



## Full wwPDB EM Validation Report ⓘ

Oct 7, 2024 – 02:11 PM JST

PDB ID : 8ISJ  
EMDB ID : EMD-35692  
Title : Pr conformer of Arabidopsis thaliana phytochrome A - AtphyA-Pr  
Authors : Zhang, Y.; Ma, C.; Zhao, J.; Gao, N.; Wang, J.  
Deposited on : 2023-03-20  
Resolution : 3.00 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](mailto: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>.

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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 : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

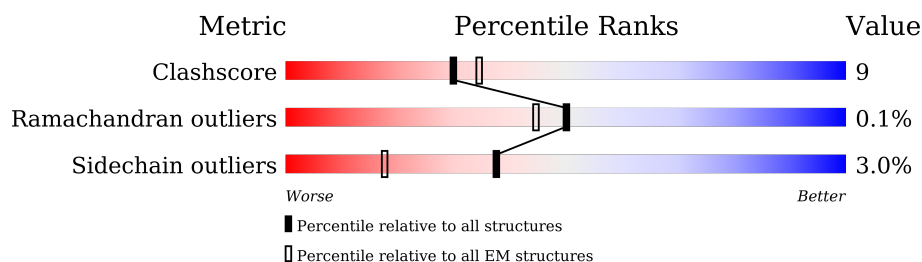
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	1120	
1	B	1120	

## 2 Entry composition [i](#)

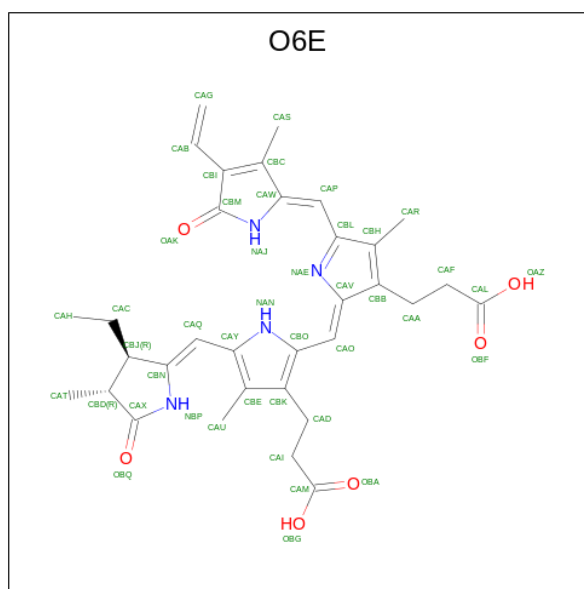
There are 2 unique types of molecules in this entry. The entry contains 13533 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phytochrome A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	859	Total	C	N	O	S	0	0
			6730	4276	1156	1245	53		
1	B	857	Total	C	N	O	S	0	0
			6717	4269	1155	1240	53		

- Molecule 2 is 3-[5-[[[(3 {R},4 {R})-3-ethyl-4-methyl-5-oxidanylidene-3,4-dihydropyrrol-2-yl)methyl]-2-[[5-[(4-ethyl-3-methyl-5-oxidanylidene-pyrrol-2-yl)methyl]-3-(3-hydroxy-3-oxopropyl)-4-methyl-1 {H}-pyrrol-2-yl)methyl]-4-methyl-1 {H}-pyrrol-3-yl]propanoic acid (three-letter code: O6E) (formula: C<sub>33</sub>H<sub>38</sub>N<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			43	33	4	6	
2	B	1	Total	C	N	O	0
			43	33	4	6	



L1050	A1051	I1055	R1056	H1059	I1064	L1069	M1072	S1080	G1083	L1084	S1085	L1086	M1087	M1096	Q1101	R1104	I1112	I1113	L1117	A1118	A1119	ALA																												
1933	1934	Q943	K946	D949	L953	N965	K966	E967	E972	A976	S977	T978	S979	Q980	N981	N982	S985	K988	S989	V990	Y1006	G1007	Q1013	Q1014	Y1015	L1016	F1019	M1022	M1025	F1026	L1033	S1036	R1040	LYS	ASP	M920	GLN	LEU	GLY	ARG	SER	VAL	HIS							
N760	D770	E771	K789	E792	L798	F803	Q806	N814	N827	S831	K836	C851	L852	V855	R861	C870	L874	A875	Q880	K895	R896	L897	L900	R905	P910	I914	M915	F916	K919	M920	I921	L926	E929	Q930																
GLN	ASN	VAL	PHE	GLU	ILE	LYS	THR	HIS	SER	ARG	ALA	ASP	ALA	ALA	GLY	PRO	ILE	SER	LEU	VAL	VAL	VAL	GLY	THR	GLN	LYS	THR	VAL	M742	D743	K744	F745	Y752	I755																
VAL	PRO	ILE	LEU	ALA	VAL	ASP	SER	GLY	LEU	VAL	ASN	GLY	THR	GLY	THR	VAL	LEU	GLY	THR	LEU	VAL	PHE	LEU	THR	GLN	VAL	ILE	LYS	ARG	MET	LEU	GLU	MET	ASN	ALA	LEU	ILE	GLU	THR	GLU	THR									
M548	H549	P550	R551	F554	T563	R564	S565	L566	P567	E572	I576	K588	ASP	SER	GLU	THR	THR	GLY	ASP	VAL	ASN	THR	LYS	THR	ILE	TYR	SER	LYS	LEU	ASN	ASP	R512	I513	D517	M518	I519	R523	S524	H525	G533	H537	D538	P539	ASP	ARG	LEU	ILE	GLU	THR	THR
L459	G460	T461	S464	E465	F466	H467	L468	Q469	E470	L475	Y478	H479	M480	D481	S482	L485	D488	S489	L490	F495	A498	L501	S504	V505	C506	R512	I513	D517	M518	I519	R523	S524	H525	G533	H537	D538	P539	ASP	ARG	LEU	ILE	GLU	THR	THR						
R318	H321	Y327	M328	A335	D347	GLY	GLU	GLY	ASP	ALA	PRO	ASP	ALA	THR	THR	GLN	PRO	GLN	K361	N373	R377	R394	Y385	L390	E403	Q407	M408	V409	I413	L419	M423	R426	I432	P437	M438	I439	M440	K444	K453											
S163	A164	K165	P166	F167	Y168	H172	R173	I178	D181	F182	V185	M192	R210	L211	C223	V227	Q228	E229	E232	Y242	H245	G250	E251	T257	K258	P259	E262	H268	Y269	P270	A271	T272	D273	N285	R288	D309	I310	T311	L312	C313	G314									
PRO	ARG	SER	ASP	LYS	VAL	THR	THR	TYR	LEU	HIS	K76	C85	A88	L89	D90	T93	F94	K95	V96	I97	A98	Y99	S100	F101	N102	L106	M109	A110	SER	HIS	ALA	VAL	PRO	SER	VAL	GLY	H120	L123	R130	S131	L132	A138	L153	R161	T162					

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	774153	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (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: O6E

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	0.27	0/6852	0.52	1/9245 (0.0%)
1	B	0.27	0/6840	0.53	0/9232
All	All	0.27	0/13692	0.52	1/18477 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	LEU	CA-CB-CG	5.10	127.03	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	384	ARG	Sidechain
1	B	384	ARG	Sidechain

## 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	6730	0	6826	114	0
1	B	6717	0	6810	136	0
2	A	43	0	0	0	0
2	B	43	0	0	0	0
All	All	13533	0	13636	243	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 9.

All (243) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:855:VAL:HG13	1:B:870:CYS:SG	1.52	1.50
1:B:855:VAL:CG1	1:B:870:CYS:SG	2.43	1.05
1:B:855:VAL:HG13	1:B:870:CYS:HG	1.24	0.93
1:A:439:ILE:HG23	1:A:521:TRP:CZ2	2.11	0.86
1:B:926:LEU:HB3	1:B:930:GLN:HE21	1.49	0.77
1:B:525:HIS:HB2	1:B:563:THR:HG23	1.70	0.74
1:A:832:GLN:HB2	1:A:857:LYS:HD3	1.71	0.72
1:A:533:GLY:HA2	1:A:556:ALA:HA	1.70	0.71
1:B:423:MET:HG2	1:B:432:ILE:HG22	1.73	0.70
1:B:257:THR:HG22	1:B:259:PRO:HD2	1.74	0.70
1:B:88:ALA:HB3	1:B:98:ALA:HB3	1.74	0.68
1:B:965:MET:CE	1:B:1007:GLY:HA2	2.23	0.68
1:A:463:PRO:HD3	1:A:505:VAL:HG11	1.76	0.67
1:B:228:GLN:NE2	1:B:232:GLU:OE2	2.28	0.66
1:A:160:CYS:HG	1:A:163:SER:HG	1.42	0.65
1:B:76:LYS:HD3	1:B:311:THR:HA	1.79	0.65
1:B:285:ASN:HD21	1:B:314:GLY:HA2	1.62	0.64
1:B:943:GLN:OE1	1:B:1013:GLN:NE2	2.31	0.64
1:B:1051:ALA:HB3	1:B:1117:LEU:O	1.98	0.63
1:A:943:GLN:OE1	1:A:1013:GLN:NE2	2.31	0.63
1:B:288:ARG:NH2	1:B:318:ARG:O	2.32	0.62
1:B:501:LEU:HB3	1:B:505:VAL:HG21	1.81	0.62
1:B:88:ALA:C	1:B:89:LEU:HD12	2.20	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1065:PRO:HD2	1:A:1068:LEU:HD12	1.80	0.61
1:B:311:THR:OG1	1:B:313:CYS:SG	2.57	0.61
1:A:439:ILE:HG23	1:A:521:TRP:HZ2	1.61	0.61
1:B:426:ARG:HH22	1:B:437:PRO:HG2	1.65	0.61
1:B:132:LEU:H	1:B:132:LEU:HD23	1.67	0.60
1:B:100:SER:OG	1:B:102:ASN:OD1	2.20	0.60
1:B:268:HIS:O	1:B:533:GLY:N	2.30	0.60
1:B:309:ASP:OD1	1:B:309:ASP:N	2.34	0.60
1:A:1016:LEU:HB3	1:A:1020:MET:HE3	1.84	0.59
1:B:1064:ILE:O	1:B:1104:ARG:NH2	2.30	0.59
1:B:311:THR:HG1	1:B:313:CYS:HG	1.49	0.59
1:A:439:ILE:CG2	1:A:521:TRP:CZ2	2.85	0.58
1:B:172:HIS:NE2	1:B:181:ASP:OD2	2.30	0.58
1:A:985:SER:OG	1:A:990:VAL:O	2.22	0.58
1:A:910:PRO:O	1:A:914:ILE:HG13	2.03	0.58
1:B:466:PHE:O	1:B:470:GLU:HG2	2.04	0.58
1:A:918:ARG:NE	1:A:922:GLU:OE2	2.35	0.57
1:A:1018:ASP:O	1:A:1022:MET:HG2	2.04	0.57
1:A:242:TYR:CZ	1:A:250:GLY:HA3	2.40	0.57
1:B:444:LYS:HG3	1:B:523:ARG:HH21	1.69	0.57
1:A:88:ALA:HB3	1:A:98:ALA:HB3	1.87	0.57
1:B:109:MET:O	1:B:165:LYS:NZ	2.38	0.57
1:B:855:VAL:HG22	1:B:870:CYS:SG	2.45	0.57
1:B:1016:LEU:HD21	1:B:1055:ILE:HD13	1.87	0.56
1:B:162:THR:HG22	1:B:163:SER:H	1.70	0.56
1:B:89:LEU:HD12	1:B:89:LEU:N	2.19	0.56
1:A:78:LYS:NZ	1:A:302:GLN:OE1	2.31	0.56
1:B:1055:ILE:HB	1:B:1113:ILE:HB	1.86	0.56
1:A:1006:TYR:HB3	1:A:1118:ALA:HB3	1.87	0.56
1:A:991:ARG:HD2	1:A:1032:GLN:HE22	1.71	0.56
1:A:532:TRP:HE1	1:A:536:LYS:HA	1.71	0.56
1:A:918:ARG:HD3	1:A:941:GLN:HE22	1.70	0.56
1:B:498:ALA:HA	1:B:501:LEU:HD12	1.88	0.55
1:B:921:ILE:HG22	1:B:934:LEU:HD11	1.87	0.55
1:A:564:ARG:HB2	1:A:564:ARG:HH11	1.71	0.55
1:B:482:SER:HB3	1:B:745:PHE:HA	1.89	0.55
1:A:1018:ASP:OD2	1:A:1085:SER:OG	2.24	0.55
1:B:1033:LEU:HD13	1:B:1059:HIS:HB3	1.89	0.55
1:B:537:HIS:CD2	1:B:539:PRO:HD3	2.42	0.55
1:B:335:ALA:HB3	1:B:373:ASN:HB3	1.89	0.54
1:A:922:GLU:HG3	1:A:934:LEU:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:LYS:HG2	1:B:259:PRO:HD3	1.88	0.54
1:B:1019:PHE:HA	1:B:1022:MET:SD	2.47	0.54
1:A:95:LYS:HB3	1:A:126:GLY:HA2	1.90	0.54
1:B:929:GLU:HG3	1:B:930:GLN:OE1	2.07	0.54
1:A:143:LYS:HD2	1:A:143:LYS:O	2.08	0.54
1:A:160:CYS:SG	1:A:165:LYS:N	2.78	0.53
1:A:918:ARG:HD3	1:A:941:GLN:NE2	2.23	0.53
1:B:438:ASN:OD1	1:B:438:ASN:N	2.40	0.53
1:A:1064:ILE:HD12	1:A:1111:PHE:CZ	2.44	0.53
1:B:495:PHE:HB3	1:B:498:ALA:HB2	1.91	0.53
1:B:814:ASN:N	1:B:814:ASN:OD1	2.42	0.53
1:B:875:ALA:O	1:B:880:GLN:NE2	2.42	0.53
1:A:492:ASP:OD2	1:A:564:ARG:NH2	2.38	0.53
1:A:1071:GLN:HG2	1:A:1079:VAL:HA	1.91	0.53
1:A:270:PRO:HA	1:A:537:HIS:HB2	1.91	0.53
1:B:229:GLU:OE1	1:B:229:GLU:HA	2.09	0.53
1:A:190:VAL:HG13	1:A:191:PRO:HD3	1.91	0.53
1:B:770:ASP:OD1	1:B:771:GLU:N	2.37	0.52
1:A:532:TRP:HZ2	1:A:537:HIS:HB3	1.73	0.52
1:A:982:MET:HA	1:A:985:SER:HB3	1.90	0.52
1:B:965:MET:HE2	1:B:1007:GLY:HA2	1.90	0.52
1:A:225:THR:O	1:A:229:GLU:HG2	2.09	0.52
1:A:530:VAL:HG12	1:A:532:TRP:HB2	1.90	0.52
1:A:1079:VAL:O	1:A:1080:SER:OG	2.17	0.52
1:B:89:LEU:HG	1:B:96:VAL:HA	1.92	0.51
1:B:168:TYR:O	1:B:182:PHE:HA	2.10	0.51
1:B:919:LYS:HD2	1:B:919:LYS:C	2.32	0.51
1:A:439:ILE:CG2	1:A:521:TRP:CE2	2.94	0.50
1:A:439:ILE:HG22	1:A:521:TRP:NE1	2.26	0.50
1:B:489:SER:HB2	1:B:564:ARG:HA	1.93	0.50
1:B:930:GLN:OE1	1:B:930:GLN:N	2.32	0.50
1:B:73:HIS:HB2	1:B:321:HIS:HD2	1.75	0.50
1:B:1006:TYR:HB2	1:B:1118:ALA:HB3	1.92	0.50
1:A:85:CYS:SG	1:A:182:PHE:HB2	2.51	0.50
1:B:985:SER:OG	1:B:990:VAL:O	2.30	0.50
1:A:748:ILE:O	1:A:748:ILE:HG13	2.12	0.50
1:A:1064:ILE:CD1	1:A:1111:PHE:HZ	2.25	0.50
1:B:438:ASN:HD22	1:B:459:LEU:HD11	1.77	0.50
1:A:438:ASN:OD1	1:A:438:ASN:N	2.45	0.50
1:A:814:ASN:OD1	1:A:814:ASN:N	2.45	0.49
1:A:982:MET:HE2	1:B:916:PHE:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:978:THR:HG22	1:B:982:MET:SD	2.53	0.49
1:B:1101:GLN:HB2	1:B:1112:ILE:HB	1.94	0.49
1:B:549:HIS:HB3	1:B:550:PRO:HD2	1.95	0.49
1:B:373:ASN:HD22	1:B:377:ARG:HB2	1.78	0.49
1:A:568:TRP:O	1:A:747:ARG:NH2	2.42	0.49
1:A:943:GLN:O	1:A:947:ILE:HG22	2.12	0.49
1:B:910:PRO:O	1:B:914:ILE:HG12	2.11	0.49
1:A:141:LEU:O	1:A:145:LEU:HD12	2.13	0.49
1:B:90:ASP:HB2	1:B:93:THR:HG22	1.95	0.48
1:A:982:MET:HE2	1:B:916:PHE:HE2	1.78	0.48
1:A:1083:GLY:HA2	1:A:1086:LEU:HD12	1.94	0.48
1:B:89:LEU:N	1:B:89:LEU:CD1	2.76	0.48
1:A:748:ILE:HG22	1:A:754:ALA:HA	1.95	0.48
1:A:267:LEU:HD23	1:A:533:GLY:HA3	1.95	0.48
1:A:915:MET:SD	1:A:941:GLN:NE2	2.87	0.48
1:B:161:ARG:NH2	1:B:162:THR:OG1	2.46	0.48
1:B:988:LYS:NZ	1:B:1025:ASN:O	2.46	0.48
1:A:933:ILE:HG21	1:B:920:MET:HB2	1.95	0.48
1:A:129:ILE:HG13	1:A:132:LEU:HD12	1.95	0.48
1:B:85:CYS:SG	1:B:182:PHE:HB2	2.54	0.48
1:A:231:PHE:HB2	1:A:239:VAL:HG21	1.96	0.48
1:A:530:VAL:HG11	1:A:532:TRP:HE3	1.79	0.47
1:B:258:LYS:CG	1:B:259:PRO:HD3	2.44	0.47
1:B:273:ASP:OD1	1:B:551:ARG:NH2	2.47	0.47
1:A:959:GLY:HA2	1:A:1091:LYS:NZ	2.30	0.47
1:B:513:ILE:HD11	1:B:519:ILE:HD11	1.97	0.47
1:B:210:ARG:NH1	1:B:229:GLU:OE2	2.47	0.47
1:B:967:GLU:HG2	1:B:1006:TYR:CE1	2.50	0.47
1:B:1069:LEU:HA	1:B:1072:MET:HG3	1.96	0.47
1:B:426:ARG:NH2	1:B:437:PRO:HG2	2.28	0.47
1:B:1056:ARG:NH2	1:B:1112:ILE:HG13	2.29	0.47
1:B:490:LEU:HD12	1:B:506:CYS:HA	1.97	0.47
1:B:976:ALA:O	1:B:980:GLN:HG3	2.15	0.46
1:B:123:LEU:HD11	1:B:132:LEU:HD13	1.97	0.46
1:B:153:LEU:H	1:B:153:LEU:HD23	1.81	0.46
1:A:1064:ILE:CD1	1:A:1111:PHE:CZ	2.99	0.46
1:B:836:LYS:HB3	1:B:852:LEU:HD23	1.96	0.46
1:A:432:ILE:HG22	1:A:439:ILE:HG13	1.98	0.46
1:A:902:TYR:CE2	1:B:953:LEU:HD13	2.50	0.46
1:A:1033:LEU:HD13	1:A:1059:HIS:HB3	1.98	0.46
1:B:173:ARG:HG2	1:B:178:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1080:SER:O	1:B:1084:LEU:N	2.44	0.46
1:A:497:ARG:O	1:A:500:SER:OG	2.33	0.45
1:B:965:MET:HE1	1:B:1007:GLY:HA2	1.98	0.45
1:A:890:GLU:OE2	1:A:890:GLU:HA	2.15	0.45
1:A:238:ARG:NH1	1:A:255:GLU:OE2	2.47	0.45
1:A:843:THR:OG1	1:A:847:LYS:HB2	2.17	0.45
1:A:506:CYS:HB2	1:A:525:HIS:HB2	1.99	0.45
1:A:572:GLU:O	1:A:576:ILE:HG13	2.17	0.45
1:A:91:GLU:HG2	1:A:92:LYS:HE2	1.98	0.45
1:B:461:THR:HG21	1:B:504:SER:HB3	1.99	0.45
1:B:93:THR:HG23	1:B:95:LYS:H	1.82	0.45
1:B:798:LEU:HD11	1:B:803:PHE:CE2	2.51	0.45
1:A:326:GLN:OE1	1:A:326:GLN:HA	2.17	0.44
1:A:532:TRP:CZ2	1:A:537:HIS:HB3	2.51	0.44
1:A:861:ARG:H	1:A:861:ARG:HG3	1.55	0.44
1:A:915:MET:O	1:A:919:LYS:HD3	2.17	0.44
1:A:452:TYR:HB3	1:A:457:TRP:CZ3	2.52	0.44
1:B:403:GLU:O	1:B:407:GLN:HG2	2.18	0.44
1:B:572:GLU:O	1:B:576:ILE:HD12	2.18	0.44
1:B:827:ASN:O	1:B:831:SER:N	2.35	0.44
1:A:564:ARG:HB2	1:A:564:ARG:NH1	2.32	0.44
1:B:270:PRO:HB2	1:B:272:THR:HG22	2.00	0.43
1:B:223:CYS:O	1:B:227:VAL:HG22	2.18	0.43
1:A:855:VAL:HG13	1:A:870:CYS:SG	2.58	0.43
1:B:409:VAL:O	1:B:413:ILE:HG13	2.17	0.43
1:B:512:ARG:HA	1:B:518:MET:HG2	2.01	0.43
1:B:1026:PHE:CD2	1:B:1064:ILE:HG12	2.53	0.43
1:A:514:SER:OG	1:A:515:SER:N	2.50	0.43
1:B:166:PRO:HG2	1:B:185:VAL:HB	1.99	0.43
1:B:490:LEU:HB2	1:B:506:CYS:HA	2.00	0.43
1:B:980:GLN:OE1	1:B:1013:GLN:NE2	2.50	0.43
1:A:859:LEU:HD23	1:A:859:LEU:HA	1.85	0.43
1:A:944:LEU:HB2	1:B:910:PRO:HB2	1.99	0.43
1:A:1065:PRO:HB2	1:A:1067:PHE:CD1	2.53	0.43
1:B:798:LEU:HD11	1:B:803:PHE:CD2	2.53	0.43
1:A:174:VAL:HG23	1:A:177:SER:HB3	2.01	0.43
1:A:478:TYR:HD1	1:A:478:TYR:HA	1.68	0.43
1:A:190:VAL:CG1	1:A:191:PRO:HD3	2.49	0.43
1:A:534:GLY:HA2	1:A:554:PHE:HA	2.00	0.43
1:B:855:VAL:CB	1:B:870:CYS:SG	3.07	0.42
1:B:930:GLN:HA	1:B:933:ILE:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:LYS:H	1:A:76:LYS:HG2	1.71	0.42
1:A:909:ASN:HB3	1:A:910:PRO:HD3	2.00	0.42
1:A:1059:HIS:NE2	1:A:1109:SER:HB2	2.35	0.42
1:B:895:LYS:H	1:B:895:LYS:HG2	1.72	0.42
1:B:900:LEU:HD12	1:B:900:LEU:HA	1.91	0.42
1:B:262:GLU:OE1	1:B:262:GLU:N	2.48	0.42
1:A:258:LYS:HG3	1:A:259:PRO:HD2	2.02	0.42
1:A:245:HIS:NE2	1:A:251:GLU:OE1	2.47	0.42
1:A:532:TRP:NE1	1:A:535:ALA:O	2.52	0.42
1:B:130:ARG:HG3	1:B:138:ALA:HB1	2.02	0.42
1:B:211:LEU:HD12	1:B:390:LEU:HD11	2.02	0.42
1:B:566:LEU:HD13	1:B:567:PRO:HD2	2.02	0.42
1:B:1022:MET:HA	1:B:1025:ASN:HB2	2.02	0.42
1:A:439:ILE:CG2	1:A:521:TRP:NE1	2.83	0.42
1:A:247:ASP:OD1	1:A:249:HIS:ND1	2.38	0.42
1:A:866:THR:O	1:A:866:THR:OG1	2.30	0.42
1:A:746:THR:HG22	1:A:756:ILE:HG12	2.02	0.42
1:B:475:LEU:HD21	1:B:485:LEU:HD21	2.01	0.42
1:A:857:LYS:HE2	1:A:859:LEU:HG	2.00	0.42
1:B:789:LYS:HB2	1:B:792:GLU:HG2	2.02	0.42
1:B:478:TYR:C	1:B:480:MET:HE1	2.40	0.42
1:B:752:TYR:HB2	1:B:755:ILE:HD11	2.01	0.42
1:A:532:TRP:NE1	1:A:536:LYS:HA	2.34	0.41
1:B:475:LEU:HD23	1:B:475:LEU:HA	1.82	0.41
1:B:488:ASP:HB2	1:B:564:ARG:O	2.20	0.41
1:B:926:LEU:HB3	1:B:930:GLN:NE2	2.26	0.41
1:B:946:LYS:HA	1:B:949:ASP:OD2	2.20	0.41
1:A:156:ILE:HG22	1:A:158:VAL:HG23	2.02	0.41
1:A:906:GLN:NE2	1:B:1014:GLN:OE1	2.54	0.41
1:A:963:LEU:HD22	1:A:1011:ARG:HG3	2.03	0.41
1:B:1036:SER:OG	1:B:1056:ARG:HB2	2.19	0.41
1:A:265:LEU:HD12	1:A:266:GLY:N	2.35	0.41
1:A:328:MET:HG2	1:A:333:SER:O	2.20	0.41
1:B:855:VAL:CG2	1:B:870:CYS:SG	3.09	0.41
1:B:897:LEU:H	1:B:897:LEU:HD23	1.84	0.41
1:A:964:GLU:N	1:A:1008:ASP:OD2	2.49	0.41
1:B:242:TYR:CZ	1:B:250:GLY:HA3	2.56	0.41
1:B:464:SER:O	1:B:468:LEU:HD13	2.21	0.41
1:B:488:ASP:OD1	1:B:488:ASP:N	2.53	0.41
1:B:742:MET:HG2	1:B:743:ASP:H	1.84	0.41
1:B:851:CYS:HB3	1:B:874:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ASP:OD1	1:A:90:ASP:N	2.53	0.41
1:A:419:LEU:HD11	1:A:441:ASP:HB3	2.03	0.41
1:A:518:MET:HE2	1:A:520:PHE:CZ	2.56	0.41
1:A:74:ILE:HG21	1:A:318:ARG:HH11	1.86	0.41
1:A:569:LYS:HB2	1:A:572:GLU:HG3	2.03	0.41
1:B:106:LEU:HD23	1:B:106:LEU:HA	1.88	0.41
1:B:453:LYS:N	1:B:517:ASP:OD2	2.42	0.41
1:B:1083:GLY:HA2	1:B:1086:LEU:HD12	2.02	0.41
1:A:97:ILE:O	1:A:303:ASP:HB2	2.21	0.40
1:A:288:ARG:HH21	1:A:318:ARG:CZ	2.34	0.40
1:B:245:HIS:NE2	1:B:251:GLU:OE1	2.48	0.40
1:A:946:LYS:HD3	1:A:946:LYS:N	2.36	0.40
1:A:311:THR:HG22	1:A:313:CYS:H	1.85	0.40
1:A:743:ASP:OD1	1:A:743:ASP:N	2.55	0.40
1:A:1082:GLU:HG3	1:B:905:ARG:HH12	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	847/1120 (76%)	811 (96%)	35 (4%)	1 (0%)	48	81
1	B	845/1120 (75%)	796 (94%)	49 (6%)	0	100	100
All	All	1692/2240 (76%)	1607 (95%)	84 (5%)	1 (0%)	50	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	428	ALA

### 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	743/968 (77%)	724 (97%)	19 (3%)	41	72
1	B	742/968 (77%)	716 (96%)	26 (4%)	31	65
All	All	1485/1936 (77%)	1440 (97%)	45 (3%)	37	69

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	CYS
1	A	153	LEU
1	A	160	CYS
1	A	261	LEU
1	A	293	CYS
1	A	385	TYR
1	A	427	ASP
1	A	430	LEU
1	A	477	GLU
1	A	478	TYR
1	A	506	CYS
1	A	546	ARG
1	A	859	LEU
1	A	890	GLU
1	A	896	ARG
1	A	902	TYR
1	A	965	MET
1	A	1006	TYR
1	A	1087	MET
1	B	85	CYS
1	B	95	LYS
1	B	153	LEU
1	B	192	MET
1	B	285	ASN
1	B	327	TYR
1	B	328	MET
1	B	385	TYR

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Mol	Chain	Res	Type
1	B	408	MET
1	B	419	LEU
1	B	440	MET
1	B	480	MET
1	B	547	ARG
1	B	548	MET
1	B	554	PHE
1	B	745	PHE
1	B	760	ASN
1	B	806	GLN
1	B	861	ARG
1	B	919	LYS
1	B	972	GLU
1	B	1022	MET
1	B	1056	ARG
1	B	1072	MET
1	B	1087	MET
1	B	1096	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	469	GLN
1	A	873	GLN
1	A	906	GLN
1	A	941	GLN
1	A	943	GLN
1	A	980	GLN
1	A	1013	GLN
1	B	330	ASN
1	B	372	HIS
1	B	577	HIS
1	B	827	ASN
1	B	906	GLN
1	B	980	GLN
1	B	1013	GLN

### 5.3.3 RNA ⓘ

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 oligosaccharides 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$
2	O6E	A	1201	1	42,46,46	1.01	3 (7%)	50,67,67	1.17	3 (6%)
2	O6E	B	1201	1	42,46,46	0.99	3 (7%)	50,67,67	1.26	4 (8%)

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	O6E	A	1201	1	-	7/25/74/74	0/4/4/4
2	O6E	B	1201	1	-	6/25/74/74	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	O6E	CAO-CAV	3.39	1.37	1.35
2	B	1201	O6E	CAO-CAV	3.15	1.37	1.35
2	B	1201	O6E	CAB-CBI	-2.96	1.39	1.47
2	A	1201	O6E	CAB-CBI	-2.93	1.39	1.47
2	A	1201	O6E	CBI-CBC	2.14	1.41	1.37
2	B	1201	O6E	CBI-CBC	2.12	1.41	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	O6E	CBO-CAO-CAV	5.12	134.92	128.81
2	A	1201	O6E	CBO-CAO-CAV	4.71	134.43	128.81
2	B	1201	O6E	CAW-CAP-CBL	3.61	136.91	128.08
2	A	1201	O6E	CAW-CAP-CBL	3.24	136.00	128.08
2	B	1201	O6E	CBD-CBJ-CBN	2.38	104.90	101.34
2	A	1201	O6E	CAO-CAV-NAE	-2.26	125.69	128.83
2	B	1201	O6E	CAO-CAV-NAE	-2.04	126.00	128.83

There are no chirality outliers.

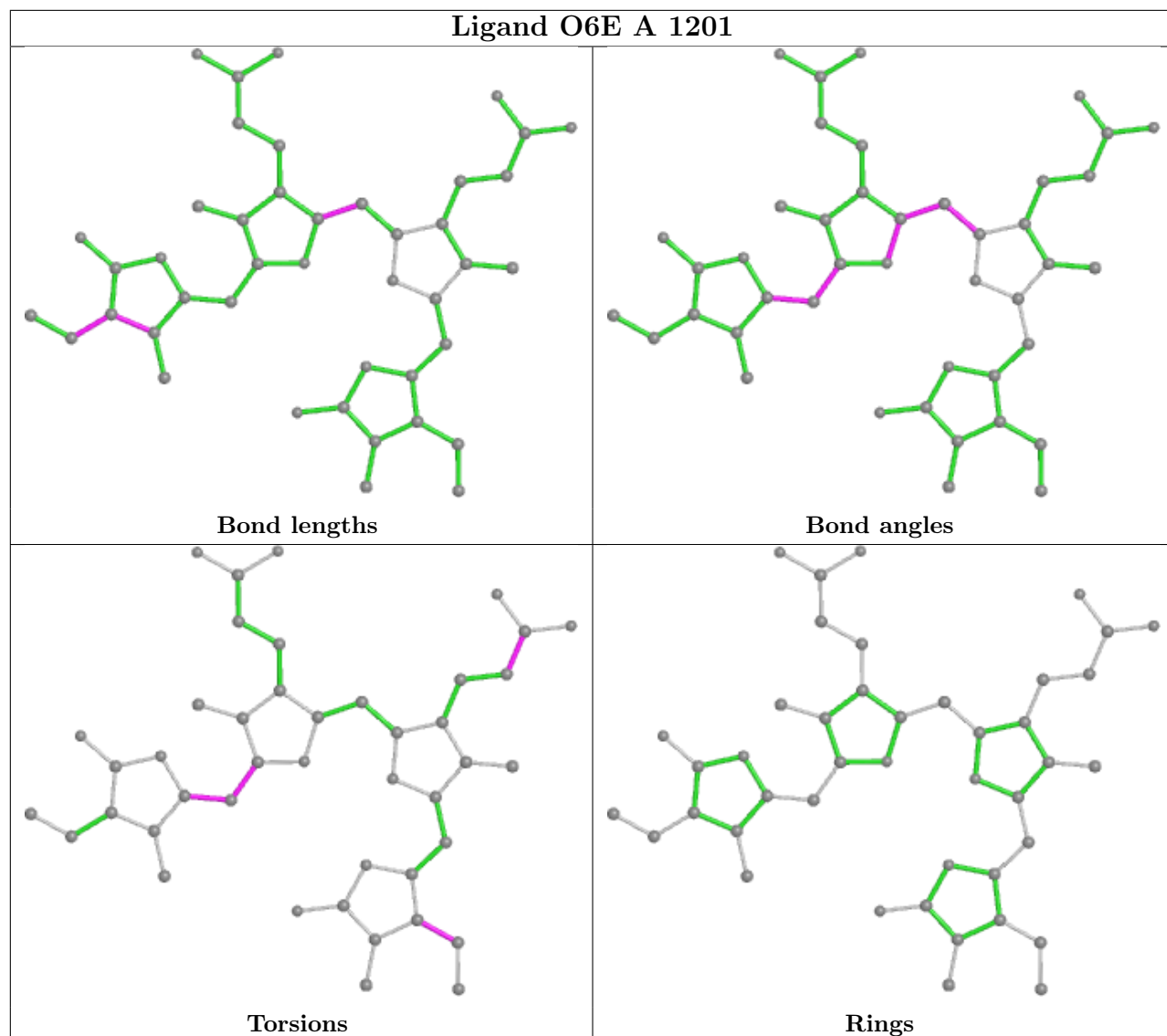
All (13) torsion outliers are listed below:

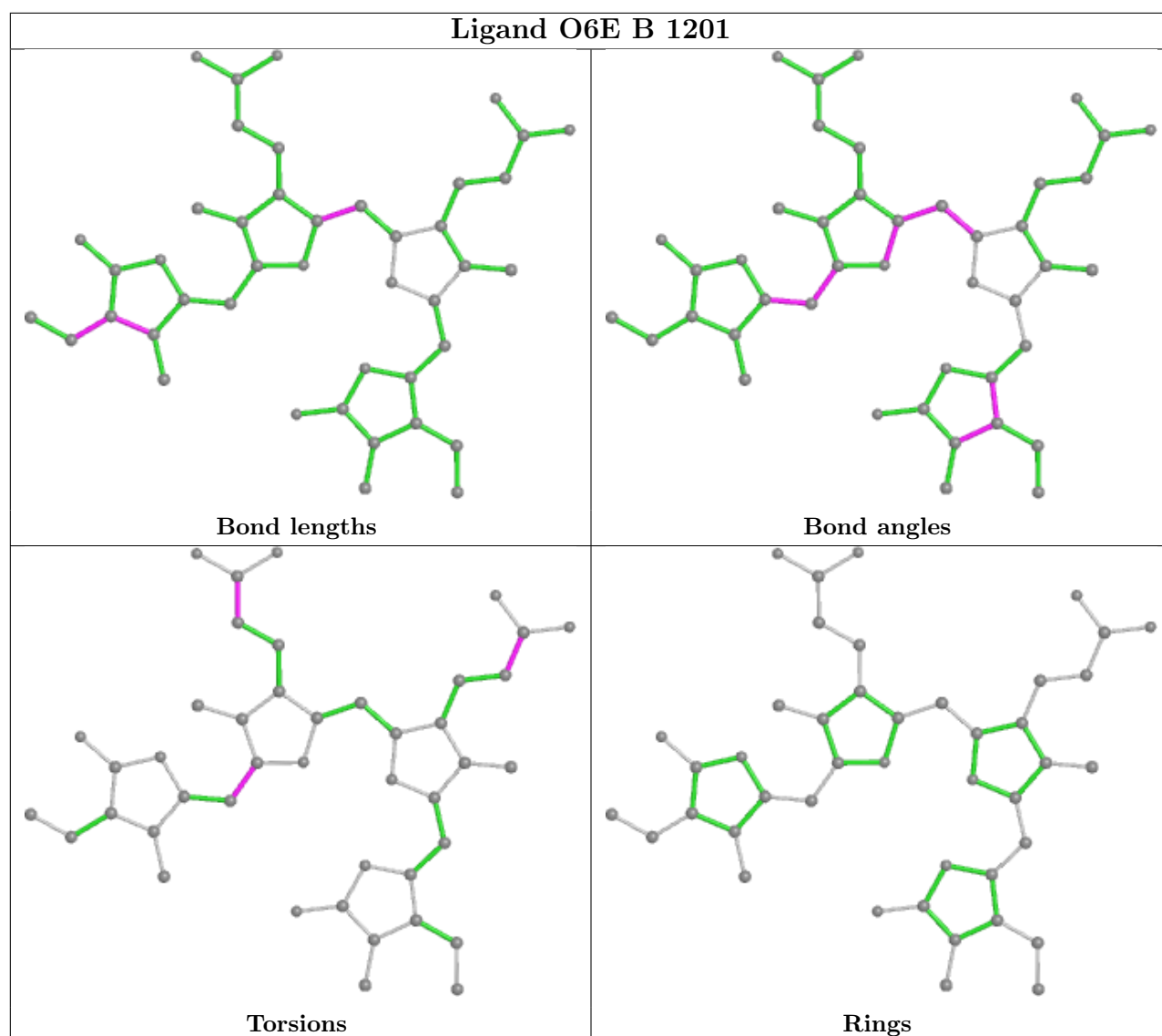
Mol	Chain	Res	Type	Atoms
2	A	1201	O6E	CAW-CAP-CBL-NAE
2	B	1201	O6E	CAW-CAP-CBL-NAE
2	A	1201	O6E	CAW-CAP-CBL-CBH
2	B	1201	O6E	CAW-CAP-CBL-CBH
2	A	1201	O6E	CAH-CAC-CBJ-CBN
2	A	1201	O6E	CAH-CAC-CBJ-CBD
2	A	1201	O6E	CAD-CAI-CAM-OBG
2	A	1201	O6E	CAD-CAI-CAM-OBA
2	B	1201	O6E	CAD-CAI-CAM-OBG
2	B	1201	O6E	CAD-CAI-CAM-OBA
2	B	1201	O6E	CAA-CAF-CAL-OAZ
2	B	1201	O6E	CAA-CAF-CAL-OBF
2	A	1201	O6E	CBL-CAP-CAW-NAJ

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 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.