



Full wwPDB EM Validation Report ⓘ

Jul 14, 2024 – 12:09 AM JST

PDB ID : 8XQS
EMDB ID : EMD-38587
Title : Structure of human class T GPCR TAS2R14-DNGi complex with Flufenamic acid.
Authors : Hu, X.L.; Wu, L.J.; Hua, T.; Liu, Z.J.
Deposited on : 2024-01-05
Resolution : 3.30 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

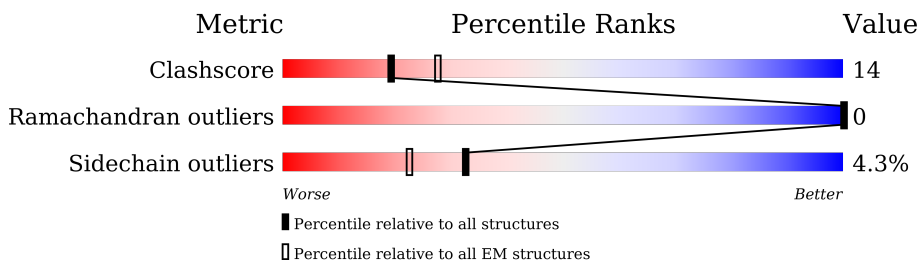
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	370	42% 18% . 39%
2	B	366	61% 29% . 8%
3	C	71	70% 8% 21%
4	S	286	54% 25% . 19%
5	R	990	18% 9% 73%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8867 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(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	225	1813	1151	300	348	14	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP P63096
A	-14	ASP	-	expression tag	UNP P63096
A	-13	TYR	-	expression tag	UNP P63096
A	-12	LYS	-	expression tag	UNP P63096
A	-11	ASP	-	expression tag	UNP P63096
A	-10	ASP	-	expression tag	UNP P63096
A	-9	ASP	-	expression tag	UNP P63096
A	-8	ASP	-	expression tag	UNP P63096
A	-7	LYS	-	expression tag	UNP P63096
A	-6	GLU	-	expression tag	UNP P63096
A	-5	ASN	-	expression tag	UNP P63096
A	-4	LEU	-	expression tag	UNP P63096
A	-3	TYR	-	expression tag	UNP P63096
A	-2	PHE	-	expression tag	UNP P63096
A	-1	GLN	-	expression tag	UNP P63096
A	0	SER	-	expression tag	UNP P63096
A	203	ALA	GLY	conflict	UNP P63096
A	326	SER	ALA	conflict	UNP P63096

- 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
			Total	C	N	O	S		
2	B	338	2600	1604	467	508	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
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
3	C	56	Total	C	N	O	S	0	0
			429	269	76	81	3		

- Molecule 4 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	232	Total	C	N	O	S	0	0
			1783	1131	295	347	10		

- 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	271	2194	1485	350	348	11	0	0

There are 50 discrepancies between the modelled and reference sequences:

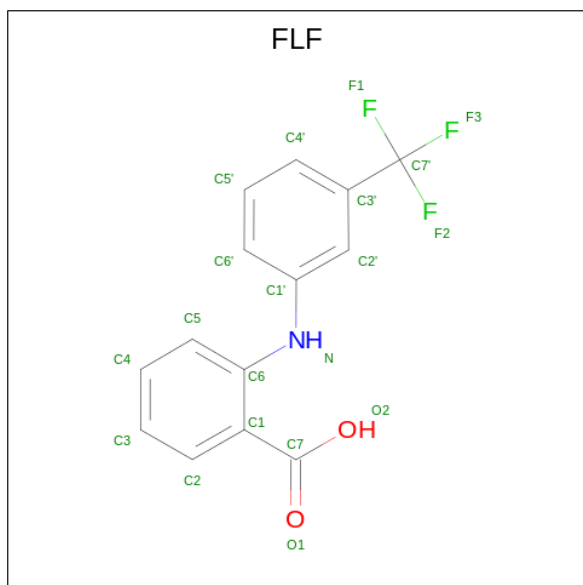
Chain	Residue	Modelled	Actual	Comment	Reference
R	-499	MET	-	initiating methionine	UNP Q59310
R	-498	LYS	-	expression tag	UNP Q59310
R	-497	THR	-	expression tag	UNP Q59310
R	-496	ILE	-	expression tag	UNP Q59310
R	-495	ILE	-	expression tag	UNP Q59310
R	-494	ALA	-	expression tag	UNP Q59310
R	-493	LEU	-	expression tag	UNP Q59310
R	-492	SER	-	expression tag	UNP Q59310
R	-491	TYR	-	expression tag	UNP Q59310
R	-490	ILE	-	expression tag	UNP Q59310
R	-489	PHE	-	expression tag	UNP Q59310
R	-488	CYS	-	expression tag	UNP Q59310
R	-487	LEU	-	expression tag	UNP Q59310
R	-486	VAL	-	expression tag	UNP Q59310
R	-485	PHE	-	expression tag	UNP Q59310
R	-484	ALA	-	expression tag	UNP Q59310
R	-483	ASP	-	expression tag	UNP Q59310
R	-482	TYR	-	expression tag	UNP Q59310
R	-481	LYS	-	expression tag	UNP Q59310
R	-480	ASP	-	expression tag	UNP Q59310
R	-479	ASP	-	expression tag	UNP Q59310
R	-478	ASP	-	expression tag	UNP Q59310
R	-477	ASP	-	expression tag	UNP Q59310
R	-476	ALA	-	expression tag	UNP Q59310
R	-475	HIS	-	expression tag	UNP Q59310
R	-474	HIS	-	expression tag	UNP Q59310
R	-473	HIS	-	expression tag	UNP Q59310
R	-472	HIS	-	expression tag	UNP Q59310
R	-471	HIS	-	expression tag	UNP Q59310
R	-470	HIS	-	expression tag	UNP Q59310
R	-469	HIS	-	expression tag	UNP Q59310
R	-468	HIS	-	expression tag	UNP Q59310
R	-467	HIS	-	expression tag	UNP Q59310
R	-466	HIS	-	expression tag	UNP Q59310
R	-465	GLU	-	expression tag	UNP Q59310
R	-464	ASN	-	expression tag	UNP Q59310
R	-463	LEU	-	expression tag	UNP Q59310

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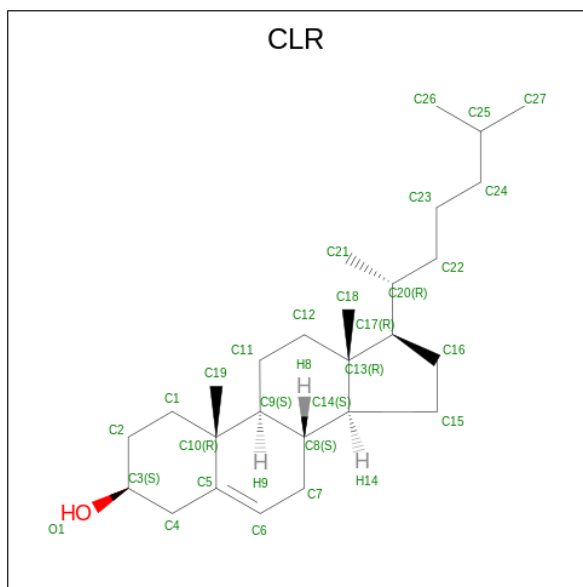
Chain	Residue	Modelled	Actual	Comment	Reference
R	-462	TYR	-	expression tag	UNP Q59310
R	-461	PHE	-	expression tag	UNP Q59310
R	-460	GLN	-	expression tag	UNP Q59310
R	-459	SER	-	expression tag	UNP Q59310
R	-458	GLY	-	expression tag	UNP Q59310
R	-457	ARG	-	expression tag	UNP Q59310
R	-456	ALA	-	expression tag	UNP Q59310
R	-305	SER	GLY	conflict	UNP Q59310
R	-3	GLY	-	linker	UNP Q59310
R	-2	SER	-	linker	UNP Q59310
R	-1	ALA	-	linker	UNP Q59310
R	0	GLY	-	linker	UNP Q59310
R	1	SER	-	linker	UNP Q59310

- Molecule 6 is 2-[[3-(TRIFLUOROMETHYL)PHENYL]AMINO] BENZOIC ACID (three-letter code: FLF) (formula: C₁₄H₁₀F₃NO₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	F	N	O	
6	R	1	20	14	3	1	2	0

- Molecule 7 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
7	R	1	Total	C	O	0
			28	27	1	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	400545	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.29	0/1843	0.48	0/2473
2	B	0.29	0/2647	0.56	1/3589 (0.0%)
3	C	0.25	0/435	0.45	0/587
4	S	0.30	0/1827	0.52	0/2477
5	R	0.28	0/2249	0.47	0/3048
All	All	0.29	0/9001	0.51	1/12174 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	258	ASP	CB-CG-OD1	5.53	123.28	118.30

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	A	1813	0	1799	46	0
2	B	2600	0	2505	76	0
3	C	429	0	441	5	0
4	S	1783	0	1717	55	0
5	R	2194	0	2326	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	R	20	0	9	2	0
7	R	28	0	46	9	0
All	All	8867	0	8843	250	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 14.

All (250) 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)
4:S:142:SER:HA	4:S:204:ILE:O	1.71	0.91
1:A:337:ASP:HB3	5:R:212:MET:SD	2.24	0.77
5:R:180:VAL:HG23	7:R:502:CLR:H213	1.68	0.74
1:A:47:SER:O	1:A:50:VAL:HB	1.88	0.73
5:R:258:GLU:HA	5:R:261:LEU:HG	1.71	0.72
1:A:33:GLU:HG2	1:A:195:HIS:HB3	1.71	0.72
1:A:34:VAL:HG21	1:A:339:VAL:HG11	1.71	0.72
2:B:331:SER:OG	2:B:333:ASP:OD1	2.08	0.71
5:R:187:ILE:HG21	7:R:502:CLR:H263	1.72	0.71
1:A:52:GLN:OE1	1:A:331:ASN:ND2	2.25	0.70
2:B:160:SER:HB3	2:B:190:LEU:HD23	1.75	0.69
1:A:335:VAL:O	1:A:339:VAL:HG23	1.92	0.68
5:R:253:THR:HG22	5:R:254:SER:H	1.59	0.68
5:R:257:LEU:HD23	5:R:260:ASN:HD22	1.57	0.68
4:S:40:ALA:HB3	4:S:43:LYS:HB2	1.73	0.68
5:R:109:LEU:HD12	5:R:129:VAL:HG11	1.75	0.67
4:S:68:PHE:CE1	4:S:83:MET:HG3	2.29	0.67
2:B:269:ILE:HG21	2:B:289:TYR:HD2	1.58	0.67
2:B:283:ARG:NH1	2:B:298:ASP:OD1	2.28	0.66
5:R:34:ASP:HA	5:R:39:ARG:HD3	1.77	0.66
4:S:153:LEU:HA	4:S:221:LEU:HD11	1.78	0.66
1:A:186:GLU:N	1:A:186:GLU:OE1	2.29	0.65
4:S:67:ARG:NH1	4:S:87:ARG:HE	1.94	0.64
2:B:191:SER:HB2	2:B:232:ILE:HG23	1.79	0.64
5:R:260:ASN:HA	5:R:263:ILE:HD12	1.78	0.64
2:B:271:CYS:HB2	2:B:290:ASP:HB3	1.78	0.63
2:B:286:LEU:HG	2:B:296:VAL:HG13	1.80	0.63
2:B:281:SER:HB3	3:C:48:ASP:HB2	1.79	0.63
2:B:93:ILE:HG12	2:B:133:VAL:HG21	1.80	0.63
2:B:251:ARG:NH1	2:B:260:GLU:OE1	2.32	0.63
4:S:6:GLU:HA	4:S:22:CYS:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:130:GLN:NE2	4:S:217:CYS:SG	2.72	0.63
2:B:320:VAL:HG22	2:B:327:VAL:HG22	1.81	0.63
5:R:72:PHE:HE1	5:R:74:ALA:HB3	1.62	0.62
5:R:277:SER:O	5:R:281:ILE:HG13	1.99	0.62
2:B:237:ASN:ND2	2:B:239:ASN:OD1	2.33	0.62
5:R:80:LYS:O	5:R:84:MET:HG2	2.00	0.61
5:R:2:GLY:HA2	5:R:257:LEU:HD21	1.82	0.61
5:R:62:ILE:HD11	5:R:89:TRP:HE1	1.66	0.61
2:B:43:ILE:HD12	2:B:284:LEU:HD21	1.83	0.60
1:A:8:GLU:OE2	4:S:163:TYR:OH	2.12	0.59
5:R:108:PHE:HD1	5:R:201:LEU:HB2	1.68	0.59
5:R:72:PHE:HD1	5:R:75:LEU:H	1.52	0.58
1:A:34:VAL:HG13	1:A:196:PHE:HA	1.85	0.58
5:R:151:HIS:HB2	5:R:175:PHE:HE1	1.69	0.58
2:B:51:LEU:HB2	2:B:336:LEU:HB2	1.85	0.57
4:S:38:ARG:HH21	4:S:48:VAL:HG22	1.69	0.57
4:S:219:GLN:HE22	4:S:222:GLU:H	1.53	0.57
2:B:58:ILE:O	2:B:316:SER:OG	2.17	0.56
2:B:18:ILE:HD11	3:C:23:ALA:HA	1.88	0.56
5:R:89:TRP:CH2	7:R:502:CLR:H20	2.41	0.56
2:B:117:LEU:HD23	2:B:145:TYR:HB3	1.88	0.56
4:S:51:ILE:HD11	4:S:79:LEU:HD13	1.87	0.56
2:B:200:VAL:HG12	2:B:234:PHE:CE2	2.41	0.55
2:B:235:PHE:HD2	2:B:237:ASN:H	1.54	0.55
1:A:227:LEU:HB3	1:A:274:PHE:CD1	2.41	0.55
2:B:304:ARG:HG3	2:B:304:ARG:HH11	1.72	0.55
5:R:13:LEU:HB2	5:R:267:VAL:HG12	1.89	0.55
1:A:35:LYS:HB3	1:A:199:PHE:HE2	1.70	0.55
2:B:264:TYR:CE2	2:B:285:LEU:HD13	2.42	0.54
5:R:72:PHE:CE1	5:R:74:ALA:HB3	2.42	0.54
2:B:121:CYS:HB3	2:B:139:LEU:HB2	1.90	0.53
1:A:211:TRP:CE3	1:A:215:PHE:HE1	2.27	0.53
4:S:29:PHE:O	4:S:72:ARG:NH2	2.42	0.53
1:A:36:LEU:HD13	1:A:222:ILE:HD11	1.90	0.53
1:A:208:ARG:NH2	1:A:252:SER:OG	2.42	0.53
1:A:15:ARG:HH21	2:B:91:HIS:HB3	1.72	0.53
1:A:344:ILE:HD12	5:R:208:HIS:CD2	2.44	0.53
5:R:35:TRP:HA	5:R:41:ILE:HD11	1.91	0.53
1:A:224:CYS:SG	1:A:269:ASN:ND2	2.83	0.52
2:B:43:ILE:HG22	2:B:45:MET:HG3	1.92	0.52
4:S:219:GLN:NE2	4:S:222:GLU:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:176:SER:HA	5:R:179:ILE:HG22	1.92	0.52
2:B:72:SER:HB3	2:B:82:TRP:HE1	1.75	0.52
4:S:137:VAL:HB	4:S:207:LEU:HD13	1.90	0.52
5:R:65:SER:HB2	7:R:502:CLR:H6	1.91	0.52
5:R:269:GLY:HA2	7:R:502:CLR:H262	1.92	0.52
2:B:264:TYR:HE2	2:B:285:LEU:HD13	1.75	0.52
2:B:311:HIS:NE2	2:B:329:THR:O	2.42	0.52
4:S:7:SER:N	4:S:21:SER:O	2.43	0.52
5:R:74:ALA:O	5:R:78:THR:HG23	2.10	0.51
5:R:187:ILE:O	5:R:190:PRO:HD2	2.10	0.51
2:B:79:LEU:HD11	2:B:114:CYS:HB3	1.92	0.51
4:S:175:LEU:HD22	4:S:184:ALA:HB2	1.93	0.51
1:A:41:ALA:HB2	1:A:249:LEU:HD23	1.91	0.51
4:S:125:ASP:OD1	4:S:125:ASP:N	2.42	0.51
4:S:219:GLN:HE22	4:S:222:GLU:HG2	1.76	0.51
5:R:94:HIS:CE1	5:R:141:LEU:HB2	2.46	0.51
4:S:128:MET:SD	4:S:219:GLN:HB3	2.51	0.50
2:B:129:ARG:NH1	4:S:109:ASP:OD2	2.44	0.50
2:B:205:ASP:OD1	2:B:205:ASP:N	2.37	0.50
5:R:73:PRO:HD2	5:R:74:ALA:H	1.76	0.50
4:S:73:ASP:HB2	4:S:80:PHE:HE2	1.75	0.50
5:R:189:ILE:O	5:R:192:THR:OG1	2.25	0.49
5:R:144:ASN:O	5:R:148:ILE:HG12	2.11	0.49
5:R:149:ASN:O	5:R:152:ILE:HG22	2.11	0.49
4:S:17:SER:HA	4:S:83:MET:O	2.12	0.49
5:R:149:ASN:HA	5:R:152:ILE:HG22	1.93	0.49
4:S:51:ILE:HD12	4:S:72:ARG:HD2	1.94	0.49
5:R:51:LEU:HD13	5:R:99:LEU:HB3	1.92	0.49
5:R:233:VAL:HG22	5:R:279:VAL:HG13	1.94	0.49
2:B:149:CYS:HB2	2:B:157:ILE:HD11	1.94	0.49
4:S:9:GLY:H	4:S:18:ARG:NH2	2.11	0.49
5:R:240:TYR:CE1	5:R:272:TYR:HB2	2.47	0.48
5:R:120:LEU:O	5:R:124:TRP:NE1	2.46	0.48
1:A:251:ASP:HB2	1:A:310:LEU:HD12	1.95	0.48
1:A:196:PHE:HE2	1:A:339:VAL:HG21	1.78	0.48
1:A:219:THR:HG21	1:A:339:VAL:HG13	1.95	0.48
2:B:168:LEU:HD22	2:B:213:VAL:HG13	1.96	0.48
4:S:219:GLN:NE2	4:S:222:GLU:HG2	2.27	0.48
5:R:82:PHE:CD1	7:R:502:CLR:H22	2.49	0.48
2:B:81:ILE:HD12	2:B:91:HIS:CD2	2.48	0.48
2:B:316:SER:HB3	2:B:332:TRP:HE1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:6:GLU:HG3	4:S:22:CYS:HB2	1.96	0.47
4:S:48:VAL:HG13	4:S:64:VAL:HG21	1.96	0.47
5:R:89:TRP:CZ2	7:R:502:CLR:H20	2.49	0.47
2:B:52:ARG:HE	2:B:335:PHE:HE2	1.62	0.47
5:R:98:TRP:CZ2	5:R:190:PRO:HG3	2.48	0.47
5:R:255:GLU:HB3	5:R:261:LEU:HD11	1.95	0.47
2:B:34:THR:HG21	2:B:300:LEU:HB3	1.97	0.47
4:S:162:LEU:HD21	4:S:164:TRP:NE1	2.29	0.47
1:A:9:ASP:O	1:A:13:VAL:HG23	2.14	0.47
2:B:147:SER:OG	2:B:160:SER:OG	2.33	0.47
1:A:230:TYR:OH	1:A:277:LYS:HG2	2.14	0.47
1:A:250:PHE:HE1	1:A:264:ILE:HG21	1.79	0.47
2:B:68:ARG:HG3	2:B:85:TYR:CD1	2.49	0.47
5:R:16:GLU:OE2	5:R:270:MET:HG3	2.15	0.47
4:S:67:ARG:HD2	4:S:87:ARG:HH21	1.80	0.47
4:S:51:ILE:HG22	4:S:58:ILE:HG12	1.96	0.47
5:R:147:LEU:O	5:R:151:HIS:ND1	2.48	0.47
1:A:348:LEU:HD22	1:A:353:LEU:HD22	1.97	0.47
4:S:223:TYR:N	4:S:224:PRO:HD2	2.30	0.46
2:B:75:GLN:O	2:B:98:SER:OG	2.32	0.46
2:B:315:VAL:HA	2:B:331:SER:HA	1.97	0.46
4:S:165:PHE:HE1	4:S:218:MET:HB2	1.80	0.46
2:B:269:ILE:HG21	2:B:289:TYR:CD2	2.43	0.46
2:B:72:SER:HB2	2:B:336:LEU:HD11	1.98	0.46
4:S:37:VAL:HG22	4:S:95:TYR:HB2	1.98	0.46
1:A:49:ILE:HA	1:A:52:GLN:HG3	1.98	0.46
4:S:6:GLU:OE1	4:S:6:GLU:N	2.49	0.46
2:B:333:ASP:OD1	2:B:333:ASP:N	2.43	0.45
4:S:2:VAL:HG22	4:S:27:PHE:HB3	1.97	0.45
2:B:207:SER:HB2	2:B:223:THR:HG22	1.97	0.45
2:B:185:GLY:HA3	2:B:204:CYS:HB3	1.98	0.45
2:B:242:ALA:HB2	2:B:278:PHE:HE1	1.81	0.45
4:S:67:ARG:NH2	4:S:90:ASP:OD2	2.49	0.45
5:R:82:PHE:HZ	5:R:175:PHE:HE2	1.64	0.45
2:B:152:LEU:HD23	2:B:192:LEU:HD13	1.98	0.45
5:R:295:LEU:HD23	5:R:298:LEU:HD12	1.99	0.45
4:S:32:PHE:HD2	4:S:98:ARG:HB2	1.82	0.45
1:A:227:LEU:HD11	1:A:268:LEU:HD23	1.99	0.45
3:C:52:THR:O	3:C:52:THR:OG1	2.35	0.45
5:R:16:GLU:HA	5:R:19:ILE:HG22	1.98	0.45
1:A:187:THR:OG1	1:A:198:MET:HB3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:147:LEU:O	5:R:151:HIS:CE1	2.71	0.44
1:A:27:GLY:HA3	2:B:55:LEU:HD13	2.00	0.44
1:A:34:VAL:HG21	1:A:339:VAL:CG1	2.45	0.44
1:A:284:THR:HG23	1:A:288:PRO:HA	1.98	0.44
2:B:225:HIS:CE1	2:B:251:ARG:HD2	2.53	0.44
5:R:62:ILE:HD11	5:R:89:TRP:NE1	2.30	0.44
5:R:268:MET:HE3	7:R:502:CLR:H232	1.99	0.44
2:B:275:SER:HB2	2:B:318:LEU:HB3	1.99	0.44
5:R:265:SER:OG	7:R:502:CLR:H17	2.17	0.44
5:R:259:GLU:OE2	5:R:260:ASN:ND2	2.51	0.44
2:B:304:ARG:HG3	2:B:304:ARG:NH1	2.31	0.44
4:S:144:SER:HG	4:S:201:THR:HG1	1.61	0.44
5:R:240:TYR:CZ	5:R:272:TYR:HB2	2.52	0.44
4:S:144:SER:HA	4:S:202:LEU:O	2.17	0.44
5:R:127:LYS:HA	5:R:127:LYS:HD3	1.72	0.44
1:A:14:GLU:OE2	4:S:52:SER:OG	2.22	0.44
4:S:43:LYS:HE2	4:S:43:LYS:HA	2.00	0.43
5:R:82:PHE:HZ	5:R:175:PHE:CE2	2.36	0.43
5:R:143:LEU:HD12	5:R:147:LEU:HD23	1.99	0.43
5:R:68:VAL:O	5:R:76:PHE:HB2	2.18	0.43
1:A:209:LYS:HG3	1:A:210:LYS:HG2	2.00	0.43
4:S:163:TYR:HB2	4:S:218:MET:HB3	2.00	0.43
1:A:54:LYS:NZ	1:A:188:HIS:O	2.52	0.43
5:R:82:PHE:CZ	5:R:175:PHE:HE2	2.36	0.43
6:R:501:FLF:H2'	6:R:501:FLF:H5	2.01	0.43
2:B:323:ASP:OD1	2:B:323:ASP:N	2.51	0.43
1:A:208:ARG:HA	1:A:211:TRP:NE1	2.34	0.43
2:B:78:LYS:NZ	2:B:94:PRO:HB3	2.33	0.43
2:B:230:ASN:ND2	2:B:246:ASP:OD1	2.43	0.43
5:R:186:PHE:O	5:R:190:PRO:HD3	2.19	0.43
5:R:263:ILE:O	5:R:267:VAL:HG13	2.17	0.43
1:A:201:VAL:HG22	1:A:201:VAL:O	2.19	0.43
2:B:311:HIS:NE2	2:B:329:THR:HG23	2.34	0.43
1:A:23:LEU:HD23	2:B:78:LYS:HD3	2.00	0.43
5:R:17:PHE:HD1	5:R:17:PHE:O	2.02	0.43
1:A:197:LYS:HE3	1:A:199:PHE:HZ	1.83	0.43
2:B:162:GLY:HA2	2:B:186:ASP:HB3	2.01	0.43
3:C:26:ASP:OD1	3:C:26:ASP:N	2.43	0.43
2:B:180:PHE:HE1	2:B:216:GLY:HA2	1.84	0.42
2:B:225:HIS:CD2	2:B:229:ILE:HD11	2.54	0.42
5:R:14:ILE:O	5:R:18:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:249:ILE:O	5:R:253:THR:OG1	2.23	0.42
4:S:126:ILE:HD13	4:S:151:LYS:HG2	2.00	0.42
4:S:211:ASP:O	4:S:215:TYR:OH	2.27	0.42
1:A:271:LYS:HD3	1:A:325:CYS:HB3	2.00	0.42
5:R:45:ASP:OD1	5:R:45:ASP:N	2.45	0.42
5:R:56:ILE:HA	5:R:59:VAL:HG22	2.02	0.42
1:A:230:TYR:O	1:A:286:CYS:HB2	2.18	0.42
2:B:283:ARG:HG2	3:C:41:CYS:HB3	2.01	0.42
4:S:47:TRP:HZ2	4:S:50:TYR:HB3	1.84	0.42
5:R:64:GLY:O	5:R:68:VAL:HG13	2.19	0.42
5:R:68:VAL:HG23	5:R:76:PHE:HD1	1.85	0.42
5:R:86:THR:O	5:R:90:THR:OG1	2.34	0.42
5:R:281:ILE:HG23	5:R:287:LEU:HB3	2.00	0.42
2:B:131:GLY:HA3	4:S:32:PHE:CE1	2.54	0.42
5:R:99:LEU:HD23	5:R:99:LEU:HA	1.72	0.42
5:R:189:ILE:HB	5:R:190:PRO:HD3	2.01	0.42
4:S:62:ASP:HA	4:S:65:LYS:HE2	2.01	0.42
5:R:126:VAL:HA	5:R:129:VAL:HG12	2.00	0.42
1:A:184:ILE:HD13	1:A:184:ILE:HA	1.88	0.42
2:B:63:TRP:HZ2	2:B:338:ILE:HD11	1.83	0.41
5:R:9:PHE:HD1	5:R:9:PHE:HA	1.77	0.41
1:A:46:LYS:HA	1:A:49:ILE:HG22	2.02	0.41
6:R:501:FLF:H5	6:R:501:FLF:C2'	2.50	0.41
4:S:34:MET:HB3	4:S:79:LEU:HD22	2.02	0.41
4:S:91:THR:OG1	4:S:118:THR:HA	2.20	0.41
5:R:51:LEU:HG	5:R:55:ARG:NH1	2.35	0.41
5:R:69:SER:HA	5:R:76:PHE:CG	2.55	0.41
5:R:98:TRP:CE2	5:R:190:PRO:HG3	2.55	0.41
5:R:172:PHE:O	5:R:176:SER:N	2.51	0.41
2:B:247:ASP:O	2:B:249:THR:HG23	2.21	0.41
4:S:29:PHE:HZ	4:S:72:ARG:HB2	1.86	0.41
4:S:39:GLN:HB3	4:S:93:MET:HB3	2.02	0.41
4:S:145:ILE:O	4:S:201:THR:HA	2.21	0.41
2:B:153:ASP:OD1	2:B:154:ASP:N	2.54	0.41
2:B:308:LEU:HG	2:B:339:TRP:CE3	2.56	0.41
2:B:338:ILE:HD13	2:B:338:ILE:HA	1.82	0.41
1:A:192:LYS:NZ	1:A:333:GLN:OE1	2.52	0.41
4:S:36:TRP:CZ3	4:S:94:TYR:HB3	2.56	0.41
2:B:200:VAL:HG21	2:B:241:PHE:CZ	2.55	0.40
2:B:45:MET:SD	2:B:308:LEU:HD11	2.62	0.40
2:B:60:ALA:HA	2:B:317:CYS:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:HIS:NE2	2:B:126:LEU:HD22	2.35	0.40
2:B:128:THR:OG1	2:B:132:ASN:O	2.34	0.40
2:B:189:SER:OG	2:B:232:ILE:HG22	2.21	0.40
2:B:277:SER:OG	2:B:278:PHE:N	2.54	0.40
4:S:145:ILE:HD13	4:S:231:THR:OG1	2.21	0.40
4:S:219:GLN:HE22	4:S:222:GLU:N	2.16	0.40
5:R:55:ARG:HH21	5:R:100:ALA:HB2	1.87	0.40
2:B:51:LEU:HD12	2:B:336:LEU:HD12	2.02	0.40
1:A:208:ARG:HA	1:A:211:TRP:CE2	2.57	0.40
1:A:210:LYS:HE3	1:A:210:LYS:HB3	1.85	0.40
1:A:214:CYS:HG	2:B:99:TRP:HE3	1.68	0.40
2:B:129:ARG:HA	2:B:129:ARG:HD2	1.79	0.40
5:R:84:MET:HG2	5:R:84:MET:H	1.69	0.40
5:R:114:PHE:HB2	5:R:119:PHE:CD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	221/370 (60%)	217 (98%)	4 (2%)	0	100	100
2	B	336/366 (92%)	321 (96%)	15 (4%)	0	100	100
3	C	54/71 (76%)	52 (96%)	2 (4%)	0	100	100
4	S	228/286 (80%)	215 (94%)	13 (6%)	0	100	100
5	R	265/990 (27%)	259 (98%)	6 (2%)	0	100	100
All	All	1104/2083 (53%)	1064 (96%)	40 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	201/322 (62%)	191 (95%)	10 (5%)	24	55
2	B	281/298 (94%)	268 (95%)	13 (5%)	27	58
3	C	45/58 (78%)	44 (98%)	1 (2%)	52	74
4	S	197/229 (86%)	187 (95%)	10 (5%)	24	54
5	R	247/864 (29%)	239 (97%)	8 (3%)	39	67
All	All	971/1771 (55%)	929 (96%)	42 (4%)	33	59

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	PHE
1	A	230	TYR
1	A	243	MET
1	A	246	SER
1	A	271	LYS
1	A	275	GLU
1	A	307	PHE
1	A	312	LYS
1	A	321	THR
1	A	323	PHE
2	B	46	ARG
2	B	52	ARG
2	B	61	MET
2	B	105	TYR
2	B	153	ASP
2	B	204	CYS
2	B	246	ASP
2	B	278	PHE
2	B	290	ASP
2	B	292	PHE
2	B	294	CYS
2	B	298	ASP
2	B	334	SER

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Mol	Chain	Res	Type
3	C	46	LYS
4	S	29	PHE
4	S	65	LYS
4	S	67	ARG
4	S	165	PHE
4	S	185	SER
4	S	192	SER
4	S	200	PHE
4	S	219	GLN
4	S	220	HIS
4	S	223	TYR
5	R	17	PHE
5	R	60	TRP
5	R	71	PHE
5	R	81	MET
5	R	82	PHE
5	R	121	TYR
5	R	151	HIS
5	R	299	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	ASN
1	A	269	ASN
1	A	331	ASN
2	B	266	HIS
5	R	260	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

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	FLF	R	501	-	21,21,21	0.54	0	30,30,30	0.74	0
7	CLR	R	502	-	31,31,31	0.48	0	48,48,48	0.80	2 (4%)

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
7	CLR	R	502	-	-	6/10/68/68	0/4/4/4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	502	CLR	C21-C20-C17	2.19	116.28	112.92
7	R	502	CLR	C13-C17-C20	2.04	122.67	119.49

There are no chirality outliers.

All (6) torsion outliers are listed below:

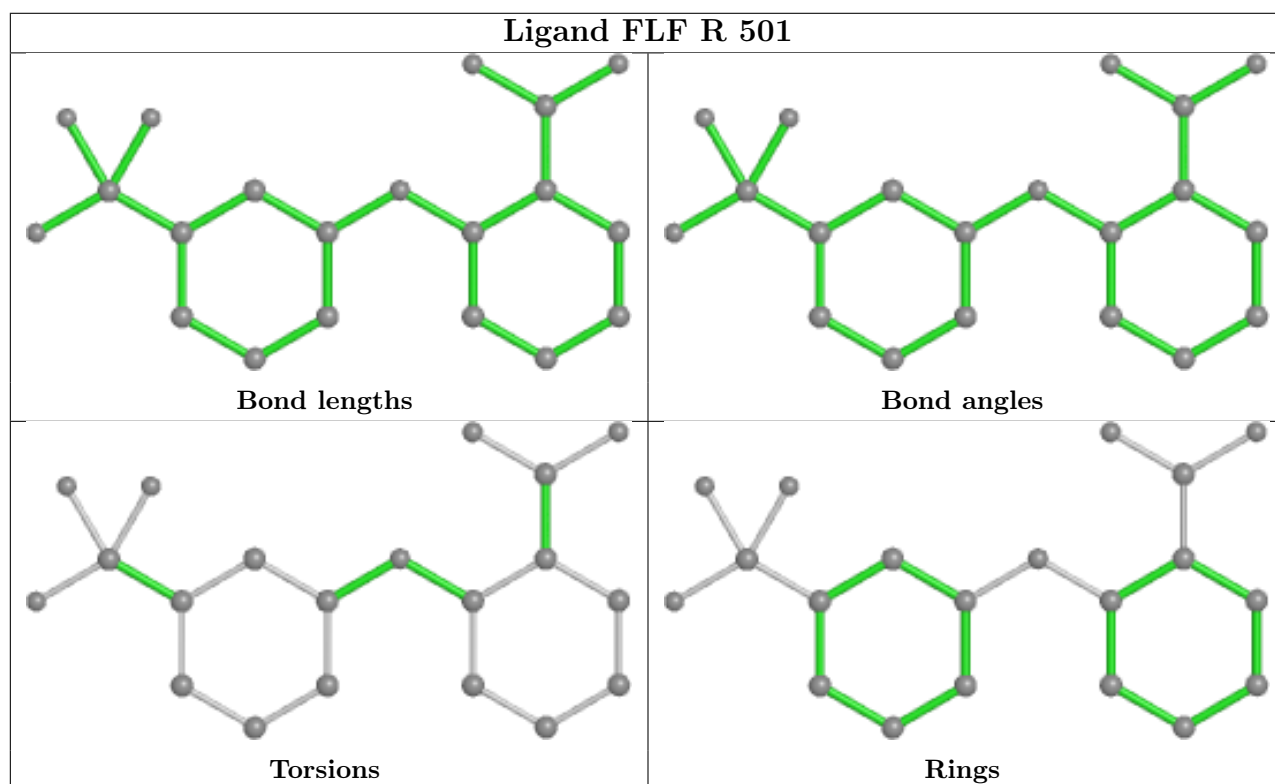
Mol	Chain	Res	Type	Atoms
7	R	502	CLR	C21-C20-C22-C23
7	R	502	CLR	C20-C22-C23-C24
7	R	502	CLR	C22-C23-C24-C25
7	R	502	CLR	C17-C20-C22-C23
7	R	502	CLR	C23-C24-C25-C26
7	R	502	CLR	C23-C24-C25-C27

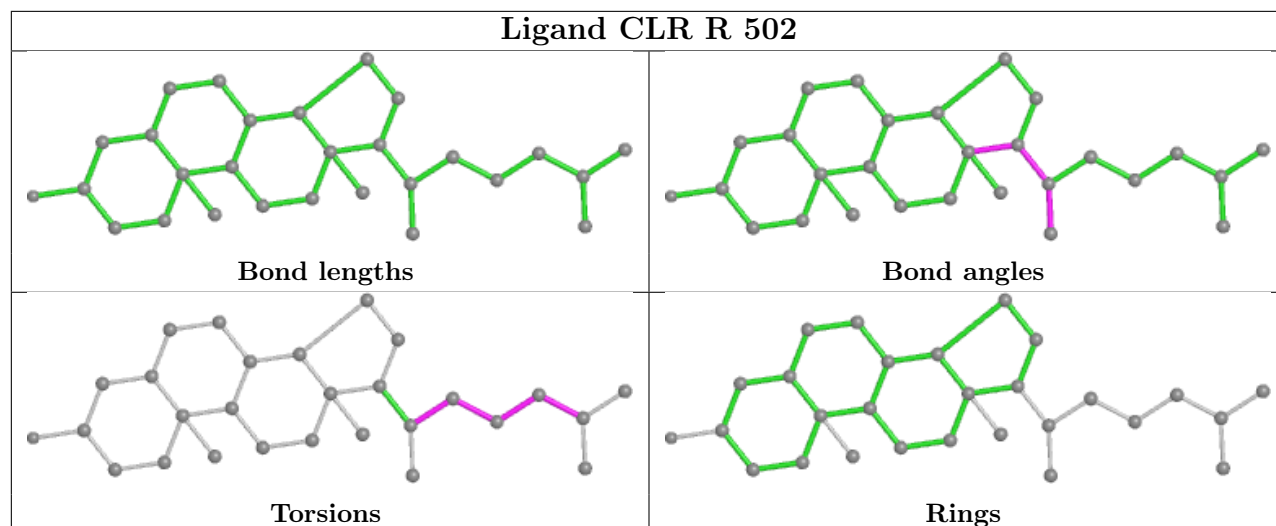
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	501	FLF	2	0
7	R	502	CLR	9	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.