



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2023 – 06:39 PM EDT

PDB ID : 1L8H  
Title : DNA PROTECTION AND BINDING BY E. COLI DPS PROTEIN  
Authors : Luo, J.; Liu, D.; White, M.A.; Fox, R.O.  
Deposited on : 2002-03-20  
Resolution : 3.20 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.35  
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) : 2.35

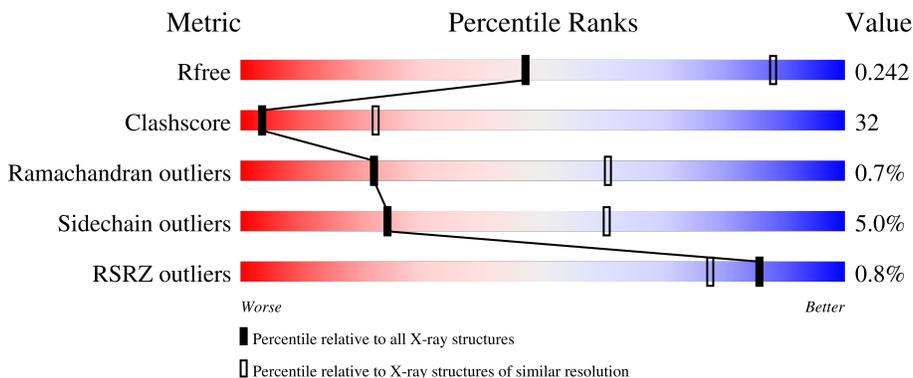
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

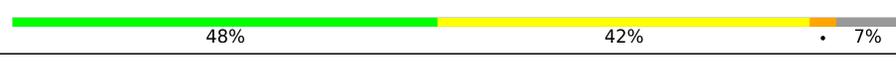
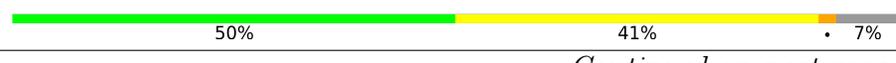
The reported resolution of this entry is 3.20 Å.

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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	167	
1	B	167	
1	C	167	
1	D	167	
1	E	167	

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Mol	Chain	Length	Quality of chain
1	F	167	 <p>2% 50% 41% • 8%</p>
1	G	167	 <p>53% 38% • 7%</p>
1	H	167	 <p>51% 40% • 7%</p>
1	I	167	 <p>2% 49% 41% • 7%</p>
1	J	167	 <p>49% 41% • 7%</p>
1	K	167	 <p>49% 40% • 7%</p>
1	L	167	 <p>47% 43% • 8%</p>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14949 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 DNA PROTECTION DURING STARVATION PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	156	1231	774	216	237	4	0	0	0
1	B	154	1216	766	213	233	4	0	0	0
1	C	158	1245	783	219	239	4	0	0	0
1	D	155	1224	770	215	235	4	0	0	0
1	E	156	1231	774	216	237	4	0	0	0
1	F	154	1216	766	213	233	4	0	0	0
1	G	156	1231	774	216	237	4	0	0	0
1	H	156	1231	774	216	237	4	0	0	0
1	I	156	1231	774	216	237	4	0	0	0
1	J	156	1231	774	216	237	4	0	0	0
1	K	155	1224	770	215	235	4	0	0	0
1	L	154	1216	766	213	233	4	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	75	CYS	ASP	engineered mutation	UNP P0ABT2
A	78	ALA	ASP	engineered mutation	UNP P0ABT2
B	75	CYS	ASP	engineered mutation	UNP P0ABT2
B	78	ALA	ASP	engineered mutation	UNP P0ABT2
C	75	CYS	ASP	engineered mutation	UNP P0ABT2

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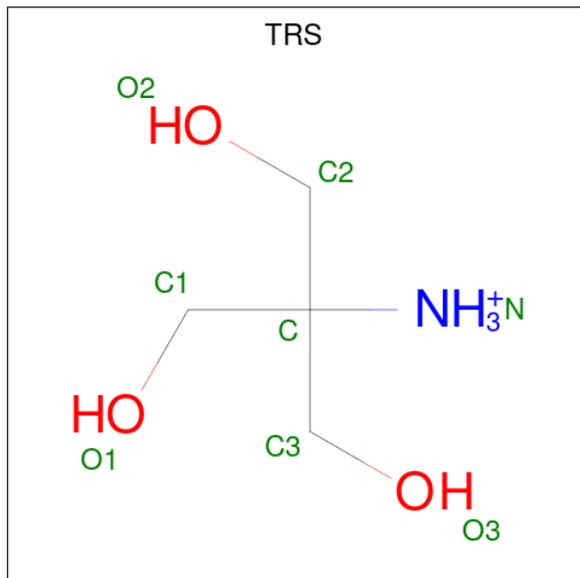
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Chain	Residue	Modelled	Actual	Comment	Reference
C	78	ALA	ASP	engineered mutation	UNP P0ABT2
D	75	CYS	ASP	engineered mutation	UNP P0ABT2
D	78	ALA	ASP	engineered mutation	UNP P0ABT2
E	75	CYS	ASP	engineered mutation	UNP P0ABT2
E	78	ALA	ASP	engineered mutation	UNP P0ABT2
F	75	CYS	ASP	engineered mutation	UNP P0ABT2
F	78	ALA	ASP	engineered mutation	UNP P0ABT2
G	75	CYS	ASP	engineered mutation	UNP P0ABT2
G	78	ALA	ASP	engineered mutation	UNP P0ABT2
H	75	CYS	ASP	engineered mutation	UNP P0ABT2
H	78	ALA	ASP	engineered mutation	UNP P0ABT2
I	75	CYS	ASP	engineered mutation	UNP P0ABT2
I	78	ALA	ASP	engineered mutation	UNP P0ABT2
J	75	CYS	ASP	engineered mutation	UNP P0ABT2
J	78	ALA	ASP	engineered mutation	UNP P0ABT2
K	75	CYS	ASP	engineered mutation	UNP P0ABT2
K	78	ALA	ASP	engineered mutation	UNP P0ABT2
L	75	CYS	ASP	engineered mutation	UNP P0ABT2
L	78	ALA	ASP	engineered mutation	UNP P0ABT2

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total K 1 1	0	0
2	B	1	Total K 1 1	0	0
2	C	1	Total K 1 1	0	0
2	D	1	Total K 1 1	0	0
2	E	1	Total K 1 1	0	0
2	G	3	Total K 3 3	0	0
2	H	1	Total K 1 1	0	0
2	J	1	Total K 1 1	0	0
2	K	1	Total K 1 1	0	0
2	L	1	Total K 1 1	0	0

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		
3	A	1	Total	C	N	O	0	0
			8	4	1	3		
3	B	1	Total	C	N	O	0	0
			8	4	1	3		
3	B	1	Total	C	N	O	0	0
			8	4	1	3		
3	C	1	Total	C	N	O	0	0
			8	4	1	3		
3	D	1	Total	C	N	O	0	0
			8	4	1	3		
3	D	1	Total	C	N	O	0	0
			8	4	1	3		
3	D	1	Total	C	N	O	0	0
			8	4	1	3		
3	E	1	Total	C	N	O	0	0
			8	4	1	3		
3	G	1	Total	C	N	O	0	0
			8	4	1	3		
3	J	1	Total	C	N	O	0	0
			8	4	1	3		
3	K	1	Total	C	N	O	0	0
			8	4	1	3		

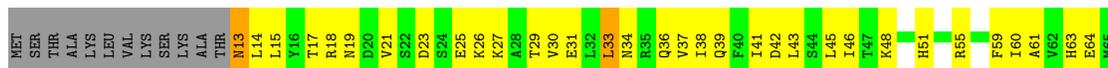
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	11	Total O 11 11	0	0
4	B	7	Total O 7 7	0	0
4	C	7	Total O 7 7	0	0
4	D	16	Total O 16 16	0	0
4	E	7	Total O 7 7	0	0
4	F	10	Total O 10 10	0	0
4	G	9	Total O 9 9	0	0
4	H	10	Total O 10 10	0	0
4	I	13	Total O 13 13	0	0
4	J	10	Total O 10 10	0	0
4	K	6	Total O 6 6	0	0
4	L	8	Total O 8 8	0	0





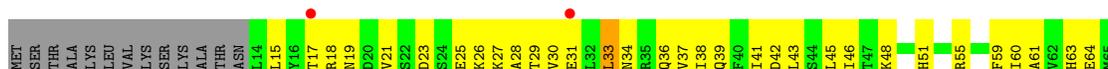
• Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN



• Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN



• Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN



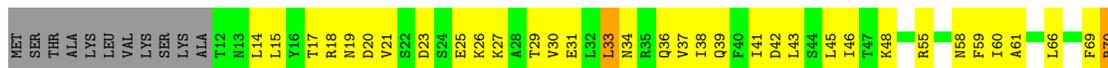
• Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN





- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain H: 51% 40% 7%



- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain I: 2% 49% 41% 7%



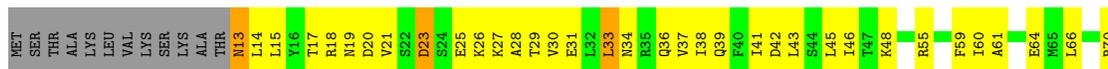
- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain J: 49% 41% 7%



- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

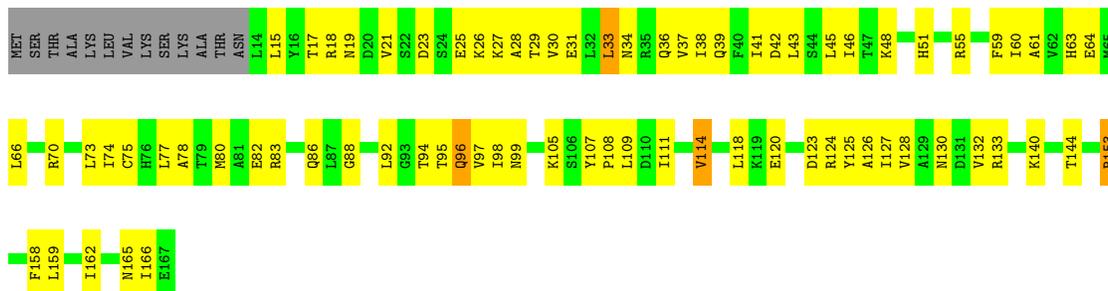
Chain K: 49% 40% 7%



E167

- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain L:  47% 43% 8%



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.27Å 91.27Å 239.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.83 – 3.20 79.04 – 3.19	Depositor EDS
% Data completeness (in resolution range)	97.6 (44.83-3.20) 97.3 (79.04-3.19)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.63 (at 3.19Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.210 , 0.250 0.204 , 0.242	Depositor DCC
$R_{free}$ test set	1835 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.5	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 86.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.044 for h,-h-k,-l 0.024 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14949	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.56% 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: TRS, K

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	0.42	0/1249	0.60	0/1691
1	B	0.43	0/1234	0.69	2/1670 (0.1%)
1	C	0.42	0/1263	0.62	0/1709
1	D	0.42	0/1242	0.60	0/1681
1	E	0.41	0/1249	0.63	0/1691
1	F	0.43	0/1234	0.61	0/1670
1	G	0.44	0/1249	0.62	0/1691
1	H	0.41	0/1249	0.71	2/1691 (0.1%)
1	I	0.43	0/1249	0.61	0/1691
1	J	0.44	0/1249	0.71	2/1691 (0.1%)
1	K	0.40	0/1242	0.61	0/1681
1	L	0.40	0/1234	0.60	0/1670
All	All	0.42	0/14943	0.64	6/20227 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	70	ARG	NE-CZ-NH1	-9.93	115.33	120.30
1	H	70	ARG	NE-CZ-NH2	9.65	125.13	120.30
1	B	70	ARG	NE-CZ-NH2	9.63	125.11	120.30
1	H	70	ARG	NE-CZ-NH1	-9.41	115.59	120.30
1	J	35	ARG	NE-CZ-NH1	-9.23	115.69	120.30

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	1231	0	1234	91	0
1	B	1216	0	1221	84	0
1	C	1245	0	1252	88	0
1	D	1224	0	1227	90	0
1	E	1231	0	1234	89	0
1	F	1216	0	1221	87	0
1	G	1231	0	1234	83	0
1	H	1231	0	1234	82	0
1	I	1231	0	1234	82	0
1	J	1231	0	1234	93	0
1	K	1224	0	1227	90	0
1	L	1216	0	1221	83	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	G	3	0	0	0	0
2	H	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	16	0	24	1	0
3	B	16	0	24	0	0
3	C	8	0	12	0	0
3	D	24	0	36	0	0
3	E	8	0	12	0	0
3	G	8	0	12	0	0
3	J	8	0	12	0	0
3	K	8	0	12	0	0
4	A	11	0	0	1	0
4	B	7	0	0	0	0
4	C	7	0	0	1	0
4	D	16	0	0	2	0
4	E	7	0	0	1	0
4	F	10	0	0	0	0
4	G	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	10	0	0	1	0
4	I	13	0	0	0	0
4	J	10	0	0	0	0
4	K	6	0	0	0	0
4	L	8	0	0	1	0
All	All	14949	0	14917	946	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 32.

The worst 5 of 946 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:109:LEU:HD23	1:F:92:LEU:HD22	1.38	1.05
1:K:109:LEU:HD23	1:L:92:LEU:HD22	1.39	1.03
1:A:92:LEU:HD22	1:B:109:LEU:HD23	1.46	0.97
1:I:92:LEU:HD22	1:J:109:LEU:HD23	1.43	0.96
1:A:109:LEU:HD23	1:B:92:LEU:HD22	1.50	0.93

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	154/167 (92%)	132 (86%)	20 (13%)	2 (1%)	12	47
1	B	152/167 (91%)	133 (88%)	18 (12%)	1 (1%)	22	61
1	C	156/167 (93%)	129 (83%)	27 (17%)	0	100	100
1	D	153/167 (92%)	131 (86%)	21 (14%)	1 (1%)	22	61
1	E	154/167 (92%)	132 (86%)	22 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	152/167 (91%)	128 (84%)	24 (16%)	0	100	100
1	G	154/167 (92%)	135 (88%)	19 (12%)	0	100	100
1	H	154/167 (92%)	133 (86%)	19 (12%)	2 (1%)	12	47
1	I	154/167 (92%)	131 (85%)	20 (13%)	3 (2%)	8	39
1	J	154/167 (92%)	130 (84%)	23 (15%)	1 (1%)	25	64
1	K	153/167 (92%)	135 (88%)	17 (11%)	1 (1%)	22	61
1	L	152/167 (91%)	128 (84%)	23 (15%)	1 (1%)	22	61
All	All	1842/2004 (92%)	1577 (86%)	253 (14%)	12 (1%)	22	61

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	I	14	LEU
1	I	164	SER
1	H	20	ASP
1	L	114	VAL

### 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	133/142 (94%)	127 (96%)	6 (4%)	27	63
1	B	131/142 (92%)	125 (95%)	6 (5%)	27	63
1	C	134/142 (94%)	126 (94%)	8 (6%)	19	54
1	D	132/142 (93%)	125 (95%)	7 (5%)	22	58
1	E	133/142 (94%)	126 (95%)	7 (5%)	22	58
1	F	131/142 (92%)	125 (95%)	6 (5%)	27	63
1	G	133/142 (94%)	127 (96%)	6 (4%)	27	63
1	H	133/142 (94%)	127 (96%)	6 (4%)	27	63
1	I	133/142 (94%)	126 (95%)	7 (5%)	22	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	133/142 (94%)	126 (95%)	7 (5%)	22	58
1	K	132/142 (93%)	125 (95%)	7 (5%)	22	58
1	L	131/142 (92%)	125 (95%)	6 (5%)	27	63
All	All	1589/1704 (93%)	1510 (95%)	79 (5%)	24	60

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	96	GLN
1	K	96	GLN
1	J	33	LEU
1	J	153	ARG
1	L	66	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	39	GLN
1	K	86	GLN
1	G	86	GLN
1	K	39	GLN
1	L	39	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

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 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	TRS	D	306	-	7,7,7	0.31	0	9,9,9	0.81	0
3	TRS	K	302	-	7,7,7	0.58	0	9,9,9	0.96	0
3	TRS	A	309	-	7,7,7	0.39	0	9,9,9	0.89	0
3	TRS	C	307	-	7,7,7	0.57	0	9,9,9	1.02	0
3	TRS	A	301	-	7,7,7	0.52	0	9,9,9	0.96	0
3	TRS	E	311	-	7,7,7	0.56	0	9,9,9	0.96	0
3	TRS	G	303	-	7,7,7	0.34	0	9,9,9	0.82	0
3	TRS	D	305	-	7,7,7	0.53	0	9,9,9	0.93	0
3	TRS	B	312	-	7,7,7	0.38	0	9,9,9	0.85	0
3	TRS	J	308	-	7,7,7	0.65	0	9,9,9	0.95	0
3	TRS	B	304	-	7,7,7	0.71	0	9,9,9	1.05	0
3	TRS	D	310	-	7,7,7	0.52	0	9,9,9	1.00	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	TRS	D	306	-	-	2/9/9/9	-
3	TRS	K	302	-	-	0/9/9/9	-
3	TRS	A	309	-	-	2/9/9/9	-
3	TRS	C	307	-	-	2/9/9/9	-
3	TRS	A	301	-	-	2/9/9/9	-
3	TRS	E	311	-	-	0/9/9/9	-
3	TRS	G	303	-	-	2/9/9/9	-
3	TRS	D	305	-	-	0/9/9/9	-
3	TRS	B	312	-	-	2/9/9/9	-
3	TRS	J	308	-	-	0/9/9/9	-
3	TRS	B	304	-	-	3/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TRS	D	310	-	-	3/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	TRS	N-C-C2-O2
3	B	304	TRS	N-C-C2-O2
3	C	307	TRS	N-C-C2-O2
3	D	310	TRS	N-C-C2-O2
3	A	301	TRS	C3-C-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	309	TRS	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	156/167 (93%)	-0.07	2 (1%) 77 65	35, 60, 81, 92	0
1	B	154/167 (92%)	0.05	6 (3%) 39 25	36, 59, 81, 86	0
1	C	158/167 (94%)	0.05	0 100 100	34, 56, 78, 112	1 (0%)
1	D	155/167 (92%)	-0.29	0 100 100	25, 48, 74, 85	0
1	E	156/167 (93%)	-0.09	0 100 100	38, 60, 82, 95	0
1	F	154/167 (92%)	0.06	3 (1%) 66 53	29, 59, 85, 94	0
1	G	156/167 (93%)	-0.12	1 (0%) 89 83	30, 53, 75, 94	0
1	H	156/167 (93%)	-0.14	0 100 100	31, 56, 77, 92	0
1	I	156/167 (93%)	0.02	3 (1%) 66 53	19, 49, 82, 113	0
1	J	156/167 (93%)	-0.12	0 100 100	21, 52, 75, 88	0
1	K	155/167 (92%)	-0.16	0 100 100	38, 61, 81, 90	0
1	L	154/167 (92%)	0.16	0 100 100	42, 66, 86, 91	0
All	All	1866/2004 (93%)	-0.06	15 (0%) 86 78	19, 58, 81, 113	1 (0%)

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	88	GLY	4.4
1	I	13	ASN	3.2
1	A	95	THR	3.0
1	B	95	THR	2.5
1	F	17	THR	2.5

### 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
2	K	C	262	1/1	-0.25	0.24	92,92,92,92	0
2	K	G	260	1/1	0.61	0.25	82,82,82,82	0
2	K	B	256	1/1	0.67	0.19	75,75,75,75	0
3	TRS	K	302	8/8	0.76	0.34	91,92,94,94	0
3	TRS	E	311	8/8	0.81	0.29	84,85,86,86	0
2	K	L	255	1/1	0.83	0.21	73,73,73,73	0
3	TRS	J	308	8/8	0.86	0.22	91,92,92,93	0
3	TRS	D	305	8/8	0.89	0.27	99,101,101,101	0
3	TRS	B	312	8/8	0.90	0.26	66,67,68,70	0
2	K	E	251	1/1	0.91	0.20	76,76,76,76	0
2	K	H	253	1/1	0.91	0.26	78,78,78,78	0
3	TRS	D	306	8/8	0.92	0.22	63,66,67,69	0
2	K	A	252	1/1	0.92	0.19	68,68,68,68	0
2	K	J	258	1/1	0.93	0.14	72,72,72,72	0
2	K	G	259	1/1	0.93	0.17	71,71,71,71	0
2	K	G	254	1/1	0.94	0.19	67,67,67,67	0
2	K	K	257	1/1	0.94	0.17	64,64,64,64	0
2	K	D	261	1/1	0.94	0.25	79,79,79,79	0
3	TRS	A	301	8/8	0.94	0.24	46,48,49,53	0
3	TRS	A	309	8/8	0.94	0.14	63,64,64,64	0
3	TRS	B	304	8/8	0.94	0.20	38,42,42,43	0
3	TRS	C	307	8/8	0.95	0.14	27,31,32,34	0
3	TRS	G	303	8/8	0.95	0.24	44,48,50,52	0
3	TRS	D	310	8/8	0.97	0.18	20,21,25,27	0

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

There are no such residues in this entry.