



## Full wwPDB EM Validation Report ⓘ

Jul 16, 2025 – 12:51 AM JST

PDB ID : 8ISK / pdb\_00008isk  
EMDB ID : EMD-35693  
Title : Pr conformer of Zea mays phytochrome A1 - ZmphyA1-Pr  
Authors : Zhang, Y.; Ma, C.; Zhao, J.; Gao, N.; Wang, J.  
Deposited on : 2023-03-20  
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](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 : 4-5-2 with Phenix2.0rc1  
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) : 2.44

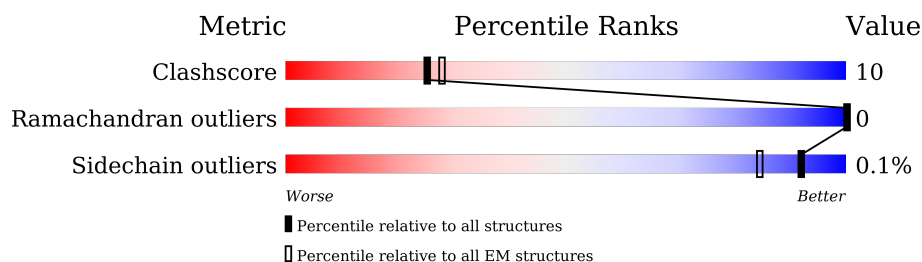
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 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	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  $\leq 5\%$ .

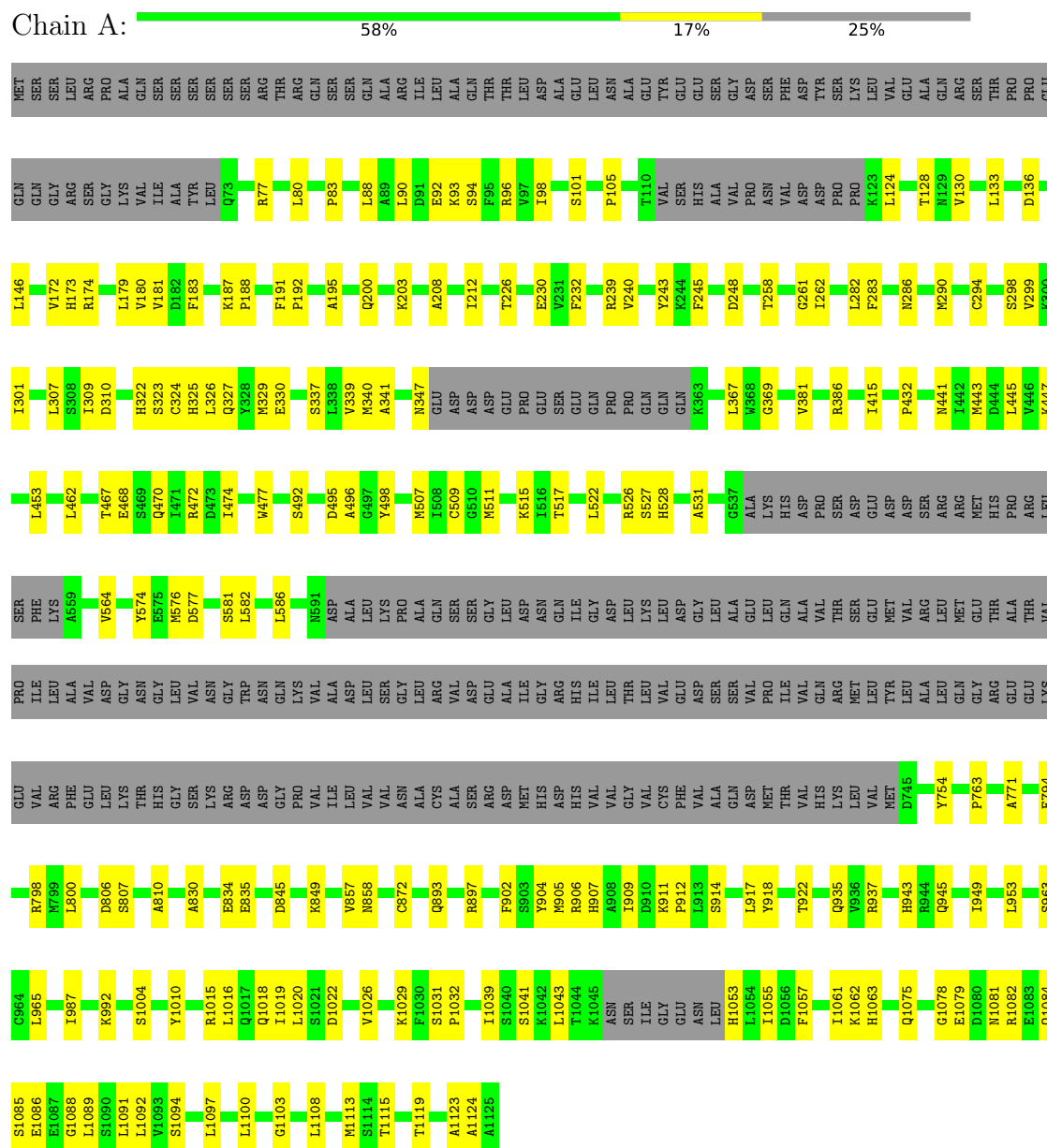
Mol	Chain	Length	Quality of chain
1	A	1125	
1	B	1125	



### 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: Phytochrome



#### • Molecule 1: Phytochrome

Chain B:

57%

19%

25%

GLN	GLN	R174	V344	F476	D573	LEU	GLY	R222	D960	L1059
GLN	GLY	A175	N345	F476	H580	VAL	SER	R222	S963	R1060
ARG	ARG	C178	E346	E480	S581	ASN	LYS	L823	L963	I1061
SER	SER	L179	N347	T486	L582	TRP	ASP	C824	L965	K1062
GLY	GLY	V180	GLU	G487	R587	ASN	ASP	N828	D966	H1063
LYS	LYS	V181	ASP	L488	N591	GLN	GLY	E837	L967	Q1064
VAL	VAL	E190	ASP	L493	N591	LYS	PRO	P840	D968	E1071
ILE	ILE	A193	ASP	L493	N591	ALA	VAL	P840	M969	I1072
ALA	ALA	T194	PRO	Y498	N591	LEU	LEU	C853	Q975	Q1075
SER	SER	T194	GLU	P499	N591	LEU	VAL	C853	V978	G1078
SER	SER	A195	SER	P499	N591	GLY	ASN	S856	V979	G1078
SER	SER	A196	GLU	P499	N591	LEU	ALA	S856	S990	N1081
ARG	ARG	G197	GLN	M507	N591	ALA	ALA	I874	Q984	R1082
THR	THR	L80	PRO	I508	N591	VAL	CYS	H875	V985	E1083
ARG	ARG	A99	PRO	M511	N591	ASP	SER	V876	L986	Q1084
GLN	GLN	L90	GLN	M511	N591	GLY	ASP	L885	L987	S1085
SER	SER	R96	GLN	V513	N591	ALA	ASP	L885	R987	E1086
SER	SER	V97	GLN	A514	N591	ILE	MET	Q889	R995	L1089
ALA	ALA	I98	GLN	I516	N591	GLY	HIS	A890	L1000	L1092
ALA	ALA	I98	GLN	I516	N591	ARG	ASP	Q893	S1004	L1098
ILE	ILE	S101	GLY	S518	N591	ILE	VAL	L896	M1005	R1099
LEU	LEU	E102	GLY	S518	N591	LEU	VAL	L896	Y1010	L1100
ALA	ALA	N103	ASP	K519	N591	THR	GLY	L899	D1012	M1101
GLN	GLN	A104	D520	D520	N591	LEU	VAL	L899	L1016	L1105
THR	THR	P105	Y387	I521	N591	LEU	VAL	L899	Q1017	G1112
THR	THR	E106	H399	I521	N591	VAL	CYS	L899	Q1018	M1113
LEU	LEU	M107	H399	L522	N591	VAL	PHE	L899	S914	S1114
ASP	ASP	L108	M401	L522	N591	GLU	ASP	R906	G915	T1115
ALA	ALA	T109	M401	L522	N591	ASP	VAL	H907	M916	F1116
GLU	GLU	T110	E403	L522	N591	LEU	ALA	L907	L917	I1117
LEU	LEU	VAL	M418	L522	N591	ALA	GLN	S919	Y918	A1123
ASN	ASN	HIS	M418	L522	N591	SER	ASP	P912	N941	A1124
GLU	GLU	VAL	V436	L522	N591	VAL	THR	L913	C942	A1125
TYR	TYR	VAL	M443	L522	N591	GLN	THR	S914	H943	
GLU	GLU	ASN	D444	L522	N591	ARG	LEU	S914	R945	
GLY	GLY	ASP	L445	L522	N591	LEU	GLY	Q945	L946	
SER	SER	ASP	L445	L522	N591	TYR	ASP	N947	K948	
ASP	ASP	PRO	A452	L522	N591	LEU	GLU	L949	P767	
SER	SER	PRO	I311	L522	N591	ALA	ALA	D952	A771	
PHE	PHE	PRO	I311	L522	N591	LEU	LEU	L953	D954	
ASP	ASP	K123	H322	L522	N591	GLN	GLN	Q955	Q955	
TYR	TYR	L124	S323	L522	N591	THR	THR	D956	D956	
SER	SER	G127	C324	L522	N591	ALA	ALA	L957	N957	
LYS	LYS	G127	H325	L522	N591	VAL	VAL	L958	L958	
LEU	LEU	I157	L462	L522	N591	THR	THR	L959	T959	
VAL	VAL	L158	Q463	L522	N591	GLU	GLU			
GLU	GLU	V159	T464	L522	N591	VAL	VAL			
ALA	ALA	Q160	A465	L522	N591	ILE	ILE			
GLN	GLN	C161	P466	L522	N591	ALA	ALA			
ARG	ARG	K166	T467	L522	N591	PHE	PHE			
SER	SER	K166	E468	L522	N591	VAL	VAL			
THR	THR	V172	S469	L522	N591	ASP	ASP			
PRO	PRO	H173	Q470	L522	N591	GLY	GLY			
GLU	GLU		I471	L522	N591	ASN	ASN			
			R472	L522	N591	GLY	GLY			

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	229726	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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.18	0/6704	0.38	0/9051
1	B	0.19	0/6728	0.39	0/9083
All	All	0.19	0/13432	0.38	0/18134

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.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1082	ARG	Sidechain
1	B	1082	ARG	Sidechain

### 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	6581	0	6617	138	0
1	B	6606	0	6649	141	0
2	A	43	0	0	1	0
2	B	43	0	0	0	0
All	All	13273	0	13266	270	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 10.

All (270) 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:1075:GLN:HA	1:A:1081:ASN:ND2	1.44	1.28
1:A:1084:GLN:HB3	1:A:1089:LEU:CD2	1.71	1.19
1:B:1064:GLN:HG2	1:B:1113:MET:SD	1.87	1.14
1:A:1084:GLN:CB	1:A:1089:LEU:HD21	1.78	1.13
1:B:1081:ASN:O	1:B:1084:GLN:HG2	1.48	1.11
1:A:1084:GLN:CB	1:A:1089:LEU:CD2	2.29	1.10
1:A:1084:GLN:HB2	1:A:1089:LEU:HD21	1.32	1.07
1:A:1075:GLN:CA	1:A:1081:ASN:HD22	1.65	1.07
1:A:1084:GLN:HB3	1:A:1089:LEU:HD23	1.40	1.01
1:B:466:PRO:O	1:B:471:ILE:HD11	1.78	0.83
1:A:1075:GLN:HA	1:A:1081:ASN:HD22	0.73	0.80
1:A:1084:GLN:HB2	1:A:1089:LEU:CD2	2.07	0.79
1:B:914:SER:HA	1:B:917:LEU:HD12	1.64	0.79
1:A:1075:GLN:CA	1:A:1081:ASN:ND2	2.33	0.77
1:A:1084:GLN:CB	1:A:1089:LEU:HD23	2.07	0.74
1:B:960:ASP:HB3	1:B:963:SER:HB2	1.69	0.73
1:B:507:MET:HG2	1:B:508:ILE:HG13	1.72	0.71
1:A:904:TYR:HB2	1:B:1089:LEU:HD21	1.71	0.71
1:B:896:LEU:HA	1:B:899:LEU:HD13	1.74	0.70
1:B:1084:GLN:OE1	1:B:1092:LEU:HD12	1.92	0.69
1:A:935:GLN:NE2	1:B:919:SER:O	2.25	0.69
1:A:1085:SER:O	1:A:1089:LEU:HG	1.92	0.69
1:B:536:GLY:HA2	1:B:559:ALA:HA	1.74	0.69
1:A:172:VAL:HG22	1:A:181:VAL:HG12	1.74	0.68
1:A:341:ALA:HB1	1:A:367:LEU:HD11	1.76	0.68
1:A:1022:ASP:OD2	1:A:1094:SER:OG	2.12	0.67
1:B:1016:LEU:O	1:B:1020:LEU:HG	1.95	0.67
1:B:158:LEU:HD22	1:B:194:THR:HG23	1.77	0.66
1:A:325:HIS:NE2	2:A:1201:O6E:OAZ	2.18	0.66
1:A:88:LEU:HD12	1:A:183:PHE:HE2	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:THR:HG22	1:A:470:GLN:HG2	1.77	0.65
1:B:466:PRO:O	1:B:471:ILE:CD1	2.45	0.64
1:B:890:ALA:H	1:B:893:GLN:H	1.44	0.64
1:A:906:ARG:O	1:A:906:ARG:NH1	2.30	0.64
1:A:806:ASP:OD1	1:A:807:SER:N	2.32	0.63
1:B:517:THR:OG1	1:B:520:ASP:OD1	2.14	0.62
1:B:1010:TYR:HB3	1:B:1123:ALA:HB3	1.81	0.62
1:A:806:ASP:HB3	1:A:810:ALA:HB2	1.82	0.62
1:A:1078:GLY:O	1:A:1092:LEU:HD21	2.00	0.61
1:B:967:LEU:HD21	1:B:1100:LEU:HD13	1.81	0.61
1:A:77:ARG:NH1	1:A:310:ASP:OD2	2.33	0.61
1:B:106:GLU:O	1:B:110:THR:OG1	2.19	0.60
1:A:124:LEU:HD21	1:A:133:LEU:HD21	1.84	0.60
1:A:904:TYR:HB2	1:B:1089:LEU:CD2	2.31	0.59
1:B:178:CYS:HB3	1:B:311:ILE:HG23	1.85	0.59
1:A:893:GLN:O	1:A:897:ARG:HG3	2.02	0.59
1:B:202:TYR:CE1	1:B:387:TYR:HB3	2.38	0.59
1:B:196:ALA:HA	1:B:200:GLN:OE1	2.03	0.59
1:B:1042:LYS:HB3	1:B:1058:GLU:HB2	1.83	0.59
1:A:918:TYR:O	1:A:922:THR:HG23	2.02	0.59
1:B:332:MET:O	1:B:333:ASN:ND2	2.37	0.58
1:B:952:ASP:OD1	1:B:957:ASN:ND2	2.36	0.58
1:B:1101:MET:N	1:B:1101:MET:SD	2.77	0.58
1:B:101:SER:OG	1:B:103:ASN:OD1	2.20	0.57
1:B:587:ARG:HH22	1:B:746:LYS:HD3	1.69	0.57
1:B:824:CYS:O	1:B:828:ASN:ND2	2.35	0.57
1:A:1103:GLY:CA	1:A:1119:THR:O	2.52	0.56
1:B:290:MET:SD	1:B:386:ARG:NH1	2.77	0.56
1:B:912:PRO:O	1:B:916:MET:HG3	2.06	0.56
1:A:98:ILE:HG21	1:A:307:LEU:HD22	1.88	0.56
1:A:1086:GLU:HB3	1:B:907:HIS:ND1	2.21	0.56
1:A:96:ARG:NH1	1:A:128:THR:O	2.39	0.56
1:A:771:ALA:HB2	1:A:800:LEU:HD22	1.87	0.56
1:A:1015:ARG:NH2	1:A:1018:GLN:OE1	2.39	0.55
1:A:945:GLN:HE21	1:A:1018:GLN:HB2	1.71	0.55
1:A:1016:LEU:O	1:A:1020:LEU:HG	2.05	0.55
1:A:191:PHE:CG	1:A:192:PRO:HD3	2.42	0.55
1:A:1032:PRO:HD2	1:A:1063:HIS:CE1	2.41	0.55
1:B:955:GLN:HA	1:B:958:ILE:HB	1.88	0.55
1:B:980:SER:HB2	1:B:1017:GLN:NE2	2.21	0.54
1:A:949:ILE:HD12	1:A:949:ILE:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:LYS:O	1:A:526:ARG:NH2	2.37	0.54
1:A:83:PRO:HG3	1:A:299:VAL:HG13	1.90	0.54
1:A:581:SER:HB3	1:A:763:PRO:O	2.07	0.54
1:B:455:TYR:HB2	1:B:520:ASP:HB3	1.88	0.54
1:B:515:LYS:HG2	1:B:521:ILE:HG22	1.88	0.54
1:A:468:GLU:OE2	1:A:472:ARG:NE	2.40	0.54
1:A:1103:GLY:HA2	1:A:1119:THR:O	2.08	0.54
1:B:345:ASN:HA	1:B:365:LYS:HA	1.91	0.53
1:A:963:SER:HB3	1:A:1100:LEU:HD21	1.90	0.53
1:B:573:ASP:OD1	1:B:573:ASP:N	2.40	0.53
1:B:294:CYS:H	1:B:335:ILE:HG23	1.73	0.53
1:B:906:ARG:HD3	1:B:953:LEU:HD23	1.90	0.53
1:A:1084:GLN:HB3	1:A:1089:LEU:CG	2.38	0.53
1:B:945:GLN:O	1:B:949:ILE:HG22	2.09	0.53
1:A:173:HIS:HB2	1:A:180:VAL:HG23	1.90	0.52
1:B:452:ALA:HB3	1:B:523:PHE:HB2	1.92	0.52
1:B:1019:ILE:HD13	1:B:1098:LEU:HG	1.90	0.52
1:A:226:THR:O	1:A:230:GLU:HG2	2.10	0.52
1:A:495:ASP:OD1	1:A:495:ASP:N	2.37	0.52
1:B:943:HIS:O	1:B:947:ASN:ND2	2.43	0.52
1:B:822:ARG:NH2	1:B:840:PRO:O	2.43	0.52
1:A:992:LYS:NZ	1:A:1029:LYS:O	2.43	0.51
1:B:488:LEU:HB2	1:B:749:ARG:NH1	2.26	0.51
1:B:965:LEU:HB3	1:B:1100:LEU:HD21	1.92	0.51
1:A:918:TYR:CE2	1:B:986:LEU:HD13	2.46	0.51
1:B:461:ARG:HD2	1:B:465:ALA:HB3	1.91	0.51
1:B:1038:ASP:OD2	1:B:1062:LYS:HB3	2.09	0.51
1:B:172:VAL:HG12	1:B:181:VAL:HG22	1.93	0.51
1:B:995:ARG:HH21	1:B:1036:SER:HB2	1.76	0.51
1:A:1043:LEU:HD23	1:A:1055:ILE:HD13	1.92	0.50
1:A:1075:GLN:NE2	1:A:1084:GLN:HA	2.26	0.50
1:A:282:LEU:O	1:A:286:ASN:N	2.36	0.50
1:B:202:TYR:HE1	1:B:387:TYR:HB3	1.77	0.50
1:A:232:PHE:HB2	1:A:240:VAL:HG21	1.93	0.50
1:A:1039:ILE:HG23	1:A:1061:ILE:HG12	1.93	0.50
1:B:980:SER:HB2	1:B:1017:GLN:HE22	1.77	0.50
1:A:507:MET:O	1:A:527:SER:OG	2.25	0.50
1:B:322:HIS:CE1	1:B:324:CYS:H	2.29	0.50
1:A:307:LEU:HG	1:A:309:ILE:H	1.75	0.50
1:B:104:ALA:O	1:B:108:LEU:HB2	2.12	0.50
1:A:381:VAL:O	1:A:386:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:937:ARG:HG3	1:A:937:ARG:HH11	1.76	0.50
1:A:290:MET:SD	1:A:386:ARG:NH1	2.85	0.49
1:A:470:GLN:O	1:A:474:ILE:HG13	2.11	0.49
1:A:531:ALA:HB3	1:A:564:VAL:HG23	1.94	0.49
1:A:1026:VAL:HG21	1:A:1091:LEU:HD21	1.92	0.49
1:A:415:ILE:HG12	1:A:574:TYR:CE1	2.48	0.49
1:B:913:LEU:O	1:B:917:LEU:HG	2.12	0.49
1:A:515:LYS:HG2	1:A:517:THR:O	2.12	0.49
1:B:1012:ASP:OD1	1:B:1012:ASP:N	2.45	0.49
1:A:200:GLN:HA	1:A:203:LYS:HD3	1.95	0.49
1:A:845:ASP:OD1	1:A:849:LYS:N	2.42	0.49
1:B:1105:ILE:HD11	1:B:1116:PHE:HD1	1.78	0.49
1:A:105:PRO:HA	1:A:124:LEU:HD12	1.94	0.49
1:A:130:VAL:HA	1:A:133:LEU:HD13	1.95	0.49
1:B:978:VAL:HG11	1:B:1000:LEU:HD11	1.94	0.49
1:B:1000:LEU:HD13	1:B:1005:MET:HE3	1.95	0.48
1:B:1081:ASN:HB3	1:B:1084:GLN:HE21	1.77	0.48
1:A:294:CYS:HB2	1:A:326:LEU:HD22	1.93	0.48
1:A:453:LEU:HG	1:A:522:LEU:HD23	1.95	0.48
1:A:443:MET:HE1	1:A:462:LEU:HB3	1.95	0.48
1:B:339:VAL:HG22	1:B:372:VAL:HG13	1.94	0.48
1:A:1108:LEU:HB2	1:A:1115:THR:HG23	1.96	0.48
1:A:283:PHE:HB3	1:A:341:ALA:HB2	1.96	0.48
1:B:767:PRO:HD2	1:B:874:ILE:O	2.13	0.47
1:A:329:MET:HE1	1:A:337:SER:HB3	1.95	0.47
1:A:347:ASN:OD1	1:A:347:ASN:N	2.47	0.47
1:B:1113:MET:HE2	1:B:1113:MET:N	2.29	0.47
1:B:853:CYS:HB3	1:B:876:VAL:HG22	1.96	0.47
1:B:493:LEU:HD11	1:B:511:MET:HB2	1.97	0.47
1:A:953:LEU:HD23	1:A:953:LEU:H	1.80	0.47
1:A:1053:HIS:HB2	1:A:1124:ALA:HB3	1.97	0.46
1:B:158:LEU:HD13	1:B:194:THR:HA	1.98	0.46
1:B:209:ILE:HG22	1:B:213:GLN:HE21	1.80	0.46
1:A:987:ILE:HG12	1:B:918:TYR:HB2	1.97	0.46
1:B:488:LEU:HB3	1:B:513:VAL:HG12	1.96	0.46
1:B:515:LYS:NZ	1:B:518:SER:O	2.37	0.46
1:B:885:LEU:HA	1:B:889:GLN:HB3	1.98	0.46
1:A:1015:ARG:O	1:A:1019:ILE:HG12	2.16	0.46
1:B:941:ASN:HD21	1:B:1017:GLN:HE21	1.63	0.46
1:A:88:LEU:HB2	1:A:181:VAL:HG23	1.96	0.46
1:A:965:LEU:HD23	1:A:965:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1079:GLU:HG2	1:A:1092:LEU:HD22	1.97	0.46
1:B:1081:ASN:HB3	1:B:1084:GLN:NE2	2.31	0.46
1:B:1112:GLY:C	1:B:1113:MET:HE2	2.41	0.46
1:A:496:ALA:HA	1:A:754:TYR:HB3	1.98	0.46
1:A:857:VAL:HG13	1:A:872:CYS:SG	2.56	0.46
1:B:226:THR:O	1:B:230:GLU:HG2	2.16	0.45
1:B:954:ASP:OD1	1:B:954:ASP:N	2.49	0.45
1:A:907:HIS:CD2	1:B:1086:GLU:HB3	2.50	0.45
1:B:96:ARG:HB3	1:B:127:GLY:HA2	1.98	0.45
1:B:975:GLN:HB2	1:B:1005:MET:HG3	1.98	0.45
1:A:94:SER:OG	1:A:96:ARG:NH2	2.49	0.45
1:A:327:GLN:O	1:A:330:GLU:HG3	2.15	0.45
1:B:986:LEU:HD23	1:B:986:LEU:O	2.17	0.45
1:A:1031:SER:HA	1:A:1063:HIS:NE2	2.31	0.45
1:A:1041:SER:HB2	1:A:1057:PHE:HE1	1.81	0.45
1:A:92:GLU:OE1	1:A:174:ARG:NH1	2.50	0.45
1:A:1010:TYR:N	1:A:1123:ALA:O	2.35	0.45
1:A:1097:LEU:HD23	1:A:1100:LEU:HD12	1.98	0.45
1:B:161:CYS:SG	1:B:166:LYS:N	2.72	0.45
1:B:175:ALA:HB3	1:B:178:CYS:HB2	1.98	0.45
1:B:1044:THR:HB	1:B:1056:ASP:HB2	1.98	0.45
1:B:1078:GLY:O	1:B:1084:GLN:NE2	2.50	0.45
1:B:1081:ASN:CB	1:B:1084:GLN:HE21	2.29	0.45
1:A:1004:SER:HB3	1:A:1043:LEU:HD13	1.99	0.44
1:B:307:LEU:HD13	1:B:311:ILE:HD11	1.99	0.44
1:B:399:HIS:O	1:B:403:GLU:HG2	2.16	0.44
1:A:239:ARG:HG3	1:A:258:THR:HG22	1.99	0.44
1:B:327:GLN:N	1:B:327:GLN:OE1	2.50	0.44
1:B:762:ASN:OD1	1:B:762:ASN:N	2.50	0.44
1:B:209:ILE:O	1:B:213:GLN:HG3	2.17	0.44
1:A:146:LEU:HG	1:A:179:LEU:HD13	1.99	0.44
1:A:835:GLU:HG2	1:A:858:ASN:HA	1.98	0.44
1:B:201:SER:O	1:B:204:LEU:HB3	2.18	0.44
1:A:93:LYS:HA	1:A:93:LYS:HD3	1.82	0.44
1:A:195:ALA:HA	1:A:200:GLN:HG2	2.00	0.44
1:A:1062:LYS:HG3	1:A:1113:MET:HE2	1.98	0.44
1:B:466:PRO:HB2	1:B:471:ILE:HG13	2.00	0.44
1:B:1075:GLN:OE1	1:B:1081:ASN:ND2	2.51	0.44
1:A:918:TYR:HB2	1:B:987:ILE:HG13	2.00	0.44
1:A:245:PHE:CD2	1:A:369:GLY:HA2	2.53	0.44
1:B:1071:GLU:HG2	1:B:1072:ILE:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:TYR:O	1:A:369:GLY:HA3	2.18	0.44
1:B:157:ILE:HG22	1:B:159:VAL:HG23	2.00	0.43
1:B:325:HIS:CD2	1:B:325:HIS:C	2.96	0.43
1:A:441:ASN:OD1	1:A:441:ASN:N	2.51	0.43
1:A:187:LYS:HE3	1:A:188:PRO:HD2	2.00	0.43
1:A:1092:LEU:HA	1:A:1092:LEU:HD23	1.54	0.43
1:B:980:SER:O	1:B:984:GLN:HG3	2.18	0.43
1:A:248:ASP:OD1	1:A:248:ASP:N	2.42	0.43
1:A:917:LEU:HD12	1:A:943:HIS:CE1	2.52	0.43
1:B:443:MET:O	1:B:443:MET:HE3	2.19	0.43
1:A:432:PRO:HG3	1:A:586:LEU:HD12	1.99	0.43
1:A:90:LEU:HB2	1:A:179:LEU:HB2	2.00	0.43
1:A:492:SER:OG	1:A:495:ASP:OD1	2.21	0.43
1:A:1075:GLN:O	1:A:1092:LEU:HD21	2.18	0.43
1:B:1106:ARG:HB2	1:B:1117:ILE:HB	2.00	0.43
1:A:576:MET:HE2	1:A:576:MET:HB2	1.63	0.43
1:B:173:HIS:HB2	1:B:180:VAL:HG12	2.01	0.43
1:B:487:GLY:HA3	1:B:748:THR:HG22	2.01	0.43
1:B:1082:ARG:C	1:B:1084:GLN:H	2.26	0.43
1:B:1084:GLN:OE1	1:B:1092:LEU:CD1	2.65	0.42
1:A:902:PHE:HE1	1:B:953:LEU:HD21	1.84	0.42
1:A:80:LEU:HD23	1:A:298:SER:HB3	2.00	0.42
1:A:509:CYS:SG	1:A:528:HIS:HB3	2.59	0.42
1:A:1084:GLN:HG2	1:A:1092:LEU:HD12	2.00	0.42
1:A:101:SER:HA	1:A:301:ILE:HG22	2.01	0.42
1:B:468:GLU:HB3	1:B:472:ARG:HH12	1.84	0.42
1:B:1000:LEU:HD22	1:B:1041:SER:HB3	2.01	0.42
1:A:208:ALA:O	1:A:212:ILE:HG13	2.19	0.42
1:B:498:TYR:CD1	1:B:499:PRO:HD2	2.54	0.42
1:A:511:MET:HE2	1:A:511:MET:HB3	1.90	0.42
1:A:911:LYS:O	1:A:914:SER:OG	2.35	0.42
1:B:97:VAL:HG21	1:B:124:LEU:HD11	2.00	0.42
1:B:198:ALA:O	1:B:199:LEU:HD23	2.20	0.42
1:A:794:GLU:O	1:A:798:ARG:NH1	2.52	0.42
1:B:211:LYS:NZ	1:B:230:GLU:OE1	2.40	0.42
1:A:124:LEU:HD23	1:A:124:LEU:HA	1.90	0.42
1:A:339:VAL:C	1:A:340:MET:HG3	2.44	0.42
1:B:79:LYS:O	1:B:80:LEU:HD13	2.20	0.42
1:B:436:VAL:HG23	1:B:462:LEU:HD11	2.02	0.42
1:B:790:TRP:CE2	1:B:811:SER:HB3	2.55	0.42
1:B:89:ALA:C	1:B:90:LEU:HD23	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:HIS:NE2	1:B:329:MET:SD	2.83	0.42
1:B:322:HIS:CG	1:B:323:SER:N	2.87	0.42
1:B:580:HIS:CD2	1:B:746:LYS:HE2	2.54	0.42
1:B:1004:SER:HB3	1:B:1043:LEU:HD22	2.02	0.42
1:B:98:ILE:HG21	1:B:307:LEU:HD21	2.01	0.41
1:B:526:ARG:HD2	1:B:571:TRP:CH2	2.55	0.41
1:A:200:GLN:O	1:A:203:LYS:HG2	2.20	0.41
1:B:190:GLU:HG2	1:B:193:ALA:HB2	2.02	0.41
1:A:905:MET:SD	1:A:909:ILE:HD11	2.60	0.41
1:B:969:MET:N	1:B:969:MET:SD	2.94	0.41
1:B:1060:ARG:HH11	1:B:1115:THR:HG21	1.86	0.41
1:A:283:PHE:HA	1:A:286:ASN:O	2.21	0.41
1:B:1084:GLN:CD	1:B:1092:LEU:CD1	2.94	0.41
1:A:261:GLY:C	1:A:262:ILE:HD13	2.46	0.41
1:B:476:PHE:O	1:B:480:GLU:HG2	2.21	0.41
1:A:1075:GLN:OE1	1:A:1088:GLY:HA3	2.21	0.41
1:B:418:MET:HE1	1:B:764:LEU:HD11	2.01	0.41
1:B:1104:ASP:OD1	1:B:1105:ILE:N	2.53	0.41
1:B:771:ALA:HB2	1:B:800:LEU:HD22	2.02	0.41
1:A:909:ILE:O	1:A:912:PRO:HD2	2.21	0.41
1:B:463:GLN:HB3	1:B:464:THR:H	1.64	0.41
1:B:486:THR:OG1	1:B:515:LYS:HD3	2.21	0.41
1:B:344:VAL:HG13	1:B:401:ASN:OD1	2.20	0.41
1:B:445:LEU:HD22	1:B:582:LEU:HD22	2.03	0.41
1:B:455:TYR:O	1:B:458:LYS:HG2	2.20	0.41
1:B:837:GLU:O	1:B:856:SER:HB3	2.21	0.41
1:A:323:SER:O	1:A:327:GLN:HG2	2.21	0.41
1:B:467:THR:HG23	1:B:470:GLN:HE22	1.86	0.41
1:A:322:HIS:CE1	1:A:324:CYS:H	2.39	0.40
1:A:477:TRP:NE1	1:A:498:TYR:HA	2.36	0.40
1:A:445:LEU:HD22	1:A:582:LEU:HD22	2.03	0.40
1:A:574:TYR:HA	1:A:577:ASP:HB2	2.03	0.40
1:B:224:CYS:O	1:B:228:VAL:HG22	2.21	0.40
1:B:443:MET:HG2	1:B:462:LEU:HD22	2.03	0.40
1:A:830:ALA:HA	1:A:834:GLU:O	2.22	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	833/1125 (74%)	799 (96%)	34 (4%)	0	100	100
1	B	836/1125 (74%)	802 (96%)	34 (4%)	0	100	100
All	All	1669/2250 (74%)	1601 (96%)	68 (4%)	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	718/962 (75%)	717 (100%)	1 (0%)	92	96
1	B	722/962 (75%)	721 (100%)	1 (0%)	92	96
All	All	1440/1924 (75%)	1438 (100%)	2 (0%)	92	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	ASP
1	B	1083	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	374	HIS

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Mol	Chain	Res	Type
1	A	762	ASN
1	A	883	HIS
1	A	907	HIS
1	A	1081	ASN
1	A	1096	ASN
1	B	160	GLN
1	B	213	GLN
1	B	277	GLN
1	B	333	ASN
1	B	399	HIS
1	B	580	HIS
1	B	858	ASN
1	B	882	GLN
1	B	883	HIS
1	B	893	GLN
1	B	947	ASN
1	B	957	ASN
1	B	1007	GLN
1	B	1017	GLN
1	B	1084	GLN

### 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 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	B	1201	1	42,46,46	0.97	3 (7%)	50,67,67	1.33	2 (4%)
2	O6E	A	1201	1	42,46,46	0.99	3 (7%)	50,67,67	1.13	5 (10%)

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	B	1201	1	-	4/25/74/74	0/4/4/4
2	O6E	A	1201	1	-	7/25/74/74	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	3.15	1.37	1.35
2	A	1201	O6E	CAB-CBI	-2.93	1.39	1.47
2	B	1201	O6E	CAB-CBI	-2.87	1.39	1.47
2	B	1201	O6E	CAO-CAV	2.87	1.37	1.35
2	B	1201	O6E	CBI-CBC	2.13	1.41	1.37
2	A	1201	O6E	CBI-CBC	2.10	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	6.39	136.44	128.81
2	A	1201	O6E	CBM-CBI-CBC	-3.31	103.68	107.92
2	A	1201	O6E	CBO-CAO-CAV	3.29	132.73	128.81
2	B	1201	O6E	CAW-CAP-CBL	3.01	135.44	128.08
2	A	1201	O6E	CAW-CAP-CBL	2.53	134.27	128.08
2	A	1201	O6E	CAO-CAV-NAE	-2.20	125.78	128.83
2	A	1201	O6E	CAV-CBB-CBH	-2.11	104.45	106.78

There are no chirality outliers.

All (11) torsion outliers are listed below:

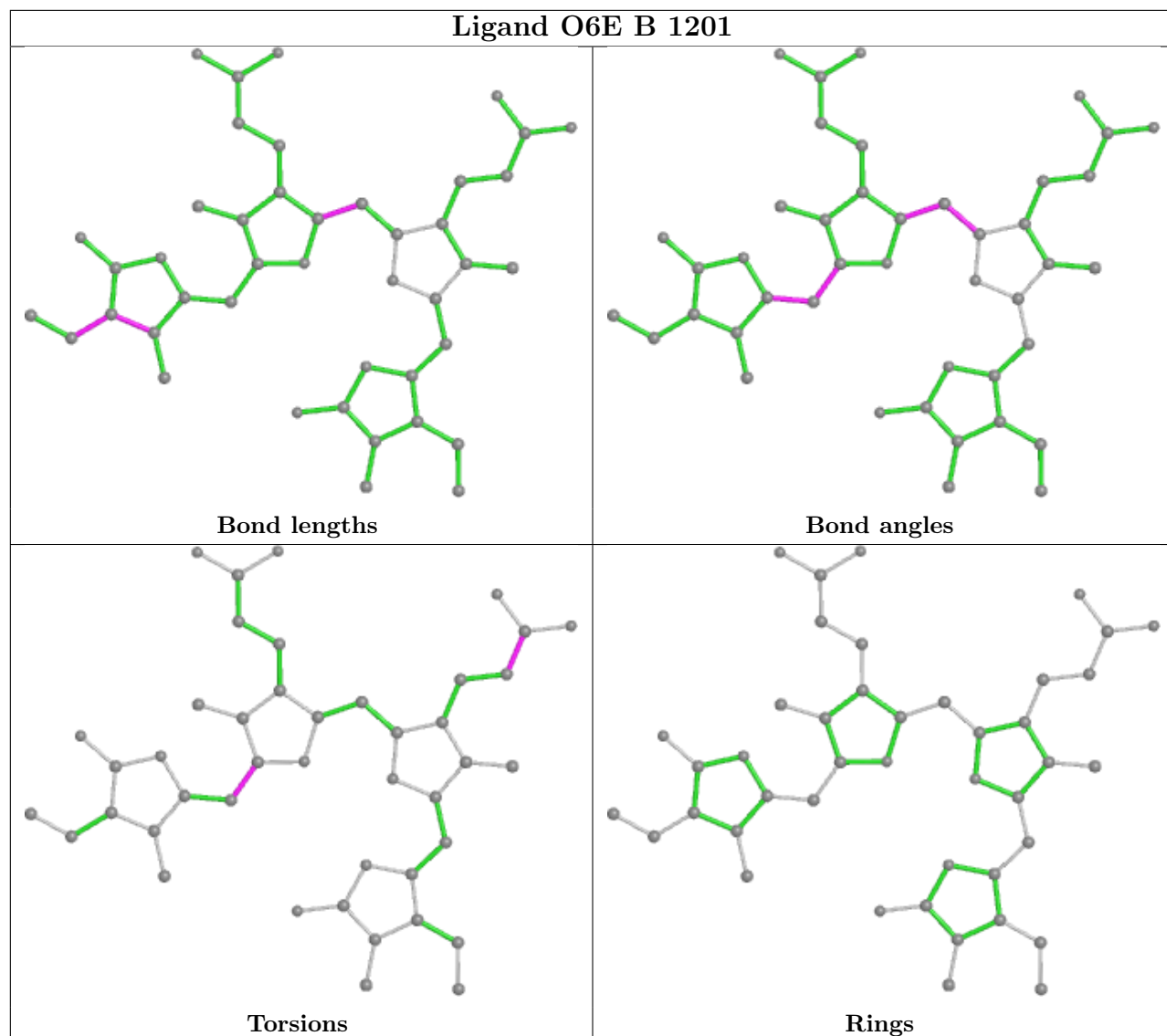
Mol	Chain	Res	Type	Atoms
2	A	1201	O6E	CAW-CAP-CBL-NAE
2	B	1201	O6E	CAW-CAP-CBL-NAE
2	A	1201	O6E	CAW-CAP-CBL-CBH
2	B	1201	O6E	CAW-CAP-CBL-CBH
2	A	1201	O6E	CAH-CAC-CBJ-CBN
2	B	1201	O6E	CAD-CAI-CAM-OBA
2	A	1201	O6E	CAH-CAC-CBJ-CBD
2	B	1201	O6E	CAD-CAI-CAM-OBG
2	A	1201	O6E	CAD-CAI-CAM-OBG
2	A	1201	O6E	CAD-CAI-CAM-OBA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

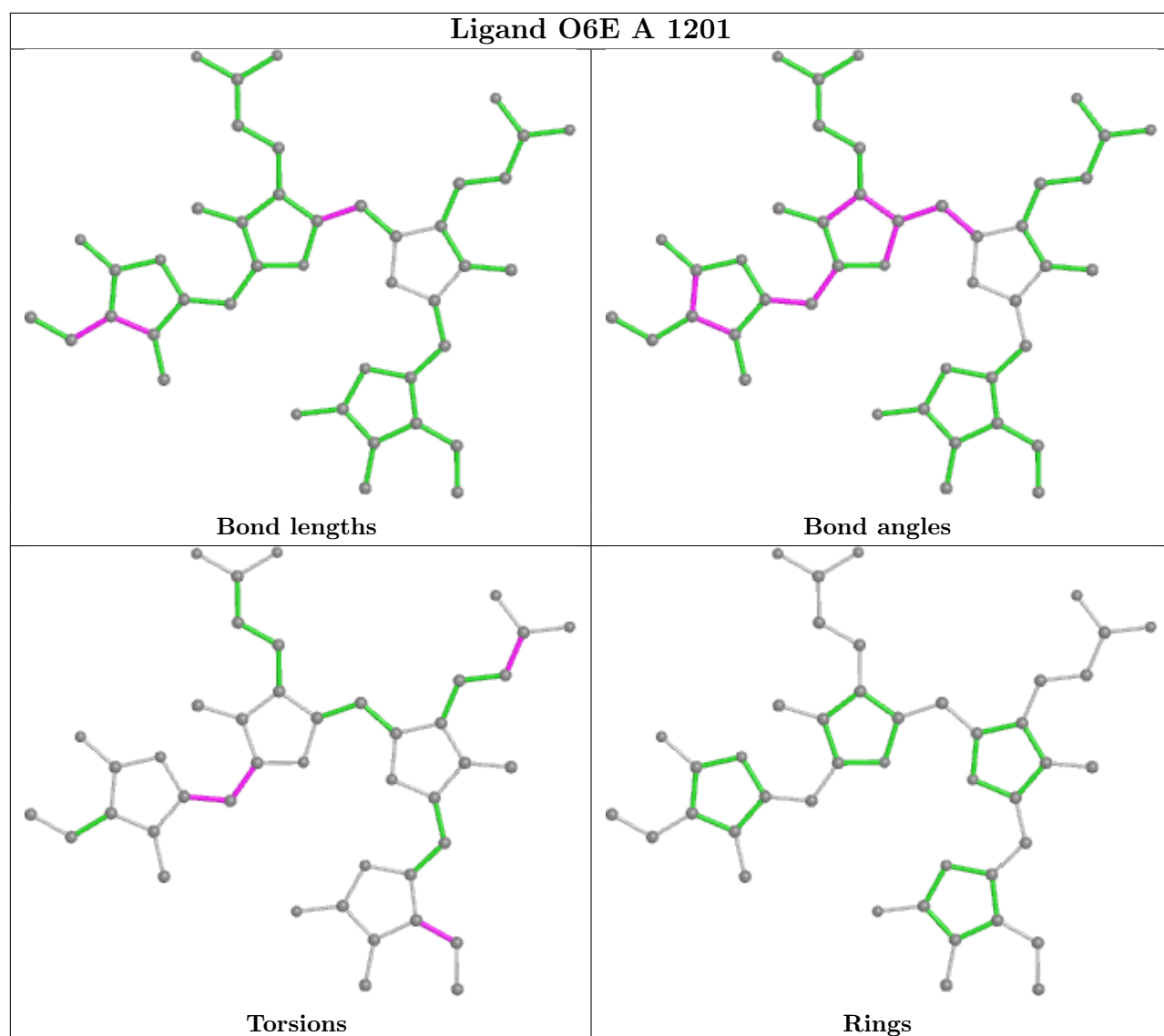
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	O6E	1	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.