN ALA GLY LEU GLY SER PHE LYS ASN ILE GLY SER GLU LEU TYR LEU CYS LEU TYR ASP SER SER GLY

LYS GLU PHE THR VAL ARG GLU ASN VAL TYR ASP ASP SER LYS THR ASN ASN LYS THR GLU THR TYR THR THR ASN ALA LEU GLY ASP ASP LEU PHE LYS ASN GLY THR ILE ASP ILE ASN SER SER ALA PRO LEU LYS ALA GLY THR TYR ILE LEU VAL SER ASP ASP

ASP GLY LYS TRP SER GLU PRO GLN ILE ASN PHE GLN LYS LYS ASP TRP MET LYS PHE LEU GLY ILE ILE ALA PRO GLY ARG GLY ILE GLN LYS LYS ASN GLU HIS LYS ARG ILE VAL VAL PRO VAL TYR THR ASN GLU LYS GLY LYS SER ALA VAL ILE

TYR SER ASP ASP SER GLY ASN TRP THR TYR THR ILE GLY SER GLU PRO ASP ASN ASP ARG LYS LEU GLU ASN ALA LEU GLY ILE ILE PRO LEU GLU MET PRO ASN GLY GLU LEU ARG SER ASP ASP SER ARG GLY VAL TYR SER ASN VAL VAL THR PRO GLN LEU LEU PHE MET ARG ASN LEU SER

GLY TYR LEU ILE ALA THR SER PHE GLY ALA GLY THR TRP GLU THR ASP GLY VAL ILE LEU GLU PRO TYR CYS GLU LEU VAL ILE ASN SER LYS ASP ASP SER ALA VAL LYS LEU PHE SER VAL ASN PRO ASN ALA ARG SER ARG ASN GLY

THR VAL ARG ILE GLY LEU ILE ASN GLN VAL GLY THR TYR GLU ASN ALA ASN LYS GLY SER ALA GLY SER ALA VAL GLU THR VAL ARG GLY LEU LEU GLY TYR GLU GLY THR PRO SER GLU GLU MET

SER TYR ILE GLU MET ASN LEU LYS TYR LEU GLU SER GLY ALA ASN LYS GLY SER ALA GLY SER G2 T10 I14 F17 I18 I19 G23 N24 S25 F26 I27 V30 N31 S42 D45 L51 A52 R55 I56 S57 L58 V59 I62 L75 T78 E79 K80

M81 F82 R83 M84 L85 T86 I92 N93 H94 F95 W98 L99 A100 T101 T105 L109 F114 F119 K123 W124 R125 V126 K127 K128 V129 V130 L131 V132 L133 L134 L135 V136 T137 S138 V139 F140 L141 N144 I148 I152 G158 TYR ARG ARG ASN LYS THR CYS SER

SER ASP SER ASN F172 S176 I179 I187 F188 I189 P190 K210 K211 M212 K217 ILE SER GLY ASP ALA SER T224 V230 V233 I234 S250 S254 I257 E258 E259 N260 L261 M268 P273 S274 C278 V279 L280 I281 N284 L287 S291

V294 R299 TYR MET PHE LYS ASP GLY GLU PRO SER GLY HIS LYS GLU PHE ARG GLU GLY SER SER GLY SER GLY SER GLY SER GLY VAL PHE THR LEU GLU GLY ASP PHE VAL GLY ASP TRP GLU GLN THR ALA ALA TYR ASN LEU ASP GLN VAL LEU GLU

GLN GLY GLY VAL SER SER LEU LEU GLN ASN LEU ALA VAL SER VAL THR PRO ILE GLN ARG ILE VAL ARG SER GLY GLU ASN ALA LEU LYS ILE ASP ILE HIS VAL ILE ILE PRO TYR GLU GLY LEU SER ALA ASP GLN MET ALA GLN ILE GLU GLU VAL PHE LYS VAL VAL TYR PRO VAL

ASP ASP HIS PHE LYS ILE LEU PRO TYR GLY THR LEU VAL ILE ASP GLY VAL THR PRO ASN MET LEU ASN TYR PHE GLY ARG PRO TYR GLU GLY ILE ALA VAL PHE ASP GLY LYS LYS ILE THR VAL THR GLY THR LEU TRP ASN GLY ASN LYS ILE ILE ASP GLU ARG LEU ILE

THR PRO ASP GLY SER MET LEU PHE ARG VAL THR ILE ASN SER

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	224762	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (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: FLF

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	0.32	0/2002	0.53	0/2694
2	B	0.30	0/2663	0.57	0/3610
3	C	0.25	0/442	0.46	0/597
4	N	0.30	0/1001	0.52	0/1355
5	R	0.27	0/2312	0.48	1/3131 (0.0%)
All	All	0.30	0/8420	0.53	1/11387 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	R	257	LEU	CA-CB-CG	6.94	131.27	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1964	0	1935	52	0
2	B	2616	0	2518	79	0
3	C	436	0	448	11	0
4	N	981	0	947	23	0
5	R	2256	0	2396	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	R	20	0	9	0	0
All	All	8273	0	8253	211	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 13.

All (211) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ARG:NH1	2:B:186:ASP:OD1	2.10	0.84
2:B:45:MET:HG2	2:B:341:GLY:HA2	1.60	0.82
2:B:153:ASP:OD1	2:B:154:ASP:N	2.16	0.78
5:R:144:ASN:O	5:R:148:ILE:HG12	1.84	0.78
2:B:295:ASN:HB3	2:B:304:ARG:HD3	1.65	0.78
5:R:210:LYS:N	5:R:210:LYS:HD3	1.99	0.78
2:B:230:ASN:ND2	2:B:273:ILE:O	2.19	0.74
5:R:257:LEU:HB2	5:R:261:LEU:HB2	1.72	0.70
1:A:96:ARG:NH2	1:A:127:ASP:OD1	2.24	0.69
4:N:52:ILE:HG13	4:N:59:ILE:HG22	1.73	0.68
2:B:162:GLY:O	2:B:186:ASP:OD1	2.13	0.66
5:R:281:ILE:HD12	5:R:287:LEU:HD23	1.77	0.66
5:R:26:PHE:HE1	5:R:281:ILE:HD11	1.60	0.66
5:R:114:PHE:HB2	5:R:119:PHE:HD2	1.60	0.65
2:B:170:ASP:HB3	2:B:173:THR:HB	1.77	0.65
5:R:284:ASN:HB3	5:R:287:LEU:HB2	1.79	0.65
2:B:96:ARG:HG2	2:B:96:ARG:HH11	1.61	0.64
5:R:51:LEU:HD21	5:R:55:ARG:HH21	1.62	0.64
5:R:278:CYS:O	5:R:281:ILE:HG22	1.98	0.64
2:B:26:ALA:HB2	2:B:259:GLN:HE22	1.61	0.64
2:B:155:ASN:O	2:B:155:ASN:ND2	2.29	0.64
5:R:94:HIS:CD2	5:R:141:LEU:HB2	2.34	0.62
2:B:271:CYS:HB2	2:B:290:ASP:HB2	1.81	0.62
4:N:53:SER:OG	4:N:54:GLN:N	2.33	0.62
1:A:187:PRO:O	1:A:190:THR:OG1	2.16	0.62
5:R:257:LEU:CD1	5:R:258:GLU:H	2.13	0.61
5:R:250:SER:O	5:R:254:SER:N	2.35	0.60
2:B:30:LEU:HD22	2:B:261:LEU:HD12	1.83	0.60
2:B:340:ASN:OD1	3:C:59:ASN:ND2	2.36	0.59
4:N:48:TRP:O	4:N:62:THR:OG1	2.20	0.58
1:A:129:LYS:HG3	1:A:203:ILE:HD12	1.85	0.57
5:R:42:SER:N	5:R:45:ASP:OD2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:257:LEU:HA	5:R:260:ASN:HB3	1.85	0.57
5:R:26:PHE:CE1	5:R:281:ILE:HD11	2.40	0.57
1:A:94:ASP:N	1:A:94:ASP:OD1	2.33	0.56
2:B:16:ASN:OD1	2:B:19:ARG:NH2	2.38	0.56
2:B:123:ILE:HG13	2:B:171:ILE:HD12	1.87	0.56
1:A:135:ARG:HA	1:A:138:ARG:HH11	1.71	0.55
2:B:105:TYR:HE1	2:B:109:GLY:HA2	1.71	0.55
2:B:81:ILE:HD12	2:B:91:HIS:HB2	1.89	0.55
5:R:82:PHE:O	5:R:86:THR:HG22	2.06	0.54
1:A:137:LEU:HA	1:A:140:ILE:HD12	1.90	0.54
1:A:7:ASP:OD1	1:A:7:ASP:N	2.38	0.54
1:A:46:ASN:HB3	1:A:120:ARG:HH21	1.72	0.54
1:A:111:PHE:HZ	1:A:127:ASP:HB3	1.73	0.53
2:B:33:ILE:HG21	3:C:34:ALA:HB1	1.90	0.53
2:B:45:MET:SD	3:C:50:LEU:HD22	2.49	0.53
2:B:271:CYS:SG	2:B:291:ASP:HB3	2.48	0.53
5:R:136:VAL:O	5:R:139:VAL:HG12	2.08	0.53
4:N:34:LYS:HD3	4:N:106:ARG:HA	1.91	0.52
5:R:125:ARG:O	5:R:129:VAL:HG23	2.09	0.52
3:C:26:ASP:OD1	3:C:26:ASP:N	2.42	0.52
5:R:233:VAL:HG22	5:R:279:VAL:HG13	1.90	0.52
2:B:248:ALA:HB1	2:B:269:ILE:HG22	1.92	0.52
2:B:104:ALA:HB3	2:B:113:ALA:HB3	1.92	0.52
3:C:21:MET:N	3:C:21:MET:SD	2.82	0.52
5:R:52:ALA:O	5:R:56:ILE:HG22	2.10	0.52
5:R:56:ILE:HA	5:R:59:VAL:HG22	1.92	0.52
5:R:75:LEU:O	5:R:78:THR:HG23	2.10	0.52
1:A:72:ILE:HG22	1:A:74:GLU:HG2	1.91	0.52
1:A:98:LYS:HD2	2:B:188:MET:CE	2.40	0.52
1:A:45:ASP:OD1	1:A:45:ASP:N	2.38	0.51
2:B:286:LEU:HD22	2:B:327:VAL:HG21	1.92	0.51
5:R:133:LEU:O	5:R:137:THR:HG23	2.11	0.51
1:A:6:GLU:HG2	1:A:9:ARG:HH21	1.76	0.51
1:A:63:SER:OG	1:A:74:GLU:O	2.29	0.51
1:A:214:CYS:O	5:R:217:LYS:NZ	2.40	0.51
2:B:79:LEU:HD11	2:B:114:CYS:HB3	1.92	0.51
2:B:5:ASP:OD1	2:B:5:ASP:N	2.44	0.50
2:B:217:MET:SD	2:B:217:MET:N	2.84	0.50
2:B:331:SER:OG	2:B:332:TRP:N	2.45	0.50
5:R:58:LEU:O	5:R:62:ILE:HG12	2.11	0.50
5:R:83:ARG:HG3	5:R:152:ILE:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:VAL:O	1:A:238:ILE:HG12	2.11	0.50
2:B:173:THR:HG22	2:B:175:GLN:HG3	1.93	0.50
2:B:327:VAL:HG13	2:B:339:TRP:HB2	1.93	0.50
1:A:185:GLU:OE2	1:A:189:VAL:HG13	2.11	0.50
5:R:176:SER:HB3	5:R:261:LEU:HD21	1.93	0.50
1:A:72:ILE:HD11	1:A:89:VAL:HG22	1.94	0.50
2:B:225:HIS:NE2	2:B:249:THR:O	2.41	0.50
5:R:109:LEU:HD12	5:R:123:LYS:HA	1.93	0.50
2:B:231:ALA:O	2:B:244:GLY:N	2.43	0.49
2:B:280:LYS:NZ	2:B:322:ASP:O	2.44	0.49
1:A:236:ASP:OD1	1:A:240:LYS:NZ	2.33	0.49
5:R:24:ASN:ND2	5:R:55:ARG:HB3	2.28	0.49
5:R:19:ILE:HG13	5:R:274:SER:HB2	1.93	0.49
4:N:30:PHE:O	4:N:73:ARG:NH2	2.45	0.49
1:A:97:ARG:HG3	1:A:98:LYS:HG2	1.95	0.48
2:B:295:ASN:ND2	2:B:307:VAL:HG22	2.28	0.48
4:N:52:ILE:HD13	4:N:73:ARG:HB2	1.95	0.48
4:N:35:MET:HB3	4:N:80:LEU:HD22	1.94	0.48
1:A:144:LEU:HB3	1:A:216:PRO:HA	1.95	0.48
1:A:150:ASP:OD1	1:A:151:LEU:N	2.46	0.48
1:A:62:GLY:HA2	1:A:75:THR:OG1	2.14	0.48
2:B:121:CYS:HB3	2:B:139:LEU:HB2	1.95	0.48
5:R:55:ARG:HD3	5:R:273:PRO:HA	1.96	0.48
5:R:109:LEU:HD13	5:R:119:PHE:HE1	1.79	0.48
1:A:239:ILE:O	1:A:243:LEU:HD13	2.14	0.47
5:R:98:TRP:CE3	5:R:137:THR:HG21	2.48	0.47
1:A:199:GLU:HA	1:A:199:GLU:OE1	2.14	0.47
2:B:67:SER:HB2	2:B:321:THR:HB	1.96	0.47
1:A:136:TRP:CH2	2:B:314:ARG:HD2	2.49	0.47
1:A:173:TYR:OH	1:A:198:ASP:OD2	2.22	0.47
2:B:295:ASN:HD22	2:B:307:VAL:HG22	1.79	0.47
2:B:158:VAL:HG22	2:B:190:LEU:HD11	1.96	0.47
2:B:241:PHE:CE1	2:B:253:PHE:HB2	2.50	0.47
2:B:61:MET:HG3	2:B:317:CYS:HB2	1.97	0.47
2:B:86:THR:O	2:B:88:ASN:ND2	2.48	0.47
4:N:52:ILE:HD12	4:N:71:ILE:HG22	1.97	0.47
5:R:257:LEU:HD13	5:R:258:GLU:H	1.78	0.47
1:A:208:GLY:HA3	1:A:211:ARG:HH22	1.80	0.47
4:N:65:VAL:HG12	4:N:68:ARG:NH2	2.30	0.47
4:N:33:TYR:O	4:N:73:ARG:NH2	2.47	0.47
4:N:33:TYR:CG	4:N:99:ARG:HD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:176:SER:HA	5:R:179:ILE:HG22	1.97	0.47
4:N:84:MET:HB3	4:N:87:LEU:HD21	1.97	0.46
5:R:94:HIS:CE1	5:R:98:TRP:CD1	3.03	0.46
4:N:68:ARG:HD2	4:N:88:LYS:NZ	2.31	0.46
2:B:119:ASN:C	2:B:120:ILE:HD13	2.36	0.46
2:B:298:ASP:HB3	2:B:301:LYS:O	2.16	0.46
2:B:253:PHE:HE1	2:B:260:GLU:HG2	1.80	0.46
2:B:68:ARG:NH1	2:B:83:ASP:OD2	2.49	0.46
2:B:276:VAL:HG13	2:B:285:LEU:HD11	1.97	0.46
5:R:126:VAL:O	5:R:130:VAL:HG22	2.16	0.46
4:N:40:GLN:HE21	4:N:46:LEU:HG	1.81	0.45
1:A:5:THR:HG23	1:A:8:GLN:HB2	1.98	0.45
1:A:136:TRP:HH2	2:B:290:ASP:HB3	1.81	0.45
5:R:55:ARG:HH11	5:R:273:PRO:HA	1.81	0.45
4:N:68:ARG:HD2	4:N:88:LYS:HZ3	1.82	0.45
1:A:201:LEU:HD23	1:A:201:LEU:HA	1.81	0.45
4:N:19:LEU:HB3	4:N:84:MET:HB2	1.99	0.45
5:R:98:TRP:CD2	5:R:137:THR:HG21	2.52	0.45
1:A:115:SER:O	1:A:115:SER:OG	2.35	0.45
2:B:147:SER:OG	2:B:160:SER:OG	2.33	0.45
3:C:41:CYS:SG	3:C:42:GLU:N	2.90	0.45
5:R:80:LYS:HD2	5:R:80:LYS:HA	1.78	0.45
1:A:73:PHE:O	1:A:87:PHE:HA	2.17	0.45
5:R:55:ARG:NH2	5:R:100:ALA:HB2	2.32	0.45
5:R:105:THR:HG23	5:R:109:LEU:HD23	1.99	0.45
1:A:25:GLN:OE1	1:A:25:GLN:HA	2.17	0.44
2:B:294:CYS:HB3	2:B:308:LEU:HB2	1.99	0.44
2:B:311:HIS:CE1	2:B:337:LYS:HD3	2.53	0.44
4:N:62:THR:HG22	4:N:64:SER:H	1.82	0.44
5:R:291:SER:O	5:R:294:VAL:HG12	2.18	0.44
3:C:13:ARG:HH21	3:C:16:VAL:HG21	1.82	0.44
2:B:249:THR:HG22	2:B:265:SER:HB3	1.98	0.44
1:A:57:ARG:O	1:A:62:GLY:N	2.48	0.44
1:A:232:ASP:HB3	5:R:212:MET:HE3	2.00	0.44
5:R:230:VAL:O	5:R:234:ILE:HG13	2.18	0.44
2:B:166:CYS:SG	2:B:187:VAL:HG11	2.58	0.43
2:B:155:ASN:HD22	2:B:155:ASN:C	2.15	0.43
2:B:320:VAL:HG12	2:B:327:VAL:HB	2.01	0.43
5:R:127:LYS:O	5:R:131:LEU:HD22	2.19	0.43
1:A:33:TYR:HB2	2:B:55:LEU:HD21	2.00	0.43
2:B:149:CYS:O	2:B:150:ARG:NH1	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:PHE:HB3	2:B:211:TRP:CE3	2.53	0.43
1:A:71:GLY:HA3	1:A:91:GLY:N	2.33	0.43
1:A:98:LYS:HD2	2:B:188:MET:HE1	1.99	0.43
2:B:125:ASN:HB3	2:B:128:THR:HG23	2.00	0.43
2:B:315:VAL:HA	2:B:331:SER:HA	2.00	0.43
5:R:109:LEU:O	5:R:123:LYS:HG3	2.19	0.43
5:R:10:THR:O	5:R:14:ILE:HG12	2.19	0.43
1:A:109:ILE:HG13	1:A:140:ILE:HG21	2.00	0.43
2:B:204:CYS:HA	2:B:228:ASP:HB2	2.01	0.43
5:R:26:PHE:O	5:R:30:VAL:HG13	2.20	0.42
2:B:189:SER:HB3	2:B:232:ILE:HG22	2.00	0.42
2:B:278:PHE:HE1	2:B:299:ALA:HB2	1.85	0.42
2:B:315:VAL:HG12	2:B:331:SER:HB2	2.01	0.42
2:B:313:ASN:HB3	2:B:332:TRP:HB2	2.00	0.42
5:R:109:LEU:HD13	5:R:119:PHE:CE1	2.54	0.42
5:R:258:GLU:O	5:R:261:LEU:HB3	2.20	0.42
1:A:138:ARG:O	1:A:212:HIS:ND1	2.53	0.42
5:R:135:LEU:O	5:R:138:SER:HB2	2.19	0.42
2:B:96:ARG:HG2	2:B:96:ARG:NH1	2.32	0.42
5:R:92:ILE:HD12	5:R:92:ILE:HA	1.84	0.42
5:R:55:ARG:HH22	5:R:100:ALA:HB2	1.86	0.41
2:B:110:ASN:N	2:B:110:ASN:OD1	2.53	0.41
5:R:85:LEU:HD12	5:R:85:LEU:HA	1.80	0.41
5:R:187:ILE:O	5:R:190:PRO:HD2	2.19	0.41
2:B:25:CYS:SG	3:C:27:ARG:HB3	2.59	0.41
5:R:23:GLY:O	5:R:27:ILE:HG13	2.20	0.41
1:A:104:ASN:OD1	2:B:57:LYS:NZ	2.41	0.41
2:B:264:TYR:CE2	2:B:285:LEU:HD22	2.56	0.41
5:R:17:PHE:CD2	5:R:18:ILE:HD13	2.56	0.41
1:A:41:LEU:HD12	1:A:110:ILE:HB	2.03	0.41
1:A:104:ASN:HA	1:A:140:ILE:HD11	2.03	0.41
2:B:187:VAL:HA	2:B:203:ALA:HA	2.01	0.41
5:R:281:ILE:HD12	5:R:287:LEU:HB3	2.02	0.41
5:R:98:TRP:CZ3	5:R:101:THR:HG21	2.56	0.41
5:R:109:LEU:HB3	5:R:126:VAL:HG12	2.03	0.41
1:A:97:ARG:HH21	2:B:204:CYS:HB3	1.84	0.41
1:A:128:PHE:HE1	1:A:142:VAL:HG11	1.86	0.41
2:B:338:ILE:HG21	3:C:61:PHE:CE2	2.56	0.41
3:C:24:ASN:O	3:C:24:ASN:ND2	2.54	0.41
2:B:328:ALA:HB1	2:B:336:LEU:HD21	2.03	0.41
4:N:8:SER:HA	4:N:123:THR:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:52:ILE:HB	4:N:71:ILE:HG21	2.03	0.41
1:A:39:LEU:HD23	1:A:110:ILE:HD11	2.02	0.40
2:B:156:GLN:HB3	2:B:168:LEU:HD11	2.03	0.40
4:N:44:LYS:HE3	4:N:44:LYS:HB3	1.72	0.40
1:A:109:ILE:HB	1:A:142:VAL:HG22	2.02	0.40
2:B:163:ASP:OD1	2:B:165:THR:HB	2.20	0.40
3:C:29:LYS:HA	3:C:29:LYS:HD3	1.93	0.40
1:A:34:ARG:HD3	1:A:34:ARG:HA	1.95	0.40
1:A:121:LEU:HA	1:A:121:LEU:HD12	1.84	0.40
4:N:34:LYS:HB3	4:N:34:LYS:HE2	1.73	0.40
4:N:37:TRP:CZ3	4:N:95:TYR:HB3	2.57	0.40
4:N:126:THR:HG22	4:N:128:SER:H	1.85	0.40
2:B:340:ASN:HD22	2:B:341:GLY:N	2.19	0.40
2:B:340:ASN:ND2	2:B:341:GLY:N	2.70	0.40
1:A:75:THR:HG23	1:A:77:PHE:HE1	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	A	236/264 (89%)	229 (97%)	7 (3%)	0	100	100
2	B	339/366 (93%)	326 (96%)	13 (4%)	0	100	100
3	C	55/71 (78%)	55 (100%)	0	0	100	100
4	N	127/135 (94%)	122 (96%)	5 (4%)	0	100	100
5	R	273/990 (28%)	266 (97%)	7 (3%)	0	100	100
All	All	1030/1826 (56%)	998 (97%)	32 (3%)	0	100	100

There are no Ramachandran outliers to report.

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 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	A	213/233 (91%)	201 (94%)	12 (6%)	21	57
2	B	283/298 (95%)	270 (95%)	13 (5%)	27	63
3	C	46/58 (79%)	44 (96%)	2 (4%)	29	64
4	N	107/113 (95%)	102 (95%)	5 (5%)	26	62
5	R	253/864 (29%)	244 (96%)	9 (4%)	35	69
All	All	902/1566 (58%)	861 (96%)	41 (4%)	31	63

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	21	LYS
1	A	23	GLU
1	A	45	ASP
1	A	54	LYS
1	A	118	TYR
1	A	127	ASP
1	A	135	ARG
1	A	145	PHE
1	A	185	GLU
1	A	199	GLU
1	A	245	ASP
2	B	59	TYR
2	B	68	ARG
2	B	70	LEU
2	B	88	ASN
2	B	110	ASN
2	B	114	CYS
2	B	125	ASN
2	B	155	ASN
2	B	160	SER
2	B	188	MET
2	B	217	MET

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Mol	Chain	Res	Type
2	B	234	PHE
2	B	340	ASN
3	C	41	CYS
3	C	62	ARG
4	N	8	SER
4	N	22	SER
4	N	53	SER
4	N	100	CYS
4	N	109	PHE
5	R	31	ASN
5	R	81	MET
5	R	82	PHE
5	R	93	ASN
5	R	95	PHE
5	R	138	SER
5	R	188	PHE
5	R	257	LEU
5	R	268	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	259	GLN
2	B	295	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	$\#|Z| > 2$
6	FLF	R	501	-	21,21,21	0.54	0	30,30,30	0.73	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
6	FLF	R	501	-	-	0/14/14/14	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand FLF R 501
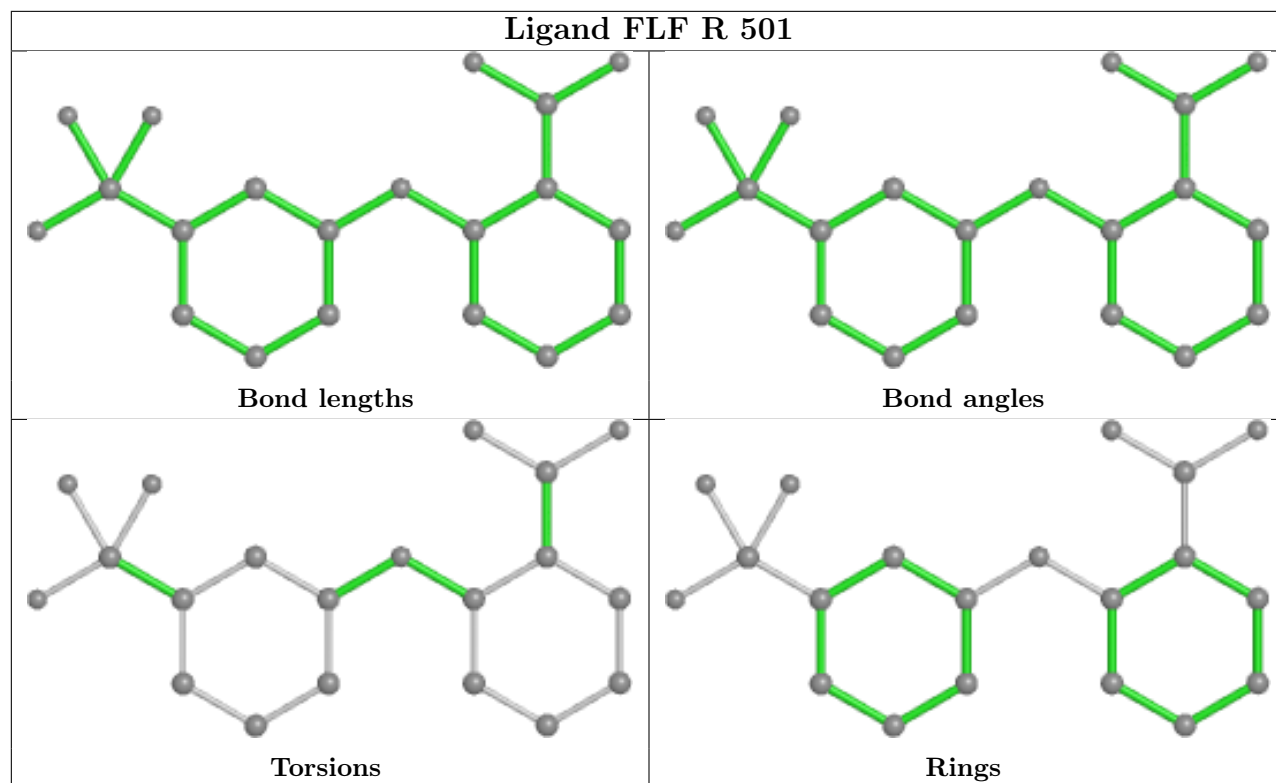
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.