



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 04:37 AM BST

PDB ID : 4H09  
Title : Crystal structure of a leucine-rich repeat protein (EUBVEN\_01088) from *Escherichia coli* strain ATCC 27560 at 2.50 Å resolution  
Authors : Joint Center for Structural Genomics (JCSG)  
Deposited on : 2012-09-07  
Resolution : 2.50 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.

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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 : 2.13.1  
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) : 2.13.1

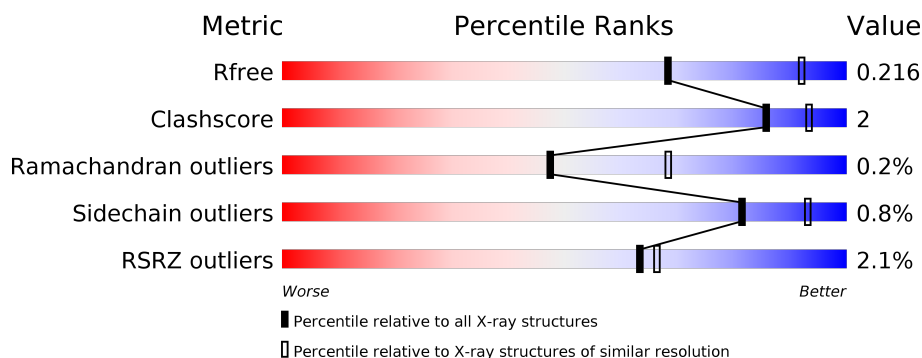
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	379	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>7%</div> </div> </div>
1	B	379	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div>5%</div> </div> </div>
1	C	379	<div> <div>2%</div> <div> <div></div> <div>95%</div> <div></div> </div> </div>
1	D	379	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>
1	E	379	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>6%</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
3	EDO	B	505	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14625 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.

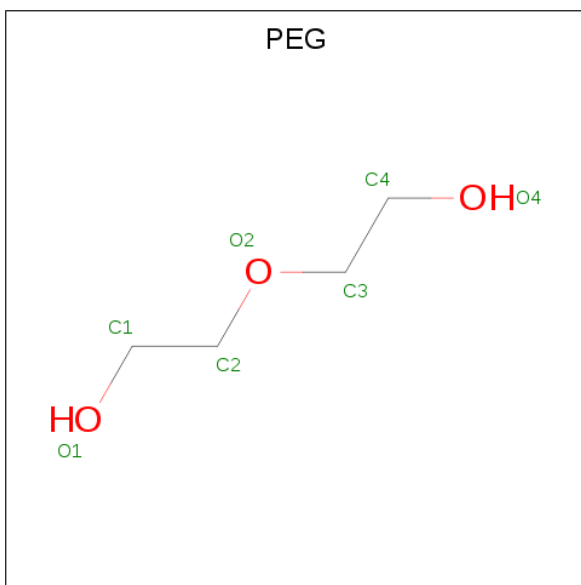
- Molecule 1 is a protein called Hypothetical leucine rich repeat protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	Se	0	1	0
			2832	1808	444	568	6	6			
1	B	372	Total	C	N	O	S	Se	0	0	0
			2778	1768	439	559	6	6			
1	C	373	Total	C	N	O	S	Se	0	0	0
			2780	1768	442	558	6	6			
1	D	377	Total	C	N	O	S	Se	0	2	0
			2849	1818	450	569	6	6			
1	E	373	Total	C	N	O	S	Se	0	0	0
			2807	1791	445	559	6	6			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	leader sequence	UNP A5Z5V6
B	0	GLY	-	leader sequence	UNP A5Z5V6
C	0	GLY	-	leader sequence	UNP A5Z5V6
D	0	GLY	-	leader sequence	UNP A5Z5V6
E	0	GLY	-	leader sequence	UNP A5Z5V6

- 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	D	1	Total	C	O	0	0
			7	4	3		
2	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	64	Total O 64 64	0	0
4	B	77	Total O 77 77	0	0
4	C	90	Total O 90 90	0	0

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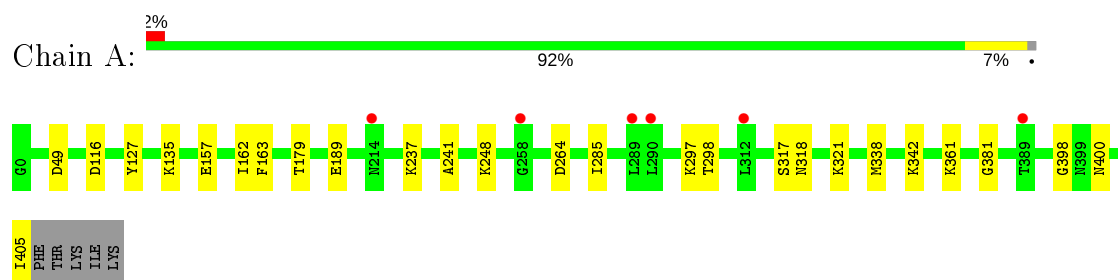
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	93	Total	O	0	0
			93	93		
4	E	75	Total	O	0	0
			75	75		



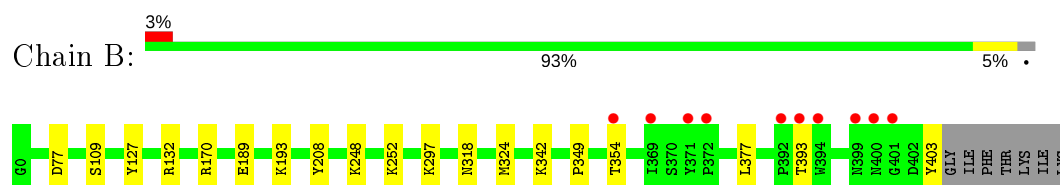
### 3 Residue-property plots [i](#)

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.

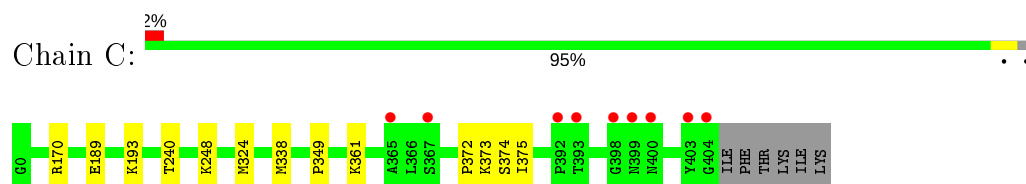
- Molecule 1: Hypothetical leucine rich repeat protein



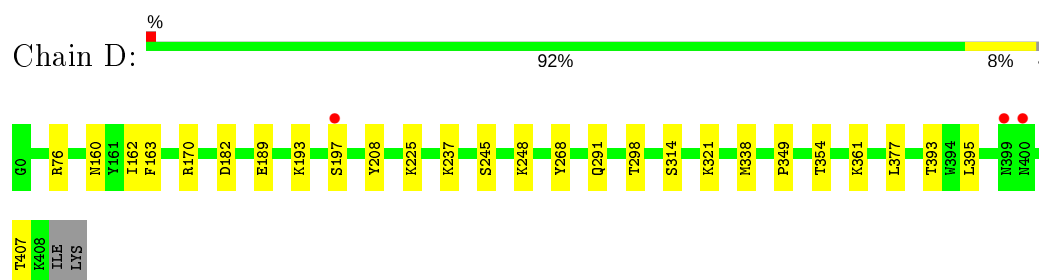
- Molecule 1: Hypothetical leucine rich repeat protein



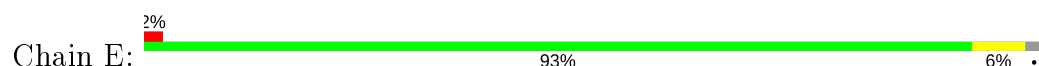
- Molecule 1: Hypothetical leucine rich repeat protein

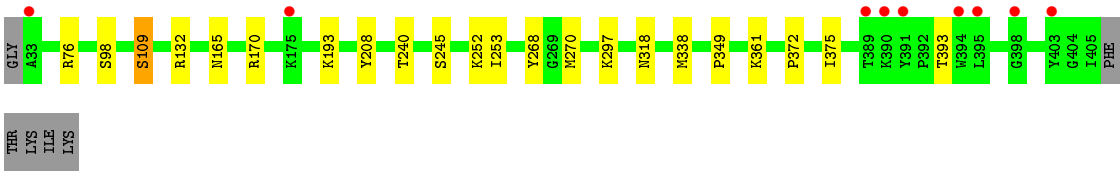


- Molecule 1: Hypothetical leucine rich repeat protein



- Molecule 1: Hypothetical leucine rich repeat protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.51Å 105.51Å 361.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.96 – 2.50 29.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.96-2.50) 99.9 (29.96-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 2.51Å)	Xtriage
Refinement program	BUSTER-TNT 2.10.0, BUSTER 2.10.0	Depositor
R, $R_{free}$	0.176 , 0.209 0.183 , 0.216	Depositor DCC
$R_{free}$ test set	3933 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.4	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 45.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.054 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14625	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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, EDO

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	0.49	0/2881	0.68	0/3907
1	B	0.47	0/2823	0.68	0/3839
1	C	0.49	0/2825	0.69	0/3836
1	D	0.51	0/2901	0.69	0/3937
1	E	0.48	0/2853	0.67	0/3871
All	All	0.49	0/14283	0.68	0/19390

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2832	0	2816	16	0
1	B	2778	0	2701	10	0
1	C	2780	0	2698	7	0
1	D	2849	0	2823	15	0
1	E	2807	0	2766	13	0
2	A	14	0	20	3	0
2	D	14	0	20	1	0
3	A	48	0	72	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	42	1	0
3	C	20	0	30	1	0
3	D	32	0	48	2	0
3	E	24	0	36	2	0
4	A	64	0	0	0	0
4	B	77	0	0	0	0
4	C	90	0	0	1	0
4	D	93	0	0	1	0
4	E	75	0	0	1	0
All	All	14625	0	14072	61	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 2.

All (61) 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:A:285:ILE:H	3:A:510:EDO:H22	1.40	0.85
1:D:395:LEU:HD22	1:D:404:GLY:O	1.78	0.84
1:E:240:THR:HA	3:E:501:EDO:H12	1.77	0.66
1:C:240:THR:HA	3:C:503:EDO:H12	1.78	0.65
1:A:116:ASP:H	2:A:501:PEG:H12	1.61	0.65
1:E:372:PRO:HD2	1:E:375:ILE:HD11	1.84	0.58
1:D:349:PRO:HB2	4:D:608:HOH:O	2.04	0.57
1:D:160:ASN:OD1	1:D:182:ASP:HB2	2.05	0.56
1:A:157[B]:GLU:HG2	1:A:179:THR:HB	1.87	0.56
1:E:338:MSE:HG3	1:E:361:LYS:HB3	1.87	0.55
1:A:135:LYS:HG2	1:A:157[B]:GLU:HB2	1.89	0.54
1:A:127:TYR:CE2	3:A:504:EDO:H21	2.44	0.53
1:D:298:THR:HG22	1:D:321:LYS:HB3	1.89	0.53
1:A:298:THR:HG22	1:A:321:LYS:HB3	1.91	0.51
1:D:245:SER:HA	1:D:268:TYR:O	2.11	0.51
1:C:338:MSE:HE1	4:C:630:HOH:O	2.10	0.51
1:E:165:ASN:HD22	3:E:506:EDO:H12	1.75	0.51
1:A:135:LYS:HG2	1:A:157[A]:GLU:HB3	1.93	0.51
3:A:506:EDO:H22	1:B:77:ASP:HB2	1.93	0.50
1:E:245:SER:HA	1:E:268:TYR:O	2.12	0.49
1:E:297:LYS:HE2	1:E:318:ASN:HB3	1.94	0.48
1:E:253:ILE:HD11	1:E:270:MSE:HE1	1.95	0.48
1:B:127:TYR:CE2	3:B:502:EDO:H12	2.49	0.48
1:A:398:GLY:C	1:A:400:ASN:H	2.16	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ILE:HG23	1:A:163:PHE:CD2	2.50	0.47
1:A:264:ASP:H	2:A:502:PEG:C2	2.28	0.47
1:E:372:PRO:HD2	1:E:375:ILE:CD1	2.45	0.47
1:A:381:GLY:H	3:A:509:EDO:H11	1.80	0.47
1:C:189:GLU:O	1:C:248:LYS:HE2	2.16	0.46
1:A:297:LYS:HE2	1:A:318:ASN:HB3	1.98	0.45
1:E:76:ARG:HD2	1:E:98:SER:O	2.16	0.45
1:B:297:LYS:HE2	1:B:318:ASN:HB3	1.99	0.44
1:D:162:ILE:HG23	1:D:163:PHE:CD2	2.53	0.44
1:A:318:ASN:HA	1:A:342:LYS:HD2	2.00	0.44
1:A:241:ALA:HB2	2:A:502:PEG:H21	2.00	0.44
1:D:291:GLN:HG3	1:D:314:SER:HB3	2.00	0.44
1:D:76:ARG:HH22	3:D:506:EDO:H12	1.83	0.43
1:A:189:GLU:O	1:A:248:LYS:HE2	2.19	0.43
1:E:170:ARG:HG3	1:E:193:LYS:HB2	2.01	0.43
1:C:338:MSE:HG3	1:C:361:LYS:HB3	2.01	0.42
1:B:354:THR:HG23	1:B:377:LEU:HD23	2.02	0.42
1:E:349:PRO:HB2	4:E:635:HOH:O	2.18	0.42
1:D:225:LYS:HG3	3:D:510:EDO:H21	2.02	0.42
1:C:324:MSE:HB3	1:C:349:PRO:HG3	2.02	0.42
1:D:170:ARG:HG3	1:D:193:LYS:HB2	2.02	0.42
1:D:193:LYS:HA	1:D:208:TYR:HB3	2.02	0.41
1:B:318:ASN:HA	1:B:342:LYS:HD2	2.02	0.41
1:D:197:SER:HA	2:D:502:PEG:H11	2.02	0.41
1:C:170:ARG:HG3	1:C:193:LYS:HB2	2.03	0.41
1:A:338:MSE:HG3	1:A:361:LYS:HB3	2.03	0.41
1:E:109:SER:O	1:E:132:ARG:HB2	2.20	0.41
1:B:109:SER:O	1:B:132:ARG:HB2	2.21	0.41
1:C:372:PRO:C	1:C:374:SER:H	2.24	0.41
1:D:338:MSE:HG3	1:D:361:LYS:HB3	2.03	0.41
1:B:193:LYS:HA	1:B:208:TYR:HB3	2.03	0.41
1:D:354:THR:HG23	1:D:377:LEU:HD23	2.03	0.41
1:B:170:ARG:HG3	1:B:193:LYS:HB2	2.02	0.40
1:B:189:GLU:O	1:B:248:LYS:HE3	2.20	0.40
1:B:324:MSE:HB3	1:B:349:PRO:HG3	2.03	0.40
1:D:189:GLU:O	1:D:248:LYS:HE3	2.21	0.40
1:E:193:LYS:HA	1:E:208:TYR:HB3	2.02	0.40

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	373/379 (98%)	360 (96%)	13 (4%)	0	100	100
1	B	370/379 (98%)	359 (97%)	11 (3%)	0	100	100
1	C	371/379 (98%)	358 (96%)	11 (3%)	2 (0%)	29	48
1	D	377/379 (100%)	365 (97%)	11 (3%)	1 (0%)	41	61
1	E	371/379 (98%)	358 (96%)	13 (4%)	0	100	100
All	All	1862/1895 (98%)	1800 (97%)	59 (3%)	3 (0%)	47	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	406	PHE
1	C	373	LYS
1	C	375	ILE

### 5.3.2 Protein sidechains [i](#)

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	315/320 (98%)	311 (99%)	4 (1%)	69	87
1	B	301/320 (94%)	298 (99%)	3 (1%)	76	90
1	C	298/320 (93%)	298 (100%)	0	100	100
1	D	314/320 (98%)	311 (99%)	3 (1%)	76	90
1	E	307/320 (96%)	304 (99%)	3 (1%)	76	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1535/1600 (96%)	1522 (99%)	13 (1%)	81	93

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASP
1	A	237	LYS
1	A	317	SER
1	A	405	ILE
1	B	252	LYS
1	B	393	THR
1	B	403	TYR
1	D	237	LYS
1	D	393	THR
1	D	407	THR
1	E	109	SER
1	E	252	LYS
1	E	393	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	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 monosaccharides in this entry.



## 5.6 Ligand geometry

42 ligands are 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	$\# Z  > 2$
3	EDO	C	505	-	3,3,3	0.74	0	2,2,2	0.11	0
3	EDO	D	507	-	3,3,3	0.69	0	2,2,2	0.11	0
3	EDO	E	502	-	3,3,3	0.46	0	2,2,2	0.40	0
3	EDO	D	506	-	3,3,3	0.66	0	2,2,2	0.17	0
3	EDO	E	503	-	3,3,3	0.66	0	2,2,2	0.31	0
3	EDO	A	508	-	3,3,3	1.08	0	2,2,2	0.23	0
3	EDO	A	514	-	3,3,3	0.60	0	2,2,2	0.34	0
3	EDO	D	509	-	3,3,3	0.74	0	2,2,2	0.05	0
3	EDO	E	505	-	3,3,3	0.53	0	2,2,2	0.33	0
3	EDO	E	501	-	3,3,3	0.37	0	2,2,2	0.42	0
3	EDO	B	503	-	3,3,3	0.76	0	2,2,2	0.10	0
2	PEG	A	501	-	6,6,6	0.37	0	5,5,5	0.28	0
3	EDO	A	506	-	3,3,3	1.00	0	2,2,2	0.23	0
3	EDO	B	502	-	3,3,3	0.47	0	2,2,2	0.43	0
2	PEG	A	502	-	6,6,6	0.19	0	5,5,5	0.26	0
2	PEG	D	501	-	6,6,6	0.18	0	5,5,5	0.11	0
3	EDO	A	507	-	3,3,3	0.85	0	2,2,2	0.34	0
3	EDO	C	504	-	3,3,3	0.72	0	2,2,2	0.04	0
3	EDO	D	504	-	3,3,3	0.42	0	2,2,2	0.32	0
3	EDO	A	504	-	3,3,3	0.69	0	2,2,2	0.09	0
3	EDO	B	504	-	3,3,3	0.94	0	2,2,2	0.12	0
3	EDO	A	512	-	3,3,3	0.35	0	2,2,2	0.48	0
3	EDO	D	510	-	3,3,3	0.60	0	2,2,2	0.12	0
3	EDO	B	506	-	3,3,3	0.69	0	2,2,2	0.09	0
3	EDO	E	506	-	3,3,3	0.48	0	2,2,2	0.63	0
3	EDO	C	502	-	3,3,3	0.75	0	2,2,2	0.16	0
3	EDO	B	505	-	3,3,3	0.66	0	2,2,2	0.22	0
3	EDO	C	503	-	3,3,3	0.50	0	2,2,2	0.45	0
3	EDO	A	503	-	3,3,3	0.84	0	2,2,2	0.08	0
3	EDO	A	509	-	3,3,3	0.78	0	2,2,2	0.08	0
3	EDO	D	508	-	3,3,3	0.57	0	2,2,2	0.25	0
3	EDO	E	504	-	3,3,3	0.67	0	2,2,2	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	D	503	-	3,3,3	0.58	0	2,2,2	0.48	0
3	EDO	C	501	-	3,3,3	0.76	0	2,2,2	0.17	0
3	EDO	B	507	-	3,3,3	0.59	0	2,2,2	0.26	0
3	EDO	A	511	-	3,3,3	0.77	0	2,2,2	0.10	0
2	PEG	D	502	-	6,6,6	0.19	0	5,5,5	0.11	0
3	EDO	A	510	-	3,3,3	0.66	0	2,2,2	0.16	0
3	EDO	B	501	-	3,3,3	0.80	0	2,2,2	0.11	0
3	EDO	D	505	-	3,3,3	0.50	0	2,2,2	0.39	0
3	EDO	A	513	-	3,3,3	0.51	0	2,2,2	0.36	0
3	EDO	A	505	-	3,3,3	0.65	0	2,2,2	0.36	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	EDO	C	505	-	-	0/1/1/1	-
3	EDO	D	507	-	-	0/1/1/1	-
3	EDO	E	502	-	-	0/1/1/1	-
3	EDO	D	506	-	-	0/1/1/1	-
3	EDO	E	503	-	-	0/1/1/1	-
3	EDO	A	508	-	-	1/1/1/1	-
3	EDO	A	514	-	-	1/1/1/1	-
3	EDO	D	509	-	-	0/1/1/1	-
3	EDO	E	505	-	-	0/1/1/1	-
3	EDO	E	501	-	-	0/1/1/1	-
3	EDO	B	503	-	-	1/1/1/1	-
2	PEG	A	501	-	-	2/4/4/4	-
3	EDO	A	506	-	-	0/1/1/1	-
3	EDO	B	502	-	-	1/1/1/1	-
2	PEG	A	502	-	-	0/4/4/4	-
2	PEG	D	501	-	-	0/4/4/4	-
3	EDO	A	507	-	-	0/1/1/1	-
3	EDO	C	504	-	-	0/1/1/1	-
3	EDO	D	504	-	-	0/1/1/1	-
3	EDO	A	504	-	-	1/1/1/1	-
3	EDO	B	504	-	-	0/1/1/1	-
3	EDO	A	512	-	-	0/1/1/1	-
3	EDO	D	510	-	-	0/1/1/1	-
3	EDO	B	506	-	-	0/1/1/1	-
3	EDO	E	506	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	C	502	-	-	1/1/1/1	-
3	EDO	B	505	-	-	0/1/1/1	-
3	EDO	C	503	-	-	1/1/1/1	-
3	EDO	A	503	-	-	0/1/1/1	-
3	EDO	A	509	-	-	1/1/1/1	-
3	EDO	D	508	-	-	0/1/1/1	-
3	EDO	E	504	-	-	0/1/1/1	-
3	EDO	D	503	-	-	0/1/1/1	-
3	EDO	C	501	-	-	0/1/1/1	-
3	EDO	B	507	-	-	0/1/1/1	-
3	EDO	A	511	-	-	1/1/1/1	-
2	PEG	D	502	-	-	0/4/4/4	-
3	EDO	A	510	-	-	0/1/1/1	-
3	EDO	B	501	-	-	0/1/1/1	-
3	EDO	D	505	-	-	1/1/1/1	-
3	EDO	A	513	-	-	1/1/1/1	-
3	EDO	A	505	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	508	EDO	O1-C1-C2-O2
3	B	503	EDO	O1-C1-C2-O2
3	C	502	EDO	O1-C1-C2-O2
3	D	505	EDO	O1-C1-C2-O2
2	A	501	PEG	C1-C2-O2-C3
3	A	509	EDO	O1-C1-C2-O2
3	B	502	EDO	O1-C1-C2-O2
3	A	514	EDO	O1-C1-C2-O2
3	A	511	EDO	O1-C1-C2-O2
2	A	501	PEG	O1-C1-C2-O2
3	A	504	EDO	O1-C1-C2-O2
3	C	503	EDO	O1-C1-C2-O2
3	A	513	EDO	O1-C1-C2-O2

There are no ring outliers.

13 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	506	EDO	1	0
3	E	501	EDO	1	0
2	A	501	PEG	1	0
3	A	506	EDO	1	0
3	B	502	EDO	1	0
2	A	502	PEG	2	0
3	A	504	EDO	1	0
3	D	510	EDO	1	0
3	E	506	EDO	1	0
3	C	503	EDO	1	0
3	A	509	EDO	1	0
2	D	502	PEG	1	0
3	A	510	EDO	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	368/379 (97%)	-0.27	6 (1%) 72 74	39, 63, 89, 121	0
1	B	366/379 (96%)	-0.16	10 (2%) 54 58	39, 67, 122, 146	0
1	C	367/379 (96%)	-0.23	9 (2%) 57 61	40, 59, 116, 153	0
1	D	371/379 (97%)	-0.39	4 (1%) 80 82	37, 58, 99, 129	0
1	E	367/379 (96%)	-0.28	9 (2%) 57 61	38, 60, 105, 134	0
All	All	1839/1895 (97%)	-0.26	38 (2%) 63 66	37, 61, 107, 153	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	392	PRO	5.1
1	B	394	TRP	4.8
1	B	399	ASN	4.7
1	C	365	ALA	4.6
1	C	398	GLY	4.2
1	C	400	ASN	4.1
1	E	33	ALA	3.9
1	E	389	THR	3.7
1	B	400	ASN	3.6
1	B	393	THR	3.4
1	C	403	TYR	3.4
1	E	391	TYR	3.3
1	C	399	ASN	3.2
1	D	400	ASN	3.1
1	B	354	THR	3.0
1	E	390	LYS	3.0
1	E	394	TRP	3.0
1	C	393	THR	3.0
1	A	258	GLY	2.9
1	C	392	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	372	PRO	2.8
1	B	371	TYR	2.8
1	E	403	TYR	2.8
1	A	289	LEU	2.7
1	C	367	SER	2.7
1	D	403	TYR	2.6
1	A	389	THR	2.5
1	E	175	LYS	2.5
1	A	290	LEU	2.4
1	D	197	SER	2.3
1	E	395	LEU	2.3
1	A	312	LEU	2.3
1	B	369	ILE	2.3
1	D	399	ASN	2.2
1	A	214	ASN	2.2
1	C	404	GLY	2.1
1	B	401	GLY	2.1
1	E	398	GLY	2.0

## 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<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
3	EDO	C	502	4/4	0.45	0.27	88,90,90,91	0
3	EDO	A	507	4/4	0.70	0.29	83,83,83,84	0
3	EDO	B	505	4/4	0.72	0.52	80,82,84,85	0
3	EDO	D	509	4/4	0.73	0.37	79,82,84,85	0
2	PEG	D	502	7/7	0.74	0.31	96,99,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	A	508	4/4	0.78	0.27	61,64,68,70	0
2	PEG	D	501	7/7	0.81	0.23	95,97,100,100	0
3	EDO	C	504	4/4	0.83	0.23	73,76,78,79	0
3	EDO	A	509	4/4	0.83	0.21	74,76,76,77	0
3	EDO	B	503	4/4	0.83	0.24	71,71,73,73	0
3	EDO	C	505	4/4	0.84	0.21	70,72,75,76	0
3	EDO	D	506	4/4	0.84	0.23	73,75,77,77	0
3	EDO	A	513	4/4	0.85	0.29	63,65,69,76	0
3	EDO	B	507	4/4	0.86	0.42	81,81,83,83	0
3	EDO	B	504	4/4	0.86	0.15	60,61,62,64	0
2	PEG	A	502	7/7	0.86	0.19	71,72,75,77	0
3	EDO	A	504	4/4	0.87	0.18	71,71,74,75	0
3	EDO	A	510	4/4	0.87	0.19	67,67,70,76	0
3	EDO	A	511	4/4	0.87	0.22	66,66,69,69	0
3	EDO	E	505	4/4	0.88	0.29	84,84,84,86	0
3	EDO	A	506	4/4	0.89	0.21	65,66,67,68	0
3	EDO	B	506	4/4	0.89	0.32	80,81,84,85	0
2	PEG	A	501	7/7	0.90	0.19	64,66,70,71	0
3	EDO	D	510	4/4	0.91	0.33	73,76,80,84	0
3	EDO	D	507	4/4	0.92	0.20	78,78,78,78	0
3	EDO	A	505	4/4	0.92	0.14	58,62,66,66	0
3	EDO	D	503	4/4	0.93	0.17	62,63,63,63	0
3	EDO	D	505	4/4	0.94	0.14	54,55,56,59	0
3	EDO	D	504	4/4	0.95	0.21	59,59,60,61	0
3	EDO	E	506	4/4	0.95	0.19	64,64,65,67	0
3	EDO	E	503	4/4	0.95	0.15	56,57,58,60	0
3	EDO	E	502	4/4	0.95	0.15	56,56,58,58	0
3	EDO	C	503	4/4	0.95	0.16	64,64,64,65	0
3	EDO	A	514	4/4	0.95	0.28	69,71,71,71	0
3	EDO	D	508	4/4	0.95	0.20	63,65,66,66	0
3	EDO	E	504	4/4	0.95	0.13	44,47,50,56	0
3	EDO	B	502	4/4	0.96	0.11	54,55,55,56	0
3	EDO	E	501	4/4	0.97	0.12	54,56,56,60	0
3	EDO	A	503	4/4	0.97	0.12	38,39,42,45	0
3	EDO	B	501	4/4	0.97	0.12	45,47,49,51	0
3	EDO	A	512	4/4	0.98	0.13	55,57,62,67	0
3	EDO	C	501	4/4	0.98	0.11	54,55,56,56	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.