



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 06:07 am BST

PDB ID : 3C1L  
Title : Crystal structure of an antioxidant defense protein (mlr4105) from mesorhizobium loti maff303099 at 2.00 Å resolution  
Authors : Joint Center for Structural Genomics (JCSG)  
Deposited on : 2008-01-23  
Resolution : 2.00 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](mailto: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 ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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	:	2.11
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)	:	2.11

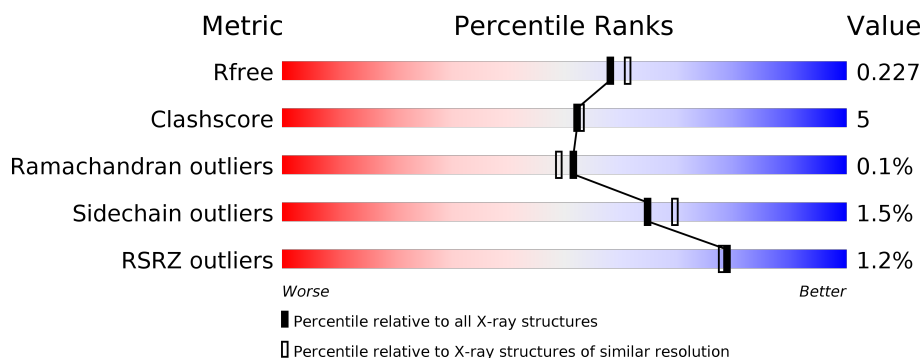
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on the lower 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  $\leq 5\%$ . 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	A	188	<div> <div>85%</div> <div>10%</div> <div>• •</div> </div>
1	B	188	<div> <div>%</div> <div>89%</div> <div>9%</div> <div>• •</div> </div>
1	C	188	<div> <div>88%</div> <div>9%</div> <div>• •</div> </div>
1	D	188	<div> <div>84%</div> <div>12%</div> <div>• •</div> </div>
1	E	188	<div> <div>88%</div> <div>9%</div> <div>•</div> </div>
1	F	188	<div> <div>89%</div> <div>7%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	188	
1	H	188	
1	I	188	
1	J	188	
1	K	188	
1	L	188	

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
2	PEG	I	190	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17569 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 Putative antioxidant defense protein Mlr4105.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	Se	0	3	0
			1408	887	243	267	3	8			
1	B	185	Total	C	N	O	S	Se	0	1	0
			1423	894	245	273	3	8			
1	C	183	Total	C	N	O	S	Se	0	3	0
			1414	891	246	266	3	8			
1	D	180	Total	C	N	O	S	Se	0	1	0
			1391	876	241	263	3	8			
1	E	181	Total	C	N	O	S	Se	0	0	0
			1392	876	239	266	3	8			
1	F	181	Total	C	N	O	S	Se	0	0	0
			1383	870	238	264	3	8			
1	G	185	Total	C	N	O	S	Se	0	0	0
			1416	893	244	267	3	9			
1	H	180	Total	C	N	O	S	Se	0	0	0
			1359	856	233	259	3	8			
1	I	181	Total	C	N	O	S	Se	0	1	0
			1393	877	241	264	3	8			
1	J	183	Total	C	N	O	S	Se	0	0	0
			1400	882	241	266	3	8			
1	K	181	Total	C	N	O	S	Se	0	0	0
			1354	848	237	258	3	8			
1	L	181	Total	C	N	O	S	Se	0	0	0
			1329	833	231	254	3	8			

There are 12 discrepancies between the modelled and reference sequences:

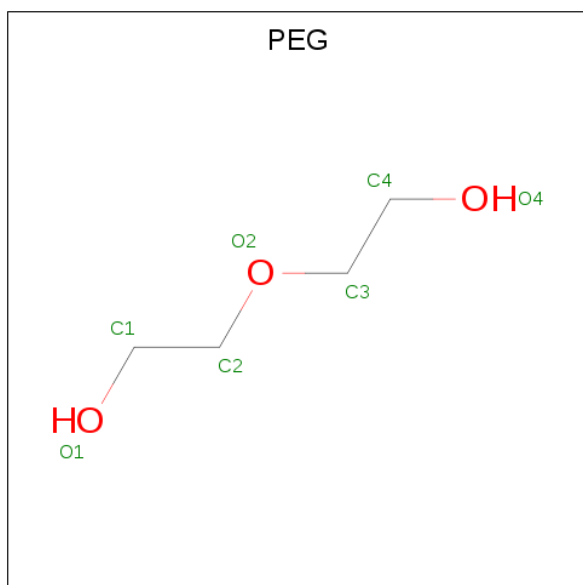
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	LEADER SEQUENCE	UNP Q98ES4
B	0	GLY	-	LEADER SEQUENCE	UNP Q98ES4
C	0	GLY	-	LEADER SEQUENCE	UNP Q98ES4
D	0	GLY	-	LEADER SEQUENCE	UNP Q98ES4
E	0	GLY	-	LEADER SEQUENCE	UNP Q98ES4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	GLY	-	LEADER SEQUENCE	UNP Q98ES4
G	0	GLY	-	LEADER SEQUENCE	UNP Q98ES4
H	0	GLY	-	LEADER SEQUENCE	UNP Q98ES4
I	0	GLY	-	LEADER SEQUENCE	UNP Q98ES4
J	0	GLY	-	LEADER SEQUENCE	UNP Q98ES4
K	0	GLY	-	LEADER SEQUENCE	UNP Q98ES4
L	0	GLY	-	LEADER SEQUENCE	UNP Q98ES4

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			7	4	3		
2	C	1	Total	C	O	0	0
			7	4	3		
2	C	1	Total	C	O	0	0
			7	4	3		
2	D	1	Total	C	O	0	0
			7	4	3		
2	D	1	Total	C	O	0	0
			7	4	3		
2	D	1	Total	C	O	0	0
			7	4	3		
2	E	1	Total	C	O	0	0
			7	4	3		
2	E	1	Total	C	O	0	0
			7	4	3		
2	G	1	Total	C	O	0	0
			7	4	3		
2	H	1	Total	C	O	0	0
			7	4	3		
2	H	1	Total	C	O	0	0
			7	4	3		
2	I	1	Total	C	O	0	0
			7	4	3		
2	I	1	Total	C	O	0	0
			7	4	3		
2	I	1	Total	C	O	0	0
			7	4	3		
2	J	1	Total	C	O	0	0
			7	4	3		
2	J	1	Total	C	O	0	0
			7	4	3		
2	J	1	Total	C	O	0	0
			7	4	3		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	1	Total	Cl	0	0
			1	1		


- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	75	Total 75	O 75	0	0
4	B	76	Total 76	O 76	0	0
4	C	76	Total 76	O 76	0	0
4	D	87	Total 87	O 87	0	0
4	E	78	Total 78	O 78	0	0
4	F	64	Total 64	O 64	0	0
4	G	57	Total 57	O 57	0	0
4	H	48	Total 48	O 48	0	0
4	I	56	Total 56	O 56	0	0
4	J	59	Total 59	O 59	0	0
4	K	33	Total 33	O 33	0	0
4	L	22	Total 22	O 22	0	0

### 3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA 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: Putative antioxidant defense protein Mlr4105

Chain A: 




- Molecule 1: Putative antioxidant defense protein Mlr4105

Chain B: 




- Molecule 1: Putative antioxidant defense protein Mlr4105

Chain C: 




- Molecule 1: Putative antioxidant defense protein Mlr4105

Chain D: 



- Molecule 1: Putative antioxidant defense protein Mlr4105

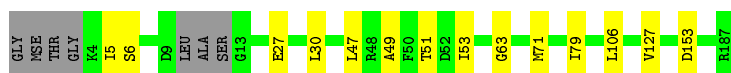
Chain E: 



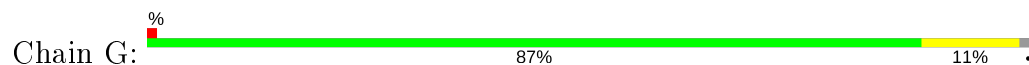
- Molecule 1: Putative antioxidant defense protein Mlr4105

Chain F: 

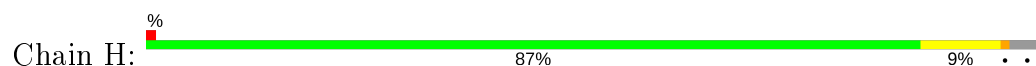




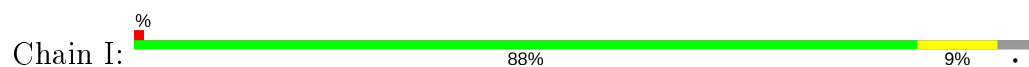
- Molecule 1: Putative antioxidant defense protein Mlr4105



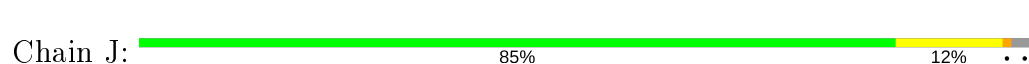
- Molecule 1: Putative antioxidant defense protein Mlr4105



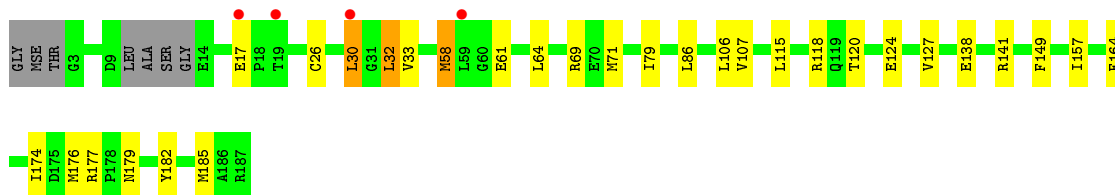
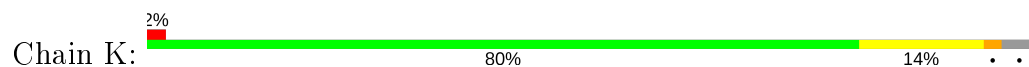
- Molecule 1: Putative antioxidant defense protein Mlr4105



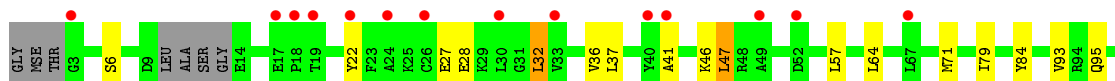
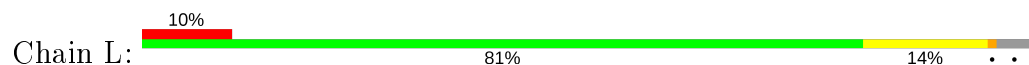
- Molecule 1: Putative antioxidant defense protein Mlr4105

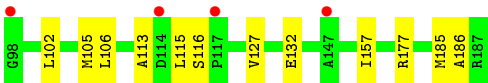


- Molecule 1: Putative antioxidant defense protein Mlr4105



- Molecule 1: Putative antioxidant defense protein Mlr4105





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.69 Å 68.06 Å 266.83 Å 90.00° 95.94° 90.00°	Depositor
Resolution (Å)	29.81 – 2.00 29.82 – 2.00	Depositor EDS
% Data completeness (in resolution range)	87.5 (29.81-2.00) 87.5 (29.82-2.00)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 2.00 Å)	Xtriage
Refinement program	REFMAC 5.4.0066, PHENIX	Depositor
R, $R_{free}$	0.171 , 0.225 0.176 , 0.227	Depositor DCC
$R_{free}$ test set	6959 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.3	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 47.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17569	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.89% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.

## 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

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	0.84	0/1432	0.80	2/1920 (0.1%)
1	B	0.78	0/1439	0.81	1/1928 (0.1%)
1	C	0.84	0/1438	0.81	1/1927 (0.1%)
1	D	0.81	0/1409	0.81	2/1886 (0.1%)
1	E	0.80	0/1407	0.81	2/1884 (0.1%)
1	F	0.77	0/1398	0.75	0/1874
1	G	0.79	1/1431 (0.1%)	0.81	1/1915 (0.1%)
1	H	0.65	0/1374	0.73	0/1845
1	I	0.78	0/1411	0.76	0/1890
1	J	0.71	0/1415	0.79	1/1895 (0.1%)
1	K	0.57	0/1369	0.71	2/1837 (0.1%)
1	L	0.82	2/1343 (0.1%)	0.66	0/1808
All	All	0.77	3/16866 (0.0%)	0.77	12/22609 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	28	GLU	CD-OE2	17.11	1.44	1.25
1	L	28	GLU	CD-OE1	12.25	1.39	1.25
1	G	26	CYS	CB-SG	-5.09	1.73	1.81

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	141	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	C	57	LEU	CA-CB-CG	6.92	131.21	115.30
1	E	169	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	G	141	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	B	141	ARG	NE-CZ-NH1	5.96	123.28	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1408	0	1392	16	0
1	B	1423	0	1396	16	0
1	C	1414	0	1396	16	0
1	D	1391	0	1376	16	0
1	E	1392	0	1369	22	0
1	F	1383	0	1352	19	0
1	G	1416	0	1407	15	0
1	H	1359	0	1312	14	0
1	I	1393	0	1369	15	0
1	J	1400	0	1379	18	0
1	K	1354	0	1288	21	0
1	L	1329	0	1243	23	0
2	A	28	0	40	1	0
2	B	28	0	40	4	0
2	C	21	0	30	1	0
2	D	21	0	30	1	0
2	E	14	0	20	0	0
2	G	7	0	10	0	0
2	H	14	0	20	0	0
2	I	21	0	30	5	0
2	J	21	0	30	0	0
3	J	1	0	0	0	0
4	A	75	0	0	1	0
4	B	76	0	0	0	0
4	C	76	0	0	1	0
4	D	87	0	0	1	0
4	E	78	0	0	1	0
4	F	64	0	0	0	0
4	G	57	0	0	2	0
4	H	48	0	0	1	0
4	I	56	0	0	1	0
4	J	59	0	0	0	0
4	K	33	0	0	2	0
4	L	22	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	17569	0	16529	183	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 5.

The worst 5 of 183 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:53:ILE:HD12	1:F:53:ILE:CD1	1.48	1.44
1:E:53:ILE:CD1	1:F:53:ILE:CD1	2.25	1.15
1:E:53:ILE:CD1	1:F:53:ILE:HD12	1.84	1.06
1:G:53:ILE:HG13	1:H:53:ILE:HD11	1.42	1.02
1:E:53:ILE:HD12	1:F:53:ILE:HD11	1.05	1.02

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	Percentiles	
1	A	181/188 (96%)	180 (99%)	1 (1%)	0	100	100
1	B	184/188 (98%)	182 (99%)	2 (1%)	0	100	100
1	C	182/188 (97%)	178 (98%)	4 (2%)	0	100	100
1	D	177/188 (94%)	175 (99%)	2 (1%)	0	100	100
1	E	177/188 (94%)	175 (99%)	2 (1%)	0	100	100
1	F	177/188 (94%)	175 (99%)	2 (1%)	0	100	100
1	G	181/188 (96%)	178 (98%)	3 (2%)	0	100	100
1	H	176/188 (94%)	172 (98%)	4 (2%)	0	100	100
1	I	178/188 (95%)	177 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	179/188 (95%)	174 (97%)	5 (3%)	0	100	100
1	K	177/188 (94%)	169 (96%)	7 (4%)	1 (1%)	25	19
1	L	177/188 (94%)	166 (94%)	10 (6%)	1 (1%)	25	19
All	All	2146/2256 (95%)	2101 (98%)	43 (2%)	2 (0%)	51	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	61	GLU
1	L	27	GLU

### 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 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	A	144/139 (104%)	138 (96%)	6 (4%)	30	27
1	B	144/139 (104%)	142 (99%)	2 (1%)	67	72
1	C	143/139 (103%)	143 (100%)	0	100	100
1	D	142/139 (102%)	139 (98%)	3 (2%)	53	57
1	E	142/139 (102%)	141 (99%)	1 (1%)	84	88
1	F	140/139 (101%)	140 (100%)	0	100	100
1	G	144/139 (104%)	144 (100%)	0	100	100
1	H	135/139 (97%)	134 (99%)	1 (1%)	84	88
1	I	141/139 (101%)	140 (99%)	1 (1%)	84	88
1	J	142/139 (102%)	139 (98%)	3 (2%)	53	57
1	K	131/139 (94%)	127 (97%)	4 (3%)	40	40
1	L	125/139 (90%)	120 (96%)	5 (4%)	31	29
All	All	1673/1668 (100%)	1647 (98%)	26 (2%)	65	67

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	48	ARG
1	J	48	ARG
1	L	57	LEU
1	H	106	LEU
1	I	132	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	119	GLN
1	L	95	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 1 is monoatomic - leaving 25 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	PEG	H	189	-	6,6,6	0.50	0	5,5,5	0.66	0
2	PEG	B	188	-	6,6,6	0.75	0	5,5,5	0.72	0
2	PEG	J	189	-	6,6,6	0.68	0	5,5,5	0.67	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PEG	J	191	-	6,6,6	0.47	0	5,5,5	0.65	0
2	PEG	B	189	-	6,6,6	0.87	0	5,5,5	0.82	0
2	PEG	H	188	-	6,6,6	0.73	0	5,5,5	0.90	0
2	PEG	B	191	-	6,6,6	0.50	0	5,5,5	0.31	0
2	PEG	I	190	-	6,6,6	0.71	0	5,5,5	0.68	0
2	PEG	I	189	-	6,6,6	0.78	0	5,5,5	0.73	0
2	PEG	D	190	-	6,6,6	0.46	0	5,5,5	0.38	0
2	PEG	E	188	-	6,6,6	0.64	0	5,5,5	0.57	0
2	PEG	E	189	-	6,6,6	0.52	0	5,5,5	0.44	0
2	PEG	A	188	-	6,6,6	0.97	0	5,5,5	0.82	0
2	PEG	C	188	-	6,6,6	0.79	0	5,5,5	0.75	0
2	PEG	C	190	-	6,6,6	0.47	0	5,5,5	0.34	0
2	PEG	D	189	-	6,6,6	0.69	0	5,5,5	0.27	0
2	PEG	I	188	-	6,6,6	0.89	0	5,5,5	0.96	0
2	PEG	A	190	-	6,6,6	0.73	0	5,5,5	0.75	0
2	PEG	A	189	-	6,6,6	0.47	0	5,5,5	0.25	0
2	PEG	A	191	-	6,6,6	0.46	0	5,5,5	0.24	0
2	PEG	D	188	-	6,6,6	0.68	0	5,5,5	0.82	0
2	PEG	B	190	-	6,6,6	0.36	0	5,5,5	0.71	0
2	PEG	J	190	-	6,6,6	0.53	0	5,5,5	0.28	0
2	PEG	G	188	-	6,6,6	0.51	0	5,5,5	0.55	0
2	PEG	C	189	-	6,6,6	0.66	0	5,5,5	0.75	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
2	PEG	H	189	-	-	3/4/4/4	-
2	PEG	B	188	-	-	4/4/4/4	-
2	PEG	J	189	-	-	4/4/4/4	-
2	PEG	J	191	-	-	2/4/4/4	-
2	PEG	B	189	-	-	4/4/4/4	-
2	PEG	H	188	-	-	3/4/4/4	-
2	PEG	B	191	-	-	4/4/4/4	-
2	PEG	I	190	-	-	2/4/4/4	-
2	PEG	I	189	-	-	3/4/4/4	-
2	PEG	D	190	-	-	3/4/4/4	-
2	PEG	E	188	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	E	189	-	-	1/4/4/4	-
2	PEG	A	188	-	-	2/4/4/4	-
2	PEG	C	188	-	-	2/4/4/4	-
2	PEG	C	190	-	-	2/4/4/4	-
2	PEG	D	189	-	-	2/4/4/4	-
2	PEG	I	188	-	-	2/4/4/4	-
2	PEG	A	190	-	-	3/4/4/4	-
2	PEG	A	189	-	-	2/4/4/4	-
2	PEG	A	191	-	-	1/4/4/4	-
2	PEG	D	188	-	-	2/4/4/4	-
2	PEG	B	190	-	-	2/4/4/4	-
2	PEG	J	190	-	-	2/4/4/4	-
2	PEG	G	188	-	-	2/4/4/4	-
2	PEG	C	189	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 61 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	188	PEG	C1-C2-O2-C3
2	C	190	PEG	O2-C3-C4-O4
2	C	189	PEG	O1-C1-C2-O2
2	H	189	PEG	C4-C3-O2-C2
2	B	190	PEG	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	189	PEG	1	0
2	B	191	PEG	3	0
2	I	190	PEG	5	0
2	C	188	PEG	1	0
2	A	190	PEG	1	0
2	D	188	PEG	1	0

## 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<sup>th</sup> 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>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	174/188 (92%)	-0.49	0 <span>100</span> <span>100</span>	25, 30, 38, 48	0
1	B	177/188 (94%)	-0.41	1 (0%) <span>89</span> <span>88</span>	25, 30, 37, 48	0
1	C	175/188 (93%)	-0.51	0 <span>100</span> <span>100</span>	22, 29, 38, 48	0
1	D	172/188 (91%)	-0.38	0 <span>100</span> <span>100</span>	25, 30, 38, 51	0
1	E	173/188 (92%)	-0.54	0 <span>100</span> <span>100</span>	25, 29, 38, 43	0
1	F	173/188 (92%)	-0.44	0 <span>100</span> <span>100</span>	26, 30, 38, 43	0
1	G	176/188 (93%)	-0.46	1 (0%) <span>89</span> <span>88</span>	21, 29, 40, 51	0
1	H	172/188 (91%)	-0.37	1 (0%) <span>89</span> <span>88</span>	26, 29, 36, 41	0
1	I	173/188 (92%)	-0.49	1 (0%) <span>89</span> <span>88</span>	24, 29, 37, 52	0
1	J	175/188 (93%)	-0.41	0 <span>100</span> <span>100</span>	23, 30, 38, 46	0
1	K	173/188 (92%)	-0.04	4 (2%) <span>60</span> <span>59</span>	25, 29, 36, 44	0
1	L	173/188 (92%)	0.54	18 (10%) <span>6</span> <span>5</span>	26, 29, 36, 43	0
All	All	2086/2256 (92%)	-0.33	26 (1%) <span>79</span> <span>78</span>	21, 29, 38, 52	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	19	THR	7.3
1	L	3	GLY	5.4
1	L	18	PRO	5.0
1	L	26	CYS	4.6
1	L	33	VAL	3.6

### 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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	PEG	A	190	7/7	0.89	0.15	32,40,44,49	0
2	PEG	I	189	7/7	0.90	0.13	40,42,48,51	0
2	PEG	E	189	7/7	0.90	0.14	52,54,57,58	0
2	PEG	J	191	7/7	0.90	0.19	33,42,46,49	0
2	PEG	H	189	7/7	0.91	0.16	41,43,48,51	0
2	PEG	B	191	7/7	0.93	0.11	43,47,52,57	0
2	PEG	I	188	7/7	0.93	0.12	32,37,42,43	0
2	PEG	E	188	7/7	0.93	0.11	33,37,44,49	0
2	PEG	G	188	7/7	0.93	0.15	28,35,39,49	0
2	PEG	B	189	7/7	0.94	0.10	27,35,42,43	0
2	PEG	D	188	7/7	0.94	0.11	33,38,43,43	0
2	PEG	J	190	7/7	0.94	0.15	43,48,56,56	0
2	PEG	B	190	7/7	0.94	0.12	40,41,48,51	0
2	PEG	A	189	7/7	0.95	0.09	36,36,39,48	0
2	PEG	C	190	7/7	0.95	0.16	36,41,48,49	0
2	PEG	D	189	7/7	0.95	0.10	34,44,46,46	0
2	PEG	B	188	7/7	0.95	0.12	25,37,42,50	0
2	PEG	H	188	7/7	0.95	0.14	35,46,53,53	0
2	PEG	A	191	7/7	0.96	0.14	29,32,43,47	0
2	PEG	I	190	7/7	0.96	0.12	30,36,42,44	0
2	PEG	J	189	7/7	0.96	0.12	31,37,47,47	0
2	PEG	A	188	7/7	0.96	0.10	19,31,37,41	0
2	PEG	C	188	7/7	0.96	0.10	33,37,41,49	0
2	PEG	D	190	7/7	0.97	0.08	39,45,49,51	0
2	PEG	C	189	7/7	0.97	0.09	29,39,45,47	0
3	CL	J	188	1/1	0.98	0.03	50,50,50,50	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.