



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2020 – 05:32 PM BST

PDB ID : 6QVX  
Title : Escherichia coli DPS  
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Deposited on : 2019-03-05  
Resolution : 2.20 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 : 2.14.6  
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) : 2.14.6

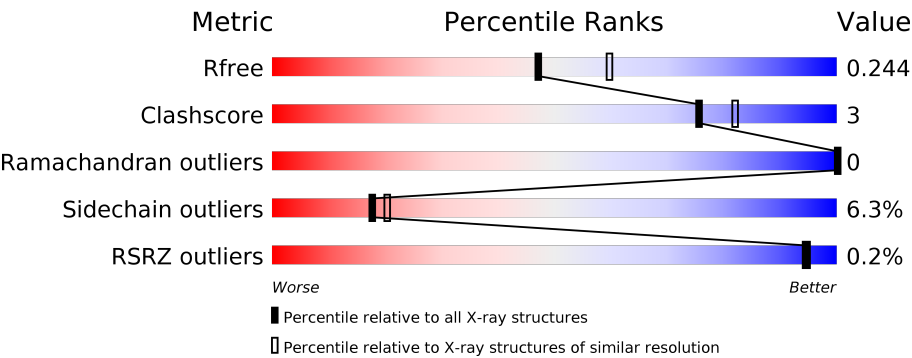
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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.















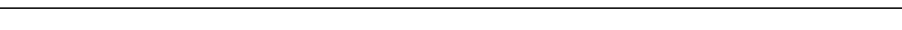


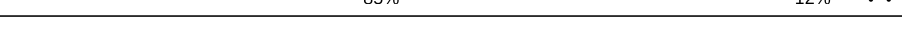


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 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	159	<div><div></div><div>84%12% . .</div></div>
1	B	159	<div><div></div><div>87%9% . .</div></div>
1	C	159	<div><div></div><div>92%5% . .</div></div>
1	D	159	<div><div></div><div>87%9% . .</div></div>
1	E	159	<div><div>%</div><div>86%9% . .</div></div>
1	F	159	<div><div></div><div>89%8% . .</div></div>

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Mol	Chain	Length	Quality of chain
1	G	159	 84% 13% ..
1	H	159	 91% 5% ..
1	I	159	 89% 8% .
1	J	159	 87% 9% ..
1	K	159	 84% 13% .
1	L	159	 87% 9% ..
1	M	159	 88% 9% ..
1	N	159	 89% 8% ..
1	O	159	 86% 11% ..
1	P	159	 86% 11% ..
1	Q	159	 81% 16% ..
1	R	159	 84% 13% ..
1	S	159	 86% 12% ..
1	T	159	 84% 14% ..
1	U	159	 85% 12% ..
1	V	159	 86% 11% .
1	W	159	 87% 9% ..
1	X	159	 87% 8% ..

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	SO4	K	201	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 33411 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
1	A	155	Total	C	N	O	S	0	1	0
			1237	776	216	242	3			
1	B	155	Total	C	N	O	S	0	0	0
			1229	772	215	239	3			
1	C	155	Total	C	N	O	S	0	0	0
			1229	772	215	239	3			
1	D	155	Total	C	N	O	S	0	0	0
			1229	772	215	239	3			
1	E	156	Total	C	N	O	S	0	0	0
			1236	776	216	241	3			
1	F	155	Total	C	N	O	S	0	0	0
			1229	772	215	239	3			
1	G	155	Total	C	N	O	S	0	0	0
			1229	772	215	239	3			
1	H	155	Total	C	N	O	S	0	0	0
			1229	772	215	239	3			
1	I	155	Total	C	N	O	S	0	0	0
			1229	772	215	239	3			
1	J	156	Total	C	N	O	S	0	1	0
			1247	782	220	242	3			
1	K	154	Total	C	N	O	S	0	0	0
			1221	768	213	237	3			
1	L	155	Total	C	N	O	S	0	0	0
			1229	772	215	239	3			
1	M	156	Total	C	N	O	S	0	0	0
			1236	776	216	241	3			
1	N	155	Total	C	N	O	S	0	1	0
			1240	778	219	240	3			
1	O	156	Total	C	N	O	S	0	0	0
			1236	776	216	241	3			
1	P	155	Total	C	N	O	S	0	0	0
			1229	772	215	239	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	155	Total	C	N	O	S	0	1	0
			1240	778	219	240	3			
1	R	156	Total	C	N	O	S	0	0	0
			1236	776	216	241	3			
1	S	158	Total	C	N	O	S	0	0	0
			1250	785	219	243	3			
1	T	156	Total	C	N	O	S	0	0	0
			1236	776	216	241	3			
1	U	155	Total	C	N	O	S	0	0	0
			1229	772	215	239	3			
1	V	155	Total	C	N	O	S	0	0	0
			1229	772	215	239	3			
1	W	156	Total	C	N	O	S	0	0	0
			1236	776	216	241	3			
1	X	155	Total	C	N	O	S	0	1	0
			1237	776	216	242	3			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0
2	D	1	Total 5	O 4	S 1	0	0
2	D	1	Total 5	O 4	S 1	0	0
2	E	1	Total 5	O 4	S 1	0	0
2	F	1	Total 5	O 4	S 1	0	0
2	F	1	Total 5	O 4	S 1	0	0
2	G	1	Total 5	O 4	S 1	0	0
2	G	1	Total 5	O 4	S 1	0	0
2	H	1	Total 5	O 4	S 1	0	0
2	H	1	Total 5	O 4	S 1	0	0
2	I	1	Total 5	O 4	S 1	0	0
2	I	1	Total 5	O 4	S 1	0	0
2	I	1	Total 5	O 4	S 1	0	0
2	J	1	Total 5	O 4	S 1	0	0
2	J	1	Total 5	O 4	S 1	0	0
2	K	1	Total 5	O 4	S 1	0	0
2	L	1	Total 5	O 4	S 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	L	1	Total 5	O 4	S 1	0	0
2	M	1	Total 5	O 4	S 1	0	0
2	M	1	Total 5	O 4	S 1	0	0
2	M	1	Total 5	O 4	S 1	0	0
2	N	1	Total 5	O 4	S 1	0	0
2	N	1	Total 5	O 4	S 1	0	0
2	O	1	Total 5	O 4	S 1	0	0
2	O	1	Total 5	O 4	S 1	0	0
2	P	1	Total 5	O 4	S 1	0	0
2	P	1	Total 5	O 4	S 1	0	0
2	P	1	Total 5	O 4	S 1	0	0
2	Q	1	Total 5	O 4	S 1	0	0
2	Q	1	Total 5	O 4	S 1	0	0
2	R	1	Total 5	O 4	S 1	0	0
2	R	1	Total 5	O 4	S 1	0	0
2	S	1	Total 5	O 4	S 1	0	0
2	S	1	Total 5	O 4	S 1	0	0
2	T	1	Total 5	O 4	S 1	0	0
2	T	1	Total 5	O 4	S 1	0	0
2	U	1	Total 5	O 4	S 1	0	0
2	U	1	Total 5	O 4	S 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	V	1	Total	O	S	0	0
			5	4	1		
2	W	1	Total	O	S	0	0
			5	4	1		
2	W	1	Total	O	S	0	0
			5	4	1		
2	X	1	Total	O	S	0	0
			5	4	1		
2	X	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	150	Total	O	0	0
			150	150		
3	B	134	Total	O	0	0
			134	134		
3	C	151	Total	O	0	0
			151	151		
3	D	145	Total	O	0	0
			145	145		
3	E	155	Total	O	0	0
			155	155		
3	F	166	Total	O	0	0
			166	166		
3	G	136	Total	O	0	0
			136	136		
3	H	136	Total	O	0	0
			136	136		
3	I	150	Total	O	0	0
			150	150		
3	J	163	Total	O	0	0
			163	163		
3	K	145	Total	O	0	0
			145	145		
3	L	142	Total	O	0	0
			142	142		
3	M	140	Total	O	0	0
			140	140		
3	N	142	Total	O	0	0
			142	142		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	154	Total 154	O 154	0	0
3	P	139	Total 139	O 139	0	0
3	Q	151	Total 151	O 151	0	0
3	R	153	Total 153	O 153	0	0
3	S	163	Total 163	O 163	0	0
3	T	153	Total 153	O 153	0	0
3	U	145	Total 145	O 145	0	0
3	V	142	Total 142	O 142	0	0
3	W	149	Total 149	O 149	0	0
3	X	150	Total 150	O 150	0	0

### 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: DNA protection during starvation protein

Chain A: 



- Molecule 1: DNA protection during starvation protein

Chain B: 




- Molecule 1: DNA protection during starvation protein

Chain C: 




- Molecule 1: DNA protection during starvation protein

Chain D: 




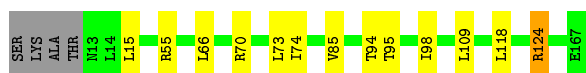
- Molecule 1: DNA protection during starvation protein

Chain E: 



- Molecule 1: DNA protection during starvation protein

Chain F: 



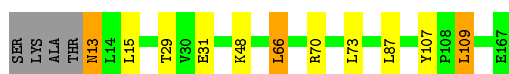
- Molecule 1: DNA protection during starvation protein

Chain G: 84% 13% ..



- Molecule 1: DNA protection during starvation protein

Chain H: 91% 5% ..



- Molecule 1: DNA protection during starvation protein

Chain I: 89% 8% .



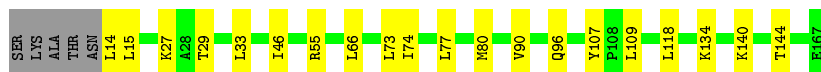
- Molecule 1: DNA protection during starvation protein

Chain J: 87% 9% ..



- Molecule 1: DNA protection during starvation protein

Chain K: 84% 13% .



- Molecule 1: DNA protection during starvation protein

Chain L: 87% 9% ..



- Molecule 1: DNA protection during starvation protein

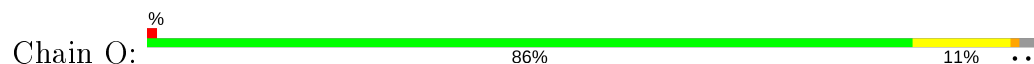
Chain M: 88% 9% ..



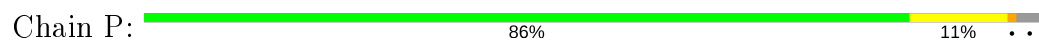
- Molecule 1: DNA protection during starvation protein



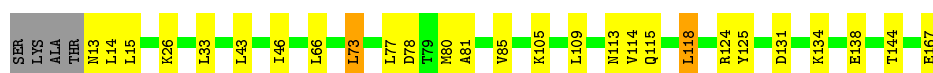
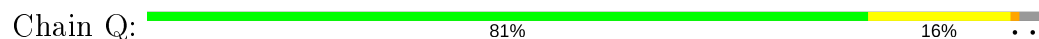
- Molecule 1: DNA protection during starvation protein



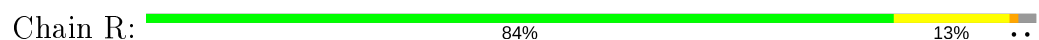
- Molecule 1: DNA protection during starvation protein



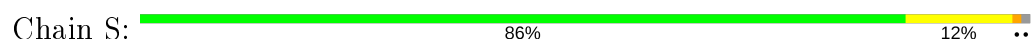
- Molecule 1: DNA protection during starvation protein



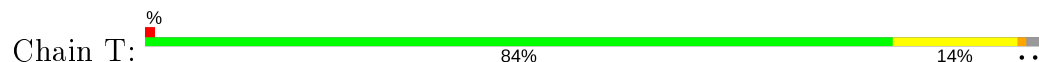
- Molecule 1: DNA protection during starvation protein

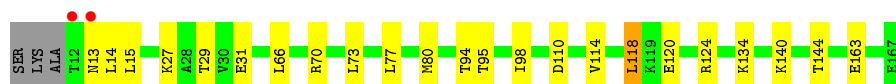


- Molecule 1: DNA protection during starvation protein



- Molecule 1: DNA protection during starvation protein





- Molecule 1: DNA protection during starvation protein

Chain U: 85% 12% ..



- Molecule 1: DNA protection during starvation protein

Chain V: 86% 11% .



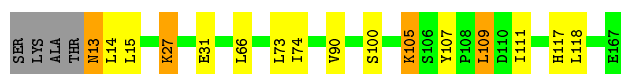
- Molecule 1: DNA protection during starvation protein

Chain W: 87% 9% ..



- Molecule 1: DNA protection during starvation protein

Chain X: 87% 8% ..



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.58Å 90.17Å 157.31Å 92.18° 104.99° 117.85°	Depositor
Resolution (Å)	149.30 – 2.20 49.77 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.2 (149.30-2.20) 98.6 (49.77-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.189 , 0.258 0.193 , 0.244	Depositor DCC
$R_{free}$ test set	13287 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.5	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 40.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for k,h,-h-k-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	33411	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.22 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.0168e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: SO4

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	0.72	0/1255	0.85	0/1699
1	B	0.76	0/1247	0.85	0/1688
1	C	0.71	0/1247	0.86	0/1688
1	D	0.71	0/1247	0.85	0/1688
1	E	0.71	0/1254	0.85	0/1698
1	F	0.73	0/1247	0.84	0/1688
1	G	0.73	0/1247	0.83	0/1688
1	H	0.72	0/1247	0.85	0/1688
1	I	0.71	0/1247	0.86	0/1688
1	J	0.71	0/1265	0.87	0/1712
1	K	0.74	0/1239	0.88	0/1677
1	L	0.72	0/1247	0.84	0/1688
1	M	0.75	0/1254	0.86	0/1698
1	N	0.72	0/1258	0.89	0/1702
1	O	0.68	0/1254	0.87	0/1698
1	P	0.70	0/1247	0.87	0/1688
1	Q	0.74	0/1258	0.86	0/1702
1	R	0.73	0/1254	0.85	0/1698
1	S	0.75	0/1268	0.84	0/1716
1	T	0.74	0/1254	0.87	0/1698
1	U	0.75	0/1247	0.88	0/1688
1	V	0.74	0/1247	0.84	0/1688
1	W	0.73	0/1254	0.84	0/1698
1	X	0.71	0/1255	0.82	0/1699
All	All	0.73	0/30039	0.86	0/40663

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	1237	0	1228	10	0
1	B	1229	0	1225	6	0
1	C	1229	0	1225	8	0
1	D	1229	0	1225	7	0
1	E	1236	0	1232	10	0
1	F	1229	0	1225	6	0
1	G	1229	0	1225	8	0
1	H	1229	0	1225	7	0
1	I	1229	0	1225	4	0
1	J	1247	0	1244	9	0
1	K	1221	0	1219	7	0
1	L	1229	0	1225	7	0
1	M	1236	0	1232	7	0
1	N	1240	0	1237	5	0
1	O	1236	0	1232	10	0
1	P	1229	0	1225	9	0
1	Q	1240	0	1237	12	0
1	R	1236	0	1232	12	0
1	S	1250	0	1250	11	0
1	T	1236	0	1232	11	0
1	U	1229	0	1225	9	0
1	V	1229	0	1225	6	0
1	W	1236	0	1232	8	0
1	X	1237	0	1228	6	0
2	A	15	0	0	0	0
2	B	15	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
2	E	5	0	0	0	0
2	F	10	0	0	0	0
2	G	10	0	0	0	0
2	H	10	0	0	0	0
2	I	15	0	0	0	0
2	J	10	0	0	0	0
2	K	5	0	0	2	0
2	L	10	0	0	0	0
2	M	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	10	0	0	0	0
2	O	10	0	0	0	0
2	P	15	0	0	1	0
2	Q	10	0	0	0	0
2	R	10	0	0	0	0
2	S	10	0	0	0	0
2	T	10	0	0	1	0
2	U	10	0	0	0	0
2	V	5	0	0	0	0
2	W	10	0	0	0	0
2	X	10	0	0	0	0
3	A	150	0	0	1	0
3	B	134	0	0	1	0
3	C	151	0	0	3	0
3	D	145	0	0	1	0
3	E	155	0	0	6	0
3	F	166	0	0	0	0
3	G	136	0	0	1	0
3	H	136	0	0	1	0
3	I	150	0	0	1	0
3	J	163	0	0	1	0
3	K	145	0	0	2	0
3	L	142	0	0	5	0
3	M	140	0	0	1	0
3	N	142	0	0	1	0
3	O	154	0	0	1	0
3	P	139	0	0	3	0
3	Q	151	0	0	0	0
3	R	153	0	0	2	0
3	S	163	0	0	5	0
3	T	153	0	0	2	0
3	U	145	0	0	3	1
3	V	142	0	0	4	0
3	W	149	0	0	2	0
3	X	150	0	0	1	1
All	All	33411	0	29510	184	1

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 3.

All (184) 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:R:76:HIS:HE1	1:R:154:ASP:OD2	1.56	0.88
1:R:76:HIS:HD2	3:R:367:HOH:O	1.73	0.72
1:S:51:HIS:HD2	1:S:63:HIS:O	1.72	0.72
1:M:76:HIS:HE1	1:M:154:ASP:OD2	1.73	0.71
1:F:124:ARG:HH21	1:F:124:ARG:HG2	1.58	0.67
1:Q:114:VAL:HG12	1:Q:118:LEU:HD22	1.78	0.66
1:R:76:HIS:CE1	1:R:154:ASP:OD2	2.47	0.63
1:Q:113:ASN:ND2	1:Q:115:GLN:H	1.98	0.61
1:C:140:LYS:HD3	3:C:443:HOH:O	2.02	0.60
1:S:92:LEU:HB2	3:S:352:HOH:O	2.01	0.59
1:U:46:ILE:HD13	1:U:124:ARG:HD3	1.85	0.59
1:B:92:LEU:HB2	3:B:321:HOH:O	2.03	0.58
1:C:161:PHE:HZ	2:K:201:SO4:O3	1.86	0.58
1:N:33:LEU:HD21	1:N:144:THR:HG23	1.85	0.58
1:R:12:THR:N	3:R:304:HOH:O	2.35	0.58
2:T:202:SO4:O2	1:V:157:LYS:NZ	2.35	0.57
1:T:70:ARG:HG2	3:T:360:HOH:O	2.04	0.57
1:E:92:LEU:HB2	3:E:353:HOH:O	2.04	0.57
1:S:27:LYS:HE2	3:S:410:HOH:O	2.03	0.57
1:O:33:LEU:HD21	1:O:144:THR:HG23	1.86	0.57
1:B:33:LEU:HD21	1:B:144:THR:HG23	1.87	0.56
1:I:70:ARG:NH1	1:J:70[A]:ARG:NH2	2.53	0.56
1:L:78:ASP:HB3	3:L:414:HOH:O	2.04	0.56
1:I:120:GLU:O	1:I:124:ARG:HG2	2.05	0.56
1:U:140:LYS:NZ	3:U:304:HOH:O	2.38	0.56
1:K:55:ARG:HD2	3:K:425:HOH:O	2.06	0.56
1:R:46:ILE:HD13	1:R:124:ARG:HD3	1.89	0.55
1:J:46:ILE:HG23	1:J:107:TYR:CD1	2.42	0.55
1:C:16:TYR:HA	3:C:323:HOH:O	2.06	0.54
1:R:77:LEU:HA	1:R:80:MET:HE2	1.89	0.54
1:J:32:LEU:HD23	1:J:32:LEU:C	2.28	0.54
1:P:46:ILE:HG23	1:P:107:TYR:CD1	2.43	0.54
1:K:33:LEU:HD21	1:K:144:THR:HG23	1.89	0.54
1:R:77:LEU:C	1:R:77:LEU:HD12	2.28	0.54
1:A:21:VAL:O	1:A:26:LYS:HE3	2.08	0.54
1:L:113:ASN:HB2	3:L:390:HOH:O	2.09	0.53
1:E:111:ILE:HD11	3:E:440:HOH:O	2.07	0.53
1:S:14:LEU:HD13	3:S:324:HOH:O	2.09	0.53
1:U:13:ASN:HA	3:U:331:HOH:O	2.09	0.53
1:E:33:LEU:HD21	1:E:144:THR:HG23	1.90	0.53
1:L:112:HIS:HB2	3:L:405:HOH:O	2.07	0.53
1:S:33:LEU:HD21	1:S:144:THR:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:55:ARG:NH2	3:O:309:HOH:O	2.42	0.52
1:U:39:GLN:OE1	1:U:131:ASP:OD2	2.28	0.51
1:O:114:VAL:HG12	1:O:118:LEU:HD22	1.93	0.51
1:P:35:ARG:HD2	3:P:381:HOH:O	2.11	0.50
1:Q:33:LEU:HD21	1:Q:144:THR:HG23	1.93	0.50
1:T:114:VAL:HG12	1:T:118:LEU:HD22	1.92	0.50
1:P:29:THR:HG23	1:P:144:THR:HG21	1.93	0.50
1:M:76:HIS:HD2	3:M:326:HOH:O	1.95	0.50
1:A:15:LEU:HD21	1:B:112:HIS:CE1	2.46	0.50
1:O:120:GLU:O	1:O:124:ARG:HG2	2.11	0.49
1:K:90:VAL:HG11	1:L:109:LEU:O	2.12	0.49
1:N:27:LYS:O	1:N:31:GLU:HG2	2.12	0.49
1:T:95:THR:HG23	3:T:413:HOH:O	2.13	0.49
1:A:33:LEU:HD21	1:A:144:THR:HG23	1.94	0.49
1:F:124:ARG:HH21	1:F:124:ARG:CG	2.23	0.49
1:I:70:ARG:HH12	1:J:70[A]:ARG:NH2	2.11	0.49
1:U:153:ARG:HD2	3:U:390:HOH:O	2.13	0.49
1:A:13:ASN:N	3:A:303:HOH:O	2.45	0.48
1:G:70:ARG:HH21	1:H:70:ARG:HH12	1.60	0.48
1:U:29:THR:HG23	1:U:144:THR:HG21	1.94	0.48
1:S:51:HIS:CD2	1:S:63:HIS:O	2.59	0.48
1:A:114:VAL:HG12	1:A:118:LEU:HD22	1.95	0.48
1:E:134:LYS:HE3	3:E:414:HOH:O	2.12	0.48
1:D:33:LEU:HD21	1:D:144:THR:HG23	1.94	0.48
1:O:78:ASP:HB3	3:P:408:HOH:O	2.13	0.48
1:T:27:LYS:HE3	1:T:27:LYS:HB3	1.45	0.48
1:A:13:ASN:C	1:A:13:ASN:HD22	2.13	0.48
1:C:46:ILE:HD13	1:C:124:ARG:HD3	1.96	0.48
1:G:78:ASP:O	1:G:82:GLU:HG3	2.13	0.48
1:P:46:ILE:HD13	1:P:124:ARG:HD3	1.96	0.48
1:S:94:THR:O	1:S:98:ILE:HG12	2.13	0.47
1:C:160:TRP:CZ3	1:C:161:PHE:HE1	2.31	0.47
1:K:29:THR:HG23	1:K:144:THR:HG21	1.97	0.47
1:U:35:ARG:CZ	1:U:35:ARG:HB3	2.44	0.47
1:G:46:ILE:HD13	1:G:124:ARG:HD3	1.96	0.47
1:C:161:PHE:CZ	2:K:201:SO4:O3	2.67	0.47
1:O:70:ARG:HG2	1:O:74:ILE:CD1	2.45	0.47
1:V:13:ASN:N	3:V:305:HOH:O	2.46	0.47
1:E:119:LYS:HG2	3:E:431:HOH:O	2.15	0.47
1:V:46:ILE:HG23	1:V:107:TYR:CD1	2.50	0.46
1:W:120:GLU:O	1:W:124:ARG:HG2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:46:ILE:HG23	1:U:107:TYR:CD1	2.51	0.46
1:B:14:LEU:HD11	1:B:27:LYS:HG3	1.97	0.46
1:C:140:LYS:HD2	3:C:390:HOH:O	2.15	0.46
1:O:83:ARG:NH2	1:O:143:ASP:HB2	2.30	0.46
1:O:70:ARG:HH11	1:P:70:ARG:HH21	1.62	0.46
1:E:111:ILE:CD1	3:E:440:HOH:O	2.64	0.46
1:J:51:HIS:CE1	1:J:67:ASP:OD1	2.68	0.46
1:C:160:TRP:CZ3	1:C:161:PHE:CE1	3.03	0.46
1:J:14:LEU:HD11	1:J:27:LYS:HG3	1.98	0.45
1:X:107:TYR:O	1:X:109:LEU:HD13	2.16	0.45
1:I:51:HIS:CE1	1:I:63:HIS:CE1	3.04	0.45
1:T:120:GLU:O	1:T:124:ARG:HG2	2.17	0.45
1:V:70:ARG:NH1	3:V:308:HOH:O	2.47	0.45
1:H:13:ASN:ND2	3:H:310:HOH:O	2.50	0.45
1:K:77:LEU:HA	1:K:80:MET:HE2	1.97	0.45
1:V:29:THR:HG23	1:V:144:THR:HG21	1.99	0.45
1:G:138:GLU:HB3	3:G:428:HOH:O	2.17	0.45
1:R:46:ILE:HG23	1:R:107:TYR:CD1	2.51	0.45
1:O:76:HIS:NE2	1:O:154:ASP:OD2	2.26	0.45
1:E:12:THR:N	3:E:310:HOH:O	2.48	0.45
1:H:107:TYR:O	1:H:109:LEU:HD13	2.17	0.45
1:M:135:ALA:HA	1:M:138:GLU:HG2	1.98	0.45
1:Q:43:LEU:HD11	1:Q:125:TYR:CD1	2.51	0.45
1:L:35:ARG:NH1	3:L:310:HOH:O	2.50	0.45
1:L:32:LEU:HD12	3:L:310:HOH:O	2.16	0.45
1:X:13:ASN:HA	1:X:13:ASN:HD22	1.63	0.45
1:Q:81:ALA:O	1:Q:85:VAL:HG23	2.17	0.44
1:M:29:THR:HG23	1:M:144:THR:HG21	1.99	0.44
1:W:113:ASN:ND2	3:W:302:HOH:O	2.44	0.44
3:I:449:HOH:O	1:J:109:LEU:HD23	2.16	0.44
1:W:14:LEU:HD22	1:W:27:LYS:HE2	2.00	0.44
1:E:98:ILE:HG22	1:F:95:THR:HG21	1.99	0.44
1:G:29:THR:HG23	1:G:144:THR:HG21	1.98	0.44
1:M:26:LYS:HG2	1:M:87:LEU:HB3	1.99	0.44
1:Q:77:LEU:HA	1:Q:80:MET:HE2	1.99	0.44
1:R:127:ILE:O	1:R:131:ASP:HB2	2.17	0.44
1:M:140:LYS:HD2	1:M:140:LYS:N	2.32	0.44
1:W:76:HIS:O	1:W:80:MET:HG3	2.17	0.44
1:T:27:LYS:O	1:T:31:GLU:HG2	2.18	0.43
1:G:113:ASN:OD1	1:G:115:GLN:HB2	2.19	0.43
1:B:118:LEU:HA	1:B:118:LEU:HD12	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:78:ASP:HB3	3:V:390:HOH:O	2.18	0.43
1:X:27:LYS:O	1:X:31:GLU:HG2	2.18	0.43
1:D:94:THR:O	1:D:98:ILE:HG12	2.18	0.43
1:A:111:ILE:HG13	1:A:117:HIS:CE1	2.54	0.43
1:E:55:ARG:HH22	1:F:85:VAL:HG13	1.84	0.43
1:D:160:TRP:CZ3	1:D:161:PHE:HE1	2.36	0.43
1:H:29:THR:HG21	1:H:87:LEU:CD1	2.48	0.43
1:Q:46:ILE:HD13	1:Q:124:ARG:HD3	1.99	0.43
1:W:109:LEU:O	1:X:90:VAL:HG11	2.18	0.43
1:H:31:GLU:HA	1:H:31:GLU:OE1	2.18	0.43
1:M:114:VAL:HG12	1:M:118:LEU:HD22	2.01	0.43
1:D:77:LEU:C	1:D:77:LEU:HD12	2.38	0.42
1:P:153:ARG:NH2	2:P:203:SO4:O3	2.48	0.42
1:S:138:GLU:HB2	3:S:390:HOH:O	2.17	0.42
1:W:114:VAL:HG12	1:W:118:LEU:HD22	2.01	0.42
1:G:38:ILE:HA	1:G:98:ILE:HD12	2.00	0.42
1:N:17:THR:OG1	1:T:163:GLU:OE2	2.36	0.42
1:H:48:LYS:HG2	1:H:70:ARG:HD2	2.01	0.42
1:Q:73:LEU:HD12	1:Q:73:LEU:HA	1.92	0.42
1:T:77:LEU:HA	1:T:80:MET:CE	2.50	0.42
1:D:114:VAL:HG12	1:D:118:LEU:HD22	2.02	0.42
1:D:29:THR:HG23	1:D:144:THR:HG21	2.02	0.42
1:N:73:LEU:HD12	1:N:73:LEU:HA	1.96	0.42
1:S:114:VAL:HG12	1:S:118:LEU:HD22	2.01	0.42
1:T:77:LEU:HA	1:T:80:MET:HE2	2.01	0.42
1:W:113:ASN:ND2	3:W:311:HOH:O	2.52	0.42
1:S:124:ARG:HD3	3:S:429:HOH:O	2.19	0.42
1:D:166:ILE:HB	3:D:354:HOH:O	2.19	0.42
1:K:46:ILE:HG23	1:K:107:TYR:CD1	2.55	0.42
1:Q:113:ASN:HD22	1:Q:115:GLN:H	1.64	0.42
1:B:114:VAL:HG12	1:B:118:LEU:HD22	2.01	0.41
1:F:70:ARG:HG2	1:F:74:ILE:CD1	2.50	0.41
1:K:134:LYS:HE3	3:K:414:HOH:O	2.20	0.41
1:N:70[A]:ARG:HD3	3:N:415:HOH:O	2.21	0.41
1:R:32:LEU:HD11	1:R:135:ALA:HB1	2.03	0.41
1:X:105:LYS:NZ	3:X:316:HOH:O	2.52	0.41
1:A:46:ILE:HD13	1:A:124:ARG:HD3	2.01	0.41
1:A:70:ARG:HG2	1:A:74:ILE:HD13	2.03	0.41
1:H:66:LEU:HD12	1:H:66:LEU:HA	1.92	0.41
1:O:112:HIS:NE2	1:P:15:LEU:HD21	2.35	0.41
1:F:94:THR:O	1:F:98:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:113:ASN:ND2	1:Q:115:GLN:HB2	2.36	0.41
1:X:111:ILE:HG13	1:X:117:HIS:CE1	2.56	0.41
1:G:29:THR:HG21	1:G:87:LEU:CD1	2.51	0.41
1:S:39:GLN:HG2	1:S:103:PRO:CG	2.50	0.41
1:L:94:THR:O	1:L:98:ILE:HG12	2.21	0.40
1:T:94:THR:O	1:T:98:ILE:HG12	2.21	0.40
1:J:46:ILE:HD13	1:J:124:ARG:HD3	2.03	0.40
1:V:39:GLN:CD	3:V:324:HOH:O	2.59	0.40
1:P:153:ARG:HD2	3:P:418:HOH:O	2.21	0.40
1:P:98:ILE:HD13	1:P:98:ILE:N	2.36	0.40
1:R:163:GLU:HA	1:R:166:ILE:HD12	2.03	0.40
1:A:27:LYS:O	1:A:31:GLU:HG2	2.22	0.40
1:E:77:LEU:C	1:E:77:LEU:HD12	2.41	0.40
1:Q:113:ASN:HD22	1:Q:115:GLN:N	2.19	0.40
1:R:51:HIS:CE1	1:R:63:HIS:CE1	3.10	0.40
1:T:29:THR:HG23	1:T:144:THR:HG21	2.03	0.40
1:J:12:THR:N	3:J:323:HOH:O	2.54	0.40
1:Q:14:LEU:HD21	1:Q:26:LYS:CB	2.52	0.40
1:W:14:LEU:HD22	1:W:27:LYS:CE	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:425:HOH:O	3:X:404:HOH:O[1_665]	2.19	0.01

## 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	154/159 (97%)	152 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	153/159 (96%)	151 (99%)	2 (1%)	0	100	100
1	C	153/159 (96%)	150 (98%)	3 (2%)	0	100	100
1	D	153/159 (96%)	150 (98%)	3 (2%)	0	100	100
1	E	154/159 (97%)	150 (97%)	4 (3%)	0	100	100
1	F	153/159 (96%)	152 (99%)	1 (1%)	0	100	100
1	G	153/159 (96%)	151 (99%)	2 (1%)	0	100	100
1	H	153/159 (96%)	152 (99%)	1 (1%)	0	100	100
1	I	153/159 (96%)	152 (99%)	1 (1%)	0	100	100
1	J	155/159 (98%)	154 (99%)	1 (1%)	0	100	100
1	K	152/159 (96%)	149 (98%)	3 (2%)	0	100	100
1	L	153/159 (96%)	151 (99%)	2 (1%)	0	100	100
1	M	154/159 (97%)	152 (99%)	2 (1%)	0	100	100
1	N	154/159 (97%)	152 (99%)	2 (1%)	0	100	100
1	O	154/159 (97%)	153 (99%)	1 (1%)	0	100	100
1	P	153/159 (96%)	152 (99%)	1 (1%)	0	100	100
1	Q	154/159 (97%)	152 (99%)	2 (1%)	0	100	100
1	R	154/159 (97%)	152 (99%)	2 (1%)	0	100	100
1	S	156/159 (98%)	155 (99%)	1 (1%)	0	100	100
1	T	154/159 (97%)	152 (99%)	2 (1%)	0	100	100
1	U	153/159 (96%)	150 (98%)	3 (2%)	0	100	100
1	V	153/159 (96%)	150 (98%)	3 (2%)	0	100	100
1	W	154/159 (97%)	152 (99%)	2 (1%)	0	100	100
1	X	154/159 (97%)	150 (97%)	4 (3%)	0	100	100
All	All	3686/3816 (97%)	3636 (99%)	50 (1%)	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	134/136 (98%)	126 (94%)	8 (6%)	19	22
1	B	133/136 (98%)	124 (93%)	9 (7%)	16	17
1	C	133/136 (98%)	129 (97%)	4 (3%)	41	53
1	D	133/136 (98%)	127 (96%)	6 (4%)	27	34
1	E	134/136 (98%)	121 (90%)	13 (10%)	8	7
1	F	133/136 (98%)	126 (95%)	7 (5%)	22	27
1	G	133/136 (98%)	124 (93%)	9 (7%)	16	17
1	H	133/136 (98%)	128 (96%)	5 (4%)	33	42
1	I	133/136 (98%)	125 (94%)	8 (6%)	19	22
1	J	135/136 (99%)	126 (93%)	9 (7%)	16	18
1	K	132/136 (97%)	122 (92%)	10 (8%)	13	14
1	L	133/136 (98%)	124 (93%)	9 (7%)	16	17
1	M	134/136 (98%)	128 (96%)	6 (4%)	27	34
1	N	134/136 (98%)	127 (95%)	7 (5%)	23	28
1	O	134/136 (98%)	127 (95%)	7 (5%)	23	28
1	P	133/136 (98%)	124 (93%)	9 (7%)	16	17
1	Q	134/136 (98%)	122 (91%)	12 (9%)	9	9
1	R	134/136 (98%)	125 (93%)	9 (7%)	16	18
1	S	135/136 (99%)	127 (94%)	8 (6%)	19	23
1	T	134/136 (98%)	125 (93%)	9 (7%)	16	18
1	U	133/136 (98%)	124 (93%)	9 (7%)	16	17
1	V	133/136 (98%)	123 (92%)	10 (8%)	13	14
1	W	134/136 (98%)	124 (92%)	10 (8%)	13	14
1	X	134/136 (98%)	123 (92%)	11 (8%)	11	11
All	All	3205/3264 (98%)	3001 (94%)	204 (6%)	18	20

All (204) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	66	LEU
1	A	73	LEU
1	A	78[A]	ASP
1	A	78[B]	ASP
1	A	118	LEU

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Mol	Chain	Res	Type
1	A	134	LYS
1	A	140	LYS
1	B	15	LEU
1	B	55	ARG
1	B	66	LEU
1	B	73	LEU
1	B	77	LEU
1	B	96	GLN
1	B	109	LEU
1	B	118	LEU
1	B	134	LYS
1	C	66	LEU
1	C	73	LEU
1	C	118	LEU
1	C	140	LYS
1	D	15	LEU
1	D	66	LEU
1	D	73	LEU
1	D	74	ILE
1	D	109	LEU
1	D	118	LEU
1	E	12	THR
1	E	15	LEU
1	E	27	LYS
1	E	66	LEU
1	E	73	LEU
1	E	74	ILE
1	E	77	LEU
1	E	96	GLN
1	E	109	LEU
1	E	111	ILE
1	E	118	LEU
1	E	119	LYS
1	E	140	LYS
1	F	15	LEU
1	F	55	ARG
1	F	66	LEU
1	F	73	LEU
1	F	109	LEU
1	F	118	LEU
1	F	124	ARG
1	G	14	LEU

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Mol	Chain	Res	Type
1	G	15	LEU
1	G	66	LEU
1	G	70	ARG
1	G	73	LEU
1	G	74	ILE
1	G	100	SER
1	G	109	LEU
1	G	118	LEU
1	H	13	ASN
1	H	15	LEU
1	H	66	LEU
1	H	73	LEU
1	H	109	LEU
1	I	15	LEU
1	I	23	ASP
1	I	66	LEU
1	I	73	LEU
1	I	74	ILE
1	I	109	LEU
1	I	118	LEU
1	I	140	LYS
1	J	15	LEU
1	J	66	LEU
1	J	70[A]	ARG
1	J	70[B]	ARG
1	J	73	LEU
1	J	74	ILE
1	J	109	LEU
1	J	118	LEU
1	J	134	LYS
1	K	14	LEU
1	K	15	LEU
1	K	27	LYS
1	K	66	LEU
1	K	73	LEU
1	K	74	ILE
1	K	96	GLN
1	K	109	LEU
1	K	118	LEU
1	K	140	LYS
1	L	14	LEU
1	L	15	LEU

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Mol	Chain	Res	Type
1	L	55	ARG
1	L	66	LEU
1	L	73	LEU
1	L	74	ILE
1	L	109	LEU
1	L	118	LEU
1	L	134	LYS
1	M	15	LEU
1	M	17	THR
1	M	27	LYS
1	M	66	LEU
1	M	73	LEU
1	M	118	LEU
1	N	15	LEU
1	N	66	LEU
1	N	73	LEU
1	N	74	ILE
1	N	100	SER
1	N	109	LEU
1	N	118	LEU
1	O	15	LEU
1	O	66	LEU
1	O	73	LEU
1	O	74	ILE
1	O	100	SER
1	O	109	LEU
1	O	118	LEU
1	P	15	LEU
1	P	55	ARG
1	P	66	LEU
1	P	73	LEU
1	P	96	GLN
1	P	109	LEU
1	P	118	LEU
1	P	134	LYS
1	P	140	LYS
1	Q	13	ASN
1	Q	15	LEU
1	Q	66	LEU
1	Q	73	LEU
1	Q	78	ASP
1	Q	105	LYS

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Mol	Chain	Res	Type
1	Q	109	LEU
1	Q	118	LEU
1	Q	131	ASP
1	Q	134	LYS
1	Q	138	GLU
1	Q	167	GLU
1	R	66	LEU
1	R	70	ARG
1	R	73	LEU
1	R	74	ILE
1	R	77	LEU
1	R	109	LEU
1	R	131	ASP
1	R	138	GLU
1	R	140	LYS
1	S	10	LYS
1	S	14	LEU
1	S	15	LEU
1	S	66	LEU
1	S	73	LEU
1	S	96	GLN
1	S	109	LEU
1	S	118	LEU
1	T	13	ASN
1	T	14	LEU
1	T	15	LEU
1	T	66	LEU
1	T	73	LEU
1	T	110	ASP
1	T	118	LEU
1	T	134	LYS
1	T	140	LYS
1	U	15	LEU
1	U	66	LEU
1	U	70	ARG
1	U	73	LEU
1	U	77	LEU
1	U	100	SER
1	U	109	LEU
1	U	118	LEU
1	U	153	ARG
1	V	15	LEU

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Mol	Chain	Res	Type
1	V	31	GLU
1	V	66	LEU
1	V	73	LEU
1	V	100	SER
1	V	105	LYS
1	V	106	SER
1	V	109	LEU
1	V	118	LEU
1	V	138	GLU
1	W	14	LEU
1	W	15	LEU
1	W	55	ARG
1	W	66	LEU
1	W	73	LEU
1	W	77	LEU
1	W	109	LEU
1	W	118	LEU
1	W	138	GLU
1	W	140	LYS
1	X	13	ASN
1	X	14	LEU
1	X	15	LEU
1	X	27	LYS
1	X	66	LEU
1	X	73	LEU
1	X	74	ILE
1	X	100	SER
1	X	105	LYS
1	X	109	LEU
1	X	118	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	B	86	GLN
1	D	99	ASN
1	G	86	GLN
1	I	96	GLN
1	J	39	GLN
1	M	39	GLN
1	M	76	HIS

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Mol	Chain	Res	Type
1	Q	113	ASN
1	R	76	HIS
1	S	51	HIS
1	V	13	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

50 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	$\# Z  > 2$
2	SO4	A	203	-	4,4,4	0.28	0	6,6,6	0.18	0
2	SO4	O	202	-	4,4,4	0.32	0	6,6,6	0.20	0
2	SO4	I	201	-	4,4,4	0.18	0	6,6,6	0.10	0
2	SO4	N	201	-	4,4,4	0.24	0	6,6,6	0.22	0
2	SO4	O	201	-	4,4,4	0.26	0	6,6,6	0.19	0
2	SO4	L	201	-	4,4,4	0.33	0	6,6,6	0.19	0
2	SO4	J	201	-	4,4,4	0.21	0	6,6,6	0.30	0
2	SO4	U	202	-	4,4,4	0.29	0	6,6,6	0.10	0
2	SO4	I	203	-	4,4,4	0.40	0	6,6,6	0.18	0
2	SO4	S	202	-	4,4,4	0.31	0	6,6,6	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	M	202	-	4,4,4	0.29	0	6,6,6	0.24	0
2	SO4	S	201	-	4,4,4	0.19	0	6,6,6	0.24	0
2	SO4	Q	202	-	4,4,4	0.27	0	6,6,6	0.22	0
2	SO4	K	201	-	4,4,4	0.32	0	6,6,6	0.05	0
2	SO4	M	201	-	4,4,4	0.27	0	6,6,6	0.21	0
2	SO4	R	201	-	4,4,4	0.28	0	6,6,6	0.13	0
2	SO4	J	202	-	4,4,4	0.27	0	6,6,6	0.23	0
2	SO4	N	202	-	4,4,4	0.32	0	6,6,6	0.15	0
2	SO4	G	201	-	4,4,4	0.27	0	6,6,6	0.29	0
2	SO4	X	201	-	4,4,4	0.26	0	6,6,6	0.24	0
2	SO4	F	202	-	4,4,4	0.30	0	6,6,6	0.19	0
2	SO4	M	203	-	4,4,4	0.25	0	6,6,6	0.11	0
2	SO4	Q	201	-	4,4,4	0.23	0	6,6,6	0.14	0
2	SO4	X	202	-	4,4,4	0.32	0	6,6,6	0.05	0
2	SO4	B	203	-	4,4,4	0.32	0	6,6,6	0.04	0
2	SO4	U	201	-	4,4,4	0.27	0	6,6,6	0.17	0
2	SO4	W	201	-	4,4,4	0.20	0	6,6,6	0.22	0
2	SO4	T	201	-	4,4,4	0.24	0	6,6,6	0.16	0
2	SO4	C	202	-	4,4,4	0.30	0	6,6,6	0.30	0
2	SO4	I	202	-	4,4,4	0.30	0	6,6,6	0.17	0
2	SO4	T	202	-	4,4,4	0.36	0	6,6,6	0.13	0
2	SO4	P	201	-	4,4,4	0.30	0	6,6,6	0.14	0
2	SO4	C	201	-	4,4,4	0.27	0	6,6,6	0.19	0
2	SO4	A	202	-	4,4,4	0.26	0	6,6,6	0.12	0
2	SO4	L	202	-	4,4,4	0.26	0	6,6,6	0.31	0
2	SO4	B	202	-	4,4,4	0.27	0	6,6,6	0.25	0
2	SO4	P	203	-	4,4,4	0.23	0	6,6,6	0.17	0
2	SO4	R	202	-	4,4,4	0.24	0	6,6,6	0.15	0
2	SO4	P	202	-	4,4,4	0.29	0	6,6,6	0.14	0
2	SO4	H	201	-	4,4,4	0.30	0	6,6,6	0.28	0
2	SO4	B	201	-	4,4,4	0.17	0	6,6,6	0.36	0
2	SO4	G	202	-	4,4,4	0.22	0	6,6,6	0.15	0
2	SO4	A	201	-	4,4,4	0.36	0	6,6,6	0.27	0
2	SO4	F	201	-	4,4,4	0.29	0	6,6,6	0.33	0
2	SO4	H	202	-	4,4,4	0.28	0	6,6,6	0.16	0
2	SO4	E	201	-	4,4,4	0.38	0	6,6,6	0.27	0
2	SO4	D	201	-	4,4,4	0.20	0	6,6,6	0.19	0
2	SO4	D	202	-	4,4,4	0.32	0	6,6,6	0.14	0
2	SO4	W	202	-	4,4,4	0.22	0	6,6,6	0.14	0
2	SO4	V	201	-	4,4,4	0.17	0	6,6,6	0.26	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.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	201	SO4	2	0
2	T	202	SO4	1	0
2	P	203	SO4	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	155/159 (97%)	-0.80	0 100 100	11, 17, 29, 40	0
1	B	155/159 (97%)	-0.78	0 100 100	10, 16, 32, 44	0
1	C	155/159 (97%)	-0.73	0 100 100	12, 17, 33, 46	0
1	D	155/159 (97%)	-0.80	0 100 100	11, 16, 29, 53	0
1	E	156/159 (98%)	-0.73	1 (0%) 89 88	11, 16, 28, 71	0
1	F	155/159 (97%)	-0.77	0 100 100	11, 16, 30, 43	0
1	G	155/159 (97%)	-0.74	0 100 100	11, 17, 31, 43	0
1	H	155/159 (97%)	-0.75	0 100 100	12, 17, 31, 42	0
1	I	155/159 (97%)	-0.78	0 100 100	10, 16, 30, 39	0
1	J	156/159 (98%)	-0.75	0 100 100	11, 16, 29, 43	0
1	K	154/159 (96%)	-0.75	0 100 100	11, 16, 30, 44	0
1	L	155/159 (97%)	-0.76	0 100 100	11, 17, 31, 47	0
1	M	156/159 (98%)	-0.69	1 (0%) 89 88	11, 17, 31, 62	0
1	N	155/159 (97%)	-0.75	0 100 100	11, 16, 31, 51	0
1	O	156/159 (98%)	-0.73	1 (0%) 89 88	10, 16, 31, 67	0
1	P	155/159 (97%)	-0.77	0 100 100	10, 16, 31, 40	0
1	Q	155/159 (97%)	-0.70	0 100 100	11, 17, 33, 46	0
1	R	156/159 (98%)	-0.74	0 100 100	10, 16, 32, 59	0
1	S	158/159 (99%)	-0.78	0 100 100	11, 15, 29, 42	0
1	T	156/159 (98%)	-0.73	2 (1%) 77 75	10, 16, 29, 43	0
1	U	155/159 (97%)	-0.74	0 100 100	13, 17, 28, 39	0
1	V	155/159 (97%)	-0.83	0 100 100	10, 16, 31, 39	0
1	W	156/159 (98%)	-0.75	1 (0%) 89 88	11, 16, 28, 65	0
1	X	155/159 (97%)	-0.78	0 100 100	12, 16, 29, 45	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	3729/3816 (97%)	-0.75	6 (0%) 95 94	10, 16, 31, 71	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	W	12	THR	4.3
1	E	12	THR	4.2
1	M	12	THR	3.9
1	O	12	THR	3.4
1	T	12	THR	3.2
1	T	13	ASN	2.8

## 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	SO4	B	203	5/5	0.82	0.26	30,30,30,30	5
2	SO4	K	201	5/5	0.87	0.24	30,30,30,30	5
2	SO4	X	202	5/5	0.90	0.27	30,30,30,30	5
2	SO4	N	201	5/5	0.91	0.11	37,44,47,48	0
2	SO4	I	203	5/5	0.93	0.17	42,44,46,48	0
2	SO4	T	201	5/5	0.93	0.09	40,41,47,48	0
2	SO4	L	202	5/5	0.93	0.12	40,40,42,42	0
2	SO4	H	202	5/5	0.93	0.12	47,49,58,59	0
2	SO4	S	202	5/5	0.94	0.11	31,33,36,39	0
2	SO4	M	201	5/5	0.94	0.11	29,32,34,34	0
2	SO4	W	201	5/5	0.94	0.09	32,33,39,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	G	201	5/5	0.94	0.12	28,32,41,43	0
2	SO4	Q	202	5/5	0.94	0.10	37,40,47,50	0
2	SO4	H	201	5/5	0.94	0.09	39,42,44,47	0
2	SO4	G	202	5/5	0.94	0.09	38,38,44,46	0
2	SO4	A	201	5/5	0.94	0.09	29,35,38,42	0
2	SO4	F	202	5/5	0.94	0.11	34,35,43,46	0
2	SO4	A	202	5/5	0.95	0.09	39,42,43,47	0
2	SO4	J	202	5/5	0.95	0.10	34,39,41,43	0
2	SO4	R	202	5/5	0.95	0.10	35,38,43,43	0
2	SO4	P	203	5/5	0.95	0.10	31,32,37,43	0
2	SO4	O	202	5/5	0.95	0.10	28,30,34,40	0
2	SO4	M	202	5/5	0.95	0.09	37,38,43,44	0
2	SO4	I	202	5/5	0.95	0.10	29,31,36,36	0
2	SO4	I	201	5/5	0.96	0.07	30,32,33,35	0
2	SO4	O	201	5/5	0.96	0.08	30,31,38,38	0
2	SO4	B	202	5/5	0.96	0.10	31,33,39,40	0
2	SO4	F	201	5/5	0.96	0.09	32,32,34,36	0
2	SO4	L	201	5/5	0.96	0.09	40,43,47,52	0
2	SO4	D	201	5/5	0.96	0.07	32,32,34,38	0
2	SO4	D	202	5/5	0.96	0.10	36,41,45,46	0
2	SO4	W	202	5/5	0.96	0.09	33,36,39,40	0
2	SO4	U	202	5/5	0.97	0.10	41,46,48,52	0
2	SO4	R	201	5/5	0.97	0.09	45,45,50,50	0
2	SO4	X	201	5/5	0.97	0.08	36,38,39,43	0
2	SO4	J	201	5/5	0.97	0.07	31,32,37,38	0
2	SO4	P	201	5/5	0.97	0.08	40,41,44,45	0
2	SO4	C	201	5/5	0.97	0.08	33,35,40,43	0
2	SO4	M	203	5/5	0.97	0.09	28,28,29,30	0
2	SO4	Q	201	5/5	0.97	0.07	34,36,37,37	0
2	SO4	N	202	5/5	0.97	0.07	32,35,36,38	0
2	SO4	V	201	5/5	0.97	0.07	33,34,35,38	0
2	SO4	U	201	5/5	0.98	0.07	37,39,40,41	0
2	SO4	T	202	5/5	0.98	0.07	34,36,36,40	0
2	SO4	B	201	5/5	0.98	0.08	32,32,33,34	0
2	SO4	E	201	5/5	0.98	0.07	24,31,33,34	0
2	SO4	A	203	5/5	0.98	0.09	38,41,43,43	0
2	SO4	P	202	5/5	0.98	0.10	38,39,40,41	0
2	SO4	S	201	5/5	0.98	0.07	28,28,30,33	0
2	SO4	C	202	5/5	0.98	0.09	32,34,36,38	0

## 6.5 Other polymers

There are no such residues in this entry.