



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 08:17 PM BST

PDB ID : 5HE8  
Title : Bacterial initiation protein  
Authors : Hood, I.V.; Berger, J.M.  
Deposited on : 2016-01-05  
Resolution : 2.60 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  
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

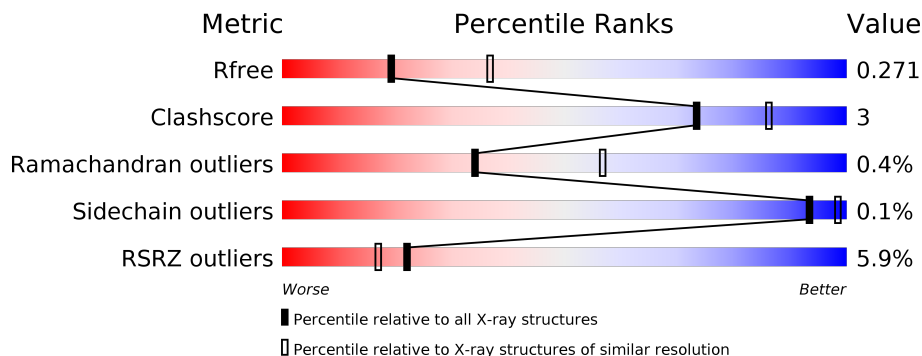
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	174	
1	B	174	
1	C	174	
1	D	174	
1	E	174	
1	F	174	

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Mol	Chain	Length	Quality of chain
1	G	174	<p>3% 93% 5%</p>
1	H	174	<p>4% 92% 5%</p>
1	I	174	<p>5% 94% 5%</p>
1	J	174	<p>4% 89% 5% 6%</p>
1	K	174	<p>15% 93% 5% 6%</p>
1	L	174	<p>18% 87% 5% 6%</p>

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	C	404	-	-	X	X

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 31944 atoms, of which 15840 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 Helicase loader.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	163	2596	830	1303	219	239	5	0	0	0
1	B	164	2611	835	1309	220	242	5	0	0	0
1	C	171	2732	872	1365	236	254	5	0	0	0
1	D	170	2716	867	1360	233	251	5	0	0	0
1	E	165	2625	839	1315	222	244	5	0	0	0
1	F	164	2611	835	1309	220	242	5	0	0	0
1	G	165	2636	841	1323	224	243	5	0	0	0
1	H	165	2635	841	1322	224	243	5	0	0	0
1	I	165	2626	839	1316	222	244	5	0	0	0
1	J	163	2597	830	1304	219	239	5	0	0	0
1	L	163	2592	829	1298	219	241	5	0	0	0
1	K	164	2620	836	1316	223	240	5	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	133	SER	-	expression tag	UNP W8TSU2
A	134	ASN	-	expression tag	UNP W8TSU2
A	135	ALA	-	expression tag	UNP W8TSU2
B	133	SER	-	expression tag	UNP W8TSU2
B	134	ASN	-	expression tag	UNP W8TSU2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	135	ALA	-	expression tag	UNP W8TSU2
C	133	SER	-	expression tag	UNP W8TSU2
C	134	ASN	-	expression tag	UNP W8TSU2
C	135	ALA	-	expression tag	UNP W8TSU2
D	133	SER	-	expression tag	UNP W8TSU2
D	134	ASN	-	expression tag	UNP W8TSU2
D	135	ALA	-	expression tag	UNP W8TSU2
E	133	SER	-	expression tag	UNP W8TSU2
E	134	ASN	-	expression tag	UNP W8TSU2
E	135	ALA	-	expression tag	UNP W8TSU2
F	133	SER	-	expression tag	UNP W8TSU2
F	134	ASN	-	expression tag	UNP W8TSU2
F	135	ALA	-	expression tag	UNP W8TSU2
G	133	SER	-	expression tag	UNP W8TSU2
G	134	ASN	-	expression tag	UNP W8TSU2
G	135	ALA	-	expression tag	UNP W8TSU2
H	133	SER	-	expression tag	UNP W8TSU2
H	134	ASN	-	expression tag	UNP W8TSU2
H	135	ALA	-	expression tag	UNP W8TSU2
I	133	SER	-	expression tag	UNP W8TSU2
I	134	ASN	-	expression tag	UNP W8TSU2
I	135	ALA	-	expression tag	UNP W8TSU2
J	133	SER	-	expression tag	UNP W8TSU2
J	134	ASN	-	expression tag	UNP W8TSU2
J	135	ALA	-	expression tag	UNP W8TSU2
L	133	SER	-	expression tag	UNP W8TSU2
L	134	ASN	-	expression tag	UNP W8TSU2
L	135	ALA	-	expression tag	UNP W8TSU2
K	133	SER	-	expression tag	UNP W8TSU2
K	134	ASN	-	expression tag	UNP W8TSU2
K	135	ALA	-	expression tag	UNP W8TSU2

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	C	1	5	4	1	0	0
2	C	1	5	4	1	0	0
2	C	1	5	4	1	0	0
2	C	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	E	1	5	4	1	0	0
2	E	1	5	4	1	0	0
2	F	1	5	4	1	0	0
2	F	1	5	4	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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	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	J	1	Total 5	O 4	S 1	0	0
2	J	1	Total 5	O 4	S 1	0	0
2	L	1	Total 5	O 4	S 1	0	0
2	L	1	Total 5	O 4	S 1	0	0
2	K	1	Total 5	O 4	S 1	0	0
2	K	1	Total 5	O 4	S 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total 8	O 8	0	0
3	B	10	Total 10	O 10	0	0
3	C	25	Total 25	O 25	0	0
3	D	19	Total 19	O 19	0	0
3	E	24	Total 24	O 24	0	0

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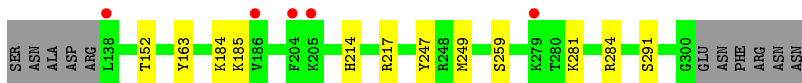
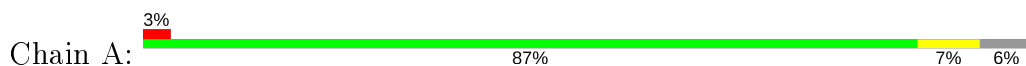
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	F	26	Total 26	O 26	0	0
3	G	24	Total 24	O 24	0	0
3	H	22	Total 22	O 22	0	0
3	I	15	Total 15	O 15	0	0
3	J	19	Total 19	O 19	0	0
3	L	5	Total 5	O 5	0	0
3	K	10	Total 10	O 10	0	0



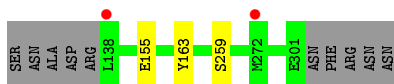
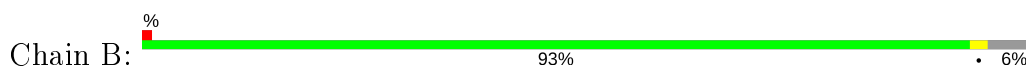
### 3 Residue-property plots [i](#)

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.

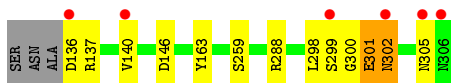
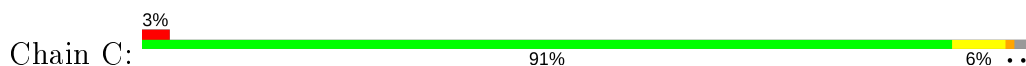
- Molecule 1: Helicase loader



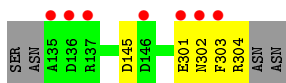
- Molecule 1: Helicase loader



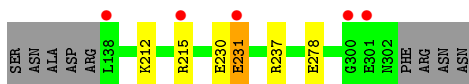
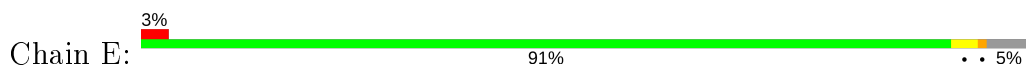
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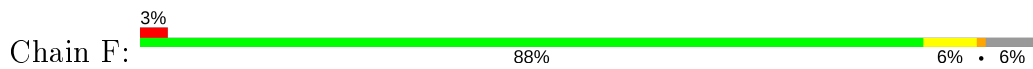
- Molecule 1: Helicase loader



- Molecule 1: Helicase loader



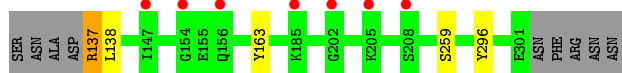
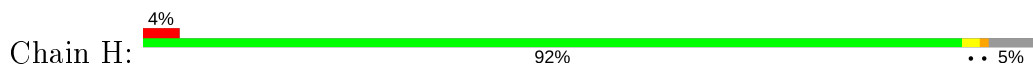
- Molecule 1: Helicase loader



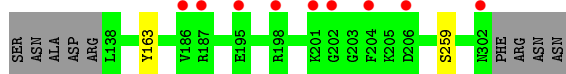
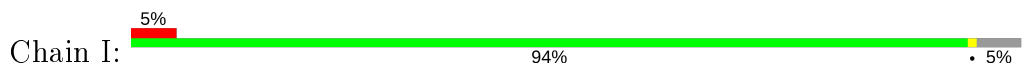
• Molecule 1: Helicase loader



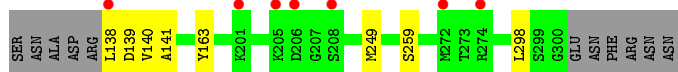
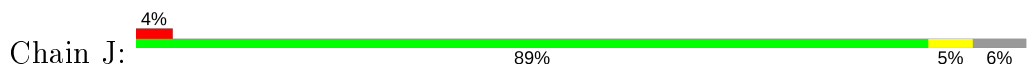
• Molecule 1: Helicase loader



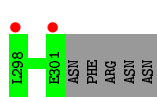
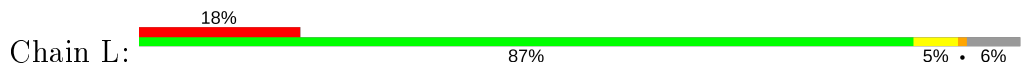
• Molecule 1: Helicase loader



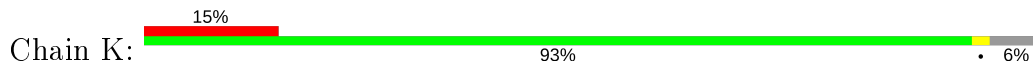
• Molecule 1: Helicase loader

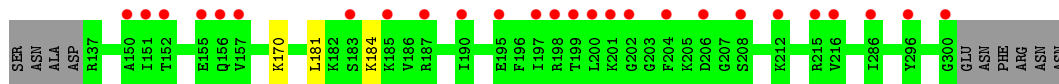


• Molecule 1: Helicase loader



• Molecule 1: Helicase loader





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.10Å 126.26Å 183.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.24 – 2.60 47.24 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.24-2.60) 89.6 (47.24-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.52 (at 2.61Å)	Xtrriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, $R_{free}$	0.225 , 0.270 0.227 , 0.271	Depositor DCC
$R_{free}$ test set	3988 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.7	Xtrriage
Anisotropy	0.571	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 43.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	31944	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.77% 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: 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	0.26	0/1320	0.42	0/1779
1	B	0.25	0/1329	0.42	0/1791
1	C	0.26	0/1395	0.43	0/1879
1	D	0.25	0/1384	0.42	0/1864
1	E	0.25	0/1337	0.42	0/1802
1	F	0.26	0/1329	0.42	0/1791
1	G	0.29	0/1340	0.42	0/1805
1	H	0.28	0/1340	0.43	0/1805
1	I	0.25	0/1337	0.42	0/1802
1	J	0.26	0/1320	0.42	0/1779
1	K	0.25	0/1331	0.41	0/1793
1	L	0.25	0/1321	0.42	0/1780
All	All	0.26	0/16083	0.42	0/21670

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	1293	1303	1303	17	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1302	1309	1309	1	1
1	C	1367	1365	1364	12	0
1	D	1356	1360	1359	10	0
1	E	1310	1315	1315	5	0
1	F	1302	1309	1309	28	0
1	G	1313	1323	1322	4	0
1	H	1313	1322	1322	8	0
1	I	1310	1316	1315	1	0
1	J	1293	1304	1303	6	0
1	K	1304	1316	1316	2	0
1	L	1294	1298	1298	15	0
2	A	15	0	0	0	0
2	B	5	0	0	0	0
2	C	20	0	0	2	0
2	D	10	0	0	0	0
2	E	10	0	0	0	0
2	F	10	0	0	0	0
2	G	10	0	0	0	0
2	H	20	0	0	0	0
2	I	10	0	0	0	0
2	J	10	0	0	0	0
2	K	10	0	0	1	0
2	L	10	0	0	0	0
3	A	8	0	0	0	0
3	B	10	0	0	0	0
3	C	25	0	0	1	0
3	D	19	0	0	0	0
3	E	24	0	0	0	0
3	F	26	0	0	1	0
3	G	24	0	0	0	0
3	H	22	0	0	0	0
3	I	15	0	0	0	0
3	J	19	0	0	2	0
3	K	10	0	0	0	0
3	L	5	0	0	0	0
All	All	16104	15840	15835	103	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 (103) 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:F:204:PHE:CE1	1:F:235:TRP:CD1	1.85	1.60
1:F:204:PHE:HE1	1:F:235:TRP:CD1	1.15	1.58
1:F:204:PHE:CE1	1:F:235:TRP:CG	1.93	1.53
1:A:281:LYS:HG2	1:A:284:ARG:NH2	1.14	1.39
1:F:204:PHE:CZ	1:F:235:TRP:CG	2.10	1.39
1:L:197:ILE:HD12	1:L:230:GLU:CD	1.58	1.21
1:A:281:LYS:CG	1:A:284:ARG:NH2	2.04	1.21
1:F:204:PHE:CZ	1:F:235:TRP:CD2	2.31	1.18
1:A:281:LYS:CG	1:A:284:ARG:HH21	1.54	1.18
1:L:197:ILE:CD1	1:L:230:GLU:CD	2.23	1.07
1:A:217:ARG:NH1	1:A:247:TYR:CD1	2.29	1.00
1:L:197:ILE:HD11	1:L:230:GLU:OE1	1.61	0.99
1:F:204:PHE:HE1	1:F:235:TRP:CG	1.51	0.97
1:F:204:PHE:CZ	1:F:235:TRP:CB	2.50	0.95
1:A:281:LYS:HG2	1:A:284:ARG:HH22	1.12	0.93
1:L:197:ILE:CD1	1:L:230:GLU:OE1	2.16	0.92
1:F:204:PHE:HZ	1:F:235:TRP:CG	1.84	0.92
1:F:204:PHE:CE1	1:F:235:TRP:CD2	2.54	0.91
1:F:204:PHE:HZ	1:F:235:TRP:CB	1.86	0.89
1:C:299:SER:O	1:C:301:GLU:N	2.08	0.86
1:F:204:PHE:CE1	1:F:235:TRP:NE1	2.43	0.86
1:A:217:ARG:NH1	1:A:247:TYR:CE1	2.47	0.82
1:J:249:MET:HE1	3:J:506:HOH:O	1.83	0.78
1:A:281:LYS:CB	1:A:284:ARG:HH21	1.97	0.77
1:F:200:LEU:O	1:F:202:GLY:N	2.17	0.76
1:L:197:ILE:HD12	1:L:230:GLU:CG	2.16	0.76
1:F:204:PHE:CD1	1:F:235:TRP:CD1	2.72	0.74
1:A:281:LYS:HA	1:A:284:ARG:HE	1.52	0.74
1:A:281:LYS:HG2	1:A:284:ARG:HH21	0.94	0.74
1:C:146:ASP:OD1	1:E:215:ARG:NH1	2.23	0.71
1:A:152:THR:HG21	1:A:184:LYS:HD2	1.71	0.71
1:F:204:PHE:CE1	1:F:235:TRP:CE2	2.80	0.70
2:C:404:SO4:O2	3:C:501:HOH:O	2.07	0.70
1:F:204:PHE:CE1	1:F:235:TRP:CB	2.70	0.69
1:J:138:LEU:O	1:J:138:LEU:HD13	1.92	0.69
1:J:249:MET:CE	3:J:506:HOH:O	2.39	0.69
1:H:137:ARG:N	1:H:137:ARG:HE	1.94	0.66
1:H:138:LEU:O	1:H:296:TYR:OH	2.04	0.63
1:C:302:ASN:HB2	1:H:137:ARG:C	2.20	0.62
1:A:281:LYS:CA	1:A:284:ARG:HH21	2.13	0.61
1:F:204:PHE:CZ	1:F:235:TRP:HB3	2.37	0.60
1:A:249:MET:HE1	1:A:291:SER:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:204:PHE:HZ	1:F:235:TRP:HB2	1.67	0.59
1:F:204:PHE:CZ	1:F:235:TRP:CE3	2.90	0.59
1:F:204:PHE:CG	1:F:204:PHE:O	2.56	0.58
1:D:301:GLU:HB3	1:D:302:ASN:HB3	1.86	0.57
1:A:281:LYS:HA	1:A:284:ARG:HH21	1.70	0.57
1:F:201:LYS:NZ	3:F:501:HOH:O	2.37	0.57
1:L:193:LEU:O	1:L:230:GLU:OE2	2.24	0.56
1:C:302:ASN:CB	1:H:137:ARG:C	2.69	0.54
1:F:196:PHE:O	1:F:199:THR:OG1	2.19	0.54
1:H:137:ARG:O	1:H:138:LEU:HD12	2.07	0.54
1:A:214:HIS:CE1	1:A:217:ARG:HH21	2.25	0.54
1:E:237:ARG:NH2	1:E:278:GLU:OE1	2.39	0.53
1:E:230:GLU:O	1:E:231:GLU:HB3	2.09	0.52
1:G:299:SER:OG	1:G:300:GLY:N	2.44	0.51
1:L:197:ILE:CD1	1:L:230:GLU:OE2	2.58	0.51
1:D:302:ASN:HD21	1:D:304:ARG:HH21	1.58	0.50
1:F:204:PHE:CE1	1:F:235:TRP:HB3	2.48	0.49
1:A:152:THR:HG21	1:A:184:LYS:CD	2.42	0.49
1:H:137:ARG:NE	1:H:137:ARG:N	2.60	0.49
1:L:197:ILE:HG13	1:L:230:GLU:OE2	2.14	0.48
1:D:301:GLU:HB3	1:D:302:ASN:CA	2.43	0.48
1:L:206:ASP:N	1:L:207:GLY:HA2	2.29	0.48
1:D:304:ARG:NH1	1:G:299:SER:HB3	2.29	0.47
1:L:197:ILE:HD12	1:L:230:GLU:OE2	2.08	0.47
1:F:204:PHE:HZ	1:F:235:TRP:CD2	2.13	0.47
1:D:301:GLU:HB3	1:D:302:ASN:HA	1.97	0.47
1:L:188:SER:HA	1:L:221:ILE:HB	1.97	0.47
1:F:204:PHE:CD2	1:F:204:PHE:O	2.68	0.46
1:J:140:VAL:HG11	1:J:298:LEU:HD21	1.97	0.46
1:J:163:TYR:HA	1:J:259:SER:O	2.15	0.46
1:C:136:ASP:CA	1:C:137:ARG:HB2	2.46	0.46
1:L:219:ALA:O	1:L:220:ASN:CB	2.64	0.46
1:C:140:VAL:CG2	1:C:298:LEU:HD13	2.46	0.45
1:C:302:ASN:HB2	1:H:138:LEU:N	2.31	0.45
1:E:212:LYS:HA	1:E:215:ARG:HE	1.81	0.45
1:D:301:GLU:HB3	1:D:302:ASN:CB	2.47	0.44
1:E:230:GLU:O	1:E:231:GLU:CB	2.65	0.44
1:F:204:PHE:CD1	1:F:235:TRP:NE1	2.81	0.44
1:L:231:GLU:O	1:L:232:VAL:HB	2.18	0.44
1:D:302:ASN:HD21	1:D:304:ARG:NH2	2.16	0.43
1:G:163:TYR:HA	1:G:259:SER:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:140:VAL:HG13	1:J:141:ALA:N	2.33	0.43
1:C:305:ASN:OD1	1:C:305:ASN:N	2.52	0.43
1:L:219:ALA:O	1:L:220:ASN:HB3	2.17	0.42
1:D:304:ARG:HH22	1:G:299:SER:H	1.68	0.42
1:H:163:TYR:HA	1:H:259:SER:O	2.19	0.42
1:B:163:TYR:HA	1:B:259:SER:O	2.19	0.42
1:F:235:TRP:CD1	1:F:239:GLU:HB2	2.54	0.42
1:A:281:LYS:HA	1:A:284:ARG:NE	2.25	0.42
1:C:136:ASP:N	1:C:137:ARG:HB2	2.35	0.41
1:F:163:TYR:HA	1:F:259:SER:O	2.20	0.41
1:C:288:ARG:NH2	2:C:404:SO4:O1	2.53	0.41
1:I:163:TYR:HA	1:I:259:SER:O	2.21	0.41
1:K:181:LEU:O	1:K:184:LYS:O	2.38	0.41
1:D:145:ASP:OD2	1:F:215:ARG:NH1	2.49	0.41
1:A:163:TYR:HA	1:A:259:SER:O	2.21	0.40
1:C:136:ASP:HA	1:C:137:ARG:HB2	2.04	0.40
1:K:170:LYS:N	2:K:401:SO4:O2	2.53	0.40
1:C:163:TYR:HA	1:C:259:SER:O	2.21	0.40
1:D:303:PHE:O	1:D:304:ARG:HB3	2.21	0.40
1:L:197:ILE:CG1	1:L:230:GLU:OE2	2.69	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)
1:A:185:LYS:NZ	1:B:155:GLU:OE2[3_555]	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	161/174 (92%)	155 (96%)	6 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	162/174 (93%)	154 (95%)	8 (5%)	0	100	100
1	C	169/174 (97%)	160 (95%)	6 (4%)	3 (2%)	8	16
1	D	168/174 (97%)	160 (95%)	8 (5%)	0	100	100
1	E	163/174 (94%)	156 (96%)	6 (4%)	1 (1%)	25	47
1	F	162/174 (93%)	151 (93%)	10 (6%)	1 (1%)	25	47
1	G	163/174 (94%)	159 (98%)	4 (2%)	0	100	100
1	H	163/174 (94%)	152 (93%)	11 (7%)	0	100	100
1	I	163/174 (94%)	158 (97%)	5 (3%)	0	100	100
1	J	161/174 (92%)	158 (98%)	2 (1%)	1 (1%)	25	47
1	K	162/174 (93%)	153 (94%)	9 (6%)	0	100	100
1	L	161/174 (92%)	153 (95%)	6 (4%)	2 (1%)	13	27
All	All	1958/2088 (94%)	1869 (96%)	81 (4%)	8 (0%)	34	57

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	300	GLY
1	F	201	LYS
1	C	301	GLU
1	C	302	ASN
1	J	139	ASP
1	L	220	ASN
1	L	232	VAL
1	E	231	GLU

### 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	139/149 (93%)	139 (100%)	0	100	100
1	B	140/149 (94%)	140 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	147/149 (99%)	147 (100%)	0	100	100
1	D	145/149 (97%)	145 (100%)	0	100	100
1	E	141/149 (95%)	141 (100%)	0	100	100
1	F	140/149 (94%)	140 (100%)	0	100	100
1	G	141/149 (95%)	141 (100%)	0	100	100
1	H	141/149 (95%)	140 (99%)	1 (1%)	84	94
1	I	141/149 (95%)	141 (100%)	0	100	100
1	J	139/149 (93%)	139 (100%)	0	100	100
1	K	140/149 (94%)	140 (100%)	0	100	100
1	L	139/149 (93%)	139 (100%)	0	100	100
All	All	1693/1788 (95%)	1692 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	137	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 [i](#)

28 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	H	403	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	J	402	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	D	401	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	L	402	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	B	401	-	4,4,4	0.15	0	6,6,6	0.04	0
2	SO4	E	402	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	L	401	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	A	402	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	C	403	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	I	402	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	C	404	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	F	402	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	H	402	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	J	401	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	C	402	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	H	404	-	4,4,4	0.13	0	6,6,6	0.05	0
2	SO4	G	401	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	I	401	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	G	402	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	K	401	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	K	402	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	D	402	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	F	401	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	A	401	-	4,4,4	0.14	0	6,6,6	0.10	0
2	SO4	C	401	-	4,4,4	0.15	0	6,6,6	0.13	0
2	SO4	E	401	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	H	401	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	A	403	-	4,4,4	0.14	0	6,6,6	0.04	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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	404	SO4	2	0
2	K	401	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 [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	163/174 (93%)	0.38	5 (3%) 49 42	45, 73, 108, 152	0
1	B	164/174 (94%)	0.35	2 (1%) 79 76	50, 70, 106, 137	0
1	C	171/174 (98%)	0.29	6 (3%) 44 36	38, 58, 96, 170	0
1	D	170/174 (97%)	0.39	7 (4%) 37 30	42, 63, 98, 147	0
1	E	165/174 (94%)	0.29	5 (3%) 50 43	43, 59, 92, 146	0
1	F	164/174 (94%)	0.37	5 (3%) 50 43	34, 54, 87, 130	0
1	G	165/174 (94%)	0.34	6 (3%) 42 35	42, 63, 92, 118	0
1	H	165/174 (94%)	0.43	7 (4%) 36 29	39, 59, 95, 119	0
1	I	165/174 (94%)	0.54	9 (5%) 25 19	46, 69, 109, 137	0
1	J	163/174 (93%)	0.43	7 (4%) 35 28	42, 65, 105, 131	0
1	K	164/174 (94%)	0.92	26 (15%) 1 1	55, 92, 128, 169	0
1	L	163/174 (93%)	1.07	32 (19%) 1 0	62, 98, 133, 156	0
All	All	1982/2088 (94%)	0.48	117 (5%) 22 17	34, 67, 116, 170	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	230	GLU	4.9
1	L	301	GLU	4.8
1	C	302	ASN	4.6
1	L	154	GLY	4.6
1	H	205	LYS	4.3
1	D	301	GLU	4.1
1	K	300	GLY	4.1
1	K	206	ASP	4.0
1	K	187	ARG	4.0
1	A	138	LEU	4.0
1	K	202	GLY	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	138	LEU	3.9
1	K	201	LYS	3.8
1	C	305	ASN	3.7
1	K	155	GLU	3.7
1	H	154	GLY	3.7
1	L	149	THR	3.6
1	A	204	PHE	3.6
1	L	211	LYS	3.6
1	K	152	THR	3.6
1	K	198	ARG	3.5
1	K	195	GLU	3.4
1	L	202	GLY	3.4
1	L	153	ASN	3.3
1	L	187	ARG	3.3
1	L	298	LEU	3.3
1	K	185	LYS	3.3
1	E	300	GLY	3.3
1	L	198	ARG	3.2
1	K	204	PHE	3.2
1	K	197	ILE	3.2
1	H	208	SER	3.2
1	G	154	GLY	3.2
1	L	186	VAL	3.2
1	L	151	ILE	3.2
1	L	157	VAL	3.1
1	K	190	ILE	3.0
1	K	183	SER	3.0
1	L	156	GLN	3.0
1	D	136	ASP	3.0
1	E	301	GLU	3.0
1	B	272	MET	2.9
1	H	147	ILE	2.9
1	F	204	PHE	2.9
1	L	181	LEU	2.9
1	G	198	ARG	2.9
1	C	306	ASN	2.9
1	J	208	SER	2.9
1	I	204	PHE	2.9
1	L	152	THR	2.8
1	K	215	ARG	2.8
1	G	204	PHE	2.8
1	H	202	GLY	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	136	ASP	2.7
1	I	186	VAL	2.7
1	I	202	GLY	2.7
1	D	137	ARG	2.7
1	I	198	ARG	2.7
1	K	208	SER	2.7
1	I	201	LYS	2.6
1	L	184	LYS	2.6
1	K	156	GLN	2.6
1	J	201	LYS	2.6
1	D	303	PHE	2.6
1	H	185	LYS	2.6
1	G	156	GLN	2.6
1	L	185	LYS	2.6
1	J	274	ARG	2.6
1	L	191	ILE	2.6
1	D	302	ASN	2.6
1	E	138	LEU	2.6
1	J	138	LEU	2.6
1	D	135	ALA	2.5
1	F	206	ASP	2.5
1	A	205	LYS	2.5
1	L	215	ARG	2.5
1	L	192	TYR	2.5
1	K	286	ILE	2.5
1	H	156	GLN	2.4
1	I	195	GLU	2.4
1	K	296	TYR	2.4
1	K	151	ILE	2.4
1	L	209	PHE	2.4
1	K	216	VAL	2.4
1	F	201	LYS	2.4
1	I	206	ASP	2.4
1	K	200	LEU	2.3
1	L	205	LYS	2.3
1	J	206	ASP	2.3
1	L	208	SER	2.3
1	L	199	THR	2.3
1	J	205	LYS	2.3
1	A	279	LYS	2.2
1	I	187	ARG	2.2
1	J	272	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	140	VAL	2.2
1	C	299	SER	2.2
1	G	157	VAL	2.2
1	K	212	LYS	2.1
1	L	220	ASN	2.1
1	L	197	ILE	2.1
1	K	199	THR	2.1
1	L	204	PHE	2.1
1	L	193	LEU	2.1
1	F	235	TRP	2.1
1	G	187	ARG	2.1
1	D	146	ASP	2.1
1	E	231	GLU	2.1
1	L	252	GLU	2.1
1	E	215	ARG	2.1
1	A	186	VAL	2.1
1	K	157	VAL	2.1
1	L	212	LYS	2.1
1	F	207	GLY	2.1
1	K	150	ALA	2.0
1	L	147	ILE	2.0
1	I	302	ASN	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
2	SO4	L	402	5/5	0.69	0.32	113,113,114,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	I	402	5/5	0.71	0.26	135,135,136,136	0
2	SO4	C	404	5/5	0.72	0.46	153,153,154,154	0
2	SO4	A	403	5/5	0.74	0.34	137,137,138,138	0
2	SO4	G	402	5/5	0.80	0.30	105,105,106,108	0
2	SO4	A	402	5/5	0.82	0.21	114,115,116,116	0
2	SO4	D	402	5/5	0.87	0.14	105,106,106,108	0
2	SO4	J	402	5/5	0.88	0.17	112,113,113,113	0
2	SO4	C	403	5/5	0.88	0.20	83,84,84,86	0
2	SO4	C	402	5/5	0.88	0.23	139,140,141,141	0
2	SO4	K	402	5/5	0.89	0.22	118,118,119,119	0
2	SO4	H	404	5/5	0.90	0.19	120,120,122,122	0
2	SO4	F	402	5/5	0.91	0.20	82,82,84,84	0
2	SO4	H	402	5/5	0.92	0.23	147,147,148,148	0
2	SO4	H	403	5/5	0.94	0.24	90,91,91,91	0
2	SO4	L	401	5/5	0.95	0.16	88,90,91,92	0
2	SO4	K	401	5/5	0.96	0.12	86,87,88,89	0
2	SO4	B	401	5/5	0.97	0.18	54,56,58,58	0
2	SO4	E	402	5/5	0.97	0.14	69,70,72,72	0
2	SO4	I	401	5/5	0.97	0.20	53,53,55,57	0
2	SO4	E	401	5/5	0.97	0.17	59,64,65,65	0
2	SO4	H	401	5/5	0.97	0.56	113,117,118,119	0
2	SO4	D	401	5/5	0.97	0.21	53,53,53,53	0
2	SO4	C	401	5/5	0.98	0.20	47,47,49,50	0
2	SO4	J	401	5/5	0.98	0.13	62,64,64,65	0
2	SO4	F	401	5/5	0.99	0.19	50,52,53,54	0
2	SO4	A	401	5/5	0.99	0.17	42,45,49,50	0
2	SO4	G	401	5/5	0.99	0.22	42,45,46,47	0

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

There are no such residues in this entry.