Full wwPDB EM Validation Report ⓘ

Jan 7, 2024 – 01:17 AM JST

PDB ID	:	8HNK
EMDB ID	:	EMD-34914
Title	:	CXCR3-DNGi complex activated by CXCL11
Authors	:	Jiao, H.Z.; Hu, H.L.
Deposited on	:	2022-12-08
Resolution	:	3.01 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:

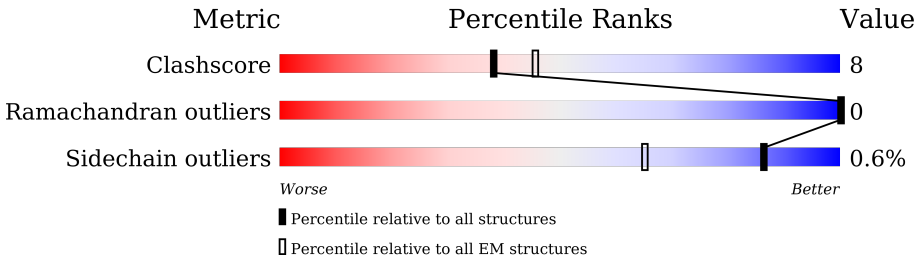
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.01 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	354	56% 5% 38%
2	B	384	73% 14% 12%
3	G	71	65% 11% 24%
4	R	657	35% 10% 55%
5	L	104	41% 26% • 30%
6	S	259	75% 15% 10%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 9492 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
1	A	218	Total	C	N	O	S	0	0
			1758	1118	294	333	13		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
2	B	336	Total	C	N	O	S	0	0
			2583	1593	465	504	21		

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	HIS	-	expression tag	UNP P62873
B	-19	HIS	-	expression tag	UNP P62873
B	-18	HIS	-	expression tag	UNP P62873
B	-17	HIS	-	expression tag	UNP P62873
B	-16	HIS	-	expression tag	UNP P62873
B	-15	HIS	-	expression tag	UNP P62873
B	-14	HIS	-	expression tag	UNP P62873
B	-13	HIS	-	expression tag	UNP P62873
B	-12	HIS	-	expression tag	UNP P62873
B	-11	HIS	-	expression tag	UNP P62873
B	-10	LEU	-	expression tag	UNP P62873
B	-9	GLU	-	expression tag	UNP P62873
B	-8	VAL	-	expression tag	UNP P62873
B	-7	LEU	-	expression tag	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	PHE	-	expression tag	UNP P62873
B	-5	GLN	-	expression tag	UNP P62873
B	-4	GLY	-	expression tag	UNP P62873
B	-3	PRO	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	GLY	-	expression tag	UNP P62873
B	341	GLY	-	expression tag	UNP P62873
B	342	ALA	-	expression tag	UNP P62873
B	343	SER	-	expression tag	UNP P62873
B	344	GLY	-	expression tag	UNP P62873
B	345	ALA	-	expression tag	UNP P62873
B	346	SER	-	expression tag	UNP P62873
B	347	GLY	-	expression tag	UNP P62873
B	348	ALA	-	expression tag	UNP P62873
B	349	SER	-	expression tag	UNP P62873
B	350	GLY	-	expression tag	UNP P62873
B	351	ALA	-	expression tag	UNP P62873
B	352	SER	-	expression tag	UNP P62873
B	353	VAL	-	expression tag	UNP P62873
B	354	SER	-	expression tag	UNP P62873
B	355	GLY	-	expression tag	UNP P62873
B	356	TRP	-	expression tag	UNP P62873
B	357	ARG	-	expression tag	UNP P62873
B	358	LEU	-	expression tag	UNP P62873
B	359	PHE	-	expression tag	UNP P62873
B	360	LYS	-	expression tag	UNP P62873
B	361	LYS	-	expression tag	UNP P62873
B	362	ILE	-	expression tag	UNP P62873
B	363	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	G	54	Total	C	N	O	S	0	0
			418	263	74	78	3		

- Molecule 4 is a protein called Soluble cytochrome b562,C-X-C chemokine receptor type 3,O plophorus-luciferin 2-monooxygenase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	297	Total	C	N	O	S	0	0
			2316	1523	400	376	17		

There are 65 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-137	MET	-	initiating methionine	UNP P0ABE7
R	-136	LYS	-	expression tag	UNP P0ABE7
R	-135	THR	-	expression tag	UNP P0ABE7
R	-134	ILE	-	expression tag	UNP P0ABE7
R	-133	ILE	-	expression tag	UNP P0ABE7
R	-132	ALA	-	expression tag	UNP P0ABE7
R	-131	LEU	-	expression tag	UNP P0ABE7
R	-130	SER	-	expression tag	UNP P0ABE7
R	-129	TYR	-	expression tag	UNP P0ABE7
R	-128	ILE	-	expression tag	UNP P0ABE7
R	-127	PHE	-	expression tag	UNP P0ABE7
R	-126	CYS	-	expression tag	UNP P0ABE7
R	-125	LEU	-	expression tag	UNP P0ABE7
R	-124	VAL	-	expression tag	UNP P0ABE7
R	-123	PHE	-	expression tag	UNP P0ABE7
R	-122	ALA	-	expression tag	UNP P0ABE7
R	-121	ASP	-	expression tag	UNP P0ABE7
R	-120	TYR	-	expression tag	UNP P0ABE7
R	-119	LYS	-	expression tag	UNP P0ABE7
R	-118	ASP	-	expression tag	UNP P0ABE7
R	-117	ASP	-	expression tag	UNP P0ABE7
R	-116	ASP	-	expression tag	UNP P0ABE7
R	-115	ASP	-	expression tag	UNP P0ABE7
R	-114	LYS	-	expression tag	UNP P0ABE7
R	-113	GLY	-	expression tag	UNP P0ABE7
R	-112	SER	-	expression tag	UNP P0ABE7
R	-105	TRP	MET	conflict	UNP P0ABE7
R	-10	ILE	HIS	conflict	UNP P0ABE7
R	-6	LEU	-	linker	UNP P0ABE7
R	-5	LEU	-	linker	UNP P0ABE7
R	-4	VAL	-	linker	UNP P0ABE7
R	-3	PRO	-	linker	UNP P0ABE7
R	-2	ARG	-	linker	UNP P0ABE7
R	-1	GLY	-	linker	UNP P0ABE7
R	0	SER	-	linker	UNP P0ABE7
R	362	VAL	THR	conflict	UNP Q9GV45
R	366	GLU	ALA	conflict	UNP Q9GV45

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Chain	Residue	Modelled	Actual	Comment	Reference
R	373	GLU	GLN	conflict	UNP Q9GV45
R	377	ALA	GLY	conflict	UNP Q9GV45
R	380	LEU	GLN	conflict	UNP Q9GV45
R	389	VAL	LEU	conflict	UNP Q9GV45
R	393	LEU	PHE	conflict	UNP Q9GV45
R	395	ASN	ALA	conflict	UNP Q9GV45
R	397	ALA	GLY	conflict	UNP Q9GV45
R	405	ARG	LYS	conflict	UNP Q9GV45
R	406	ILE	VAL	conflict	UNP Q9GV45
R	408	ARG	LEU	conflict	UNP Q9GV45
R	413	ALA	GLY	conflict	UNP Q9GV45
R	416	ILE	ALA	conflict	UNP Q9GV45
R	429	ALA	GLY	conflict	UNP Q9GV45
R	430	ASP	PHE	conflict	UNP Q9GV45
R	433	ALA	GLY	conflict	UNP Q9GV45
R	434	GLN	LEU	conflict	UNP Q9GV45
R	437	GLU	MET	conflict	UNP Q9GV45
R	438	VAL	ILE	conflict	UNP Q9GV45
R	452	VAL	ILE	conflict	UNP Q9GV45
R	455	PRO	HIS	conflict	UNP Q9GV45
R	469	LEU	ILE	conflict	UNP Q9GV45
R	470	ASN	ASP	conflict	UNP Q9GV45
R	477	GLU	PRO	conflict	UNP Q9GV45
R	486	LYS	GLN	conflict	UNP Q9GV45
R	500	ILE	TYR	conflict	UNP Q9GV45
R	506	THR	ASN	conflict	UNP Q9GV45
R	511	MET	LEU	conflict	UNP Q9GV45
R	519	SER	GLY	conflict	UNP Q9GV45

- Molecule 5 is a protein called C-X-C motif chemokine 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	L	73	578	368	107	97	6	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	74	HIS	-	expression tag	UNP O14625
L	75	HIS	-	expression tag	UNP O14625
L	76	HIS	-	expression tag	UNP O14625
L	77	HIS	-	expression tag	UNP O14625

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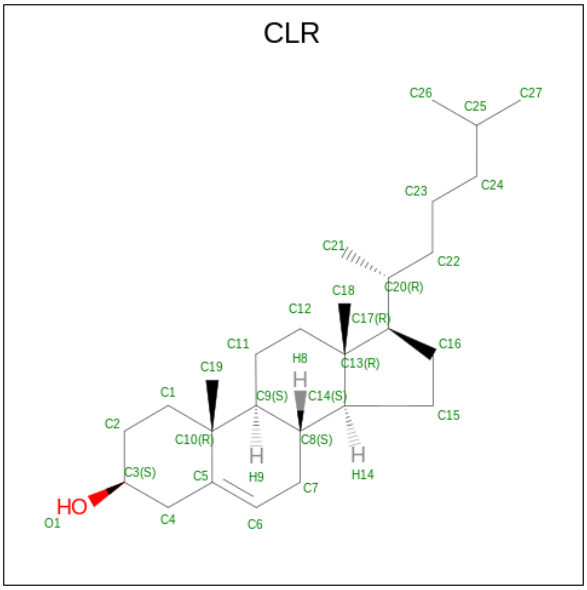
Chain	Residue	Modelled	Actual	Comment	Reference
L	78	HIS	-	expression tag	UNP O14625
L	79	HIS	-	expression tag	UNP O14625
L	80	HIS	-	expression tag	UNP O14625
L	81	HIS	-	expression tag	UNP O14625
L	82	HIS	-	expression tag	UNP O14625
L	83	HIS	-	expression tag	UNP O14625

- Molecule 6 is a protein called single-chain variable fragment scFv16.

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

- Molecule 7 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



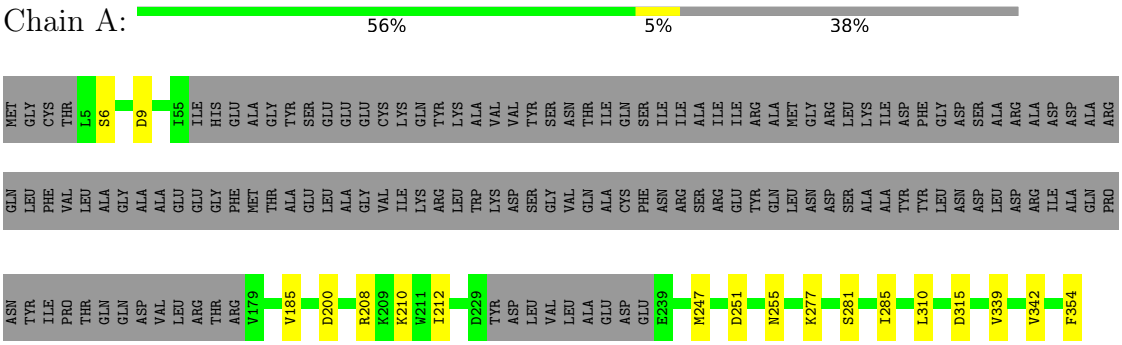
Mol	Chain	Residues	Atoms			AltConf
7	R	1	Total	C	O	0
			28	27	1	
7	R	1	Total	C	O	0
			28	27	1	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

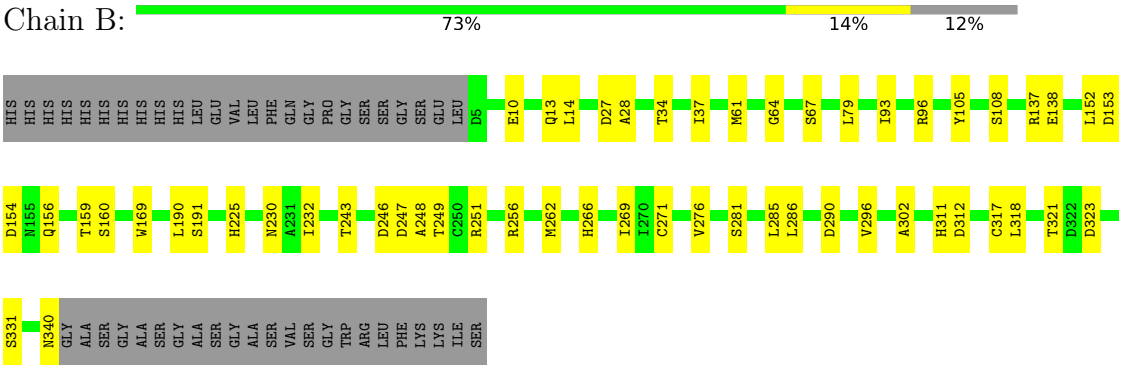
• Molecule 1: Guanine nucleotide-binding protein G(i) subunit alpha-1

Chain A:



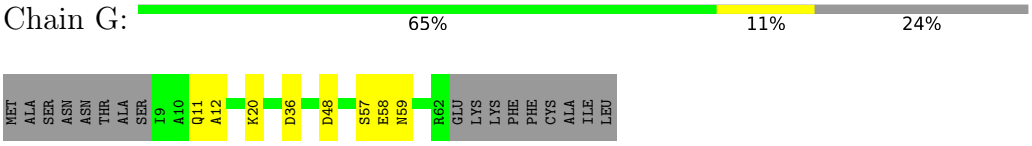
• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B:



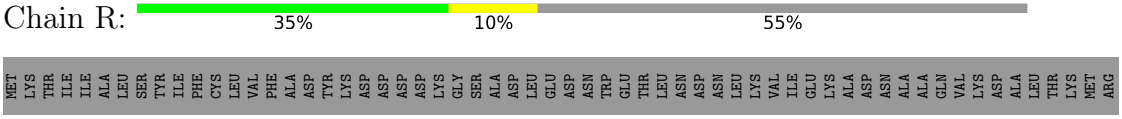
• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

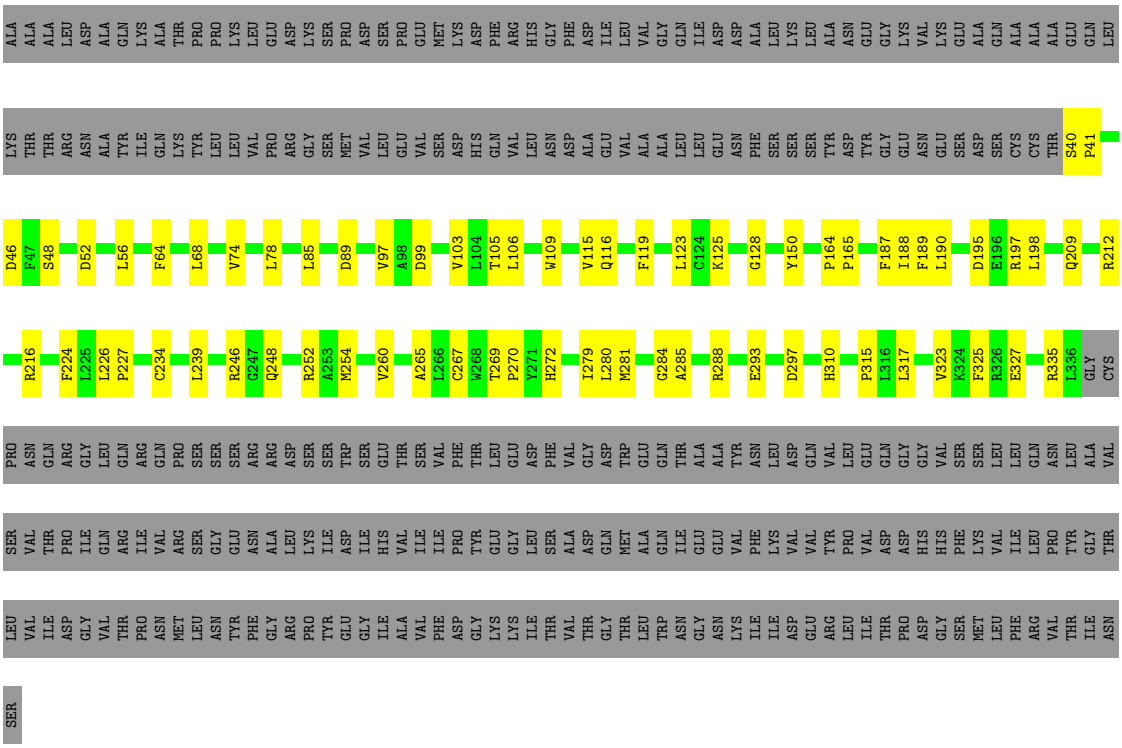
Chain G:



• Molecule 4: Soluble cytochrome b562,C-X-C chemokine receptor type 3,Oplophorus-luciferin 2-monooxygenase catalytic subunit

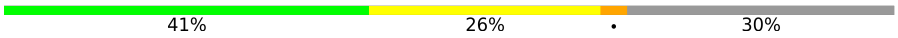
Chain R:

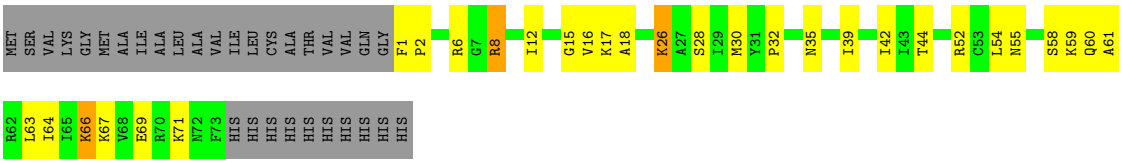




- Molecule 5: C-X-C motif chemokine 11

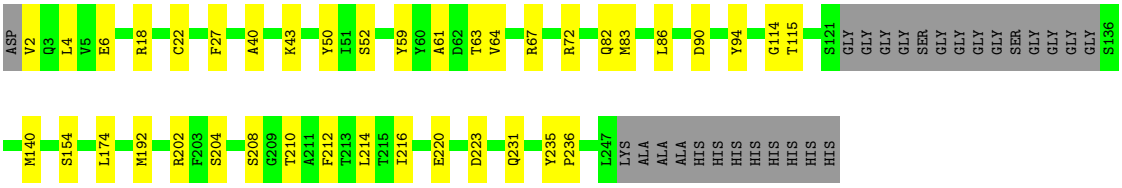
Chain L:





- Molecule 6: single-chain variable fragment scFv16

Chain S:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	96877	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	56.25	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
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: 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	0.26	0/1786	0.42	0/2391
2	B	0.28	0/2630	0.49	0/3566
3	G	0.24	0/424	0.37	0/572
4	R	0.27	0/2372	0.44	0/3237
5	L	0.25	0/585	0.51	0/778
6	S	0.29	0/1827	0.49	0/2477
All	All	0.27	0/9624	0.46	0/13021

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1758	0	1761	12	0
2	B	2583	0	2488	34	0
3	G	418	0	431	5	0
4	R	2316	0	2407	65	0
5	L	578	0	630	27	0
6	S	1783	0	1717	21	0
7	R	56	0	92	19	0
All	All	9492	0	9526	152	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 8.

All (152) 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:R:187:PHE:CZ	7:R:601:CLR:H17	1.86	1.09
4:R:269:THR:HG22	4:R:270:PRO:HD3	1.36	1.08
4:R:269:THR:CG2	4:R:270:PRO:HD3	1.84	1.06
4:R:187:PHE:CE2	7:R:601:CLR:H17	1.91	1.05
4:R:187:PHE:CE2	7:R:601:CLR:H122	2.05	0.91
4:R:187:PHE:HZ	7:R:601:CLR:H14	1.33	0.90
4:R:187:PHE:CZ	7:R:601:CLR:H14	2.08	0.87
4:R:187:PHE:HZ	7:R:601:CLR:C14	1.88	0.87
4:R:187:PHE:CZ	7:R:601:CLR:C17	2.59	0.84
2:B:247:ASP:OD1	2:B:249:THR:HG22	1.82	0.78
4:R:269:THR:HG23	4:R:270:PRO:HD3	1.67	0.77
4:R:269:THR:CG2	4:R:270:PRO:CD	2.64	0.76
4:R:52:ASP:HA	4:R:56:LEU:HD13	1.66	0.75
4:R:188:ILE:HG13	4:R:189:PHE:HD1	1.51	0.74
1:A:251:ASP:OD1	1:A:255:ASN:ND2	2.22	0.71
4:R:269:THR:HG23	4:R:270:PRO:CD	2.21	0.70
2:B:271:CYS:HB2	2:B:290:ASP:HB2	1.74	0.69
4:R:187:PHE:HZ	7:R:601:CLR:C17	2.03	0.68
6:S:52:SER:O	6:S:72:ARG:NH1	2.27	0.68
6:S:94:TYR:O	6:S:114:GLY:HA2	1.93	0.68
4:R:197:ARG:HH11	5:L:30:MET:HE1	1.59	0.67
2:B:312:ASP:OD1	4:R:335:ARG:NH2	2.29	0.66
4:R:212:ARG:NH2	5:L:35:ASN:OD1	2.29	0.64
2:B:67:SER:HB2	2:B:321:THR:HB	1.78	0.64
5:L:26:LYS:HE3	5:L:44:THR:HB	1.80	0.64
5:L:64:ILE:HD12	5:L:67:LYS:HE3	1.81	0.63
4:R:280:LEU:O	4:R:284:GLY:N	2.32	0.62
3:G:57:SER:OG	3:G:58:GLU:OE1	2.18	0.61
2:B:160:SER:HB3	2:B:190:LEU:HD23	1.83	0.60
4:R:187:PHE:CZ	7:R:601:CLR:C14	2.76	0.60
2:B:108:SER:OG	2:B:154:ASP:OD1	2.20	0.59
2:B:256:ARG:NH2	3:G:36:ASP:OD2	2.33	0.59
1:A:315:ASP:O	4:R:248:GLN:NE2	2.34	0.59
4:R:187:PHE:CZ	7:R:601:CLR:H122	2.37	0.59
4:R:119:PHE:HB3	4:R:123:LEU:HD12	1.85	0.59
5:L:28:SER:HB2	5:L:42:ILE:HG22	1.86	0.58
1:A:185:VAL:HB	1:A:200:ASP:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:SER:HB3	1:A:9:ASP:HB2	1.85	0.57
5:L:16:VAL:HB	5:L:52:ARG:HD3	1.86	0.57
6:S:4:LEU:HD12	6:S:22:CYS:SG	2.45	0.57
5:L:17:LYS:NZ	5:L:58:SER:OG	2.37	0.57
4:R:68:LEU:HD22	4:R:103:VAL:HG23	1.87	0.56
4:R:74:VAL:HG21	4:R:315:PRO:HB3	1.86	0.56
2:B:311:HIS:CG	2:B:331:SER:HG	2.24	0.56
5:L:32:PRO:HD3	5:L:39:ILE:HB	1.87	0.56
1:A:251:ASP:O	1:A:255:ASN:ND2	2.39	0.55
4:R:97:VAL:HG11	7:R:602:CLR:H112	1.87	0.55
4:R:187:PHE:HE2	7:R:601:CLR:H122	1.65	0.54
4:R:150:TYR:HB2	4:R:234:CYS:HB3	1.88	0.54
4:R:106:LEU:HA	4:R:109:TRP:HD1	1.73	0.53
4:R:115:VAL:HG23	4:R:116:GLN:H	1.73	0.53
4:R:125:LYS:NZ	4:R:188:ILE:O	2.42	0.53
5:L:15:GLY:H	5:L:55:ASN:HB3	1.73	0.53
4:R:188:ILE:HG13	4:R:189:PHE:CD1	2.39	0.52
5:L:63:LEU:O	5:L:66:LYS:HG3	2.09	0.52
6:S:208:SER:O	6:S:210:THR:N	2.38	0.52
2:B:153:ASP:OD1	2:B:156:GLN:HG2	2.11	0.51
2:B:96:ARG:NH1	2:B:138:GLU:OE1	2.44	0.51
4:R:187:PHE:HZ	7:R:601:CLR:C13	2.23	0.51
6:S:63:THR:HG23	6:S:64:VAL:HG13	1.92	0.51
4:R:187:PHE:CE2	7:R:601:CLR:C12	2.86	0.51
4:R:99:ASP:O	4:R:103:VAL:HG22	2.11	0.50
4:R:209:GLN:HB3	5:L:6:ARG:HH12	1.75	0.50
2:B:159:THR:HG1	2:B:169:TRP:HE1	1.59	0.50
1:A:354:PHE:O	4:R:252:ARG:NE	2.45	0.49
4:R:48:SER:HB2	4:R:297:ASP:OD2	2.12	0.49
6:S:83:MET:SD	6:S:86:LEU:HD21	2.53	0.49
2:B:14:LEU:HD11	3:G:20:LYS:HG3	1.94	0.48
4:R:187:PHE:CZ	7:R:601:CLR:C13	2.96	0.48
2:B:27:ASP:OD1	2:B:28:ALA:N	2.47	0.48
2:B:64:GLY:HA2	2:B:105:TYR:CD2	2.49	0.48
2:B:286:LEU:HD13	2:B:296:VAL:HG22	1.96	0.48
5:L:6:ARG:HD2	5:L:35:ASN:HB3	1.95	0.48
5:L:16:VAL:HG12	5:L:18:ALA:H	1.77	0.48
5:L:54:LEU:HD21	5:L:60:GLN:HG2	1.95	0.48
4:R:85:LEU:HD22	4:R:89:ASP:HB3	1.95	0.47
4:R:216:ARG:HB3	4:R:279:ILE:HD11	1.95	0.47
6:S:192:MET:O	6:S:192:MET:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:ASP:CG	2:B:249:THR:HG22	2.35	0.47
6:S:140:MET:SD	6:S:231:GLN:HB3	2.54	0.47
5:L:63:LEU:O	5:L:67:LYS:HG2	2.15	0.47
6:S:2:VAL:HG23	6:S:27:PHE:CD1	2.50	0.47
6:S:61:ALA:HB3	6:S:64:VAL:HG22	1.97	0.47
4:R:224:PHE:HB2	4:R:272:HIS:CE1	2.50	0.47
2:B:248:ALA:HB1	2:B:269:ILE:HG22	1.97	0.46
4:R:46:ASP:N	4:R:46:ASP:OD1	2.48	0.46
6:S:40:ALA:HB3	6:S:43:LYS:HB2	1.98	0.46
2:B:311:HIS:HD1	2:B:331:SER:HG	1.54	0.46
2:B:323:ASP:OD1	2:B:323:ASP:N	2.49	0.46
4:R:226:LEU:HB3	4:R:227:PRO:HD3	1.98	0.46
5:L:1:PHE:HA	5:L:2:PRO:HD3	1.84	0.46
4:R:269:THR:HG23	4:R:270:PRO:N	2.31	0.45
5:L:66:LYS:O	5:L:69:GLU:HG2	2.17	0.45
1:A:285:ILE:HD12	1:A:285:ILE:H	1.82	0.45
1:A:247:MET:HE3	1:A:310:LEU:HD11	1.99	0.45
2:B:225:HIS:CE1	2:B:251:ARG:HG2	2.52	0.45
2:B:262:MET:SD	2:B:302:ALA:HB2	2.57	0.45
4:R:195:ASP:HB2	4:R:198:LEU:HB2	1.99	0.45
5:L:58:SER:OG	5:L:60:GLN:OE1	2.28	0.45
6:S:6:GLU:HB3	6:S:115:THR:HB	1.98	0.45
2:B:281:SER:OG	3:G:48:ASP:OD2	2.26	0.44
6:S:67:ARG:NH1	6:S:90:ASP:OD2	2.32	0.44
2:B:10:GLU:O	2:B:13:GLN:HG3	2.18	0.44
5:L:15:GLY:N	5:L:55:ASN:HB3	2.31	0.44
4:R:164:PRO:HA	4:R:165:PRO:HD3	1.82	0.44
4:R:267:CYS:HB3	4:R:310:HIS:HB2	1.99	0.44
6:S:50:TYR:HD2	6:S:59:TYR:HD2	1.66	0.44
2:B:34:THR:O	2:B:37:ILE:HG22	2.16	0.44
4:R:64:PHE:O	4:R:68:LEU:HD23	2.18	0.44
4:R:288:ARG:HG3	5:L:12:ILE:HD13	2.00	0.44
2:B:191:SER:HB2	2:B:232:ILE:HG23	1.99	0.43
5:L:67:LYS:O	5:L:71:LYS:HB2	2.18	0.43
2:B:61:MET:HG2	2:B:317:CYS:HB2	2.00	0.43
2:B:286:LEU:HB3	2:B:318:LEU:HD21	2.00	0.43
4:R:187:PHE:HE2	7:R:601:CLR:H17	1.72	0.43
2:B:230:ASN:ND2	2:B:246:ASP:OD1	2.45	0.43
4:R:187:PHE:CE2	7:R:601:CLR:C17	2.81	0.43
4:R:197:ARG:NH1	5:L:30:MET:HE1	2.31	0.43
3:G:11:GLN:HG2	3:G:12:ALA:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:40:SER:HB3	4:R:41:PRO:HD3	2.01	0.43
5:L:61:ALA:HA	5:L:64:ILE:HG22	2.00	0.42
6:S:202:ARG:NE	6:S:223:ASP:OD2	2.48	0.42
2:B:79:LEU:HB2	2:B:93:ILE:HB	2.02	0.42
6:S:18:ARG:O	6:S:82:GLN:NE2	2.51	0.42
5:L:59:LYS:HA	5:L:59:LYS:HD2	1.84	0.42
7:R:602:CLR:H162	7:R:602:CLR:H222	1.71	0.42
6:S:202:ARG:NH1	6:S:220:GLU:OE1	2.53	0.42
4:R:281:MET:HA	4:R:285:ALA:O	2.20	0.41
1:A:208:ARG:O	1:A:212:ILE:HB	2.20	0.41
2:B:152:LEU:HD23	2:B:156:GLN:HG3	2.02	0.41
6:S:154:SER:HA	6:S:216:ILE:O	2.20	0.41
6:S:235:TYR:N	6:S:236:PRO:HD2	2.35	0.41
1:A:277:LYS:O	1:A:281:SER:N	2.37	0.41
1:A:339:VAL:HA	1:A:342:VAL:HG12	2.02	0.41
4:R:128:GLY:HA3	4:R:190:LEU:HD11	2.02	0.41
4:R:209:GLN:CB	5:L:6:ARG:HH12	2.34	0.41
4:R:260:VAL:HG22	4:R:317:LEU:HD13	2.01	0.41
6:S:174:LEU:HD22	6:S:212:PHE:CG	2.55	0.41
4:R:239:LEU:HD23	4:R:254:MET:HG2	2.03	0.41
4:R:265:ALA:O	4:R:269:THR:HB	2.21	0.41
4:R:293:GLU:OE1	5:L:8:ARG:NH1	2.53	0.41
4:R:323:VAL:O	4:R:327:GLU:HG2	2.21	0.41
1:A:210:LYS:HD3	1:A:210:LYS:HA	1.76	0.40
2:B:276:VAL:HG13	2:B:285:LEU:HD11	2.03	0.40
4:R:187:PHE:HE2	7:R:601:CLR:C12	2.29	0.40
2:B:232:ILE:HG13	2:B:243:THR:HG22	2.03	0.40
4:R:105:THR:HG22	4:R:109:TRP:HE1	1.86	0.40
5:L:16:VAL:HG21	5:L:52:ARG:HH11	1.85	0.40
2:B:137:ARG:HG3	2:B:138:GLU:N	2.37	0.40
2:B:266:HIS:HB3	2:B:269:ILE:HD12	2.03	0.40
4:R:78:LEU:HG	4:R:325:PHE:HE1	1.87	0.40
6:S:204:SER:O	6:S:214:LEU:HD12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	212/354 (60%)	206 (97%)	6 (3%)	0	100	100
2	B	334/384 (87%)	322 (96%)	12 (4%)	0	100	100
3	G	52/71 (73%)	51 (98%)	1 (2%)	0	100	100
4	R	295/657 (45%)	280 (95%)	15 (5%)	0	100	100
5	L	71/104 (68%)	67 (94%)	4 (6%)	0	100	100
6	S	228/259 (88%)	215 (94%)	13 (6%)	0	100	100
All	All	1192/1829 (65%)	1141 (96%)	51 (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	195/306 (64%)	195 (100%)	0	100	100
2	B	279/315 (89%)	278 (100%)	1 (0%)	91	97
3	G	44/58 (76%)	43 (98%)	1 (2%)	50	79
4	R	246/556 (44%)	245 (100%)	1 (0%)	91	97
5	L	65/90 (72%)	62 (95%)	3 (5%)	27	62
6	S	197/209 (94%)	197 (100%)	0	100	100
All	All	1026/1534 (67%)	1020 (99%)	6 (1%)	86	95

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	340	ASN
3	G	59	ASN
4	R	246	ARG
5	L	8	ARG
5	L	26	LYS
5	L	66	LYS

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	340	ASN
3	G	59	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\|>2$
7	CLR	R	601	-	31,31,31	0.28	0	48,48,48	0.39	0
7	CLR	R	602	-	31,31,31	0.31	0	48,48,48	0.55	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CLR	R	601	-	-	10/10/68/68	0/4/4/4
7	CLR	R	602	-	-	10/10/68/68	0/4/4/4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

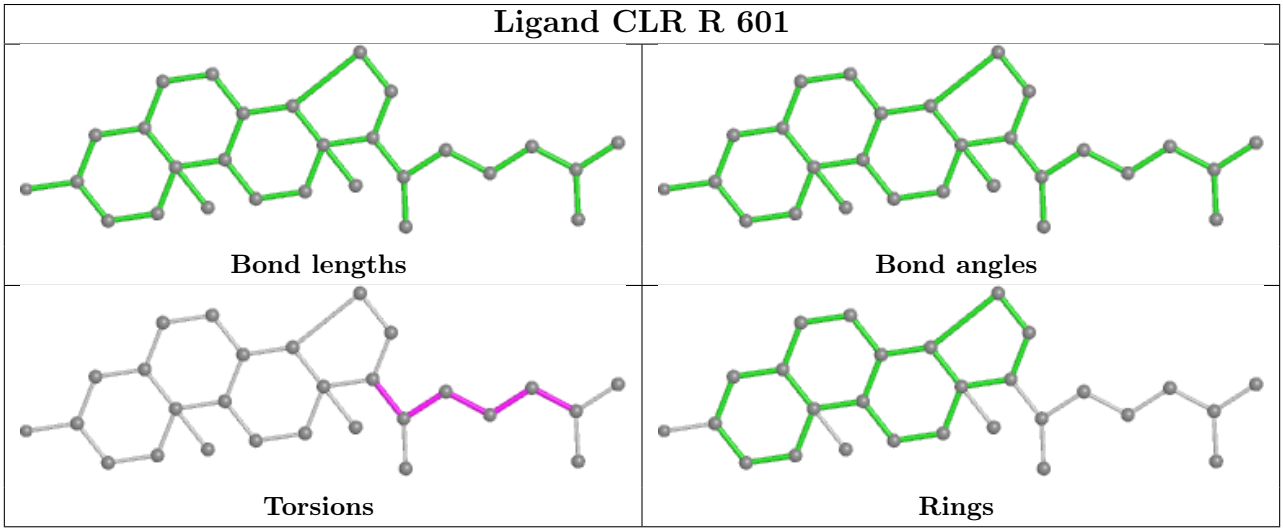
Mol	Chain	Res	Type	Atoms
7	R	601	CLR	C21-C20-C22-C23
7	R	601	CLR	C13-C17-C20-C22
7	R	601	CLR	C13-C17-C20-C21
7	R	601	CLR	C16-C17-C20-C21
7	R	601	CLR	C16-C17-C20-C22
7	R	602	CLR	C17-C20-C22-C23
7	R	601	CLR	C23-C24-C25-C27
7	R	601	CLR	C23-C24-C25-C26
7	R	602	CLR	C21-C20-C22-C23
7	R	602	CLR	C13-C17-C20-C22
7	R	602	CLR	C16-C17-C20-C21
7	R	602	CLR	C13-C17-C20-C21
7	R	601	CLR	C17-C20-C22-C23
7	R	602	CLR	C16-C17-C20-C22
7	R	602	CLR	C22-C23-C24-C25
7	R	602	CLR	C20-C22-C23-C24
7	R	602	CLR	C23-C24-C25-C26
7	R	601	CLR	C22-C23-C24-C25
7	R	602	CLR	C23-C24-C25-C27
7	R	601	CLR	C20-C22-C23-C24

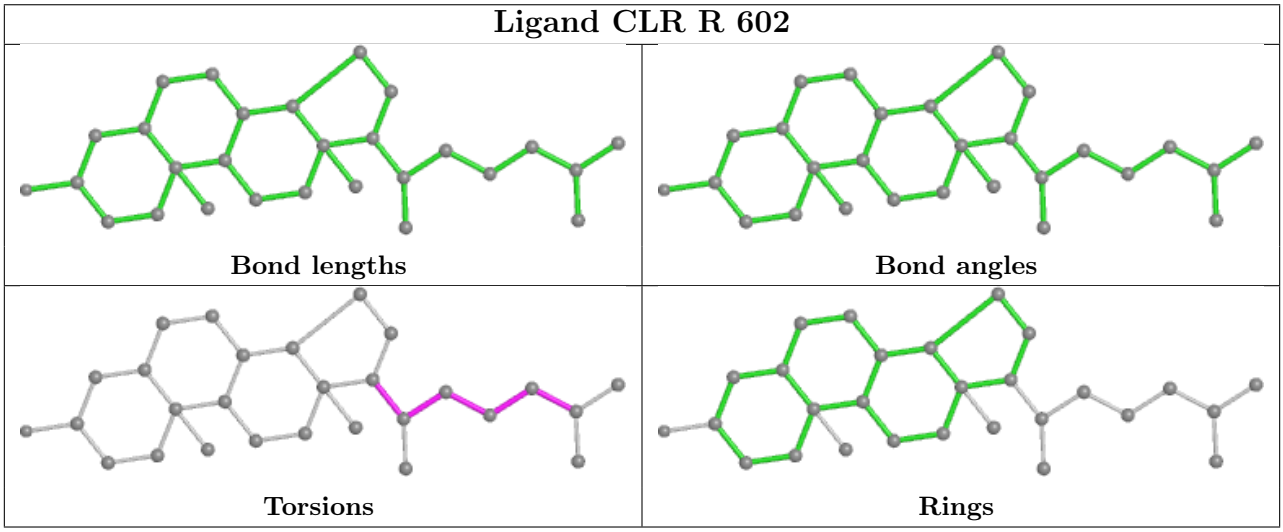
There are no ring outliers.

2 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	R	601	CLR	17	0
7	R	602	CLR	2	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.





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.