



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 04:14 PM GMT

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 full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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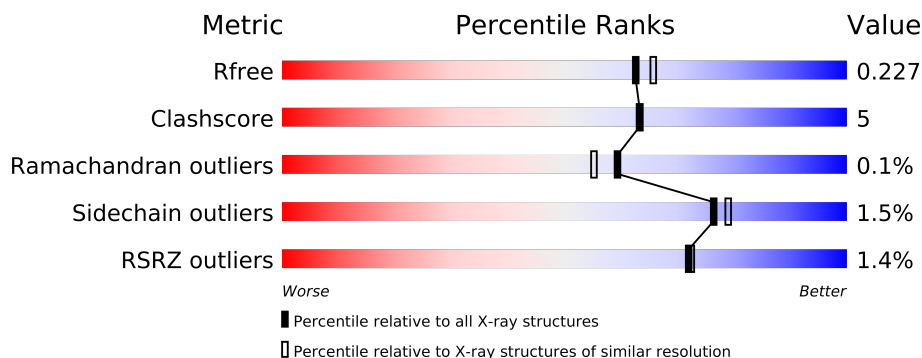
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **FAILED**  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance












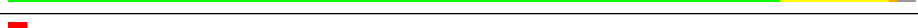
The reported resolution of this entry is 2.00 Å.

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))
$R_{free}$	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	188	
1	B	188	
1	C	188	
1	D	188	
1	E	188	
1	F	188	
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 that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	CL	J	188	-	X
3	PEG	A	190	-	X
3	PEG	B	188	-	X
3	PEG	B	189	-	X
3	PEG	D	188	-	X
3	PEG	G	188	-	X
3	PEG	I	188	-	X
3	PEG	I	190	-	X
3	PEG	J	189	-	X
3	PEG	J	191	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17569 atoms, of which 0 are hydrogen and 0 are deuterium.

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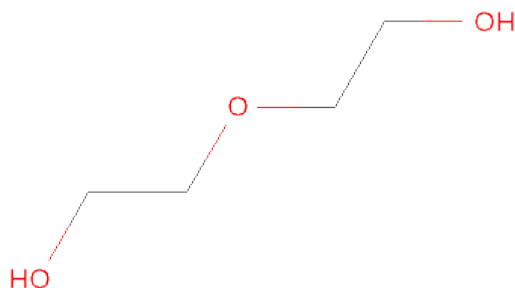
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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	GLY	-	LEADER SEQUENCE	UNP Q98ES4
G	0	GLY	-	LEADER SEQUENCE	UNP Q98ES4
H	0	GLY	-	LEADER SEQUENCE	UNP Q98ES4
I	0	GLY	-	LEADER SEQUENCE	UNP Q98ES4
J	0	GLY	-	LEADER SEQUENCE	UNP Q98ES4
K	0	GLY	-	LEADER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

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 3 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
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0

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

- 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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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



Chain G:



- Molecule 1: Putative antioxidant defense protein Mlr4105

Chain H:



- Molecule 1: Putative antioxidant defense protein Mlr4105

Chain I:



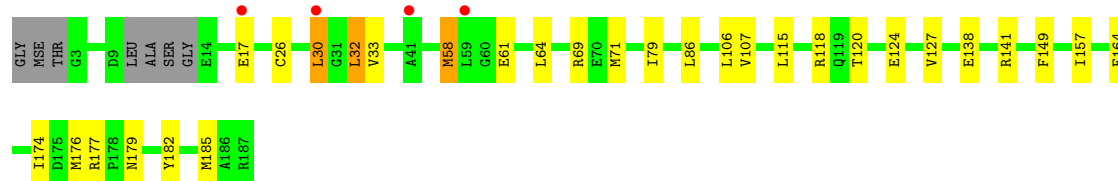
- Molecule 1: Putative antioxidant defense protein Mlr4105

Chain J:



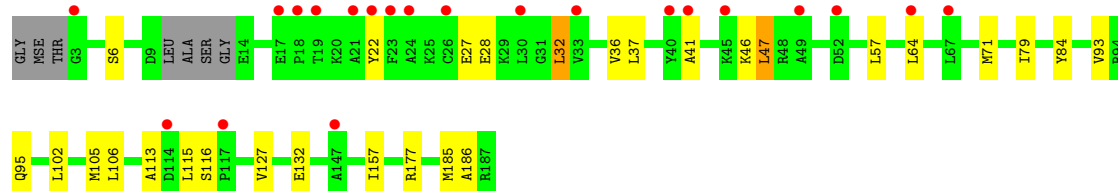
- Molecule 1: Putative antioxidant defense protein Mlr4105

Chain K:



- Molecule 1: Putative antioxidant defense protein Mlr4105

Chain L:



## 4 Data and refinement statistics

Xtriage (Phenix) failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.69Å 68.06Å 266.83Å 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
Refinement program	REFMAC 5.4.0066	Depositor
R, $R_{free}$	0.171 , 0.225 0.176 , 0.227	Depositor DCC
$R_{free}$ test set	6959 reflections (5.28%)	DCC
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 62.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17569	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

All (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
1	E	169	ARG	NE-CZ-NH2	-5.95	117.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	111	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	D	118[A]	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	D	118[B]	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	K	69	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	K	69	ARG	NE-CZ-NH2	-5.23	117.68	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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	J	1	0	0	0	0
3	A	28	0	40	1	0
3	B	28	0	40	4	0
3	C	21	0	30	1	0
3	D	21	0	30	1	0
3	E	14	0	20	0	0
3	G	7	0	10	0	0
3	H	14	0	20	0	0
3	I	21	0	30	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	21	0	30	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
All	All	17569	0	16529	183	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (183) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:E:53:ILE:HD12	1:F:53:ILE:HD11	1.05	1.02
1:G:53:ILE:HG13	1:H:53:ILE:HD11	1.42	1.02
1:E:53:ILE:HD12	1:F:53:ILE:HD12	1.42	0.93
1:A:16:SER:OG	1:A:19[A]:THR:HG23	1.70	0.91
1:K:79:ILE:HD11	1:K:127:VAL:HG22	1.59	0.84
1:B:71:MSE:HG2	1:B:106:LEU:HD21	1.61	0.80
1:I:53:ILE:HG13	1:J:53:ILE:HD11	1.65	0.79
1:E:53:ILE:CD1	1:F:53:ILE:HD11	2.00	0.78
1:D:79:ILE:HD11	1:D:127:VAL:HG22	1.66	0.77
1:L:71:MSE:HE3	1:L:106:LEU:HD11	1.68	0.76
1:E:57:LEU:HD21	1:E:160:THR:HA	1.68	0.74
1:J:101:ALA:HB1	1:J:105:MSE:HE3	1.70	0.74
1:E:71:MSE:HE3	1:E:106:LEU:HD21	1.69	0.74
1:G:53:ILE:CG1	1:H:53:ILE:HD11	2.17	0.73
1:L:71:MSE:HE1	1:L:115:LEU:HD21	1.73	0.69
1:G:79:ILE:HD11	1:G:127:VAL:HG22	1.74	0.69
1:H:79:ILE:HD11	1:H:127:VAL:HG22	1.72	0.69
1:L:93:VAL:HG11	1:L:106:LEU:HD12	1.75	0.69
1:G:114:ASP:HB3	4:G:528:HOH:O	1.93	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:71:MSE:HE1	1:I:115:LEU:HD22	1.77	0.67
1:K:71:MSE:HE1	1:K:115:LEU:HD22	1.76	0.67
1:C:71:MSE:HG2	1:C:106[A]:LEU:CD1	2.26	0.66
1:F:5:ILE:HD12	1:F:5:ILE:C	2.17	0.65
1:C:71:MSE:HG2	1:C:106[A]:LEU:HD13	1.79	0.63
1:G:71:MSE:HE2	1:G:106:LEU:HD11	1.80	0.62
1:K:174:ILE:HD11	1:K:176:MSE:HE3	1.81	0.62
1:G:71:MSE:CE	1:G:106:LEU:HD11	2.28	0.62
1:A:118:ARG:NH1	4:A:232:HOH:O	2.32	0.62
1:B:119:GLN:HE22	3:B:191:PEG:C3	2.13	0.62
4:K:711:HOH:O	1:L:46:LYS:CB	2.49	0.61
1:C:36:VAL:HG21	3:C:188:PEG:H32	1.81	0.61
1:J:5:ILE:CD1	1:J:39:ALA:HB2	2.31	0.61
1:A:112:ALA:O	1:C:177[B]:ARG:NH2	2.33	0.60
1:C:53:ILE:HD11	1:D:53:ILE:HG13	1.82	0.60
1:G:15:LEU:HD22	1:G:41:ALA:HB1	1.83	0.60
1:F:47:LEU:O	1:F:51:THR:HG23	2.01	0.59
1:D:19:THR:HG21	1:D:44:ASP:OD1	2.02	0.58
1:B:79:ILE:HD11	1:B:127:VAL:HG22	1.86	0.58
1:F:27:GLU:O	1:F:30:LEU:O	2.22	0.58
1:H:71:MSE:HG2	1:H:106:LEU:HD21	1.85	0.58
1:K:118:ARG:HB2	4:K:717:HOH:O	2.04	0.58
1:F:5:ILE:HD12	1:F:6:SER:N	2.20	0.57
1:I:36:VAL:HG21	3:I:190:PEG:H21	1.86	0.57
1:C:124:GLU:OE1	1:C:124:GLU:HA	2.05	0.56
1:D:36:VAL:HG21	3:D:188:PEG:H22	1.87	0.56
1:B:71:MSE:HG2	1:B:106:LEU:CD2	2.31	0.56
1:C:93:VAL:HG11	1:C:106[A]:LEU:HD12	1.88	0.56
1:C:57:LEU:HD23	1:C:58:MSE:SE	2.56	0.56
1:A:79:ILE:HD11	1:A:127:VAL:HG22	1.88	0.56
1:J:47:LEU:O	1:J:51:THR:HG23	2.07	0.55
1:K:118:ARG:HG2	1:K:149:PHE:CZ	2.42	0.54
1:L:32:LEU:HD12	1:L:185:MSE:HE1	1.90	0.54
1:H:71:MSE:HG2	1:H:106:LEU:CD2	2.37	0.54
1:A:33:VAL:HB	1:A:38:LYS:HE3	1.89	0.53
1:B:35:ASN:OD1	1:B:38:LYS:NZ	2.36	0.53
1:L:32:LEU:HD22	1:L:32:LEU:C	2.29	0.53
1:K:32:LEU:HD23	1:K:179:ASN:ND2	2.24	0.52
1:L:41:ALA:HA	1:L:47:LEU:HD12	1.90	0.52
1:I:71:MSE:HG2	1:I:106:LEU:CD1	2.40	0.52
1:J:5:ILE:HD13	1:J:39:ALA:HB2	1.91	0.52
1:L:71:MSE:HE2	1:L:106:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:71:MSE:HE1	1:K:115:LEU:CD2	2.40	0.52
1:K:182:TYR:HA	1:K:185:MSE:HE3	1.91	0.52
1:B:16:SER:OG	1:B:44:ASP:OD2	2.17	0.52
1:I:81:HIS:ND1	4:I:624:HOH:O	2.33	0.52
1:L:36:VAL:HG13	1:L:37:LEU:N	2.25	0.51
1:E:49:ALA:HB1	1:F:53:ILE:HG12	1.93	0.51
1:L:116:SER:HB2	4:L:741:HOH:O	2.09	0.51
1:L:71:MSE:HE1	1:L:115:LEU:CD2	2.41	0.51
1:E:71:MSE:CE	1:E:106:LEU:HD21	2.40	0.51
1:B:53:ILE:O	1:B:57:LEU:HB2	2.11	0.51
1:L:22:TYR:HE2	1:L:37:LEU:HD13	1.74	0.51
1:J:123:LEU:O	1:J:127:VAL:HG23	2.11	0.51
1:H:141:ARG:NH2	4:H:554:HOH:O	2.44	0.50
1:I:36:VAL:CG2	3:I:190:PEG:H32	2.41	0.50
1:H:17:GLU:HB2	1:H:18:PRO:HD3	1.94	0.49
1:F:71:MSE:HG2	1:F:106:LEU:CD2	2.42	0.49
1:D:57:LEU:HD21	1:D:160:THR:HA	1.94	0.49
1:L:71:MSE:HE3	1:L:102:LEU:HD11	1.94	0.49
1:J:112:ALA:HB1	1:K:177:ARG:HH12	1.78	0.49
1:A:19[A]:THR:HG21	1:A:44:ASP:OD1	2.12	0.49
1:C:70:GLU:O	1:C:74:VAL:HG23	2.13	0.49
1:A:36:VAL:HG11	3:A:190:PEG:H31	1.95	0.49
1:F:79:ILE:HD11	1:F:127:VAL:HG22	1.95	0.49
1:D:32:LEU:HD12	1:D:32:LEU:C	2.33	0.49
1:L:79:ILE:HD11	1:L:127:VAL:HG22	1.95	0.48
1:C:118[B]:ARG:NH1	1:C:118[B]:ARG:HB3	2.27	0.48
1:E:113:ALA:O	1:E:114:ASP:HB2	2.14	0.48
1:G:70:GLU:HG3	1:G:96:LEU:HD12	1.96	0.48
1:D:71:MSE:HE1	1:D:115:LEU:HD22	1.94	0.48
1:L:93:VAL:HG11	1:L:106:LEU:CD1	2.43	0.47
1:G:53:ILE:CD1	1:H:53:ILE:HD11	2.45	0.47
1:L:102:LEU:HD11	1:L:106:LEU:HD11	1.97	0.47
1:B:119:GLN:HE22	3:B:191:PEG:H32	1.79	0.47
1:J:70:GLU:OE1	1:J:89:HIS:ND1	2.36	0.47
1:A:71:MSE:HG2	1:A:106:LEU:HD21	1.97	0.47
1:K:30:LEU:CD1	1:K:30:LEU:N	2.78	0.47
1:E:5:ILE:CD1	1:E:39:ALA:HB2	2.45	0.47
1:J:71:MSE:HG2	1:J:106:LEU:CD1	2.44	0.47
1:L:71:MSE:HG2	1:L:106:LEU:HD13	1.97	0.46
1:J:105:MSE:SE	1:J:113:ALA:HA	2.65	0.46
1:J:5:ILE:HD11	1:J:39:ALA:HA	1.97	0.46
1:G:59:LEU:HD23	1:G:66:LYS:HD2	1.96	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:138:GLU:HA	1:K:141:ARG:NH1	2.31	0.46
1:B:64:LEU:HD11	1:B:157:ILE:HG13	1.98	0.46
1:K:26:CYS:HB2	1:K:33:VAL:HG22	1.97	0.45
1:F:5:ILE:CD1	1:F:5:ILE:C	2.84	0.45
1:C:146:LYS:HD2	4:C:264:HOH:O	2.16	0.45
1:D:71:MSE:HE3	1:D:106:LEU:HD11	1.97	0.45
1:K:174:ILE:HD11	1:K:176:MSE:CE	2.44	0.45
1:K:58:MSE:SE	1:K:164:PHE:CE2	3.20	0.45
1:L:177:ARG:HD2	4:L:733:HOH:O	2.16	0.45
1:G:111:ARG:HG2	4:G:530:HOH:O	2.16	0.44
1:E:71:MSE:HG2	1:E:106:LEU:CD2	2.48	0.44
1:H:105:MSE:SE	1:H:113:ALA:HA	2.67	0.44
1:E:53:ILE:HG12	1:F:49:ALA:HB1	1.99	0.44
1:I:22:TYR:HE2	1:I:37:LEU:HD13	1.83	0.44
1:A:49:ALA:HB1	1:B:53:ILE:CD1	2.48	0.43
1:A:5:ILE:HD11	1:A:39:ALA:HA	1.99	0.43
1:B:84:TYR:CE2	1:B:178:PRO:HA	2.53	0.43
1:H:104:GLU:O	1:H:108:MSE:HG3	2.18	0.43
1:D:21:ALA:O	1:D:24:ALA:HB3	2.18	0.43
1:B:167:SER:HB3	3:B:189:PEG:H32	1.99	0.43
1:I:36:VAL:HG23	3:I:190:PEG:H32	2.01	0.43
1:D:113:ALA:O	1:D:114:ASP:HB2	2.17	0.43
1:K:120:THR:O	1:K:124:GLU:HG2	2.18	0.43
1:A:49:ALA:HB1	1:B:53:ILE:HD13	2.00	0.43
1:L:84:TYR:C	1:L:84:TYR:CD1	2.91	0.43
1:E:53:ILE:CD1	1:F:53:ILE:CG1	2.95	0.43
1:L:105:MSE:SE	1:L:113:ALA:HA	2.68	0.43
1:B:119:GLN:HE22	3:B:191:PEG:H31	1.83	0.43
1:I:79:ILE:HD11	1:I:127:VAL:HG22	2.01	0.43
1:H:24:ALA:O	1:H:28:GLU:HG3	2.19	0.43
1:A:53:ILE:CD1	1:B:53:ILE:HG13	2.49	0.43
1:D:32:LEU:HD23	1:D:181:GLU:HB2	2.01	0.43
1:E:105:MSE:SE	1:E:113:ALA:HA	2.69	0.42
1:J:152:ARG:HA	1:J:152:ARG:HD2	1.95	0.42
1:L:64:LEU:HD11	1:L:157:ILE:HG13	2.01	0.42
1:K:86:LEU:HD22	1:K:107:VAL:HG22	2.00	0.42
1:I:53:ILE:HG13	1:J:53:ILE:CD1	2.43	0.42
1:A:53:ILE:HD11	1:B:53:ILE:HG13	2.01	0.42
1:C:79:ILE:HD11	1:C:127:VAL:HG22	2.01	0.42
1:K:71:MSE:HG2	1:K:106:LEU:HD13	2.02	0.42
1:I:37:LEU:HD22	1:I:47:LEU:HD11	2.01	0.42
1:D:48:ARG:O	1:D:49:ALA:C	2.57	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:71:MSE:HG2	1:A:106:LEU:CD2	2.50	0.42
1:L:71:MSE:CE	1:L:106:LEU:HD21	2.49	0.42
1:F:63:GLY:HA3	1:F:153:ASP:OD1	2.20	0.42
1:H:21:ALA:O	1:H:24:ALA:HB3	2.19	0.42
1:E:152:ARG:NH2	4:E:395:HOH:O	2.53	0.42
1:K:64:LEU:HD11	1:K:157:ILE:HG13	2.02	0.41
1:J:113:ALA:O	1:J:114:ASP:HB2	2.20	0.41
1:D:90:GLY:HA3	4:D:284:HOH:O	2.20	0.41
1:E:71:MSE:HG2	1:E:106:LEU:HD21	2.01	0.41
1:A:32:LEU:HD23	1:A:32:LEU:O	2.21	0.41
1:E:174:ILE:HD11	1:E:176:MSE:HB2	2.02	0.41
1:C:73:ALA:HB2	1:C:164:PHE:CE2	2.55	0.41
1:I:39:ALA:CB	1:I:176:MSE:HE2	2.51	0.41
1:H:19:THR:HG23	1:H:47:LEU:HD21	2.02	0.41
1:K:58:MSE:HE3	1:K:58:MSE:HB2	1.87	0.41
1:G:47:LEU:O	1:G:51:THR:HG23	2.20	0.41
1:I:167:SER:HA	3:I:190:PEG:H41	2.02	0.41
1:J:17:GLU:HB2	1:J:18:PRO:HD3	2.03	0.41
1:K:30:LEU:HD12	1:K:30:LEU:N	2.36	0.41
1:L:95:GLN:HE21	1:L:186:ALA:HB2	1.84	0.41
1:G:25:LYS:O	1:G:28:GLU:HB3	2.20	0.41
1:I:36:VAL:HG21	3:I:190:PEG:H32	2.02	0.41
1:J:71:MSE:HG2	1:J:106:LEU:HD11	2.02	0.41
1:K:58:MSE:SE	1:K:164:PHE:HE2	2.53	0.41
1:E:53:ILE:HD11	1:F:53:ILE:HG13	2.03	0.40
1:G:53:ILE:HG13	1:H:53:ILE:CD1	2.31	0.40
1:C:53:ILE:CD1	1:D:53:ILE:CD1	2.99	0.40
1:C:53:ILE:HD11	1:D:53:ILE:CD1	2.51	0.40
1:G:33:VAL:HB	1:G:38:LYS:HE3	2.02	0.40
1:C:53:ILE:HD11	1:D:53:ILE:CG1	2.47	0.40
1:J:79:ILE:HD11	1:J:127:VAL:HG22	2.03	0.40
1:E:174:ILE:HD11	1:E:176:MSE:CE	2.52	0.40
1:A:64:LEU:HD11	1:A:157:ILE:HG13	2.02	0.40
1:E:53:ILE:HD11	1:F:53:ILE:CD1	2.39	0.40
1:I:166:MSE:HB2	1:J:166:MSE:HB2	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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
1	J	179/188 (95%)	174 (97%)	5 (3%)	0	100	100
1	K	177/188 (94%)	169 (96%)	7 (4%)	1 (1%)	33	24
1	L	177/188 (94%)	166 (94%)	10 (6%)	1 (1%)	33	24
All	All	2146/2256 (95%)	2101 (98%)	43 (2%)	2 (0%)	59	55

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%)	40	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	144/139 (104%)	142 (99%)	2 (1%)	78	81
1	C	143/139 (103%)	143 (100%)	0	100	100
1	D	142/139 (102%)	139 (98%)	3 (2%)	66	67
1	E	142/139 (102%)	141 (99%)	1 (1%)	91	93
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%)	91	93
1	I	141/139 (101%)	140 (99%)	1 (1%)	91	93
1	J	142/139 (102%)	139 (98%)	3 (2%)	66	67
1	K	131/139 (94%)	127 (97%)	4 (3%)	52	49
1	L	125/139 (90%)	120 (96%)	5 (4%)	42	36
All	All	1673/1668 (100%)	1647 (98%)	26 (2%)	76	77

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	19[A]	THR
1	A	19[B]	THR
1	A	32	LEU
1	A	53	ILE
1	A	132	GLU
1	B	30	LEU
1	B	57	LEU
1	D	5	ILE
1	D	6	SER
1	D	53	ILE
1	E	48	ARG
1	H	106	LEU
1	I	132	GLU
1	J	48	ARG
1	J	57	LEU
1	J	152	ARG
1	K	17	GLU
1	K	30	LEU
1	K	32	LEU
1	K	58	MSE
1	L	6	SER

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Mol	Chain	Res	Type
1	L	32	LEU
1	L	47	LEU
1	L	57	LEU
1	L	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 ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	$\# Z  > 2$
3	PEG	A	188	-	6,6,6	0.97	0	5,5,5	0.72	0
3	PEG	A	189	-	6,6,6	0.46	0	5,5,5	0.25	0
3	PEG	A	190	-	6,6,6	0.72	0	5,5,5	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PEG	A	191	-	6,6,6	0.46	0	5,5,5	0.27	0
3	PEG	B	188	-	6,6,6	0.74	0	5,5,5	0.68	0
3	PEG	B	189	-	6,6,6	0.87	0	5,5,5	0.69	0
3	PEG	B	190	-	6,6,6	0.36	0	5,5,5	0.67	0
3	PEG	B	191	-	6,6,6	0.50	0	5,5,5	0.26	0
3	PEG	C	188	-	6,6,6	0.79	0	5,5,5	0.66	0
3	PEG	C	189	-	6,6,6	0.66	0	5,5,5	0.71	0
3	PEG	C	190	-	6,6,6	0.46	0	5,5,5	0.35	0
3	PEG	D	188	-	6,6,6	0.67	0	5,5,5	0.72	0
3	PEG	D	189	-	6,6,6	0.68	0	5,5,5	0.21	0
3	PEG	D	190	-	6,6,6	0.46	0	5,5,5	0.40	0
3	PEG	E	188	-	6,6,6	0.63	0	5,5,5	0.55	0
3	PEG	E	189	-	6,6,6	0.51	0	5,5,5	0.41	0
3	PEG	G	188	-	6,6,6	0.51	0	5,5,5	0.50	0
3	PEG	H	188	-	6,6,6	0.72	0	5,5,5	0.80	0
3	PEG	H	189	-	6,6,6	0.50	0	5,5,5	0.60	0
3	PEG	I	188	-	6,6,6	0.89	0	5,5,5	0.81	0
3	PEG	I	189	-	6,6,6	0.78	0	5,5,5	0.60	0
3	PEG	I	190	-	6,6,6	0.71	0	5,5,5	0.61	0
3	PEG	J	189	-	6,6,6	0.67	0	5,5,5	0.60	0
3	PEG	J	190	-	6,6,6	0.52	0	5,5,5	0.24	0
3	PEG	J	191	-	6,6,6	0.47	0	5,5,5	0.58	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	A	188	-	-	0/4/4/4	0/0/0/0
3	PEG	A	189	-	-	0/4/4/4	0/0/0/0
3	PEG	A	190	-	-	0/4/4/4	0/0/0/0
3	PEG	A	191	-	-	0/4/4/4	0/0/0/0
3	PEG	B	188	-	-	0/4/4/4	0/0/0/0
3	PEG	B	189	-	-	0/4/4/4	0/0/0/0
3	PEG	B	190	-	-	0/4/4/4	0/0/0/0
3	PEG	B	191	-	-	0/4/4/4	0/0/0/0
3	PEG	C	188	-	-	0/4/4/4	0/0/0/0
3	PEG	C	189	-	-	0/4/4/4	0/0/0/0
3	PEG	C	190	-	-	0/4/4/4	0/0/0/0
3	PEG	D	188	-	-	0/4/4/4	0/0/0/0
3	PEG	D	189	-	-	0/4/4/4	0/0/0/0
3	PEG	D	190	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	E	188	-	-	0/4/4/4	0/0/0/0
3	PEG	E	189	-	-	0/4/4/4	0/0/0/0
3	PEG	G	188	-	-	0/4/4/4	0/0/0/0
3	PEG	H	188	-	-	0/4/4/4	0/0/0/0
3	PEG	H	189	-	-	0/4/4/4	0/0/0/0
3	PEG	I	188	-	-	0/4/4/4	0/0/0/0
3	PEG	I	189	-	-	0/4/4/4	0/0/0/0
3	PEG	I	190	-	-	0/4/4/4	0/0/0/0
3	PEG	J	189	-	-	0/4/4/4	0/0/0/0
3	PEG	J	190	-	-	0/4/4/4	0/0/0/0
3	PEG	J	191	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	182/188 (96%)	-0.30	0 100 100	25, 30, 37, 48	0
1	B	185/188 (98%)	-0.24	1 (0%) 88 89	25, 30, 37, 48	0
1	C	183/188 (97%)	-0.30	0 100 100	22, 29, 37, 48	0
1	D	180/188 (95%)	-0.19	0 100 100	25, 30, 38, 51	0
1	E	181/188 (96%)	-0.35	0 100 100	25, 29, 38, 43	0
1	F	181/188 (96%)	-0.27	0 100 100	26, 30, 38, 43	0
1	G	185/188 (98%)	-0.28	1 (0%) 88 89	21, 29, 40, 51	0
1	H	180/188 (95%)	-0.20	1 (0%) 86 88	26, 30, 36, 41	0
1	I	181/188 (96%)	-0.30	1 (0%) 86 88	24, 29, 37, 52	0
1	J	183/188 (97%)	-0.24	1 (0%) 88 89	23, 30, 37, 46	0
1	K	181/188 (96%)	0.06	4 (2%) 59 59	25, 30, 36, 44	0
1	L	181/188 (96%)	0.66	21 (11%) 5 5	26, 29, 35, 43	0
All	All	2183/2256 (96%)	-0.16	30 (1%) 72 72	21, 30, 38, 52	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	19	THR	7.5
1	L	26	CYS	5.3
1	L	18	PRO	5.2
1	L	3	GLY	4.2
1	L	22	TYR	4.1
1	L	33	VAL	3.8
1	L	24	ALA	3.4
1	L	30	LEU	3.3
1	L	17	GLU	3.3
1	K	59	LEU	3.2
1	L	41	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	L	49	ALA	3.0
1	I	3	GLY	2.8
1	H	15	LEU	2.7
1	B	3	GLY	2.6
1	L	21	ALA	2.5
1	L	67	LEU	2.5
1	K	41	ALA	2.5
1	L	147	ALA	2.5
1	J	30	LEU	2.4
1	K	30	LEU	2.4
1	L	114	ASP	2.3
1	L	23	PHE	2.3
1	L	117	PRO	2.3
1	L	40	TYR	2.2
1	G	13	GLY	2.2
1	L	64	LEU	2.2
1	K	17	GLU	2.2
1	L	45	LYS	2.0
1	L	52	ASP	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	PEG	J	191	7/7	0.17	4.84	33,42,46,49	0
3	PEG	G	188	7/7	0.13	4.77	28,35,39,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PEG	A	190	7/7	0.15	4.47	32,40,44,49	0
3	PEG	B	188	7/7	0.13	4.30	25,37,42,50	0
3	PEG	J	189	7/7	0.14	4.16	31,37,47,47	0
3	PEG	D	188	7/7	0.14	2.97	33,38,43,43	0
3	PEG	I	188	7/7	0.14	2.65	32,37,42,43	0
3	PEG	I	190	7/7	0.12	2.59	30,36,42,44	0
3	PEG	B	189	7/7	0.12	2.33	27,35,42,43	0
2	CL	J	188	1/1	0.14	2.06	50,50,50,50	0
3	PEG	E	189	7/7	0.13	1.81	52,54,57,58	0
3	PEG	E	188	7/7	0.11	1.61	33,37,44,49	0
3	PEG	C	190	7/7	0.12	1.43	36,41,48,49	0
3	PEG	B	190	7/7	0.11	1.13	40,41,48,51	0
3	PEG	H	188	7/7	0.12	0.97	35,46,53,53	0
3	PEG	I	189	7/7	0.13	0.80	40,42,48,51	0
3	PEG	C	188	7/7	0.11	0.65	33,37,41,49	0
3	PEG	D	189	7/7	0.11	0.55	34,44,46,46	0
3	PEG	A	188	7/7	0.11	0.50	19,31,37,41	0
3	PEG	J	190	7/7	0.12	0.13	43,48,56,56	0
3	PEG	B	191	7/7	0.11	0.01	43,47,52,57	0
3	PEG	C	189	7/7	0.10	-0.03	29,39,45,47	0
3	PEG	H	189	7/7	0.12	-0.08	41,43,48,51	0
3	PEG	A	189	7/7	0.10	-0.09	36,36,39,48	0
3	PEG	A	191	7/7	0.10	-0.56	29,32,43,47	0
3	PEG	D	190	7/7	0.09	-1.57	39,45,49,51	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.