

wwPDB X-ray Structure Validation Summary Report (i)

Nov 7, 2023 – 06:33 PM JST

) :	8HQ8
e :	Bry-LHCII homotrimer of Bryopsis corticulans
3 :	Li, Z.H.; Shen, J.R.; Wang, W.D.
ı :	2022-12-13
:	2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
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 (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.60 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain		
			6%		
1	A	249	69%	20%	10%
			6%		
1	В	249	71%	18%	10%
			7%		
1	С	249	72%	17%	11%
			7%		
1	D	249	73%	16%	10%
			14%		
1	E	249	66%	22%	• 10%
			6%		
1	F	249	71%	17%	• 10%



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	BET	В	321	-	-	-	Х
11	LMG	F	319	-	-	-	Х
3	NEX	А	303	-	-	-	Х
3	NEX	D	303	-	-	_	Х
4	LMU	А	304	-	-	-	Х
4	LMU	В	305	-	-	-	Х
5	CHL	А	305	Х	-	-	-
5	CHL	А	306	Х	-	-	-
5	CHL	А	309	Х	-	-	-
5	CHL	А	310	Х	-	-	-
5	CHL	А	311	Х	-	-	-
5	CHL	А	312	Х	-	-	-
5	CHL	А	313	Х	-	-	-
5	CHL	А	318	Х	-	-	-
5	CHL	В	306	Х	-	-	-
5	CHL	В	307	Х	-	-	-
5	CHL	В	310	Х	-	-	-
5	CHL	В	311	Х	-	-	-
5	CHL	В	312	Х	-	-	-
5	CHL	В	313	Х	-	-	-
5	CHL	В	314	X	-	-	-
5	CHL	В	319	Х	-	-	-
5	CHL	С	305	X	-	-	-
5	CHL	С	306	Х	-	-	-
5	CHL	С	309	Х	_	-	-
5	CHL	С	310	Х	-	-	-
5	CHL	С	311	Х	-	-	-
5	CHL	С	312	Х	_	-	-
5	CHL	С	313	Х	-	-	-
5	CHL	С	318	Х	_	-	-
5	CHL	D	305	X	-	-	-
5	CHL	D	306	X	-	_	-
5	CHL	D	309	Х	_	-	-
5	CHL	D	310	X	-	-	-
5	CHL	D	311	X	-	-	-
5	CHL	D	312	X	-	-	-
5	CHL	D	313	X	_	-	-
5	CHL	D	318	X	-	-	-
5	CHL	Е	304	X	-	-	-
5	CHL	Е	305	X	-	-	-

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CHL	Е	308	X	-	_	-
5	CHL	E	309	X	_	_	_
5	CHL	Е	310	X	_	-	_
5	CHL	Е	311	X	-	-	-
5	CHL	Е	312	X	-	_	-
5	CHL	Е	317	X	-	_	_
5	CHL	F	304	X	-	_	_
5	CHL	F	305	X	-	-	-
5	CHL	F	308	Х	-	-	-
5	CHL	F	309	X	-	-	-
5	CHL	F	310	X	-	-	-
5	CHL	F	311	Х	_	-	-
5	CHL	F	312	X	-	-	-
5	CHL	F	317	Х	-	-	-
6	CLA	А	307	X	-	-	-
6	CLA	А	308	X	-	-	-
6	CLA	А	314	Х	_	-	-
6	CLA	А	315	X	-	-	-
6	CLA	А	316	Х	_	-	_
6	CLA	А	317	Х	-	-	-
6	CLA	В	308	Х	-	-	_
6	CLA	В	309	Х	-	-	-
6	CLA	В	315	Х	-	-	-
6	CLA	В	316	Х	_	-	_
6	CLA	В	317	Х	-	-	-
6	CLA	В	318	Х	-	-	-
6	CLA	С	307	Х	_	-	-
6	CLA	С	308	Х	-	-	_
6	CLA	С	314	Х	_	-	-
6	CLA	С	315	Х	_	-	_
6	CLA	С	316	Х	_	-	_
6	CLA	С	317	Х	_	-	-
6	CLA	D	307	Х	_	-	_
6	CLA	D	308	Х	_	-	_
6	CLA	D	314	Х	-	-	-
6	CLA	D	315	Х	-	-	-
6	CLA	D	316	Х	-	-	-
6	CLA	D	317	Х	-	-	-
6	CLA	Е	306	Х	-	-	-
6	CLA	Е	307	Х	-	-	-
6	CLA	Е	313	Х	-	_	-
6	CLA	Е	314	Х	-	-	-
<u>.</u>		,				Conti	nued on next page



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CLA	Е	315	Х	-	-	-
6	CLA	Е	316	Х	-	-	-
6	CLA	F	306	Х	-	-	-
6	CLA	F	307	Х	-	-	-
6	CLA	F	313	Х	-	-	-
6	CLA	F	314	Х	-	-	-
6	CLA	F	315	Х	-	-	-
6	CLA	F	316	Х	-	-	-

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2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 16480 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 siphonaxanthin chlorophyll a/b binding light-harvesting complex II, Bry-Lhcb1.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	222	Total	С	Ν	0	S	0	0	0
1	Π	223	1672	1083	265	314	10	0	0	0
1	В	003	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	D	220	1669	1083	266	310	10	0	0	0
1	C	<u> </u>	Total	С	Ν	0	S	0	0	0
1			1659	1075	264	310	10	0		
1	П	202	Total	С	Ν	0	S	0	0	0
1	D	220	1682	1090	267	315	10	0	0	U
1	F	223	Total	С	Ν	0	S	0	0	0
			1684	1095	267	312	10	0	0	0
1	F	002	Total	C	Ν	0	S	0	0	0
	I.	220	1685	1094	267	314	10	0	0	

• Molecule 2 is Siphonaxanthin (three-letter code: 0IE) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).





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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total C O 44 40 4	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 44 & 40 & 4 \end{array}$	0	0
2	В	1	Total C O 44 40 4	0	0
2	С	1	Total C O 44 40 4	0	0
2	С	1	Total C O 44 40 4	0	0
2	D	1	Total C O 44 40 4	0	0
2	D	1	Total C O 44 40 4	0	0
2	Е	1	Total C O 44 40 4	0	0
2	Е	1	Total C O 44 40 4	0	0
2	F	1	Total C O 44 40 4	0	0
2	F	1	Total C O 44 40 4	0	0

• Molecule 3 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2, 2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1, 3-DIOL (three-letter code: NEX) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total C O 44 40 4	0	0
3	В	1	Total C O 44 40 4	0	0
3	С	1	Total C O 44 40 4	0	0
3	D	1	Total C O 44 40 4	0	0
3	Е	1	Total C O 44 40 4	0	0
3	F	1	Total C O 44 40 4	0	0

• Molecule 4 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total C O 35 24 11	0	0
4	В	1	Total C O 33 23 10	0	0
4	В	1	Total C O 35 24 11	0	0
4	D	1	Total C O 35 24 11	0	0
4	Е	1	Total C O 35 24 11	0	0



• Molecule 5 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf
E	٨	1	Total	С	Mg	Ν	0	0	0
0	A	1	66	55	1	4	6	0	0
E	٨	1	Total	С	Mg	Ν	Ο	0	0
5	A	1	64	53	1	4	6	0	0
Б	Λ	1	Total	С	Mg	Ν	Ο	0	0
0	A	1	43	34	1	4	4	0	0
5	Λ	1	Total	С	Mg	Ν	Ο	0	0
5	A	1	51	40	1	4	6	0	0
5	Λ	1	Total	С	Mg	Ν	Ο	0	0
0	Л	1	61	50	1	4	6	0	0
5	Δ	1	Total	С	Mg	Ν	Ο	0	0
0	Π	1	56	45	1	4	6	0	0
5	Δ	1	Total	С	Mg	Ν	Ο	0	0
0	Π	1	66	55	1	4	6	0	0
5	Δ	1	Total	С	Mg	Ν	Ο	0	0
0	Π	1	42	33	1	4	4	0	0
5	В	1	Total	С	Mg	Ν	Ο	0	0
0	D	1	66	55	1	4	6	0	0
5	В	1	Total	С	Mg	Ν	Ο	0	0
0	D	1	65	54	1	4	6	0	0
5	B	1	Total	\mathbf{C}	Mg	Ν	0	0	0
0	D	I	43	34	1	4	4	0	0
5	B	1	Total	С	Mg	Ν	0	0	0
0	D	L	51	40	1	4	6	U	0



Mol	Chain	Residues	5	At	oms			ZeroOcc	AltConf
-	D	1	Total	С	Mg	Ν	0	0	0
5	В	1	62	51	1	4	6	0	0
-	D	1	Total	С	Mg	Ν	Ο	0	0
5	В	1	57	46	1	4	6	0	0
	D	1	Total	С	Mg	Ν	Ο	0	0
6	В	1	66	55	1	4	6	0	0
F	р	1	Total	С	Mg	Ν	0	0	0
0	D	1	47	36	1	4	6	0	0
E	C	1	Total	С	Mg	Ν	Ο	0	0
0	U	1	66	55	1	4	6	0	0
5	C	1	Total	С	Mg	Ν	Ο	0	0
5	C	1	66	55	1	4	6	0	0
5	C	1	Total	С	Mg	Ν	Ο	0	0
0	U	1	42	33	1	4	4	0	0
5	С	1	Total	С	Mg	Ν	Ο	0	0
5	U	1	44	35	1	4	4	0	0
5	С	1	Total	С	Mg	Ν	Ο	0	0
0	U	1	61	50	1	4	6	0	0
5	С	1	Total	С	Mg	Ν	Ο	0	0
5	U	1	56	45	1	4	6	0	0
5	С	1	Total	С	Mg	Ν	Ο	0	0
0	U	1	66	55	1	4	6	0	0
5	С	1	Total	С	Mg	Ν	Ο	0	0
0	U	T	44	35	1	4	4	0	0
5	Л	1	Total	С	Mg	Ν	Ο	0	0
0	D	1	66	55	1	4	6	0	0
5	Л	1	Total	\mathbf{C}	Mg	Ν	Ο	0	0
0	D	Ĩ	65	54	1	4	6	0	0
5	Л	1	Total	С	Mg	Ν	Ο	0	0
		1	42	33	1	4	4	0	0
5	D	1	Total	С	Mg	Ν	Ο	0	0
		-	45	35	1	4	5	Ŭ	
5	D	1	Total	С	Mg	Ν	Ο	0	0
		-	62	51	1	4	6	Ŭ	
5	D	1	Total	С	Mg	Ν	Ο	0	0
		_	57	46	1	4	6		
5	D	1	'Total	C	Mg	N	0	0	0
		_	66	55	1	4	6		
5	D	1	'I'otal	C	Mg	N	O	0	0
		_	46	35	1	4	6		
5	Е	1	'I'otal	C	Mg	N	O	0	0
		-	66	55	1	4	6		



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Mol	Chain	Residues		At	oms			ZeroOcc	AltConf
5	E	1	Total	С	Mg	Ν	Ο	0	0
5	Ľ	1	64	53	1	4	6	0	0
5	F	1	Total	С	Mg	Ν	Ο	0	0
5	Ľ	1	41	32	1	4	4	0	0
F	F	1	Total	С	Mg	Ν	0	0	0
5	Ľ	1	43	34	1	4	4	0	0
K	Б	1	Total	С	Mg	Ν	Ο	0	0
5	E	1	61	50	1	4	6	0	0
F	F	1	Total	С	Mg	Ν	Ο	0	0
5	Ľ	1	56	45	1	4	6	0	0
F	F	1	Total	С	Mg	Ν	0	0	0
Э	E	1	66	55	1	4	6	0	0
۲	F	1	Total	С	Mg	Ν	0	0	0
Э	E	1	41	32	1	4	4	0	0
F	F	1	Total	С	Mg	Ν	0	0	0
5	Г	1	66	55	1	4	6	0	
F	F	1	Total	С	Mg	Ν	0	0	0
5	Г	1	66	55	1	4	6	0	0
۲	F	1	Total	С	Mg	Ν	0	0	0
б	F	1	42	33	1	4	4	0	0
۲	F	1	Total	С	Mg	Ν	Ο	0	0
б	F	1	42	33	1	4	4	0	0
۲	F	1	Total	С	Mg	Ν	0	0	0
Э	F	1	61	50	1	4	6	0	0
٣	Б	1	Total	С	Mg	Ν	0	0	0
б	F	1	56	45	1	4	6	0	0
۲	Г	1	Total	С	Mg	Ν	Ο	0	0
Э	F	1	66	55	1	4	6	U	0
۲	Г	1	Total	С	Mg	Ν	Ο	0	0
Э	L, L,	1	46	35	1	4	6	U	U

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• Molecule 6 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		At	oms			ZeroOcc	AltConf
C	Δ	1	Total	С	Mg	Ν	0	0	0
0	A	1	65	55	1	4	5	0	0
6	Δ	1	Total	С	Mg	Ν	Ο	0	0
0	A	L	50	40	1	4	5	0	0
6	Λ	1	Total	С	Mg	Ν	Ο	0	0
0	A	L	55	45	1	4	5	0	0
6	Λ	1	Total	С	Mg	Ν	Ο	0	0
0	A	L	63	53	1	4	5	0	0
6	Δ	1	Total	С	Mg	Ν	Ο	0	0
0	A	L	45	35	1	4	5	0	0
6	Δ	1	Total	С	Mg	Ν	Ο	0	0
0	A	L	55	45	1	4	5	0	0
6	D	1	Total	С	Mg	Ν	Ο	0	0
0	D	L	65	55	1	4	5	0	0
6	D	1	Total	С	Mg	Ν	Ο	0	0
0	D	L	46	36	1	4	5	0	0
6	D	1	Total	С	Mg	Ν	Ο	0	0
0	D	L	58	48	1	4	5	0	0
6	D	1	Total	С	Mg	Ν	Ο	0	0
0	D	L	65	55	1	4	5	0	0
6	D	1	Total	С	Mg	Ν	Ο	0	0
0	D	L	45	35	1	4	5	0	0
6	D	1	Total	С	Mg	Ν	Ο	0	0
	D		65	55	1	4	5	U	U
6	C	1	Total	С	Mg	Ν	0	0	0
U		L	65	55	1	4	5	U	0
6	C	1	Total	С	Mg	Ν	0	0	0
			46	36	1	4	5	U	U



Mol	Chain	Residues	5	At	oms			ZeroOcc	AltConf
C	C	1	Total	С	Mg	Ν	0	0	0
0	C	1	53	43	1	4	5	0	0
C	C	1	Total	С	Mg	Ν	Ο	0	0
0	C	1	65	55	1	4	5	0	0
0	C	1	Total	С	Mg	Ν	0	0	0
0	C	1	45	35	1	4	5	0	0
C	C	1	Total	С	Mg	Ν	Ο	0	0
0	C	1	56	46	1	4	5	0	0
G	D	1	Total	С	Mg	Ν	Ο	0	0
0	D	1	65	55	1	4	5	0	0
G	D	1	Total	С	Mg	Ν	Ο	0	0
0	D	1	46	36	1	4	5	0	0
6	р	1	Total	С	Mg	Ν	Ο	0	0
0	D	1	58	48	1	4	5	0	0
6	Л	1	Total	С	Mg	Ν	Ο	0	0
0	D	1	65	55	1	4	5	0	0
6	Л	1	Total	С	Mg	Ν	0	0	0
0	D	1	45	35	1	4	5	0	0
G	D	1	Total	С	Mg	Ν	Ο	0	0
0	D	1	65	55	1	4	5	0	0
G	F	1	Total	С	Mg	Ν	Ο	0	0
0	E	1	65	55	1	4	5	0	0
6	Б	1	Total	С	Mg	Ν	Ο	0	0
0	E	1	50	40	1	4	5	0	0
6	F	1	Total	С	Mg	Ν	0	0	0
0	Ľ	1	55	45	1	4	5	0	0
6	F	1	Total	С	Mg	Ν	Ο	0	0
0	Ľ	T	63	53	1	4	5	0	0
6	F	1	Total	С	Mg	Ν	Ο	0	0
0	Ľ	1	45	35	1	4	5	0	0
6	E	1	Total	С	Mg	Ν	Ο	0	0
0	Ľ	1	55	45	1	4	5	0	0
6	F	1	Total	С	Mg	Ν	0	0	Ο
0	Ľ	1	65	55	1	4	5	0	0
6	F	1	Total	С	Mg	Ν	Ο	0	0
0	Ľ	1	46	36	1	4	5	0	0
6	F	1	Total	\mathbf{C}	Mg	Ν	0	0	0
	T.	1	58	48	1	4	5	0	0
6	F	1	Total	\mathbf{C}	Mg	Ν	0	0	Ο
	T.	1	55	45	1	4	5	0	0
6	F	1	Total	\mathbf{C}	Mg	Ν	Ō	0	Ο
	T,	L	45	35	1	4	5	U	



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf
6	\mathbf{F}	1	Total 56	C 46	Mg 1	N 4	O 5	0	0

• Molecule 7 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	Δ	1	Total C O P	0	0
1	Π	T	47 36 10 1	0	0
7	В	1	Total C O P	0	0
	D	I	46 35 10 1	0	0
7	В	1	Total C O P	0	0
-	D	I	31 20 10 1	0	0
7	С	1	Total C O P	0	0
•	0	T	25 14 10 1	0	
7	С	1	Total C O P	0	0
-	0	T	45 34 10 1	0	0
7	Л	1	Total C O P	0	0
-		T	46 35 10 1	0	0
7	E	1	Total C O P	0	0
·	Е	T	41 30 10 1	0	0
7	F	1	Total C O P	0	0
	T		45 34 10 1	0	0

• Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	2	Total Mg 2 2	0	0
8	D	1	Total Mg 1 1	0	0

• Molecule 9 is Siphonein (three-letter code: 0UR) (formula: $C_{52}H_{76}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	А	1	Total C O 52 47 5	0	0
9	В	1	Total C O 50 45 5	0	0
9	В	1	Total C O 52 47 5	0	0
9	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 52 & 47 & 5 \end{array}$	0	0
9	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 52 & 47 & 5 \end{array}$	0	0
9	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 52 & 47 & 5 \end{array}$	0	0
9	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 52 & 47 & 5 \end{array}$	0	0

• Molecule 10 is TRIMETHYL GLYCINE (three-letter code: BET) (formula: $C_5H_{12}NO_2$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	В	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{N} & \text{O} \\ 8 & 5 & 1 & 2 \end{array}$	0	0
10	В	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{N} & \text{O} \\ 8 & 5 & 1 & 2 \end{array}$	0	0
10	С	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{N} & \text{O} \\ 8 & 5 & 1 & 2 \end{array}$	0	0

• Molecule 11 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	В	1	Total C O 30 20 10	0	0
11	F	1	Total C O 30 20 10	0	0

• Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	А	8	Total O 8 8	0	0
12	В	7	Total O 7 7	0	0
12	С	8	Total O 8 8	0	0
12	D	4	Total O 4 4	0	0
12	Ε	6	Total O 6 6	0	0
12	F	8	Total O 8 8	0	0



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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: siphonaxanthin chlorophyll a/b binding light-harvesting complex II, Bry-Lhcb1













 \bullet Molecule 1: siphonaxanthin chlorophyll a/b binding light-harvesting complex II, Bry-Lhcb1



 \bullet Molecule 1: siphonaxanthin chlorophyll a/b binding light-harvesting complex II, Bry-Lhcb1



• Molecule 1: siphonaxanthin chlorophyll a/b binding light-harvesting complex II, Bry-Lhcb1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	109.72Å 91.61Å 169.22Å	Depositor
a, b, c, α , β , γ	90.00° 103.52° 90.00°	Depositor
Bosolution (Å)	39.90 - 2.60	Depositor
	47.58 - 2.45	EDS
% Data completeness	66.2 (39.90-2.60)	Depositor
(in resolution range)	56.8(47.58-2.45)	EDS
R_{merge}	0.06	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.20 (at 2.45 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.18_3861: ???)	Depositor
B B.	0.207 , 0.249	Depositor
n, n_{free}	0.214 , 0.248	DCC
R_{free} test set	2000 reflections $(2.93%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	75.7	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent $k_{sol}(e/A^3)$, $B_{sol}(A^2)$	0.32 , 70.9	EDS
L-test for twinning ²	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	16480	wwPDB-VP
Average B, all atoms $(Å^2)$	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: 0UR, LMU, CLA, LMG, LHG, CHL, MG, NEX, BET, 0IE

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	
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.30	0/1725	0.47	0/2350
1	В	0.29	0/1722	0.47	0/2345
1	С	0.30	0/1712	0.45	0/2332
1	D	0.29	0/1735	0.46	0/2361
1	Е	0.28	0/1737	0.45	0/2364
1	F	0.31	0/1738	0.49	0/2366
All	All	0.30	0/10369	0.46	0/14118

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 (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	А	1672	0	1547	47	0
1	В	1669	0	1552	43	0
1	С	1659	0	1523	44	0
1	D	1682	0	1572	35	0
1	Е	1684	0	1581	52	0
1	F	1685	0	1579	40	0
2	А	88	0	0	1	0



Conti	nuea fron	<i>previous</i>		TT(11 1)		a al l
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	44	0	0	1	0
2	C	88	0	0	3	0
2	D	88	0	0	0	0
2	E	88	0	0	1	0
2	F	88	0	0	0	0
3	A	44	0	56	3	0
3	В	44	0	54	4	0
3	С	44	0	55	4	0
3	D	44	0	55	4	0
3	Е	44	0	55	3	0
3	F	44	0	53	2	0
4	A	35	0	46	4	0
4	В	68	0	85	3	0
4	D	35	0	46	3	0
4	E	35	0	46	3	0
5	А	449	0	397	26	0
5	В	457	0	407	35	0
5	С	445	0	403	36	0
5	D	449	0	402	35	0
5	Е	438	0	384	33	0
5	F	445	0	397	34	0
6	А	333	0	305	21	0
6	В	344	0	337	23	0
6	С	330	0	306	29	0
6	D	344	0	337	21	0
6	Е	333	0	305	21	0
6	F	325	0	293	25	0
7	А	47	0	67	3	0
7	В	77	0	97	13	0
7	С	70	0	83	4	0
7	D	46	0	65	5	0
7	Е	41	0	52	7	0
7	F	45	0	63	8	0
8	А	2	0	0	0	0
8	D	1	0	0	0	0
9	А	52	0	0	0	0
9	В	102	0	0	5	0
9	С	52	0	0	3	0
9	D	52	0	0	0	0
9	Е	52	0	0	3	0
9	F	52	0	0	2	0
10	В	16	0	22	1	0

J fa α n tin



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	С	8	0	11	0	0
11	В	30	0	30	0	0
11	F	30	0	30	1	0
12	А	8	0	0	0	0
12	В	7	0	0	1	0
12	С	8	0	0	1	0
12	D	4	0	0	1	0
12	Ε	6	0	0	0	0
12	F	8	0	0	2	0
All	All	16480	0	14698	449	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.

The worst 5 of 449 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:E:83:GLU:H	1:E:92:GLN:HE21	1.12	0.94
6:F:313:CLA:H43	6:F:315:CLA:HBA1	1.50	0.89
3:D:303:NEX:H42	4:D:304:LMU:H6'2	1.56	0.88
5:D:311:CHL:H62	5:D:313:CHL:H193	1.61	0.81
1:B:150:PHE:HD1	5:B:313:CHL:H2	1.47	0.79

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 X-ray entries followed by that with respect to entries of similar resolution.

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	Perce	ntiles
1	А	221/249~(89%)	213 (96%)	7 (3%)	1 (0%)	29	52
1	В	221/249~(89%)	213 (96%)	6 (3%)	2(1%)	17	35



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	С	220/249~(88%)	212 (96%)	7 (3%)	1 (0%)	29	52
1	D	221/249~(89%)	214 (97%)	6 (3%)	1 (0%)	29	52
1	Ε	221/249~(89%)	211 (96%)	7 (3%)	3~(1%)	11	22
1	F	221/249~(89%)	214 (97%)	5(2%)	2(1%)	17	35
All	All	1325/1494~(89%)	1277 (96%)	38~(3%)	10 (1%)	19	39

 $5~{\rm of}~10$ Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Ε	17	GLU
1	F	27	GLU
1	В	17	GLU
1	С	108	VAL
1	Ε	92	GLN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percer	ntiles
1	А	160/184~(87%)	158~(99%)	2(1%)	69	86
1	В	159/184~(86%)	155~(98%)	4 (2%)	47	73
1	С	156/184~(85%)	155~(99%)	1 (1%)	86	95
1	D	163/184~(89%)	161 (99%)	2(1%)	71	87
1	Ε	162/184~(88%)	160 (99%)	2(1%)	71	87
1	F	163/184~(89%)	160 (98%)	3 (2%)	59	80
All	All	963/1104 (87%)	949~(98%)	14 (2%)	65	83

5 of 14 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	D	75	LYS
1	D	160	GLU



Continued from previous page...

Mol	Chain	Res	Type
1	F	141	THR
1	F	7	ASP
1	F	99	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	186	GLN
1	Е	92	GLN
1	F	49	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)

Of 129 ligands modelled in this entry, 3 are monoatomic - leaving 126 for Mogul analysis.

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).

Mal	Type	Chain	Dec	Tink	В	ond leng	gths	Bo	ond angl	es
IVIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
4	LMU	В	304	-	34,34,36	0.39	0	42,44,47	1.07	3 (7%)
3	NEX	А	303	-	38,46,46	0.96	2 (5%)	50,70,70	4.90	19 (38%)



Mol	Type	Chain	Dog	Link	В	ond leng	gths	Bo	ond angl	es
	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
5	CHL	С	309	1	42,50,74	<mark>3.27</mark>	17 (40%)	44,85,114	3.37	24 (54%)
5	CHL	В	310	1	43,51,74	3.21	17 (39%)	45,86,114	3.54	22 (48%)
5	CHL	А	312	12	56,64,74	2.82	19 (33%)	61,102,114	2.98	28 (45%)
9	0UR	Е	320	-	50,53,58	0.99	1 (2%)	58,72,77	2.05	19 (32%)
6	CLA	D	314	1	58,66,73	1.56	11 (18%)	67,104,113	1.54	12 (17%)
5	CHL	С	305	1	66,74,74	2.57	20 (30%)	73,114,114	2.74	26 (35%)
5	CHL	D	312	12	57,65,74	2.74	19 (33%)	62,103,114	2.67	28 (45%)
9	0UR	В	325	-	50,53,58	1.01	2 (4%)	58,72,77	2.09	18 (31%)
6	CLA	F	307	12	46,54,73	1.74	5 (10%)	53,90,113	1.60	7 (13%)
6	CLA	D	317	1	65,73,73	1.50	7 (10%)	76,113,113	1.36	8 (10%)
5	CHL	В	313	12	57,65,74	2.73	19 (33%)	62,103,114	<mark>3.39</mark>	26 (41%)
5	CHL	С	313	1	66,74,74	2.49	18 (27%)	73,114,114	2.45	25 (34%)
6	CLA	С	314	1	53,61,73	1.66	5 (9%)	61,98,113	1.56	10 (16%)
5	CHL	D	309	1	42,50,74	<mark>3.31</mark>	18 (42%)	44,85,114	5.62	27 (61%)
9	0UR	В	302	-	48,51,58	1.14	3 (6%)	56,70,77	2.80	19 (33%)
5	CHL	С	318	-	44,52,74	3.23	18 (40%)	46,87,114	3.82	23 (50%)
5	CHL	С	311	12	61,69,74	<mark>3.18</mark>	19 (31%)	67,108,114	2.76	27 (40%)
5	CHL	В	312	12	62,70,74	2.89	18 (29%)	68,109,114	2.76	28 (41%)
6	CLA	D	307	-	65,73,73	1.47	5 (7%)	76,113,113	1.44	7 (9%)
5	CHL	Е	311	12	56,64,74	2.82	19 (33%)	61,102,114	2.85	27 (44%)
5	CHL	D	313	1	66,74,74	2.60	16 (24%)	73,114,114	2.45	26 (35%)
5	CHL	Е	305	1	64,72,74	2.42	18 (28%)	70,111,114	2.33	27 (38%)
5	CHL	В	306	1	66,74,74	2.75	18 (27%)	73,114,114	3.60	28 (38%)
6	CLA	А	314	1	55,63,73	1.58	12 (21%)	64,101,113	1.68	14 (21%)
6	CLA	F	306	-	65,73,73	1.51	5 (7%)	76,113,113	1.41	7 (9%)
5	CHL	А	318	-	42,50,74	<mark>3.39</mark>	19 (45%)	44,85,114	3.03	24 (54%)
6	CLA	А	308	12	50,58,73	1.72	5 (10%)	58,95,113	1.58	8 (13%)
6	CLA	В	316	7	65,73,73	1.53	5 (7%)	76,113,113	1.42	9 (11%)
9	0UR	С	321	-	50,53,58	0.97	1 (2%)	58,72,77	1.98	16 (27%)
6	CLA	Е	306	-	65,73,73	1.53	5 (7%)	76,113,113	1.39	10 (13%)
7	LHG	Е	318	6	40,40,48	0.67	1 (2%)	43,46,54	1.30	6 (13%)
3	NEX	С	303	-	38,46,46	0.96	1 (2%)	50,70,70	6.57	19 (38%)
5	CHL	F	311	12	56,64,74	2.60	20 (35%)	61,102,114	3.72	27 (44%)
9	0UR	А	322	-	50,53,58	1.01	2 (4%)	58,72,77	2.10	21 (36%)
7	LHG	F	318	6	44,44,48	0.67	1 (2%)	47,50,54	1.33	8 (17%)



Mol	Type	Chain	Dog	Link	В	ond leng	gths	Bo	ond angl	es
	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
6	CLA	Е	316	1	55,63,73	1.61	6 (10%)	63,100,113	1.47	7 (11%)
6	CLA	А	307	-	65,73,73	1.49	5 (7%)	76,113,113	1.37	8 (10%)
6	CLA	А	317	1	55,63,73	1.67	6 (10%)	63,100,113	1.45	9 (14%)
9	0UR	D	321	-	$50,\!53,\!58$	0.88	1 (2%)	58,72,77	1.92	14 (24%)
5	CHL	А	309	1	43,51,74	3.24	17 (39%)	45,86,114	3.71	24 (53%)
7	LHG	В	324	-	30,30,48	1.18	2 (6%)	33,36,54	1.40	4 (12%)
5	CHL	F	305	1	66,74,74	2.15	16 (24%)	73,114,114	3.24	31 (42%)
6	CLA	В	309	12	46,54,73	1.82	6 (13%)	53,90,113	1.57	7 (13%)
6	CLA	Е	315	1	45,53,73	1.75	6 (13%)	52,89,113	1.57	6 (11%)
2	OIE	Е	302	-	42,45,45	1.49	5 (11%)	49,63,63	1.76	9 (18%)
5	CHL	Е	312	1	66,74,74	2.50	18 (27%)	73,114,114	3.00	29 (39%)
5	CHL	В	319	-	47,55,74	3.24	19 (40%)	50,91,114	4.04	24 (48%)
6	CLA	В	308	-	65,73,73	1.50	6 (9%)	76,113,113	1.47	9 (11%)
5	CHL	D	306	1	65,73,74	2.29	16 (24%)	71,112,114	2.83	30 (42%)
6	CLA	F	316	-	56,64,73	1.60	6 (10%)	65,102,113	1.48	7 (10%)
11	LMG	В	323	-	30,30,55	1.05	0	38,38,63	1.12	5 (13%)
6	CLA	Е	313	1	55,63,73	1.60	5 (9%)	64,101,113	1.46	8 (12%)
2	OIE	F	301	-	42,45,45	1.44	6 (14%)	49,63,63	1.74	10 (20%)
6	CLA	С	315	7	65,73,73	1.50	5 (7%)	76,113,113	1.39	9 (11%)
6	CLA	D	316	1	45,53,73	1.80	7 (15%)	52,89,113	1.62	7 (13%)
2	OIE	С	302	-	42,45,45	1.45	6 (14%)	49,63,63	1.67	9 (18%)
11	LMG	F	319	-	30,30,55	0.93	0	38,38,63	1.21	3 (7%)
2	OIE	В	301	-	42,45,45	1.41	6 (14%)	49,63,63	1.70	9 (18%)
5	CHL	А	306	1	64,72,74	2.35	17 (26%)	70,111,114	2.57	29 (41%)
5	CHL	А	311	12	61,69,74	2.90	18 (29%)	66,107,114	3.78	30 (45%)
6	CLA	В	317	1	45,53,73	1.79	8 (17%)	52,89,113	1.59	7 (13%)
5	CHL	Е	317	-	40,49,74	<mark>3.39</mark>	17 (42%)	42,83,114	5.25	22 (52%)
6	CLA	D	315	7	65,73,73	1.51	6 (9%)	76,113,113	1.36	9 (11%)
5	CHL	А	313	1	66,74,74	2.47	18 (27%)	73,114,114	2.30	23 (31%)
3	NEX	Е	303	-	38,46,46	0.94	1 (2%)	50,70,70	<mark>6.17</mark>	19 (38%)
6	CLA	F	315	1	45,53,73	1.78	6 (13%)	52,89,113	1.64	7 (13%)
3	NEX	F	303	-	38,46,46	0.96	1 (2%)	50,70,70	6.25	22 (44%)
5	CHL	F	312	1	66,74,74	2.27	18 (27%)	73,114,114	2.31	27 (36%)
5	CHL	D	318	-	46,54,74	<mark>3.23</mark>	19 (41%)	49,90,114	3.02	23 (46%)
2	0IE	С	301	-	42,45,45	1.47	6 (14%)	49,63,63	1.71	9 (18%)



Mol	Type	Chain	Bos	Link	B	ond leng	gths	Bo	ond ang	es
	туре	Chan	Ites		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	LHG	В	320	6	45,45,48	0.67	1 (2%)	48,51,54	1.30	6 (12%)
3	NEX	В	303	-	38,46,46	0.94	2 (5%)	50,70,70	<mark>5.77</mark>	22 (44%)
7	LHG	С	304	-	24,24,48	0.87	0	27,30,54	1.22	2 (7%)
6	CLA	Е	314	7	63,71,73	1.57	5 (7%)	73,110,113	1.38	8 (10%)
6	CLA	F	313	1	$58,\!66,\!73$	1.52	12 (20%)	67,104,113	1.71	12 (17%)
5	CHL	D	305	1	66,74,74	2.97	19 (28%)	73,114,114	2.66	26 (35%)
6	CLA	Е	307	-	50,58,73	1.69	6 (12%)	58,95,113	1.65	9 (15%)
6	CLA	С	307	-	65,73,73	1.48	6 (9%)	76,113,113	1.49	9 (11%)
5	CHL	В	311	-	51,59,74	<mark>3.09</mark>	19 (37%)	55,96,114	<mark>5.12</mark>	29 (52%)
2	OIE	Е	301	-	42,45,45	1.46	5 (11%)	49,63,63	1.79	10 (20%)
5	CHL	Е	309	-	43,51,74	<mark>3.29</mark>	17 (39%)	45,86,114	5.92	24 (53%)
5	CHL	F	309	-	42,50,74	<mark>3.60</mark>	18 (42%)	44,85,114	3.43	26 (59%)
5	CHL	Е	310	-	61,69,74	<mark>3.03</mark>	18 (29%)	66,107,114	2.85	26 (39%)
5	CHL	F	317	-	46,54,74	<mark>3.43</mark>	19 (41%)	49,90,114	<mark>3.54</mark>	26 (53%)
6	CLA	С	316	1	45,53,73	1.78	6 (13%)	52,89,113	1.59	6 (11%)
10	BET	В	322	-	7,7,7	1.02	0	10,10,10	0.87	1 (10%)
5	CHL	D	311	-	62,70,74	2.99	20 (32%)	68,109,114	2.92	30 (44%)
5	CHL	А	305	1	66,74,74	2.73	18 (27%)	73,114,114	3.24	31 (42%)
6	CLA	А	316	1	45,53,73	1.81	6 (13%)	52,89,113	1.62	7 (13%)
6	CLA	С	317	-	56,64,73	1.57	11 (19%)	65,102,113	1.53	10 (15%)
5	CHL	С	306	1	66,74,74	2.38	18 (27%)	73,114,114	2.73	30 (41%)
5	CHL	С	310	-	44,52,74	3.20	18 (40%)	46,87,114	3.01	20 (43%)
2	OIE	А	301	-	42,45,45	1.50	10 (23%)	49,63,63	2.07	13 (26%)
6	CLA	В	315	1	58,66,73	1.57	12 (20%)	67,104,113	1.75	13 (19%)
7	LHG	D	319	6	45,45,48	0.69	1 (2%)	48,51,54	1.28	7 (14%)
4	LMU	D	304	_	36,36,36	0.50	0	47,47,47	1.19	4 (8%)
5	CHL	С	312	12	56,64,74	3.04	19 (33%)	61,102,114	2.70	26 (42%)
5	CHL	В	307	1	65,73,74	2.22	18 (27%)	71,112,114	2.96	27 (38%)
3	NEX	D	303	-	38,46,46	0.95	2 (5%)	50,70,70	5.96	20 (40%)
6	CLA	В	318	1	65,73,73	1.47	6 (9%)	76,113,113	1.40	8 (10%)
6	CLA	F	314	7	55,63,73	1.68	5 (9%)	64,101,113	1.46	8 (12%)
5	CHL	А	310	_	51,59,74	3.18	17 (33%)	55,96,114	3.26	26 (47%)
4	LMU	Е	319	-	36,36,36	0.38	0	47,47,47	0.91	1 (2%)
2	0IE	F	302	-	42,45,45	1.43	6 (14%)	49,63,63	1.71	9 (18%)
5	CHL	В	314	1	66,74,74	2.29	18 (27%)	73,114,114	2.54	25 (34%)



Mol	Type	Chain	Bos	Link	B	ond leng	gths	Bond angles		
	туре	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
7	LHG	А	319	6	46,46,48	0.64	1 (2%)	49,52,54	1.22	3 (6%)
6	CLA	D	308	12	46,54,73	1.76	6 (13%)	53,90,113	1.58	7 (13%)
4	LMU	А	304	-	36,36,36	0.40	0	47,47,47	0.91	1 (2%)
9	0UR	F	320	-	50,53,58	1.09	3 (6%)	58,72,77	1.89	16 (27%)
5	CHL	F	304	1	66,74,74	2.54	18 (27%)	73,114,114	<mark>3.38</mark>	30 (41%)
5	CHL	D	310	12	45,53,74	3.16	17 (37%)	46,88,114	<mark>3.18</mark>	20 (43%)
6	CLA	А	315	7	63,71,73	1.55	6 (9%)	73,110,113	1.41	8 (10%)
6	CLA	С	308	12	46,54,73	1.76	5 (10%)	53,90,113	1.57	6 (11%)
10	BET	С	320	-	7,7,7	1.01	0	10,10,10	0.75	0
5	CHL	F	308	1	42,50,74	3.28	18 (42%)	44,85,114	<mark>3.85</mark>	26 (59%)
2	OIE	А	302	-	42,45,45	1.53	7 (16%)	49,63,63	2.04	10 (20%)
5	CHL	Е	304	1	66,74,74	2.42	18 (27%)	73,114,114	<mark>3.63</mark>	31 (42%)
2	OIE	D	302	-	42,45,45	1.43	6 (14%)	49,63,63	1.68	11 (22%)
5	CHL	Е	308	1	40,49,74	<mark>3.57</mark>	18 (45%)	42,83,114	<mark>3.07</mark>	19 (45%)
7	LHG	С	319	6	44,44,48	0.73	1 (2%)	47,50,54	1.30	7 (14%)
4	LMU	В	305	-	36,36,36	0.38	0	47,47,47	1.09	5 (10%)
2	OIE	D	301	-	42,45,45	1.43	5 (11%)	49,63,63	1.86	10 (20%)
10	BET	В	321	-	7,7,7	1.03	0	10,10,10	0.85	1 (10%)
5	CHL	F	310	12	61,69,74	2.82	21 (34%)	67,108,114	<mark>3.09</mark>	25 (37%)

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
4	LMU	В	304	-	-	9/20/56/61	1/2/2/2
3	NEX	А	303	-	-	5/27/83/83	0/3/3/3
5	CHL	С	309	1	3/3/15/26	4/10/108/137	-
5	CHL	В	310	1	3/3/15/26	6/12/110/137	-
5	CHL	А	312	12	3/3/18/26	7/27/125/137	-
9	0UR	Е	320	-	-	6/42/81/86	0/2/2/2
6	CLA	D	314	1	1/1/13/20	9/29/107/115	-
5	CHL	С	305	1	3/3/20/26	24/39/137/137	-
5	CHL	D	312	12	3/3/18/26	5/29/127/137	-
9	0UR	В	325	-	-	7/42/81/86	0/2/2/2



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CLA	F	307	12	1/1/11/20	4/15/93/115	-
6	CLA	D	317	1	1/1/15/20	8/37/115/115	-
5	CHL	В	313	12	3/3/18/26	7/29/127/137	-
5	CHL	С	313	1	3/3/20/26	11/39/137/137	-
6	CLA	С	314	1	1/1/12/20	5/23/101/115	-
5	CHL	D	309	1	3/3/15/26	4/10/108/137	-
9	0UR	В	302	-	-	16/40/79/86	0/2/2/2
5	CHL	С	318	-	3/3/15/26	4/13/111/137	-
5	CHL	С	311	12	3/3/19/26	15/33/131/137	-
5	CHL	В	312	12	3/3/19/26	9/35/133/137	-
6	CLA	D	307	-	1/1/15/20	10/37/115/115	-
5	CHL	Е	311	12	3/3/18/26	8/27/125/137	-
5	CHL	D	313	1	3/3/20/26	18/39/137/137	-
5	CHL	Е	305	1	3/3/19/26	12/37/135/137	-
5	CHL	В	306	1	3/3/20/26	16/39/137/137	-
6	CLA	А	314	1	1/1/13/20	6/25/103/115	-
6	CLA	F	306	-	1/1/15/20	15/37/115/115	-
5	CHL	А	318	-	3/3/15/26	5/10/108/137	-
6	CLA	А	308	12	1/1/12/20	6/19/97/115	-
6	CLA	В	316	7	1/1/15/20	6/37/115/115	-
9	0UR	С	321	-	-	7/42/81/86	0/2/2/2
6	CLA	Е	306	-	1/1/15/20	10/37/115/115	-
7	LHG	Е	318	6	-	15/45/45/53	-
3	NEX	С	303	-	-	2/27/83/83	0/3/3/3
5	CHL	F	311	12	3/3/18/26	12/27/125/137	-
9	0UR	А	322	-	-	8/42/81/86	0/2/2/2
7	LHG	F	318	6	-	23/49/49/53	-
6	CLA	Е	316	1	1/1/12/20	7/25/103/115	-
6	CLA	А	307	-	1/1/15/20	13/37/115/115	-
6	CLA	А	317	1	1/1/12/20	10/25/103/115	-
9	0UR	D	321	-	-	7/42/81/86	0/2/2/2
5	CHL	А	309	1	3/3/15/26	6/12/110/137	-
7	LHG	В	324	-	-	24/35/35/53	-
5	CHL	F	305	1	3/3/20/26	18/39/137/137	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CLA	В	309	12	1/1/11/20	4/15/93/115	-
6	CLA	Е	315	1	1/1/11/20	6/13/91/115	-
5	CHL	Е	312	1	3/3/20/26	9/39/137/137	-
2	0IE	Е	302	-	-	12/33/72/72	0/2/2/2
5	CHL	В	319	-	3/3/16/26	5/17/115/137	-
6	CLA	В	308	-	1/1/15/20	14/37/115/115	-
5	CHL	D	306	1	3/3/19/26	18/38/136/137	-
6	CLA	F	316	-	1/1/13/20	6/27/105/115	-
11	LMG	В	323	-	-	9/25/45/70	0/1/1/1
6	CLA	Е	313	1	1/1/13/20	4/25/103/115	-
2	0IE	F	301	-	-	12/33/72/72	0/2/2/2
6	CLA	С	315	7	1/1/15/20	15/37/115/115	-
6	CLA	D	316	1	1/1/11/20	2/13/91/115	-
2	0IE	С	302	-	-	14/33/72/72	0/2/2/2
11	LMG	F	319	-	-	11/25/45/70	0/1/1/1
2	0IE	В	301	-	-	11/33/72/72	0/2/2/2
5	CHL	А	306	1	3/3/19/26	15/37/135/137	-
5	CHL	А	311	12	3/3/18/26	14/33/131/137	-
6	CLA	В	317	1	1/1/11/20	2/13/91/115	-
5	CHL	Е	317	-	3/3/14/26	3/10/104/137	-
6	CLA	D	315	7	1/1/15/20	9/37/115/115	-
5	CHL	А	313	1	3/3/20/26	14/39/137/137	-
3	NEX	Е	303	-	-	4/27/83/83	0/3/3/3
6	CLA	F	315	1	1/1/11/20	4/13/91/115	-
3	NEX	F	303	-	-	3/27/83/83	0/3/3/3
5	CHL	F	312	1	3/3/20/26	16/39/137/137	-
5	CHL	D	318	-	3/3/16/26	4/15/113/137	-
2	0IE	С	301	-	-	9/33/72/72	0/2/2/2
7	LHG	В	320	6	-	24/50/50/53	-
3	NEX	В	303	-	-	2/27/83/83	0/3/3/3
7	LHG	С	304	-	-	16/29/29/53	-
6	CLA	Е	314	7	1/1/14/20	9/35/113/115	-
6	CLA	F	313	1	1/1/13/20	12/29/107/115	-
5	CHL	D	305	1	3/3/20/26	20/39/137/137	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CLA	Е	307	-	1/1/12/20	2/19/97/115	-
6	CLA	С	307	-	1/1/15/20	7/37/115/115	-
5	CHL	В	311	-	3/3/17/26	5/21/119/137	-
2	0IE	Е	301	-	-	7/33/72/72	0/2/2/2
5	CHL	Е	309	-	3/3/15/26	4/12/110/137	-
5	CHL	F	309	-	3/3/15/26	5/10/108/137	-
5	CHL	Е	310	-	3/3/18/26	14/33/131/137	-
5	CHL	F	317	-	3/3/16/26	5/15/113/137	-
6	CLA	С	316	1	1/1/11/20	4/13/91/115	-
10	BET	В	322	-	-	5/5/5/5	-
5	CHL	D	311	-	3/3/19/26	15/35/133/137	-
5	CHL	А	305	1	3/3/20/26	21/39/137/137	-
6	CLA	А	316	1	1/1/11/20	4/13/91/115	-
6	CLA	С	317	-	1/1/13/20	5/27/105/115	-
5	CHL	С	306	1	3/3/20/26	16/39/137/137	-
5	CHL	С	310	-	3/3/15/26	7/13/111/137	-
6	CLA	В	315	1	1/1/13/20	6/29/107/115	-
2	0IE	А	301	-	-	10/33/72/72	0/2/2/2
7	LHG	D	319	6	-	16/50/50/53	-
4	LMU	D	304	-	-	14/21/61/61	0/2/2/2
5	CHL	С	312	12	3/3/18/26	11/27/125/137	-
5	CHL	В	307	1	3/3/19/26	13/38/136/137	-
3	NEX	D	303	-	-	6/27/83/83	0/3/3/3
6	CLA	В	318	1	1/1/15/20	16/37/115/115	-
6	CLA	F	314	7	1/1/13/20	4/25/103/115	-
5	CHL	А	310	-	3/3/17/26	4/21/119/137	-
4	LMU	Е	319	-	-	15/21/61/61	0/2/2/2
2	0IE	F	302	-	-	12/33/72/72	0/2/2/2
5	CHL	В	314	1	3/3/20/26	19/39/137/137	-
7	LHG	А	319	6	-	18/51/51/53	-
6	CLA	D	308	12	1/1/11/20	6/15/93/115	-
4	LMU	А	304	-	-	14/21/61/61	0/2/2/2
9	OUR	F	320	-	-	7/42/81/86	0/2/2/2
5	CHL	F	304	1	3/3/20/26	16/39/137/137	-



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CHL	D	310	12	3/3/15/26	2/13/112/137	-
6	CLA	А	315	7	1/1/14/20	9/35/113/115	-
6	CLA	С	308	12	1/1/11/20	7/15/93/115	-
10	BET	С	320	-	-	5/5/5/5	-
5	CHL	F	308	1	3/3/15/26	4/10/108/137	-
5	CHL	Е	304	1	3/3/20/26	17/39/137/137	-
2	0IE	А	302	-	-	11/33/72/72	0/2/2/2
2	0IE	D	302	-	-	16/33/72/72	0/2/2/2
5	CHL	Е	308	1	3/3/14/26	4/10/104/137	-
7	LHG	С	319	6	-	18/49/49/53	-
4	LMU	В	305	-	-	14/21/61/61	0/2/2/2
2	0IE	D	301	-	-	14/33/72/72	0/2/2/2
10	BET	В	321	-	-	5/5/5/5	-
5	CHL	F	310	12	3/3/19/26	17/33/131/137	-

The worst 5 of 1204 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Ε	310	CHL	MG-ND	-13.99	1.78	2.05
5	С	311	CHL	MG-ND	-13.00	1.80	2.05
5	Ε	308	CHL	MG-NA	12.97	2.37	2.06
5	С	311	CHL	MG-NA	12.90	2.36	2.06
5	D	313	CHL	MG-NA	12.84	2.36	2.06

The worst 5 of 1981 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	В	311	CHL	O2A-C1-C2	26.61	178.56	108.64
3	F	303	NEX	C15-C35-C34	26.60	177.96	123.47
3	Е	303	NEX	C35-C15-C14	25.85	176.43	123.47
3	С	303	NEX	C15-C35-C34	24.82	174.32	123.47
5	Е	309	CHL	CMD-C2D-C1D	24.02	167.04	124.71

5 of 180 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	А	305	CHL	NA
5	А	305	CHL	NC
5	А	305	CHL	ND



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Mol	Chain	Res	Type	Atom
5	А	306	CHL	NA
5	А	306	CHL	NC

5 of 1237 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	302	OIE	C5-C6-C7-C21
2	А	302	0IE	C5-C6-C7-C8
2	А	302	0IE	C3-C4-C5-C6
2	А	302	0IE	C15-C16-C17-C18
2	А	302	0IE	C23-C16-C17-C18

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	В	304	LMU	C1'-C2'-C3'-C4'-C5'-O5'

111 monomers are involved in 359 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	В	304	LMU	2	0
3	А	303	NEX	3	0
5	С	309	CHL	5	0
5	В	310	CHL	1	0
5	А	312	CHL	2	0
9	Е	320	0UR	3	0
6	D	314	CLA	4	0
5	С	305	CHL	5	0
5	D	312	CHL	3	0
9	В	325	0UR	5	0
6	F	307	CLA	3	0
6	D	317	CLA	10	0
5	В	313	CHL	6	0
5	С	313	CHL	10	0
6	С	314	CLA	3	0
5	D	309	CHL	2	0
5	С	318	CHL	3	0
5	С	311	CHL	3	0
5	В	312	CHL	9	0
6	D	307	CLA	2	0
5	Е	311	CHL	6	0
5	D	313	CHL	12	0



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	Chain		\mathbf{Type}	Clashos	Symm_Clashos
5	F	205	СШ	5 Clashes	
5	D	206		0	0
5		300 214			0
6	A F	206		4	0
5	<u>Г</u> Л	300 219	CUI	0	0
5	A	200		1	0
6	A D	300 216		ა ე	0
0	D C	010 201	OUP	2	0
9	E E	321		3 4	0
7	E F	300 219		4	0
1	E C	310	LIIG NEV	1	0
о Б	E E	000 211	OUI CUI	4	0
5	Г	011 010		0 0	0
(F F	318		0 6	0
0 6		$\frac{310}{207}$		0 5	0
0 C	A	307	CLA	0 F	0
0 7	A	$\frac{317}{294}$		0	0
	B	324	LHG	8	0
C C	r D	305	CHL	1	0
0 C	B	309	CLA	1	0
0	E	315	OLE	2	0
2	E	302	OIE	1	0
5	E	312	CHL	8	0
5	B	319	CHL	3	0
0	B	308	CLA	5	0
5	D	306	CHL	5	0
6	F D	310	CLA	5	0
6	E	313	CLA	3	0
6	C	315	CLA	3	0
0		316	ULA OID	3	0
2		302		2	0
11		319		1	0
2	В	301	UIE	 	0
5	A	306	CHL	b 4	0
5 C	A	311 917	CHL	4	0
6	В	317	CLA		0
5 C		317	CHL	<u>న</u>	0
6	D	315	CLA	3	0
5	A	313	CHL	6	0
3		303	NEX	3	0
6	F F	315	CLA	2	0
3	F T	303	NEX	2	0
5	F'	312	CHL	5	0



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	Chain	Res	Type	Clashes	Symm-Clashes
5	D	219	СШ		0
<u> </u>	D C	201		1	0
	D	200		5	0
1	D	320	LIIG NEV	0	0
3 6	D E	000 214		4	0
0 6	E	014 019		3	0
5	F D	313 205	CUI	1	0
0 6	D E	303		3	0
0 6	E C	307		4	0
0 5	D	307	CLA	11	0
0 F	B	311	CHL	4	0
5 F	E	309	CHL	3	0
5 F	F	309	CHL	2	0
5	E	310	CHL	3	0
5	F C	317	CHL	2	0
6	C	316	CLA	4	0
10	B	322	BEL	1	0
5	D	311	CHL	9	0
5	A	305	CHL	6	0
6	A	316	CLA	3	0
6	C	317	CLA	7	0
5	C	306	CHL	4	0
5	C	310	CHL	4	0
6	B	315	CLA	7	0
7	D	319	LHG	5	0
4	D	304	LMU	3	0
5	С	312	CHL	3	0
5	В	307	CHL	4	0
3	D	303	NEX	4	0
6	В	318	CLA	7	0
6	F	314	CLA	1	0
5	A	310	CHL	4	0
4	E	319	LMU	3	0
5	В	314	CHL	10	0
7	A	319	LHG	3	0
4	A	304	LMU	4	0
9	F	320	OUR	2	0
5	F	304	CHL	8	0
5	D	310	CHL	5	0
6	A	315	CLA	3	0
6	С	308	CLA	3	0
5	F	308	CHL	1	0
2	А	302	OIE	1	0


	v	1	1 0		
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Е	304	CHL	4	0
5	Е	308	CHL	3	0
7	С	319	LHG	4	0
4	В	305	LMU	1	0
5	F	310	CHL	7	0

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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 sufficient 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.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<rsrz></rsrz>	#RSRZ:	>2	$OWAB(Å^2)$	Q<0.9
1	А	223/249~(89%)	0.39	15 (6%) 17	13	37, 79, 118, 154	0
1	В	223/249~(89%)	0.19	14 (6%) 20	15	38, 79, 117, 137	0
1	С	222/249~(89%)	0.15	18 (8%) 12	8	39, 84, 122, 158	0
1	D	223/249~(89%)	0.32	18 (8%) 12	8	43, 80, 120, 151	0
1	Е	223/249~(89%)	0.55	34 (15%) 2	1	46, 100, 145, 161	0
1	F	223/249~(89%)	0.25	14 (6%) 20	15	34, 76, 109, 126	0
All	All	1337/1494 (89%)	0.31	113 (8%) 10) 7	34, 83, 127, 161	0

The worst 5 of 113 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	1	VAL	17.1
1	F	1	VAL	12.1
1	Е	76	TYR	8.3
1	Е	1	VAL	7.4
1	Е	165	LEU	6.7

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.



6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	\mathbf{Res}	Atoms	RSCC	RSR	$B-factors(A^2)$	Q < 0.9
11	LMG	F	319	30/55	0.53	0.41	127,171,183,186	0
4	LMU	В	305	35/35	0.58	0.45	107,181,190,195	0
10	BET	В	322	8/8	0.66	0.21	90,114,123,132	0
4	LMU	Е	319	35/35	0.67	0.33	117,171,194,195	0
7	LHG	С	304	25/49	0.68	0.35	132,176,208,243	0
4	LMU	А	304	35/35	0.69	0.50	115,156,181,187	0
4	LMU	В	304	33/35	0.70	0.35	116,148,174,180	0
10	BET	С	320	8/8	0.72	0.28	112,121,126,133	0
9	0UR	В	325	52/57	0.72	0.32	$66,\!89,\!116,\!126$	0
3	NEX	А	303	44/44	0.73	0.42	$78,\!96,\!144,\!152$	0
4	LMU	D	304	35/35	0.73	0.40	86,132,160,170	0
11	LMG	В	323	30/55	0.74	0.39	122,164,179,181	0
10	BET	В	321	8/8	0.75	0.49	85,102,109,114	0
3	NEX	D	303	44/44	0.76	0.46	65,81,126,145	0
9	0UR	D	321	52/57	0.77	0.26	66,89,116,126	0
9	0UR	Е	320	52/57	0.80	0.32	66,89,116,126	0
3	NEX	Е	303	44/44	0.80	0.36	101,120,167,186	0
9	0UR	А	322	52/57	0.80	0.24	66,89,116,126	0
9	0UR	F	320	52/57	0.81	0.26	66,89,116,126	0
7	LHG	В	324	31/49	0.81	0.26	$56,\!98,\!121,\!145$	0
8	MG	А	321	1/1	0.81	0.77	74,74,74,74	0
8	MG	А	320	1/1	0.84	0.18	83,83,83,83	0
9	0UR	С	321	52/57	0.84	0.22	66, 89, 116, 126	0
3	NEX	В	303	44/44	0.85	0.24	$76,\!95,\!144,\!165$	0
2	0IE	А	301	44/44	0.85	0.32	$37,\!50,\!66,\!77$	0
6	CLA	D	317	65/65	0.85	0.24	66,85,110,114	0
2	OIE	D	302	44/44	0.86	0.17	74,87,104,108	0
7	LHG	А	319	47/49	0.87	0.26	49,74,99,106	0
3	NEX	F	303	44/44	0.87	0.22	$71,\!92,\!168,\!179$	0
2	0IE	А	302	44/44	0.88	0.21	55,73,85,103	0
9	0UR	В	302	50/57	0.88	0.26	$67,\!87,\!107,\!123$	0
5	CHL	Е	310	61/66	0.88	0.22	62,79,92,98	0
5	CHL	E	312	66/66	0.88	0.24	46,76,90,100	0
7	LHG	C	319	45/49	0.89	0.20	$59,\!84,\!\overline{108,\!139}$	0
5	CHL	А	312	56/66	0.89	0.23	$51,\!74,\!104,\!117$	0
2	0IE	F	301	44/44	0.89	0.26	$29,\!43,\!65,\!81$	0
5	CHL	Е	311	56/66	0.89	0.33	$9\overline{4,}112,141,146$	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
5	CHL	А	310	51/66	0.89	0.22	59,90,124,133	0
5	CHL	F	309	42/66	0.90	0.18	62,80,94,103	0
7	LHG	F	318	45/49	0.90	0.22	42,63,78,85	0
6	CLA	А	308	50/65	0.90	0.20	68,88,102,119	0
6	CLA	А	315	63/65	0.90	0.26	66,86,99,109	0
5	CHL	D	306	65/66	0.90	0.29	42,58,76,89	0
2	OIE	В	301	44/44	0.90	0.26	33,46,75,79	0
5	CHL	В	310	43/66	0.90	0.38	95,121,136,143	0
5	CHL	С	311	61/66	0.90	0.24	51,68,84,92	0
2	0IE	F	302	44/44	0.91	0.17	50,64,77,81	0
5	CHL	D	318	46/66	0.91	0.16	86,105,120,121	0
5	CHL	А	318	42/66	0.91	0.18	66,89,100,101	0
2	0IE	Е	302	44/44	0.91	0.27	57,75,105,125	0
5	CHL	В	311	51/66	0.91	0.22	71,90,122,134	0
5	CHL	С	310	44/66	0.91	0.20	66,86,104,107	0
2	0IE	Е	301	44/44	0.91	0.20	44,68,86,99	0
5	CHL	С	312	56/66	0.91	0.25	62,90,116,122	0
6	CLA	В	318	65/65	0.91	0.23	58,84,98,101	0
6	CLA	С	315	65/65	0.91	0.39	72,104,124,139	0
3	NEX	С	303	44/44	0.92	0.30	75,94,147,175	0
2	0IE	D	301	44/44	0.92	0.26	44,58,74,85	0
5	CHL	F	308	42/66	0.92	0.43	93,110,123,128	0
5	CHL	D	305	66/66	0.92	0.20	$59,\!85,\!100,\!108$	0
7	LHG	D	319	46/49	0.92	0.19	$66,\!87,\!101,\!108$	0
5	CHL	В	313	57/66	0.92	0.20	$59,\!84,\!104,\!105$	0
5	CHL	D	313	66/66	0.92	0.24	$33,\!50,\!74,\!96$	0
5	CHL	В	314	66/66	0.92	0.24	41,61,77,91	0
5	CHL	Е	305	64/66	0.92	0.23	44,65,79,95	0
2	0IE	С	301	44/44	0.92	0.22	$35,\!54,\!75,\!81$	0
5	CHL	A	313	66/66	0.93	0.34	43,58,76,95	0
2	OIE	С	302	44/44	0.93	0.20	57,77,101,107	0
5	CHL	D	309	42/66	0.93	0.25	86,109,121,128	0
5	CHL	F	304	66/66	0.93	0.21	41,58,70,84	0
5	CHL	D	310	45/66	0.93	0.15	52,77,90,91	0
5	CHL	D	311	62/66	0.93	0.19	40,72,88,94	0
5	CHL	F	310	61/66	0.93	0.20	49,65,80,89	0
5	CHL	F	311	56/66	0.93	0.20	55,83,110,118	0
5	CHL	F	312	66/66	0.93	0.25	45,61,77,86	0
5	CHL	F	317	46/66	0.93	0.20	63,83,106,122	0
5	CHL	A	311	61/66	0.93	0.19	51,70,82,97	0
6	CLA	A	314	55/65	0.93	0.15	60,71,85,87	0
5	CHL	A	309	43/66	0.93	0.28	103,123,135,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	CLA	В	315	58/65	0.93	0.23	65,76,100,107	0
5	CHL	Е	304	66/66	0.93	0.21	54,75,102,137	0
5	CHL	В	312	62/66	0.93	0.19	51,68,84,93	0
6	CLA	D	314	58/65	0.93	0.23	60,76,97,101	0
5	CHL	Е	308	41/66	0.93	0.26	119,142,157,160	0
6	CLA	Е	307	50/65	0.93	0.17	89,108,130,132	0
6	CLA	Е	314	63/65	0.93	0.29	89,121,136,151	0
6	CLA	F	314	55/65	0.94	0.23	51,63,93,103	0
6	CLA	F	316	56/65	0.94	0.17	54,68,79,90	0
5	CHL	С	309	42/66	0.94	0.34	92,113,122,129	0
7	LHG	В	320	46/49	0.94	0.18	50,74,88,106	0
5	CHL	F	305	66/66	0.94	0.29	29,43,59,71	0
6	CLA	А	317	55/65	0.94	0.16	48,77,87,97	0
6	CLA	В	309	46/65	0.94	0.16	72,88,99,103	0
5	CHL	А	305	66/66	0.94	0.20	45,73,91,106	0
7	LHG	Е	318	41/49	0.94	0.16	55,85,121,144	0
6	CLA	В	317	45/65	0.94	0.19	74,82,99,112	0
5	CHL	С	305	66/66	0.94	0.19	$51,\!71,\!86,\!102$	0
6	CLA	С	314	53/65	0.94	0.20	79,97,118,126	0
5	CHL	С	306	66/66	0.94	0.24	34,58,71,87	0
6	CLA	С	316	45/65	0.94	0.20	77,95,118,123	0
5	CHL	E	309	43/66	0.94	0.15	89,105,127,130	0
6	CLA	D	315	65/65	0.94	0.26	79,95,107,112	0
6	CLA	D	316	45/65	0.94	0.17	81,85,101,105	0
5	CHL	С	313	66/66	0.94	0.21	46,63,80,86	0
5	CHL	D	312	57/66	0.94	0.17	44,63,94,103	0
6	CLA	E	313	55/65	0.94	0.22	100,112,130,140	0
5	CHL	С	318	44/66	0.94	0.15	70, 96, 112, 129	0
6	CLA	E	315	45/65	0.94	0.20	100,118,132,138	0
6	CLA	F	307	46/65	0.94	0.14	$61,\!79,\!91,\!96$	0
6	CLA	F	313	58/65	0.94	0.19	58,70,101,102	0
5	CHL	E	317	41/66	0.95	0.15	83,96,113,116	0
6	CLA	E	316	55/65	0.95	0.16	$65,\!78,\!89,\!95$	0
6	CLA	F	306	65/65	0.95	0.36	$36,\!53,\!75,\!90$	0
6	CLA	C	308	46/65	0.95	0.14	65,86,94,100	0
5	CHL	В	319	47/66	0.95	0.17	80,96,112,117	0
6	CLA	E	306	65/65	0.95	0.36	48,63,78,86	0
6	CLA	F	315	45/65	0.95	0.16	58,74,92,100	0
5	CHL	В	307	65/66	0.95	0.27	32,45,64,88	0
6	CLA	В	316	65/65	0.95	0.22	63,79,109,139	0
5	CHL	В	306	66/66	0.95	0.22	45,63,77,93	0
6	$CL\overline{A}$	C	307	$65/\overline{65}$	$0.9\overline{6}$	$0.2\overline{6}$	$33,\!51,\!75,\!92$	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
6	CLA	С	317	56/65	0.96	0.16	57,75,89,96	0
6	CLA	D	307	65/65	0.96	0.38	34,51,81,90	0
6	CLA	D	308	46/65	0.96	0.15	$68,\!84,\!96,\!104$	0
5	CHL	А	306	64/66	0.96	0.27	30,51,64,82	0
8	MG	D	320	1/1	0.96	0.21	$63,\!63,\!63,\!63$	0
6	CLA	А	307	65/65	0.97	0.42	31,47,79,85	0
6	CLA	В	308	65/65	0.97	0.35	35,49,75,84	0
6	CLA	А	316	45/65	0.97	0.14	74,80,98,116	0

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The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.














































































































































































































































































































































































6.5 Other polymers (i)

There are no such residues in this entry.

