



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 09:52 pm BST

PDB ID : 4I1M  
Title : Crystal structure of the Legionella pneumophila GAP domain of LepB  
Authors : Streller, A.; Gazdag, E.M.; Vetter, I.R.; Goody, R.S.; Itzen, A.  
Deposited on : 2012-11-21  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

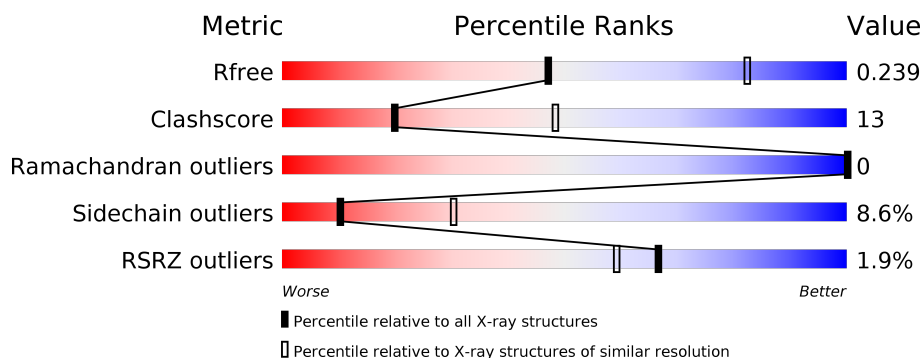
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	302	<div> <div>75%</div> <div>18%</div> <div>• 6%</div> </div>
1	B	302	<div> <div>%</div> <div>71%</div> <div>19%</div> <div>• 9%</div> </div>
1	C	302	<div> <div>4%</div> <div>68%</div> <div>26%</div> <div>• •</div> </div>

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	A	701	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6534 atoms, of which 10 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 LepB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2240	1448	368	417	7			
1	B	276	Total	C	N	O	S	0	1	0
			2130	1379	346	398	7			
1	C	293	Total	C	N	O	S	0	0	0
			2119	1355	350	407	7			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	457	ALA	LYS	ENGINEERED MUTATION	UNP Q5ZSM7
A	458	ALA	GLU	ENGINEERED MUTATION	UNP Q5ZSM7
A	460	ALA	LYS	ENGINEERED MUTATION	UNP Q5ZSM7
B	457	ALA	LYS	ENGINEERED MUTATION	UNP Q5ZSM7
B	458	ALA	GLU	ENGINEERED MUTATION	UNP Q5ZSM7
B	460	ALA	LYS	ENGINEERED MUTATION	UNP Q5ZSM7
C	457	ALA	LYS	ENGINEERED MUTATION	UNP Q5ZSM7
C	458	ALA	GLU	ENGINEERED MUTATION	UNP Q5ZSM7
C	460	ALA	LYS	ENGINEERED MUTATION	UNP Q5ZSM7

- 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	H	O	0	0
			17	4	10	3		

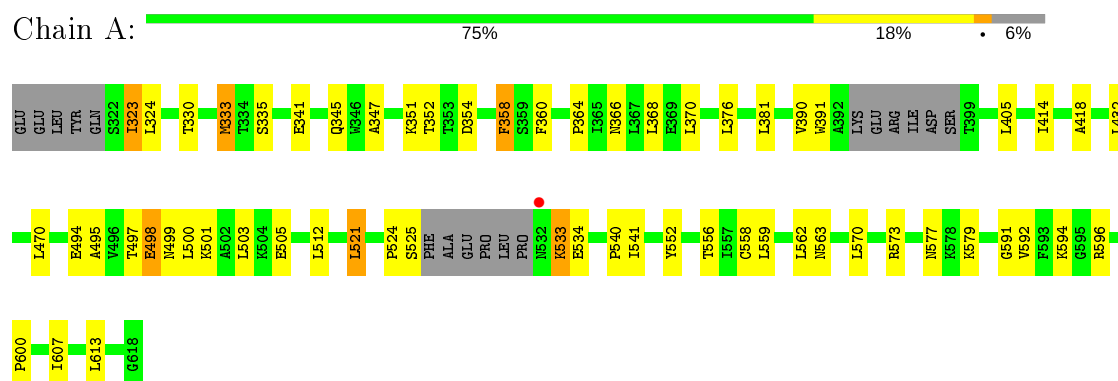
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	24	Total	O	0	0
			24	24		
3	B	4	Total	O	0	0
			4	4		

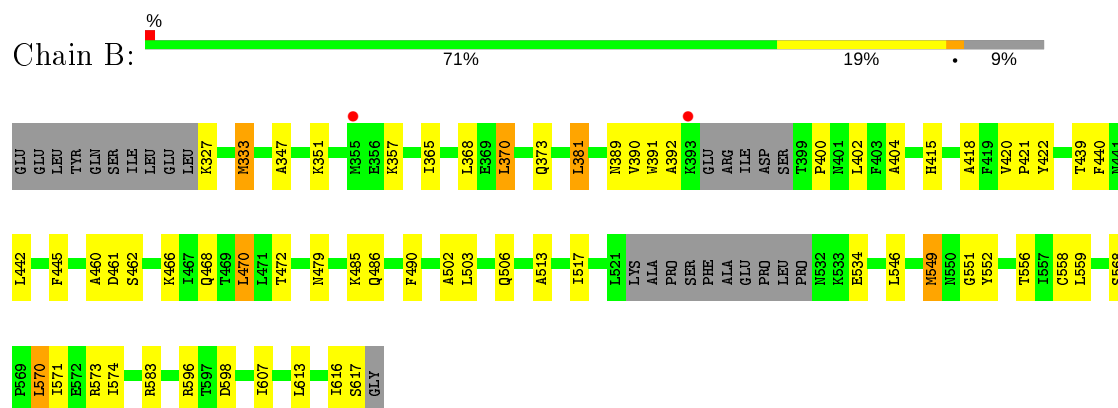
### 3 Residue-property plots

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

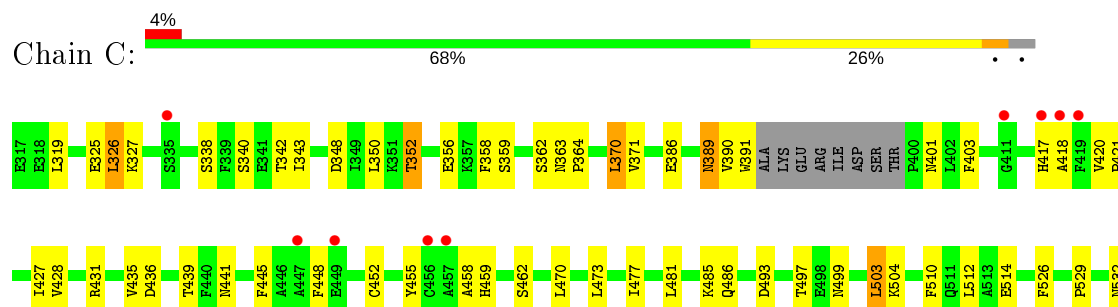
#### • Molecule 1: LepB

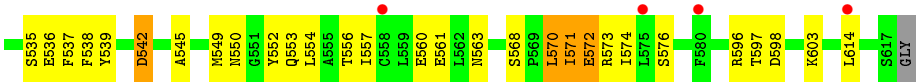


#### • Molecule 1: LepB



#### • Molecule 1: LepB





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 <sub>2</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	152.70 Å   152.70 Å   129.50 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	49.83 – 2.80 49.83 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.83-2.80) 99.9 (49.83-2.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.47 (at 2.81 Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, $R_{free}$	0.200   ,   0.238 0.204   ,   0.239	Depositor DCC
$R_{free}$ test set	1903 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.9	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 56.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6534	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG

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	0.26	0/2288	0.42	0/3101
1	B	0.23	0/2180	0.39	0/2966
1	C	0.23	0/2170	0.39	0/2968
All	All	0.24	0/6638	0.40	0/9035

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

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	2240	0	2224	42	0
1	B	2130	0	2045	42	0
1	C	2119	0	1849	77	0
2	A	7	10	9	1	0
3	A	24	0	0	3	0
3	B	4	0	0	1	0
All	All	6524	10	6127	159	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 13.

All (159) 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:C:535:SER:HB2	1:C:570:LEU:HD12	1.33	1.10
1:A:533:LYS:HD3	1:A:533:LYS:H	1.12	1.07
1:C:570:LEU:HD22	1:C:574:ILE:HD11	1.36	1.03
1:C:570:LEU:CD2	1:C:574:ILE:HD11	1.89	1.02
1:C:570:LEU:O	1:C:574:ILE:HD12	1.63	0.97
1:C:532:ASN:ND2	1:C:538:PHE:O	2.00	0.94
1:B:418:ALA:H	1:B:556:THR:HG21	1.36	0.91
1:C:568:SER:O	1:C:571:ILE:HG22	1.69	0.90
1:A:533:LYS:H	1:A:533:LYS:CD	1.85	0.88
1:A:418:ALA:H	1:A:556:THR:HG21	1.37	0.88
1:A:596:ARG:HB2	1:A:600:PRO:HG3	1.57	0.86
1:C:418:ALA:HB3	1:C:556:THR:HG21	1.56	0.86
1:A:495:ALA:O	1:A:499:ASN:ND2	2.10	0.83
1:B:333:MET:HE3	1:B:370:LEU:HD23	1.61	0.80
1:A:323:ILE:HD13	1:A:324:LEU:N	1.98	0.78
1:B:365:ILE:O	1:B:485:LYS:NZ	2.16	0.78
1:C:536:GLU:HG3	1:C:537:PHE:CE1	2.19	0.77
1:A:552:TYR:O	1:A:556:THR:HG23	1.86	0.75
1:C:570:LEU:HD22	1:C:574:ILE:CD1	2.15	0.74
1:C:535:SER:CB	1:C:570:LEU:HD12	2.14	0.73
1:C:436:ASP:HB3	1:C:439:THR:HG22	1.72	0.72
1:A:541:ILE:O	1:A:573:ARG:NH2	2.19	0.72
1:A:534:GLU:OE1	3:A:808:HOH:O	2.07	0.71
1:C:390:VAL:HG12	1:C:391:TRP:H	1.57	0.70
1:C:549:MET:CE	1:C:550:ASN:H	2.04	0.69
1:A:533:LYS:N	1:A:533:LYS:HD3	1.97	0.69
1:B:460:ALA:O	1:B:461:ASP:HB2	1.93	0.69
1:B:558:CYS:HB3	1:B:607:ILE:HD13	1.74	0.68
1:B:613:LEU:O	1:B:613:LEU:HD23	1.93	0.67
1:C:371:VAL:HG13	1:C:435:VAL:HG13	1.75	0.67
1:C:401:ASN:HB2	1:C:421:PRO:O	1.95	0.67
1:C:549:MET:HE3	1:C:550:ASN:H	1.58	0.67
1:C:348:ASP:O	1:C:352:THR:HG23	1.95	0.66
1:A:323:ILE:HD13	1:A:323:ILE:C	2.15	0.66
1:C:572:GLU:HG3	1:C:573:ARG:N	2.13	0.63
1:C:481:LEU:O	1:C:485:LYS:HG3	2.00	0.62
1:C:350:LEU:HB3	1:C:504:LYS:HZ1	1.66	0.61
1:B:389:ASN:O	1:B:392:ALA:HB3	2.01	0.61
1:C:338:SER:O	1:C:342:THR:HG23	2.00	0.60
1:A:494:GLU:OE2	1:A:498:GLU:HG2	2.00	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:537:PHE:HD2	1:C:560:GLU:HG3	1.66	0.60
1:A:333:MET:HE1	1:A:366:ASN:H	1.65	0.60
1:A:591:GLY:O	1:A:594:LYS:HG2	2.01	0.60
1:C:536:GLU:HG3	1:C:537:PHE:CD1	2.35	0.60
1:C:390:VAL:HG12	1:C:391:TRP:N	2.18	0.59
1:C:549:MET:SD	1:C:553:GLN:CB	2.90	0.59
1:C:363:ASN:HB2	1:C:364:PRO:HD3	1.86	0.58
1:C:350:LEU:O	1:C:504:LYS:NZ	2.36	0.58
1:C:470:LEU:HD23	1:C:470:LEU:C	2.23	0.57
1:B:558:CYS:HA	1:B:571:ILE:HD13	1.87	0.57
1:C:439:THR:HG23	1:C:441:ASN:H	1.70	0.56
1:B:327:LYS:N	3:B:702:HOH:O	2.37	0.56
1:B:347:ALA:O	1:B:351:LYS:HG3	2.04	0.56
1:C:340:SER:OG	1:C:514:GLU:OE2	2.18	0.56
1:A:596:ARG:CB	1:A:600:PRO:HG3	2.34	0.56
1:C:549:MET:HE2	1:C:550:ASN:N	2.20	0.56
1:C:554:LEU:O	1:C:557:ILE:HG22	2.05	0.55
1:A:540:PRO:HA	3:A:808:HOH:O	2.06	0.55
1:A:501:LYS:HE3	1:A:505:GLU:HG3	1.88	0.55
1:C:549:MET:CE	1:C:550:ASN:N	2.70	0.54
1:C:542:ASP:O	1:C:545:ALA:N	2.40	0.54
1:C:418:ALA:HB3	1:C:556:THR:CG2	2.33	0.54
1:A:501:LYS:HE3	1:A:505:GLU:CG	2.38	0.53
1:C:371:VAL:HG13	1:C:435:VAL:CG1	2.38	0.53
1:C:570:LEU:O	1:C:574:ILE:CD1	2.48	0.53
1:B:568:SER:O	1:B:571:ILE:HG22	2.08	0.52
1:B:381:LEU:HG	1:C:526:PHE:CZ	2.44	0.52
1:B:390:VAL:HG12	1:B:391:TRP:N	2.25	0.52
1:A:347:ALA:O	1:A:351:LYS:HG3	2.09	0.51
1:C:549:MET:CE	1:C:553:GLN:CB	2.88	0.51
1:A:360:PHE:HB2	1:A:500:LEU:HD11	1.93	0.51
1:B:552:TYR:O	1:B:556:THR:HG23	2.10	0.51
1:B:470:LEU:HD23	1:B:513:ALA:HB3	1.92	0.51
1:C:561:GLU:OE1	1:C:568:SER:OG	2.23	0.51
1:B:502:ALA:O	1:B:506:GLN:HG3	2.11	0.51
1:C:427:ILE:O	1:C:431:ARG:HG2	2.11	0.51
1:A:323:ILE:CD1	1:A:323:ILE:C	2.77	0.50
1:B:613:LEU:C	1:B:613:LEU:HD23	2.31	0.50
1:A:390:VAL:HG23	1:A:391:TRP:CD2	2.47	0.50
1:C:418:ALA:CB	1:C:556:THR:HG21	2.36	0.50
1:A:505:GLU:HG2	3:A:818:HOH:O	2.12	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:GLN:O	1:B:472:THR:HG23	2.12	0.50
1:B:460:ALA:O	1:B:461:ASP:CB	2.57	0.50
1:B:439:THR:O	1:B:440:PHE:HB2	2.12	0.49
1:A:358:PHE:H	1:A:358:PHE:HD1	1.61	0.49
1:A:558:CYS:HB3	1:A:607:ILE:HD13	1.95	0.49
1:C:327:LYS:O	1:C:359:SER:N	2.31	0.49
1:C:537:PHE:CE2	1:C:563:ASN:HB2	2.48	0.49
1:B:333:MET:HE2	1:B:373:GLN:OE1	2.13	0.48
1:B:391:TRP:CB	1:B:402:LEU:HD11	2.43	0.48
1:B:616:ILE:HG13	1:B:617:SER:N	2.28	0.48
1:C:538:PHE:CZ	1:C:557:ILE:HG13	2.49	0.48
1:C:570:LEU:HD23	1:C:574:ILE:HD11	1.89	0.48
1:A:533:LYS:HE2	1:A:534:GLU:N	2.28	0.48
1:C:326:LEU:HD12	1:C:358:PHE:C	2.34	0.48
1:C:362:SER:O	1:C:485:LYS:NZ	2.47	0.48
1:B:551:GLY:N	1:B:583:ARG:HG2	2.29	0.47
1:C:499:ASN:O	1:C:503:LEU:HB2	2.15	0.47
1:B:534:GLU:CD	1:B:573:ARG:HH21	2.17	0.47
1:C:537:PHE:CD2	1:C:560:GLU:HG3	2.49	0.47
1:C:596:ARG:NH2	1:C:598:ASP:OD2	2.45	0.47
1:C:326:LEU:HA	1:C:326:LEU:HD13	1.77	0.47
1:B:551:GLY:CA	1:B:583:ARG:HG2	2.45	0.46
1:B:400:PRO:HB2	1:B:404:ALA:HB2	1.97	0.46
1:A:577:ASN:OD1	1:A:579:LYS:HG2	2.16	0.46
1:C:455:TYR:O	1:C:458:ALA:HB3	2.16	0.46
1:C:549:MET:HG3	1:C:553:GLN:CB	2.46	0.46
1:A:333:MET:CE	1:A:366:ASN:H	2.26	0.46
1:B:534:GLU:O	1:B:570:LEU:HB2	2.15	0.46
1:B:596:ARG:NH2	1:B:598:ASP:OD2	2.43	0.45
1:C:568:SER:O	1:C:571:ILE:CG2	2.54	0.45
1:C:571:ILE:HG23	1:C:572:GLU:N	2.32	0.45
1:B:327:LYS:NZ	1:B:357:LYS:O	2.42	0.44
1:C:343:ILE:HG21	1:C:510:PHE:CD1	2.52	0.44
1:A:390:VAL:HG23	1:A:391:TRP:CE2	2.53	0.44
1:B:486:GLN:NE2	1:B:490:PHE:HE2	2.14	0.44
1:C:470:LEU:HD23	1:C:470:LEU:O	2.18	0.44
1:C:570:LEU:CD2	1:C:574:ILE:CD1	2.79	0.44
1:A:521:LEU:HA	1:A:521:LEU:HD12	1.80	0.44
1:B:570:LEU:O	1:B:574:ILE:HG13	2.17	0.44
1:A:358:PHE:CZ	1:A:500:LEU:HD13	2.53	0.43
1:A:501:LYS:HE3	1:A:505:GLU:OE2	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:VAL:HA	1:C:421:PRO:HD3	1.83	0.43
1:C:459:HIS:CD2	1:C:462:SER:HB3	2.53	0.43
1:C:549:MET:CG	1:C:553:GLN:CB	2.96	0.43
1:A:501:LYS:HD2	1:A:501:LYS:O	2.17	0.43
1:A:562:LEU:HD11	1:A:607:ILE:HG13	2.00	0.43
1:A:323:ILE:O	1:A:323:ILE:HG12	2.18	0.43
1:B:390:VAL:HG12	1:B:391:TRP:H	1.83	0.43
1:B:462:SER:O	1:B:466:LYS:HG2	2.19	0.43
1:C:350:LEU:HB3	1:C:504:LYS:NZ	2.32	0.42
1:C:532:ASN:HD22	1:C:539:TYR:HA	1.85	0.42
1:A:524:PRO:O	1:A:525:SER:C	2.57	0.42
1:C:389:ASN:OD1	1:C:529:PRO:HB3	2.20	0.42
1:C:537:PHE:HE2	1:C:563:ASN:HB2	1.84	0.42
1:B:370:LEU:HA	1:B:370:LEU:HD23	1.86	0.42
1:C:493:ASP:O	1:C:497:THR:HG22	2.20	0.42
1:A:563:ASN:HB3	2:A:701:PEG:H31	2.01	0.42
1:C:596:ARG:O	1:C:597:THR:OG1	2.17	0.42
1:C:390:VAL:CG1	1:C:391:TRP:H	2.31	0.41
1:A:335:SER:HB2	1:A:345:GLN:OE1	2.20	0.41
1:C:552:TYR:O	1:C:556:THR:HG23	2.21	0.41
1:C:598:ASP:CG	1:C:603:LYS:HZ2	2.23	0.41
1:B:420:VAL:HA	1:B:421:PRO:HD3	1.89	0.41
1:B:549:MET:HE2	1:B:549:MET:HB2	1.86	0.41
1:C:370:LEU:HD23	1:C:370:LEU:HA	1.92	0.41
1:C:552:TYR:H	1:C:552:TYR:HD2	1.69	0.41
1:B:546:LEU:HA	1:B:549:MET:HE2	2.02	0.41
1:C:403:PHE:CE1	1:C:452:CYS:HA	2.56	0.41
1:C:439:THR:HG23	1:C:441:ASN:N	2.33	0.41
1:A:341:GLU:OE1	1:A:345:GLN:NE2	2.45	0.41
1:A:330:THR:HG21	1:A:364:PRO:HG2	2.03	0.40
1:B:598:ASP:N	1:B:598:ASP:OD1	2.50	0.40
1:A:351:LYS:HE3	1:B:440:PHE:CZ	2.56	0.40
1:A:501:LYS:HA	1:A:501:LYS:HD2	1.87	0.40
1:B:418:ALA:N	1:B:556:THR:HG21	2.18	0.40
1:C:473:LEU:O	1:C:477:ILE:HG13	2.21	0.40
1:B:420:VAL:HG12	1:B:422:TYR:H	1.87	0.40
1:C:428:VAL:HG11	1:C:448:PHE:HD2	1.86	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	279/302 (92%)	270 (97%)	9 (3%)	0	100	100
1	B	271/302 (90%)	259 (96%)	12 (4%)	0	100	100
1	C	289/302 (96%)	257 (89%)	32 (11%)	0	100	100
All	All	839/906 (93%)	786 (94%)	53 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	239/262 (91%)	216 (90%)	23 (10%)	8	24
1	B	218/262 (83%)	204 (94%)	14 (6%)	17	45
1	C	192/262 (73%)	173 (90%)	19 (10%)	8	23
All	All	649/786 (83%)	593 (91%)	56 (9%)	10	30

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	323	ILE
1	A	333	MET
1	A	352	THR
1	A	354	ASP
1	A	358	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	368	LEU
1	A	370	LEU
1	A	376	LEU
1	A	381	LEU
1	A	405	LEU
1	A	414	ILE
1	A	432	LEU
1	A	470	LEU
1	A	497	THR
1	A	498	GLU
1	A	503	LEU
1	A	512	LEU
1	A	521	LEU
1	A	533	LYS
1	A	559	LEU
1	A	570	LEU
1	A	592	VAL
1	A	613	LEU
1	B	333	MET
1	B	368	LEU
1	B	370	LEU
1	B	381	LEU
1	B	415	HIS
1	B	442	LEU
1	B	445	PHE
1	B	470	LEU
1	B	479	ASN
1	B	503	LEU
1	B	517	ILE
1	B	549	MET
1	B	559	LEU
1	B	570	LEU
1	C	319	LEU
1	C	325	GLU
1	C	326	LEU
1	C	352	THR
1	C	356	GLU
1	C	370	LEU
1	C	386	GLU
1	C	389	ASN
1	C	417	HIS
1	C	445	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	486	GLN
1	C	503	LEU
1	C	512	LEU
1	C	542	ASP
1	C	570	LEU
1	C	571	ILE
1	C	572	GLU
1	C	576	SER
1	C	614	LEU

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

Mol	Chain	Res	Type
1	A	344	ASN
1	C	532	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	PEG	A	701	-	6,6,6	0.83	0	5,5,5	0.66	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	A	701	-	-	0/4/4/4	-

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	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 ⓘ

### 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	285/302 (94%)	0.02	1 (0%) 92 91	30, 47, 93, 145	0
1	B	276/302 (91%)	-0.07	2 (0%) 87 84	35, 63, 112, 142	0
1	C	293/302 (97%)	0.26	13 (4%) 34 24	64, 112, 150, 166	4 (1%)
All	All	854/906 (94%)	0.07	16 (1%) 66 59	30, 72, 140, 166	4 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	418	ALA	4.5
1	C	456	CYS	3.8
1	C	457	ALA	3.6
1	C	447	ALA	3.1
1	B	355	MET	3.1
1	C	419	PHE	3.0
1	C	614	LEU	2.9
1	C	449	GLU	2.6
1	C	580	PHE	2.6
1	C	575	LEU	2.6
1	B	393	LYS	2.6
1	C	335	SER	2.6
1	C	417	HIS	2.5
1	C	411	GLY	2.4
1	C	558	CYS	2.3
1	A	532	ASN	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 [i](#)

There are no carbohydrates 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<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( $\text{\AA}^2$ )	Q<0.9
2	PEG	A	701	7/7	0.64	0.42	97,117,129,130	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.