

# wwPDB X-ray Structure Validation Summary Report (i)

#### Oct 24, 2023 - 10:41 pm BST

PDB ID	:	80JE
Title	:	Arabidopsis thaliana Phosphoenolpyruvate carboxylase PPC1 in complex with
		L-malate
Authors	:	Haesaerts, S.; Loris, R.; Larsen, P.B.
Deposited on	:	2023-03-24
Resolution	:	3.14  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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	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 3.14 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.



Motrie	Whole archive	Similar resolution		
	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$		
R <sub>free</sub>	130704	1626 (3.18-3.10)		
Clashscore	141614	1735 (3.18-3.10)		
Ramachandran outliers	138981	1677 (3.18-3.10)		
Sidechain outliers	138945	1677 (3.18-3.10)		
RSRZ outliers	127900	1588 (3.18-3.10)		

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			
1	А	974	.% 81%	14%	·	
1	В	974	% • 79%	16%	•	•
1	С	974	79%	15%	•	•
1	D	974	% • 77%	17%	• •	-
1	Е	974	% <b>7</b> 9%	16%	•	•



Mol	Chain	Length	Quality of chain		
1	F	974	<b>% 7</b> 9%	15%	••
1	G	974	<b>% 7</b> 9%	15%	•••
1	Н	974	77%	18%	•••

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
3	PEG	А	1005	-	-	-	Х
3	PEG	Е	1005	-	-	-	Х
4	CL	В	1006	-	-	-	Х
4	CL	С	1009	-	-	-	Х



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 59093 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.

Mol	Chain	Residues		Α	toms			ZeroOcc	AltConf	Trace	
1	Δ	032	Total	С	Ν	Ο	$\mathbf{S}$	0	9	0	
	A	932	7262	4622	1249	1362	29	0	Δ	0	
1	В	032	Total	С	Ν	Ο	S	0	9	2	
	D	932	7228	4603	1246	1350	29	0	2		
1	С	032	Total	С	Ν	Ο	$\mathbf{S}$	0	3	1	
	U	932	7395	4696	1279	1390	30	0	5		
1	а	033	Total	С	Ν	Ο	$\mathbf{S}$	0	4	0	
	D	900	7415	4709	1281	1395	30	0	Т	0	
1	F	033	Total	С	Ν	Ο	$\mathbf{S}$	0	3	0	
1		500	7326	4658	1255	1383	30	0	5	0	
1	F	033	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	4	0	
	Ľ	900	7298	4642	1254	1372	30	0	4	0	
1	G	033	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	9	1	
	G	900	7346	4662	1276	1378	30	0	2	L	
1	н	033	Total	С	Ň	Ō	S	0	1	0	
	11	300	7395	4694	1276	1395	30			0	

• Molecule 1 is a protein called Phosphoenolpyruvate carboxylase 1.

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-6	MET	-	initiating methionine	UNP Q9MAH0
А	-5	HIS	-	expression tag	UNP Q9MAH0
А	-4	HIS	-	expression tag	UNP Q9MAH0
А	-3	HIS	-	expression tag	UNP Q9MAH0
А	-2	HIS	-	expression tag	UNP Q9MAH0
А	-1	HIS	-	expression tag	UNP Q9MAH0
А	0	HIS	-	expression tag	UNP Q9MAH0
В	-6	MET	-	initiating methionine	UNP Q9MAH0
В	-5	HIS	-	expression tag	UNP Q9MAH0
В	-4	HIS	-	expression tag	UNP Q9MAH0
В	-3	HIS	-	expression tag	UNP Q9MAH0
В	-2	HIS	-	expression tag	UNP Q9MAH0
В	-1	HIS	-	expression tag	UNP Q9MAH0



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Chain	Residue	Modelled	Actual	Comment	Reference
В	0	HIS	-	expression tag	UNP Q9MAH0
С	-6	MET	-	initiating methionine	UNP Q9MAH0
С	-5	HIS	-	expression tag	UNP Q9MAH0
С	-4	HIS	-	expression tag	UNP Q9MAH0
С	-3	HIS	-	expression tag	UNP Q9MAH0
С	-2	HIS	-	expression tag	UNP Q9MAH0
С	-1	HIS	-	expression tag	UNP Q9MAH0
С	0	HIS	-	expression tag	UNP Q9MAH0
D	-6	MET	-	initiating methionine	UNP Q9MAH0
D	-5	HIS	-	expression tag	UNP Q9MAH0
D	-4	HIS	-	expression tag	UNP Q9MAH0
D	-3	HIS	-	expression tag	UNP Q9MAH0
D	-2	HIS	-	expression tag	UNP Q9MAH0
D	-1	HIS	-	expression tag	UNP Q9MAH0
D	0	HIS	-	expression tag	UNP Q9MAH0
Е	-6	MET	-	initiating methionine	UNP Q9MAH0
Е	-5	HIS	-	expression tag	UNP Q9MAH0
Е	-4	HIS	-	expression tag	UNP Q9MAH0
Е	-3	HIS	-	expression tag	UNP Q9MAH0
Е	-2	HIS	-	expression tag	UNP Q9MAH0
Е	-1	HIS	-	expression tag	UNP Q9MAH0
Е	0	HIS	-	expression tag	UNP Q9MAH0
F	-6	MET	-	initiating methionine	UNP Q9MAH0
F	-5	HIS	-	expression tag	UNP Q9MAH0
F	-4	HIS	-	expression tag	UNP Q9MAH0
F	-3	HIS	-	expression tag	UNP Q9MAH0
F	-2	HIS	-	expression tag	UNP Q9MAH0
F	-1	HIS	-	expression tag	UNP Q9MAH0
F	0	HIS	-	expression tag	UNP Q9MAH0
G	-6	MET	-	initiating methionine	UNP Q9MAH0
G	-5	HIS	-	expression tag	UNP Q9MAH0
G	-4	HIS	-	expression tag	UNP Q9MAH0
G	-3	HIS	-	expression tag	UNP Q9MAH0
G	-2	HIS	-	expression tag	UNP Q9MAH0
G	-1	HIS	-	expression tag	UNP Q9MAH0
G	0	HIS	-	expression tag	UNP Q9MAH0
Н	-6	MET	-	initiating methionine	UNP Q9MAH0
Н	-5	HIS	-	expression tag	UNP Q9MAH0
H	-4	HIS	_	expression tag	UNP Q9MAH0
Н	-3	HIS	-	expression tag	UNP Q9MAH0
H	-2	HIS	-	expression tag	UNP Q9MAH0
Н	-1	HIS	-	expression tag	UNP Q9MAH0



Chain	Residue	Modelled	Actual	Comment	Reference
Н	0	HIS	-	expression tag	UNP Q9MAH0

• Molecule 2 is (2S)-2-hydroxybutanedioic acid (three-letter code: LMR) (formula:  $C_4H_6O_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 9  4  5 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 9  4  5 \end{array}$	0	0
2	С	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 9  4  5 \end{array}$	0	0
2	D	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 9  4  5 \end{array}$	0	0
2	Ε	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 9  4  5 \end{array}$	0	0
2	F	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 9  4  5 \end{array}$	0	0
2	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 9 & 4 & 5 \end{array}$	0	0
2	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 9 & 4 & 5 \end{array}$	0	0

• Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 7  4  3 \end{array}$	0	0
3	А	1	Total C 2 2	0	0
3	А	1	Total C 2 2	0	0
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  4  2 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 7  4  3 \end{array}$	0	0
3	А	1	Total C 2 2	0	0
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 7  4  3 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 7  4  3 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 7  4  3 \end{array}$	0	0
3	В	1	Total C 2 2	0	0
3	С	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 7  4  3 \end{array}$	0	0
3	С	1	Total C 2 2	0	0
3	С	1	Total C 2 2	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 4 & 2 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	С	1	Total C 2 2	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 7  4  3 \end{array}$	0	0
3	D	1	$\begin{array}{cc} \text{Total} & \text{C} \\ 2 & 2 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
3	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
3	Е	1	$\begin{array}{cc} \text{Total} & \text{C} \\ 2 & 2 \end{array}$	0	0
3	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 4 & 2 \end{array}$	0	0
3	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 4 & 2 \end{array}$	0	0
3	Ε	1	$\begin{array}{cc} \text{Total} & \text{C} \\ 2 & 2 \end{array}$	0	0
3	Ε	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
3	F	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 7  4  3 \end{array}$	0	0
3	F	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 7  4  3 \end{array}$	0	0
3	F	1	$\begin{array}{cc} \text{Total} & \text{C} \\ 2 & 2 \end{array}$	0	0
3	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
3	G	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 7  4  3 \end{array}$	0	0
3	G	1	$\begin{array}{cc} \text{Total} & \text{C} \\ 2 & 2 \end{array}$	0	0
3	G	1	$\begin{array}{cc} \text{Total} & \text{C} \\ 2 & 2 \end{array}$	0	0
3	G	1	$\begin{array}{ccc} \overline{\text{Total}} & \mathrm{C} & \mathrm{O} \\ 6 & 4 & 2 \end{array}$	0	0
3	G	1	TotalCO743	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total C 2 2	0	0
3	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
3	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
3	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 7 & 4 & 3 \end{array}$	0	0
3	Н	1	Total C 2 2	0	0

• Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	2	Total Cl 2 2	0	0
4	В	4	Total Cl 4 4	0	0
4	С	4	Total Cl 4 4	0	0
4	D	4	Total Cl 4 4	0	0
4	Ε	3	Total Cl 3 3	0	0
4	F	2	Total Cl 2 2	0	0
4	G	2	Total Cl 2 2	0	0
4	Н	2	$\begin{array}{cc} \text{Total} & \text{Cl} \\ 2 & 2 \end{array}$	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	5	$\begin{array}{cc} \text{Total} & \text{O} \\ 5 & 5 \end{array}$	0	0
5	В	17	Total         O           17         17	0	0
5	С	27	TotalO2727	0	0
5	D	19	Total O 19 19	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Е	18	Total O 18 18	0	0
5	F	18	Total         O           18         18	0	0
5	G	12	Total         O           12         12	0	0
5	Н	17	TotalO1717	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: Phosphoenolpyruvate carboxylase 1





# TTR N802 Head PR03 PR03 Head PR04 L805 Head E449 V820 T640 G653 K831 T640 G654 K831 F656 L963 W820 H649 G654 K831 F656 L963 W820 H649 G654 K831 F656 L963 W820 H649 G654 K831 F656 L964 F656 F656 L964 F738 F656 L965 K890 L1673 L866 K749 F746 L876 F744 L889 L147 L890 L172 R890 L172 R890 L172 R890 L172 R890 L1745 L915 F746 L915 F746 L914 F746 L914</

• Molecule 1: Phosphoenolpyruvate carboxylase 1



# K884 R90 190 H91 • Molecule 1: Phosphoenolpyruvate carboxylase 1 Chain G: 79% 15% MET HIS HIS HIS HIS HIS HIS MET ALA ASN ARG K923 GLU GLU GLU GLU GLU GLU SER LYS SER JLYS GLU LLEU TLE U LLEU TLE C GLU TTR TTR TTR TTR TTR PRO • Molecule 1: Phosphoenolpyruvate carboxylase 1 Chain H: 77% 18% • MET HIS HIS HIS HIS HIS HIS HIS ALA ALA ASN

 D4 60

 V401

 V401

 V401

 R475

 R475

 R475

 R480

 R481

 R482

 R482

 R482

 R482

 R483

 R483

 R483

 R484

 R484

 R484

 R484

 R484

 R484

 R484

 R534

 R535

 R536

 R536

#### P657 P657 P658 R658 R7565 R710 R710 R710 R710 R710 R712 R739 R756 R759 R759 R756 R759 R756 R759 R756 R759 R756 R759 R756 R7567 R756 R756 R756 R756 R756 R756 R756 R756 R756 R756

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# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	116.08Å 352.20Å 176.04Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $101.84^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution(Å)	48.93 - 3.14	Depositor
Resolution (A)	48.93 - 3.14	EDS
% Data completeness	99.3 (48.93-3.14)	Depositor
(in resolution range)	99.2 (48.93 - 3.14)	EDS
R <sub>merge</sub>	0.29	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.99 (at 3.12 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
D D .	0.202 , $0.240$	Depositor
$n, n_{free}$	0.212 , $0.248$	DCC
$R_{free}$ test set	11858  reflections  (5.00%)	wwPDB-VP
Wilson B-factor $(Å^2)$	81.6	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.31, 56.6	EDS
L-test for $twinning^2$	$ < L >=0.45, < L^2>=0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	59093	wwPDB-VP
Average B, all atoms $(Å^2)$	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 33.14 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.3954e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: PEG, CL, LMR

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).

Mal	Chain	Bond lengths		Bond angles	
1VIOI	Unain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.33	0/7426	0.51	0/10091
1	В	0.32	0/7391	0.50	0/10047
1	С	0.34	0/7563	0.53	1/10257~(0.0%)
1	D	0.35	0/7586	0.54	0/10287
1	Е	0.35	0/7494	0.53	0/10178
1	F	0.34	0/7469	0.52	0/10148
1	G	0.33	0/7510	0.51	0/10195
1	Н	0.33	0/7566	0.52	0/10265
All	All	0.34	0/60005	0.52	1/81468~(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	А	0	1
1	D	0	1
1	Ε	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	876	LEU	CA-CB-CG	5.17	127.20	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	А	750	MET	Peptide
1	D	750	MET	Peptide
1	Е	750	MET	Peptide

#### 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	7262	0	6975	79	0
1	В	7228	0	6951	85	0
1	С	7395	0	7240	95	0
1	D	7415	0	7261	105	0
1	Е	7326	0	7095	97	0
1	F	7298	0	7044	86	0
1	G	7346	0	7136	94	0
1	Н	7395	0	7200	100	0
2	А	9	0	4	0	0
2	В	9	0	4	0	0
2	С	9	0	4	1	0
2	D	9	0	4	1	0
2	Е	9	0	4	0	0
2	F	9	0	4	0	0
2	G	9	0	4	0	0
2	Н	9	0	4	1	0
3	А	33	0	35	0	0
3	В	16	0	18	1	0
3	С	26	0	26	0	0
3	D	23	0	27	1	0
3	Е	30	0	32	0	0
3	F	23	0	27	2	0
3	G	33	0	35	0	0
3	Н	16	0	18	2	0
4	А	2	0	0	0	0
4	В	4	0	0	1	0
4	С	4	0	0	1	0
4	D	4	0	0	0	0
4	Е	3	0	0	1	0
4	F	2	0	0	0	0
4	G	2	0	0	1	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Η	2	0	0	1	0
5	А	5	0	0	0	0
5	В	17	0	0	2	0
5	С	27	0	0	0	0
5	D	19	0	0	0	0
5	Ε	18	0	0	1	0
5	F	18	0	0	0	0
5	G	12	0	0	0	0
5	Н	17	0	0	0	0
All	All	59093	0	57152	712	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 6.

The worst 5 of 712 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:301[A]:ARG:NH2	1:B:388:LEU:O	2.11	0.84
1:F:169:VAL:HG22	1:F:282:SER:HB2	1.64	0.80
1:H:461:VAL:HG22	1:H:507:ILE:HG23	1.65	0.78
1:A:301:ARG:NH2	1:A:388:LEU:O	2.17	0.78
1:H:206:LYS:HE3	3:H:1003:PEG:H31	1.67	0.76

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	926/974~(95%)	885 (96%)	34 (4%)	7 (1%)	19	53
1	В	926/974~(95%)	882 (95%)	38~(4%)	6 (1%)	25	59



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	С	927/974~(95%)	882~(95%)	37~(4%)	8 (1%)	17 50
1	D	929/974~(95%)	882~(95%)	38 (4%)	9(1%)	15 47
1	Е	928/974~(95%)	882~(95%)	39 (4%)	7 (1%)	19 53
1	F	929/974~(95%)	884 (95%)	38 (4%)	7 (1%)	19 53
1	G	927/974~(95%)	882~(95%)	40 (4%)	5~(0%)	29 63
1	Н	929/974~(95%)	884 (95%)	40 (4%)	5(0%)	29 63
All	All	7421/7792~(95%)	7063 (95%)	304 (4%)	54 (1%)	22 56

5 of 54 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	395	ASP
1	В	227	LYS
1	В	395	ASP
1	В	922	SER
1	С	395	ASP

#### 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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	А	743/849~(88%)	717~(96%)	26~(4%)	36 67		
1	В	738/849~(87%)	715~(97%)	23 (3%)	40 69		
1	С	784/849~(92%)	755~(96%)	29 (4%)	34 65		
1	D	787/849~(93%)	757~(96%)	30 (4%)	33 64		
1	Ε	767/849~(90%)	742 (97%)	25 (3%)	38 68		
1	F	757/849~(89%)	731~(97%)	26 (3%)	37 67		
1	G	769/849~(91%)	739~(96%)	30 (4%)	32 63		
1	Н	780/849~(92%)	749~(96%)	31 (4%)	31 62		
All	All	6125/6792~(90%)	5905 (96%)	220 (4%)	36 66		



5 of 220 residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	Ε	301	ARG
1	F	322	LEU
1	Н	915	VAL
1	Н	226	ILE
1	Е	328	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	D	585	ASN
1	D	751	ASN
1	F	751	ASN
1	Е	751	ASN
1	В	100	HIS

#### 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 71 ligands modelled in this entry, 23 are monoatomic - leaving 48 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).



N/-1	<b>T</b>	Chain	Dag	T : 1-	В	ond leng	$_{\mathrm{gths}}$	B	ond ang	gles
IVI01	Type	Chain	Res	Link	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PEG	В	1004	3	1,1,6	0.48	0	-		
3	PEG	G	1004	3	1,1,6	0.36	0	-		
3	PEG	Е	1004	3	$5,\!5,\!6$	0.34	0	$4,\!4,\!5$	2.59	1 (25%)
2	LMR	G	1001	-	8,8,8	1.44	1 (12%)	10,10,10	1.59	1 (10%)
3	PEG	В	1003	3	6,6,6	0.46	0	$5,\!5,\!5$	0.50	0
3	PEG	F	1004	3	1,1,6	0.41	0	-		<u> </u>
3	PEG	F	1005	3	6,6,6	0.49	0	$5,\!5,\!5$	0.41	0
3	PEG	G	1002	3	6,6,6	0.50	0	$5,\!5,\!5$	0.64	0
3	PEG	А	1006	3	$6,\!6,\!6$	0.48	0	$5,\!5,\!5$	0.31	0
3	PEG	А	1003	3	$1,\!1,\!6$	0.43	0	-		
3	PEG	G	1006	3	$6,\!6,\!6$	0.49	0	$5,\!5,\!5$	0.45	0
2	LMR	Ε	1001	-	8,8,8	1.43	1 (12%)	10,10,10	1.58	2 (20%)
3	PEG	G	1005	-	$5,\!5,\!6$	0.55	0	$4,\!4,\!5$	0.49	0
3	PEG	Е	1005	3	$5,\!5,\!6$	0.70	0	$4,\!4,\!5$	1.26	0
3	PEG	Н	1002	3	6,6,6	0.47	0	$5,\!5,\!5$	0.42	0
2	LMR	С	1001	-	8,8,8	1.38	1 (12%)	10,10,10	1.64	1 (10%)
2	LMR	Н	1001	-	8,8,8	1.45	1 (12%)	10,10,10	1.59	1 (10%)
3	PEG	С	1005	-	$5,\!5,\!6$	0.55	0	4,4,5	0.59	0
3	PEG	С	1002	3	$6,\!6,\!6$	0.48	0	$5,\!5,\!5$	0.36	0
2	LMR	В	1001	-	8,8,8	1.47	1 (12%)	10,10,10	1.40	1 (10%)
3	PEG	С	1006	3	1,1,6	0.54	0	-		<u> </u>
3	PEG	С	1003	3	1,1,6	0.57	0	-		
2	LMR	D	1001	-	8,8,8	1.39	1 (12%)	10,10,10	1.49	1 (10%)
3	PEG	А	1005	-	$5,\!5,\!6$	0.57	0	4,4,5	0.45	0
2	LMR	А	1001	-	8,8,8	1.39	1 (12%)	10,10,10	1.48	1 (10%)
3	PEG	А	1002	3	6,6,6	0.50	0	$5,\!5,\!5$	0.51	0
3	PEG	D	1005	3	6,6,6	0.50	0	$5,\!5,\!5$	0.42	0
3	PEG	G	1008	-	$6,\!6,\!6$	0.50	0	$5,\!5,\!5$	0.50	0
3	PEG	D	1003	3	6,6,6	0.46	0	$5,\!5,\!5$	0.64	0
3	PEG	Н	1004	3	1,1,6	0.41	0	-		
3	PEG	С	1004	3	1,1,6	0.45	0	-		
3	PEG	E	1007	-	6,6,6	0.45	0	$5,\!5,\!5$	0.28	0
3	PEG	D	1004	3	1,1,6	0.46	0	-		
3	PEG	E	1006	3	1,1,6	0.67	0	-		
3	PEG	G	1007	3	1,1,6	0.49	0	-	0.55	
3	PEG	A	1008	-	6,6,6	0.48	0	5,5,5	0.36	0
3	PEG	H	1003	3	6,6,6	0.45	0	$5,\!5,\!5$	0.52	0
3	PEG		1003	3	1,1,6	0.48	0	-	<u> </u>	
3	PEG	F'	1002	3	6,6,6	0.48	0	$5,\!5,\!5$	0.44	0
3	PEG	A	1004	3	1,1,6	0.41	0	-	0 = 1	
3	PEG	F	1003	3	$6,\!6,\!6$	0.46	0	$5,\!5,\!5$	0.51	0



Mol Type		Chain	Dog	Ros Link		Bond lengths			Bond angles		
WIOI	Moi Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2	
3	PEG	В	1002	3	$6,\!6,\!6$	0.47	0	$5,\!5,\!5$	0.45	0	
3	PEG	Е	1002	3	$6,\!6,\!6$	0.50	0	$5,\!5,\!5$	0.41	0	
3	PEG	С	1007	-	$6,\!6,\!6$	0.49	0	$5,\!5,\!5$	0.47	0	
2	LMR	F	1001	-	8,8,8	1.55	1 (12%)	10,10,10	1.57	2 (20%)	
3	PEG	G	1003	3	$1,\!1,\!6$	0.50	0	-			
3	PEG	А	1007	3	$1,\!1,\!6$	0.46	0	-			
3	PEG	D	1002	3	$6,\!6,\!6$	0.47	0	$5,\!5,\!5$	0.40	0	

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	Е	1004	3	-	3/3/3/4	-
2	LMR	G	1001	-	-	0/8/8/8	-
3	PEG	В	1003	3	-	3/4/4/4	-
3	PEG	F	1005	3	-	2/4/4/4	-
3	PEG	G	1002	3	-	2/4/4/4	-
3	PEG	А	1006	3	-	2/4/4/4	-
3	PEG	G	1006	3	-	3/4/4/4	-
2	LMR	Е	1001	-	-	1/8/8/8	-
3	PEG	G	1005	-	-	2/3/3/4	-
3	PEG	Е	1005	3	-	3/3/3/4	-
3	PEG	Н	1002	3	-	0/4/4/4	-
2	LMR	С	1001	-	-	2/8/8/8	-
2	LMR	Н	1001	-	-	2/8/8/8	-
3	PEG	С	1005	-	-	1/3/3/4	-
3	PEG	С	1002	3	-	2/4/4/4	-
2	LMR	В	1001	-	-	2/8/8/8	-
2	LMR	D	1001	-	-	2/8/8/8	-
3	PEG	А	1005	-	-	2/3/3/4	-
2	LMR	А	1001	-	-	3/8/8/8	-
3	PEG	А	1002	3	-	2/4/4/4	-
3	PEG	D	1005	3	-	2/4/4/4	-
3	PEG	G	1008	-	-	2/4/4/4	-
3	PEG	D	1003	3	-	4/4/4/4	-
3	PEG	Е	1007	-	-	2/4/4/4	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	А	1008	-	-	2/4/4/4	-
3	PEG	Н	1003	3	-	3/4/4/4	-
3	PEG	F	1002	3	-	1/4/4/4	-
3	PEG	F	1003	3	-	3/4/4/4	-
3	PEG	В	1002	3	-	0/4/4/4	-
3	PEG	Е	1002	3	-	2/4/4/4	-
3	PEG	С	1007	-	-	3/4/4/4	-
2	LMR	F	1001	-	-	6/8/8/8	-
3	PEG	D	1002	3	-	2/4/4/4	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(Å)	Ideal(Å)
2	F	1001	LMR	C2-C1	-3.09	1.47	1.52
2	Е	1001	LMR	C2-C1	-2.93	1.47	1.52
2	G	1001	LMR	C2-C1	-2.77	1.48	1.52
2	С	1001	LMR	C2-C1	-2.75	1.48	1.52
2	Н	1001	LMR	C2-C1	-2.73	1.48	1.52

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	Е	1004	PEG	C2-O2-C3	4.89	130.44	112.90
2	G	1001	LMR	O1B-C1-C2	3.52	120.45	112.72
2	Н	1001	LMR	O1B-C1-C2	3.45	120.31	112.72
2	С	1001	LMR	O1B-C1-C2	3.39	120.16	112.72
2	D	1001	LMR	O1B-C1-C2	3.24	119.84	112.72

There are no chirality outliers.

5 of 71 torsion outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	Atoms
2	F	1001	LMR	O1A-C1-C2-O2
2	F	1001	LMR	O1B-C1-C2-O2
3	Е	1004	PEG	O2-C3-C4-O4
3	Е	1007	PEG	O1-C1-C2-O2
3	Е	1007	PEG	O2-C3-C4-O4

There are no ring outliers.

9 monomers are involved in 9 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	В	1003	PEG	1	0
3	Н	1002	PEG	1	0
2	С	1001	LMR	1	0
2	Н	1001	LMR	1	0
2	D	1001	LMR	1	0
3	Н	1003	PEG	1	0
3	F	1002	PEG	1	0
3	F	1003	PEG	1	0
3	D	1002	PEG	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

































# 5.7 Other polymers (i)

There are no such residues in this entry.

# 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 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 $>$	#RS	RZ>	>2	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	А	932/974~(95%)	-0.30	10 (1%)	80	66	50, 76, 125, 207	0
1	В	932/974~(95%)	-0.26	11 (1%)	79	64	52, 78, 133, 226	0
1	С	932/974~(95%)	-0.41	1 (0%)	95	93	38, 65, 116, 227	0
1	D	933/974~(95%)	-0.38	7 (0%)	86	74	39, 64, 115, 209	0
1	Е	933/974~(95%)	-0.40	7 (0%)	86	74	39, 64, 119, 223	0
1	F	933/974~(95%)	-0.38	9 (0%)	82	70	42, 68, 124, 217	0
1	G	933/974~(95%)	-0.38	8 (0%)	84	72	47, 74, 130, 269	0
1	Н	933/974~(95%)	-0.37	5 (0%)	91	83	47, 73, 128, 227	0
All	All	7461/7792~(95%)	-0.36	58 (0%)	86	74	38, 71, 124, 269	0

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	761	PRO	6.0
1	G	752	ILE	6.0
1	А	912	SER	5.8
1	Е	172	ALA	4.7
1	Е	757	SER	4.3

# 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	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
4	CL	С	1009	1/1	0.34	1.48	233,233,233,233	0
3	PEG	А	1005	6/7	0.71	0.64	77,88,90,92	0
3	PEG	Е	1005	6/7	0.75	0.49	85,88,96,97	0
3	PEG	С	1003	2/7	0.77	0.26	49,49,49,69	0
4	CL	В	1006	1/1	0.79	0.44	125,125,125,125	0
3	PEG	Н	1002	7/7	0.79	0.39	77,83,95,98	0
4	CL	Е	1009	1/1	0.80	0.30	114,114,114,114	0
3	PEG	С	1004	2/7	0.81	0.32	49,49,49,72	0
3	PEG	G	1005	6/7	0.81	0.33	75,89,90,98	0
3	PEG	В	1002	7/7	0.82	0.41	80,92,101,103	0
3	PEG	G	1003	2/7	0.84	0.32	$62,\!62,\!62,\!78$	0
4	CL	В	1007	1/1	0.84	0.51	71,71,71,71	0
3	PEG	D	1002	7/7	0.84	0.28	66,74,84,85	0
3	PEG	С	1005	6/7	0.84	0.46	46,78,84,93	0
3	PEG	Ε	1004	6/7	0.85	0.25	80,83,89,90	0
3	PEG	А	1002	7/7	0.85	0.31	70,74,83,84	0
3	PEG	В	1004	2/7	0.85	0.35	87,87,87,98	0
3	PEG	G	1007	2/7	0.86	0.31	$58,\!58,\!58,\!65$	0
3	PEG	С	1002	7/7	0.87	0.22	33,53,68,86	0
3	PEG	F	1002	7/7	0.87	0.35	$76,\!81,\!95,\!96$	0
3	PEG	А	1003	2/7	0.87	0.35	75,75,75,85	0
4	CL	В	1005	1/1	0.87	0.12	$63,\!63,\!63,\!63$	0
4	CL	G	1009	1/1	0.87	0.12	$65,\!65,\!65,\!65$	0
3	PEG	Е	1002	7/7	0.88	0.26	$60,\!68,\!77,\!77$	0
4	CL	D	1008	1/1	0.88	0.34	66,66,66,66	0
4	CL	G	1010	1/1	0.88	0.11	$57,\!57,\!57,\!57$	0
4	CL	С	1011	1/1	0.89	0.17	71,71,71,71	0
3	PEG	G	1002	7/7	0.89	0.23	58,70,82,86	0
4	CL	D	1009	1/1	0.89	0.30	64,64,64,64	0
4	CL	D	1007	1/1	0.90	0.14	62,62,62,62	0
2	LMR	В	1001	9/9	0.90	0.28	89,93,97,101	0
3	PEG	В	1003	7/7	0.90	0.20	79,82,84,86	0
3	PEG	A	1006	7/7	0.90	0.20	$66,\!80,\!\overline{102,\!102}$	0
3	PEG	G	1008	7/7	0.90	0.20	72,75,82,85	0
3	PEG	Е	1003	2/7	0.90	0.12	56, 56, 56, 69	0
4	CL	A	1010	1/1	0.91	0.26	81,81,81,81	0
3	PEG	A	1004	2/7	0.91	0.46	64,64,64,77	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	CL	F	1007	1/1	0.91	0.14	66,66,66,66	0
3	PEG	С	1007	7/7	0.91	0.21	55,64,85,92	0
3	PEG	F	1005	7/7	0.91	0.24	56,58,66,73	0
4	CL	Е	1010	1/1	0.92	0.10	76,76,76,76	0
3	PEG	F	1003	7/7	0.92	0.27	64,68,88,94	0
3	PEG	D	1003	7/7	0.92	0.28	59,70,89,95	0
3	PEG	С	1006	2/7	0.92	0.25	39,39,39,53	0
3	PEG	Н	1003	7/7	0.93	0.27	63,64,75,84	0
3	PEG	Ε	1006	2/7	0.93	0.35	52,52,52,54	0
4	CL	F	1006	1/1	0.93	0.20	56, 56, 56, 56	0
3	PEG	А	1008	7/7	0.93	0.25	70,70,72,79	0
3	PEG	D	1004	2/7	0.93	0.44	56, 56, 56, 79	0
3	PEG	G	1004	2/7	0.93	0.35	63,63,63,75	0
2	LMR	Н	1001	9/9	0.94	0.23	74,79,84,84	0
4	CL	С	1010	1/1	0.94	0.15	64,64,64,64	0
3	PEG	G	1006	7/7	0.94	0.19	71,73,87,90	0
3	PEG	D	1005	7/7	0.94	0.24	61,66,71,75	0
2	LMR	D	1001	9/9	0.94	0.17	63,65,68,71	0
3	PEG	F	1004	2/7	0.94	0.21	46,46,46,69	0
3	PEG	Е	1007	7/7	0.95	0.23	56,58,66,75	0
2	LMR	G	1001	9/9	0.95	0.18	71,76,80,81	0
2	LMR	А	1001	9/9	0.95	0.19	68,70,79,79	0
3	PEG	А	1007	2/7	0.96	0.24	43,43,43,56	0
3	PEG	Н	1004	2/7	0.96	0.24	48,48,48,64	0
4	CL	В	1008	1/1	0.96	0.08	67,67,67,67	0
2	LMR	F	1001	9/9	0.96	0.20	64,71,76,79	0
2	LMR	С	1001	9/9	0.96	0.23	64,67,73,74	0
2	LMR	Е	1001	9/9	0.97	0.20	57,61,69,69	0
4	CL	С	1008	1/1	0.97	0.19	53,53,53,53	0
4	CL	D	1006	1/1	0.97	0.28	70,70,70,70	0
4	CL	А	1009	1/1	0.97	0.21	66,66,66,66	0
4	CL	Н	1005	1/1	0.97	0.24	68,68,68,68	0
4	CL	Е	1008	1/1	0.98	0.25	64,64,64,64	0
4	CL	Н	1006	1/1	0.98	0.07	83,83,83,83	0

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.

