



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2023 – 10:43 pm GMT

PDB ID : 4A1I  
Title : ykud from B.subtilis  
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Deposited on : 2011-09-15  
Resolution : 1.76 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

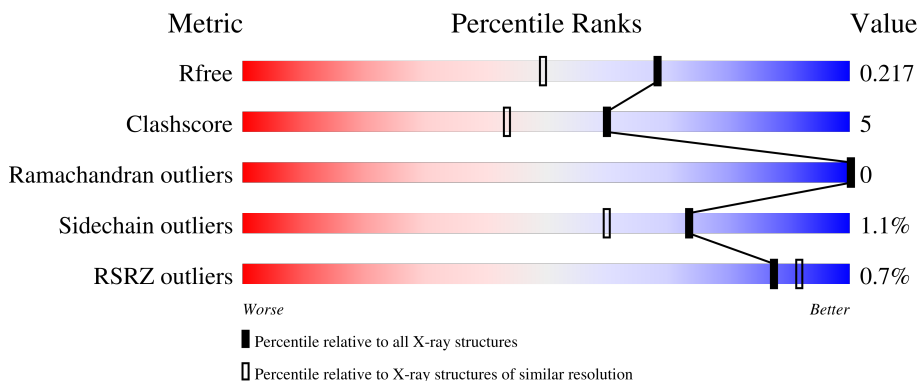
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.76 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.



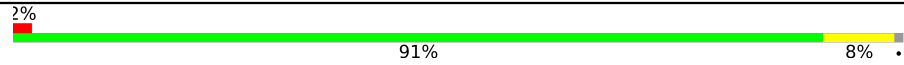
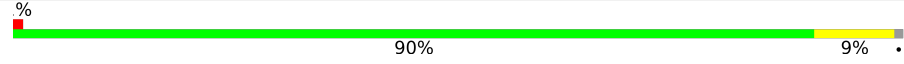
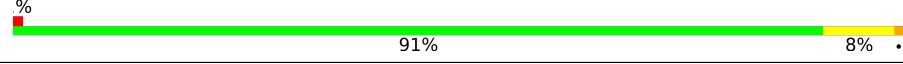
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	165	92% 7%
1	B	165	92% 8%
1	C	165	83% 17%
1	D	165	92% 8%
1	E	165	92% 8%

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Mol	Chain	Length	Quality of chain
1	F	165	 2% 91% 8% .
1	G	165	 % 90% 9% .
1	H	165	 % 91% 8% ..

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11563 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 PUTATIVE L, D-TRANSPEPTIDASE YKUD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	165	1239	787	220	228	4	0	0	0
1	B	165	1239	787	220	228	4	0	0	0
1	C	165	1239	787	220	228	4	1	0	0
1	D	165	1239	787	220	228	4	1	0	0
1	E	164	1235	785	219	227	4	0	0	0
1	F	164	1235	785	219	227	4	1	0	0
1	G	164	1235	785	219	227	4	0	0	0
1	H	164	1235	785	219	227	4	1	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP O34816
A	117	ALA	LYS	engineered mutation	UNP O34816
A	118	ALA	GLN	engineered mutation	UNP O34816
B	0	GLY	-	expression tag	UNP O34816
B	117	ALA	LYS	engineered mutation	UNP O34816
B	118	ALA	GLN	engineered mutation	UNP O34816
C	0	GLY	-	expression tag	UNP O34816
C	117	ALA	LYS	engineered mutation	UNP O34816
C	118	ALA	GLN	engineered mutation	UNP O34816
D	0	GLY	-	expression tag	UNP O34816
D	117	ALA	LYS	engineered mutation	UNP O34816
D	118	ALA	GLN	engineered mutation	UNP O34816
E	0	GLY	-	expression tag	UNP O34816

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Chain	Residue	Modelled	Actual	Comment	Reference
E	117	ALA	LYS	engineered mutation	UNP O34816
E	118	ALA	GLN	engineered mutation	UNP O34816
F	0	GLY	-	expression tag	UNP O34816
F	117	ALA	LYS	engineered mutation	UNP O34816
F	118	ALA	GLN	engineered mutation	UNP O34816
G	0	GLY	-	expression tag	UNP O34816
G	117	ALA	LYS	engineered mutation	UNP O34816
G	118	ALA	GLN	engineered mutation	UNP O34816
H	0	GLY	-	expression tag	UNP O34816
H	117	ALA	LYS	engineered mutation	UNP O34816
H	118	ALA	GLN	engineered mutation	UNP O34816

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



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

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

- Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cd	0	0
			1	1		
3	B	1	Total	Cd	0	0
			1	1		
3	C	1	Total	Cd	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Cd 1 1	0	0
3	E	1	Total Cd 1 1	0	0
3	F	1	Total Cd 1 1	0	0
3	G	1	Total Cd 1 1	0	0
3	H	1	Total Cd 1 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	B	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0
4	E	1	Total Cl 1 1	0	0
4	F	1	Total Cl 1 1	0	0
4	G	1	Total Cl 1 1	0	0
4	H	1	Total Cl 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	225	Total O 225 225	0	0
5	B	205	Total O 205 205	0	0
5	C	203	Total O 203 203	0	0
5	D	211	Total O 211 211	0	0

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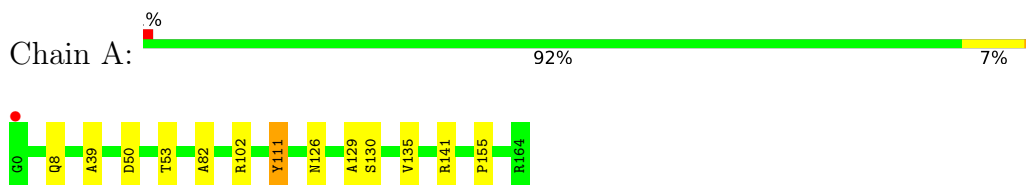
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	E	170	Total 170	O 170	0	0
5	F	194	Total 194	O 194	0	0
5	G	162	Total 162	O 162	0	0
5	H	171	Total 171	O 171	0	0



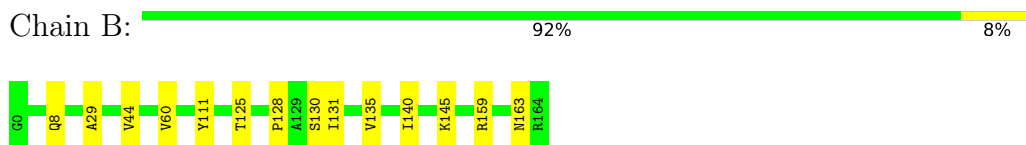
### 3 Residue-property plots [i](#)

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.

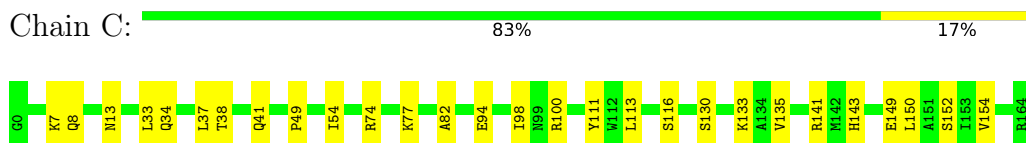
- Molecule 1: PUTATIVE L, D-TRANSPEPTIDASE YKUD



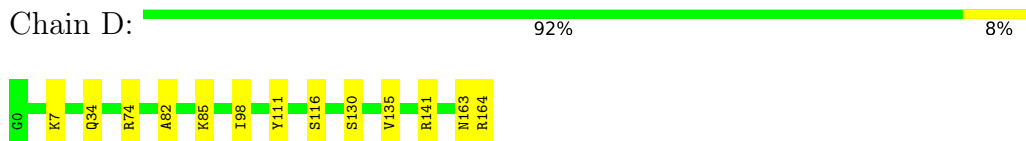
- Molecule 1: PUTATIVE L, D-TRANSPEPTIDASE YKUD



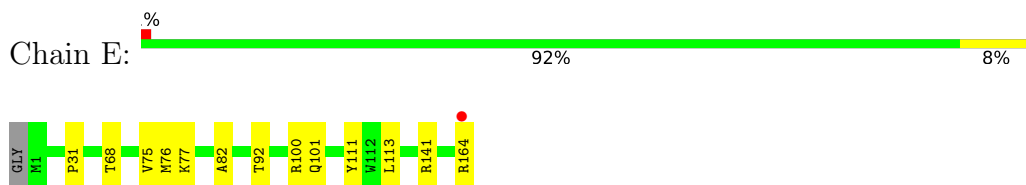
- Molecule 1: PUTATIVE L, D-TRANSPEPTIDASE YKUD



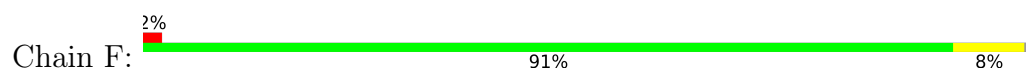
- Molecule 1: PUTATIVE L, D-TRANSPEPTIDASE YKUD



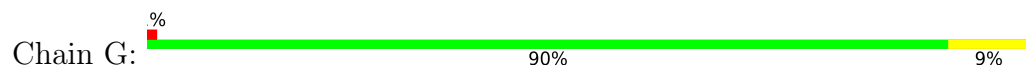
- Molecule 1: PUTATIVE L, D-TRANSPEPTIDASE YKUD



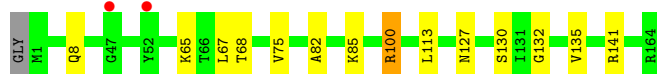
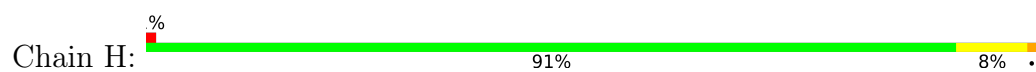
- Molecule 1: PUTATIVE L, D-TRANSPEPTIDASE YKUD



• Molecule 1: PUTATIVE L, D-TRANSPEPTIDASE YKUD



• Molecule 1: PUTATIVE L, D-TRANSPEPTIDASE YKUD



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.45Å 91.85Å 123.70Å 90.00° 90.25° 90.00°	Depositor
Resolution (Å)	51.30 – 1.76 51.30 – 1.76	Depositor EDS
% Data completeness (in resolution range)	97.8 (51.30-1.76) 96.5 (51.30-1.76)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 1.76Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.173 , 0.218 0.172 , 0.217	Depositor DCC
$R_{free}$ test set	2006 reflections (1.67%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.0	Xtrriage
Anisotropy	0.337	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 36.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.327 for h,-k,-l	Xtrriage
Reported twinning fraction	0.330 for h,-k,-l	Depositor
Outliers	3 of 120001 reflections (0.002%)	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	11563	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.73 % 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 4.4027e-03. 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, SO4, CD

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	0.28	0/1265	0.49	0/1723
1	B	0.28	0/1265	0.49	0/1723
1	C	0.28	0/1265	0.49	0/1723
1	D	0.28	0/1265	0.49	0/1723
1	E	0.27	0/1261	0.50	0/1718
1	F	0.27	0/1261	0.49	0/1718
1	G	0.28	0/1261	0.50	0/1718
1	H	0.27	0/1261	0.49	0/1718
All	All	0.28	0/10104	0.49	0/13764

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	1239	0	1273	10	0
1	B	1239	0	1273	12	0
1	C	1239	0	1273	19	0
1	D	1239	0	1273	8	1
1	E	1235	0	1270	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1235	0	1270	10	0
1	G	1235	0	1270	9	0
1	H	1235	0	1270	11	0
2	A	20	0	0	1	1
2	B	10	0	0	1	0
2	C	15	0	0	1	0
2	D	5	0	0	1	0
2	E	15	0	0	1	0
2	F	15	0	0	1	0
2	G	15	0	0	1	0
2	H	15	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	225	0	0	6	0
5	B	205	0	0	5	3
5	C	203	0	0	8	0
5	D	211	0	0	4	0
5	E	170	0	0	4	1
5	F	194	0	0	4	3
5	G	162	0	0	4	1
5	H	171	0	0	3	0
All	All	11563	0	10172	92	5

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 5.

All (92) 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:127:ASN:ND2	5:F:2167:HOH:O	2.04	0.90
1:B:125:THR:HG21	1:B:131:ILE:HD11	1.54	0.90
2:H:1165:SO4:O1	5:H:2136:HOH:O	1.90	0.87
2:B:1165:SO4:O4	5:B:2170:HOH:O	1.93	0.86
2:C:1165:SO4:O2	5:C:2173:HOH:O	1.95	0.82
2:G:1165:SO4:O1	5:G:2133:HOH:O	1.96	0.81
2:D:1165:SO4:O3	5:D:2175:HOH:O	1.98	0.81
2:E:1165:SO4:O1	5:E:2144:HOH:O	1.96	0.80
1:B:8:GLN:NE2	5:B:2032:HOH:O	2.15	0.78
2:A:1165:SO4:O2	5:A:2184:HOH:O	2.03	0.76
1:D:130:SER:HB2	1:D:135:VAL:HG21	1.67	0.76
1:G:85:LYS:HE2	5:G:2098:HOH:O	1.82	0.76
1:H:127:ASN:OD1	5:H:2141:HOH:O	2.05	0.74
2:F:1165:SO4:O1	5:F:2162:HOH:O	2.05	0.74
1:F:7:LYS:HE3	5:F:2011:HOH:O	1.87	0.73
1:C:34:GLN:NE2	5:C:2089:HOH:O	2.19	0.71
1:C:13:ASN:CG	1:F:164:ARG:HH22	1.94	0.71
5:A:2030:HOH:O	1:H:8:GLN:O	2.10	0.68
1:A:129:ALA:O	5:A:2192:HOH:O	2.12	0.67
1:A:8:GLN:HG2	1:A:39:ALA:HB2	1.78	0.66
1:B:130:SER:HB2	1:B:135:VAL:HG11	1.78	0.66
1:G:2:LEU:HD12	1:G:51:PRO:HG3	1.77	0.65
1:D:163:ASN:ND2	5:D:2208:HOH:O	2.18	0.64
1:C:8:GLN:O	5:C:2031:HOH:O	2.15	0.63
1:C:143:HIS:HE1	5:C:2188:HOH:O	1.81	0.63
1:A:130:SER:HB2	1:A:135:VAL:HG11	1.82	0.62
1:G:82:ALA:HB3	1:G:141:ARG:HB2	1.79	0.62
1:F:92:THR:HG21	1:F:164:ARG:HE	1.66	0.61
1:D:82:ALA:HB3	1:D:141:ARG:HB2	1.83	0.61
1:B:128:PRO:HA	1:B:131:ILE:HD13	1.83	0.60
1:C:74:ARG:NH1	5:C:2125:HOH:O	2.30	0.60
1:H:65:LYS:HD3	1:H:132:GLY:O	2.02	0.60
1:B:131:ILE:HD12	1:B:131:ILE:N	2.17	0.59
1:F:62:ILE:O	1:F:65:LYS:HD2	2.02	0.59
1:E:101:GLN:HG2	5:E:2128:HOH:O	2.03	0.58
1:C:133:LYS:HE2	5:C:2180:HOH:O	2.04	0.57
1:A:126:ASN:OD1	5:A:2187:HOH:O	2.17	0.57
1:H:100:ARG:HB3	1:H:113:LEU:HD23	1.87	0.57
1:E:92:THR:HG21	1:E:164:ARG:HD3	1.86	0.56
5:A:2149:HOH:O	1:D:34:GLN:NE2	2.37	0.56
1:C:130:SER:HB2	1:C:135:VAL:HG11	1.86	0.56
1:G:72:ASN:ND2	5:G:2085:HOH:O	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ASN:ND2	5:B:2201:HOH:O	2.33	0.54
1:C:135:VAL:HG22	5:C:2184:HOH:O	2.07	0.53
1:G:85:LYS:HG2	1:G:135:VAL:HA	1.90	0.51
1:H:130:SER:HB2	1:H:135:VAL:HG11	1.93	0.50
1:D:7:LYS:HD3	5:D:2013:HOH:O	2.11	0.50
1:C:7:LYS:HD3	5:C:2020:HOH:O	2.11	0.50
1:A:135:VAL:O	1:A:135:VAL:HG22	2.13	0.49
1:C:49:PRO:HG2	1:C:54:ILE:HD11	1.95	0.49
1:D:74:ARG:NH1	5:D:2127:HOH:O	2.45	0.49
1:G:50:ASP:OD1	1:G:52:TYR:HD1	1.94	0.48
1:A:82:ALA:HB3	1:A:141:ARG:HB2	1.95	0.48
1:F:102:ARG:NH2	5:F:2150:HOH:O	2.47	0.48
5:A:2204:HOH:O	1:B:145:LYS:HG2	2.13	0.48
1:E:31:PRO:HD2	5:E:2064:HOH:O	2.13	0.48
1:B:131:ILE:N	1:B:131:ILE:CD1	2.77	0.47
1:E:68:THR:HG23	1:E:75:VAL:HG23	1.95	0.47
1:F:82:ALA:HB3	1:F:141:ARG:HB2	1.96	0.47
1:E:82:ALA:HB3	1:E:141:ARG:HB2	1.97	0.47
1:H:82:ALA:HB3	1:H:141:ARG:HB2	1.96	0.47
1:C:33:LEU:HD22	1:C:37:LEU:HD23	1.97	0.47
1:C:100:ARG:HB3	1:C:113:LEU:HD23	1.98	0.46
1:H:85:LYS:HG2	1:H:135:VAL:HA	1.98	0.46
1:F:71:LEU:C	1:F:71:LEU:HD13	2.35	0.46
1:C:38:THR:O	1:C:41:GLN:HG2	2.16	0.45
1:C:77:LYS:HE2	1:C:149:GLU:OE1	2.17	0.45
1:H:135:VAL:O	1:H:135:VAL:HG22	2.16	0.45
1:A:155:PRO:HG3	1:C:152:SER:O	2.17	0.44
5:B:2196:HOH:O	1:G:49:PRO:HG3	2.18	0.44
1:G:130:SER:HB2	1:G:135:VAL:HG21	1.98	0.44
1:H:68:THR:HG23	1:H:75:VAL:HG13	1.99	0.44
1:A:50:ASP:HB3	1:A:53:THR:HG23	2.00	0.44
1:C:98:ILE:HD11	1:C:116:SER:HB3	1.98	0.44
1:E:76:MET:HB3	5:E:2055:HOH:O	2.18	0.44
1:H:85:LYS:HE2	5:H:2044:HOH:O	2.18	0.43
1:C:94:GLU:HG3	5:G:2112:HOH:O	2.17	0.43
1:C:82:ALA:HB3	1:C:141:ARG:HB2	2.01	0.43
1:A:102:ARG:NH1	1:A:111:TYR:OH	2.52	0.42
1:C:150:LEU:O	1:C:154:VAL:HG22	2.19	0.42
1:B:159:ARG:HD2	5:B:2149:HOH:O	2.18	0.42
1:F:164:ARG:HA	1:F:164:ARG:HD3	1.88	0.42
1:E:76:MET:HG3	1:E:77:LYS:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:54:ILE:HG22	1:G:56:TYR:H	1.83	0.41
1:H:67:LEU:C	1:H:67:LEU:HD23	2.40	0.41
1:D:85:LYS:HG2	1:D:135:VAL:HA	2.02	0.41
1:B:29:ALA:HB1	1:B:44:VAL:HG23	2.01	0.41
1:A:50:ASP:O	1:A:53:THR:OG1	2.29	0.41
1:B:60:VAL:HG21	1:B:140:ILE:HD13	2.02	0.41
1:F:130:SER:HB2	1:F:135:VAL:HG21	2.02	0.41
1:D:98:ILE:HD11	1:D:116:SER:HB3	2.02	0.41
1:B:135:VAL:O	1:B:135:VAL:HG22	2.21	0.40

All (5) 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:D:164:ARG:NH1	2:A:1168:SO4:O1[1_655]	1.81	0.39
5:B:2186:HOH:O	5:G:2120:HOH:O[2_646]	2.02	0.18
5:E:2088:HOH:O	5:F:2150:HOH:O[2_545]	2.05	0.15
5:B:2077:HOH:O	5:F:2119:HOH:O[2_546]	2.15	0.05
5:B:2076:HOH:O	5:F:2119:HOH:O[2_546]	2.16	0.04

## 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	163/165 (99%)	157 (96%)	6 (4%)	0	100 100
1	B	163/165 (99%)	159 (98%)	4 (2%)	0	100 100
1	C	163/165 (99%)	159 (98%)	4 (2%)	0	100 100
1	D	163/165 (99%)	159 (98%)	4 (2%)	0	100 100
1	E	162/165 (98%)	158 (98%)	4 (2%)	0	100 100
1	F	162/165 (98%)	157 (97%)	5 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	162/165 (98%)	158 (98%)	4 (2%)	0	100	100
1	H	162/165 (98%)	158 (98%)	4 (2%)	0	100	100
All	All	1300/1320 (98%)	1265 (97%)	35 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	133/133 (100%)	132 (99%)	1 (1%)	81	72
1	B	133/133 (100%)	132 (99%)	1 (1%)	81	72
1	C	133/133 (100%)	132 (99%)	1 (1%)	81	72
1	D	133/133 (100%)	132 (99%)	1 (1%)	81	72
1	E	133/133 (100%)	130 (98%)	3 (2%)	50	28
1	F	133/133 (100%)	131 (98%)	2 (2%)	65	49
1	G	133/133 (100%)	131 (98%)	2 (2%)	65	49
1	H	133/133 (100%)	132 (99%)	1 (1%)	81	72
All	All	1064/1064 (100%)	1052 (99%)	12 (1%)	73	60

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	TYR
1	B	111	TYR
1	C	111	TYR
1	D	111	TYR
1	E	100	ARG
1	E	111	TYR
1	E	113	LEU
1	F	100	ARG
1	F	111	TYR

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Mol	Chain	Res	Type
1	G	7	LYS
1	G	100	ARG
1	H	100	ARG

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

Mol	Chain	Res	Type
1	C	143	HIS

### 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](#)

Of 38 ligands modelled in this entry, 16 are monoatomic - leaving 22 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	$\# Z  > 2$
2	SO4	E	1165	3	4,4,4	0.14	0	6,6,6	0.26	0
2	SO4	F	1165	3	4,4,4	0.15	0	6,6,6	0.12	0
2	SO4	E	1166	-	4,4,4	0.13	0	6,6,6	0.06	0
2	SO4	H	1167	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	C	1165	3	4,4,4	0.15	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	1167	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	D	1165	3	4,4,4	0.18	0	6,6,6	0.09	0
2	SO4	C	1167	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	C	1166	-	4,4,4	0.13	0	6,6,6	0.09	0
2	SO4	E	1167	-	4,4,4	0.14	0	6,6,6	0.10	0
2	SO4	F	1166	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	B	1165	3	4,4,4	0.17	0	6,6,6	0.13	0
2	SO4	G	1167	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	H	1165	3	4,4,4	0.17	0	6,6,6	0.12	0
2	SO4	H	1166	-	4,4,4	0.13	0	6,6,6	0.08	0
2	SO4	B	1166	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	F	1167	-	4,4,4	0.15	0	6,6,6	0.12	0
2	SO4	A	1165	3	4,4,4	0.16	0	6,6,6	0.07	0
2	SO4	A	1168	-	4,4,4	0.13	0	6,6,6	0.09	0
2	SO4	A	1166	-	4,4,4	0.13	0	6,6,6	0.09	0
2	SO4	G	1165	3	4,4,4	0.14	0	6,6,6	0.19	0
2	SO4	G	1166	-	4,4,4	0.15	0	6,6,6	0.07	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.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1165	SO4	1	0
2	F	1165	SO4	1	0
2	C	1165	SO4	1	0
2	D	1165	SO4	1	0
2	B	1165	SO4	1	0
2	H	1165	SO4	1	0
2	A	1165	SO4	1	0
2	A	1168	SO4	0	1
2	G	1165	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	165/165 (100%)	-0.34	1 (0%) 89   92	10, 18, 31, 43	0
1	B	165/165 (100%)	-0.48	0 100   100	9, 15, 27, 44	0
1	C	165/165 (100%)	-0.39	0 100   100	10, 18, 29, 38	2 (1%)
1	D	165/165 (100%)	-0.46	0 100   100	9, 15, 27, 41	1 (0%)
1	E	164/165 (99%)	-0.44	1 (0%) 89   92	10, 16, 29, 52	0
1	F	164/165 (99%)	-0.31	3 (1%) 68   76	10, 17, 30, 55	1 (0%)
1	G	164/165 (99%)	-0.45	2 (1%) 79   84	8, 15, 30, 49	0
1	H	164/165 (99%)	-0.27	2 (1%) 79   84	8, 17, 33, 62	1 (0%)
All	All	1316/1320 (99%)	-0.39	9 (0%) 87   92	8, 16, 30, 62	5 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	52	TYR	5.2
1	A	0	GLY	3.2
1	G	52	TYR	2.8
1	E	164	ARG	2.7
1	H	47	GLY	2.4
1	F	164	ARG	2.2
1	F	74	ARG	2.1
1	G	164	ARG	2.0
1	F	52	TYR	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( $\text{\AA}^2$ )	Q<0.9
2	SO4	F	1167	5/5	0.82	0.14	41,41,42,45	1
2	SO4	E	1166	5/5	0.95	0.11	46,46,47,48	1
2	SO4	E	1167	5/5	0.95	0.14	31,32,36,37	2
2	SO4	A	1167	5/5	0.95	0.13	48,49,49,51	1
2	SO4	C	1167	5/5	0.96	0.10	43,44,45,45	3
2	SO4	H	1167	5/5	0.96	0.13	40,41,41,42	3
2	SO4	A	1166	5/5	0.97	0.09	23,24,25,28	1
2	SO4	G	1166	5/5	0.97	0.11	33,35,35,36	4
2	SO4	G	1167	5/5	0.97	0.08	34,34,34,35	4
2	SO4	F	1166	5/5	0.97	0.09	39,39,40,42	0
2	SO4	B	1166	5/5	0.98	0.08	23,24,25,28	2
4	CL	F	1169	1/1	0.98	0.08	16,16,16,16	1
2	SO4	F	1165	5/5	0.99	0.06	14,16,18,20	0
2	SO4	C	1166	5/5	0.99	0.07	20,20,20,23	3
2	SO4	B	1165	5/5	0.99	0.05	13,15,16,17	1
2	SO4	G	1165	5/5	0.99	0.05	7,10,11,17	4
2	SO4	D	1165	5/5	0.99	0.04	14,15,18,18	0
2	SO4	E	1165	5/5	0.99	0.06	14,14,15,22	0
2	SO4	H	1165	5/5	0.99	0.08	12,13,14,15	3
2	SO4	H	1166	5/5	0.99	0.08	31,32,33,34	1
2	SO4	A	1168	5/5	0.99	0.08	12,14,16,19	4
4	CL	A	1170	1/1	0.99	0.05	17,17,17,17	0
4	CL	B	1168	1/1	0.99	0.04	14,14,14,14	0
4	CL	D	1167	1/1	0.99	0.07	17,17,17,17	0
4	CL	E	1169	1/1	0.99	0.04	10,10,10,10	1
2	SO4	C	1165	5/5	0.99	0.06	16,17,19,20	0
4	CL	G	1169	1/1	0.99	0.06	15,15,15,15	1
4	CL	H	1169	1/1	0.99	0.05	9,9,9,9	1
3	CD	G	1168	1/1	1.00	0.06	13,13,13,13	1
3	CD	H	1168	1/1	1.00	0.06	15,15,15,15	1
2	SO4	A	1165	5/5	1.00	0.04	12,13,13,18	2
3	CD	A	1169	1/1	1.00	0.06	14,14,14,14	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CL	C	1169	1/1	1.00	0.03	10,10,10,10	1
3	CD	B	1167	1/1	1.00	0.05	14,14,14,14	1
3	CD	C	1168	1/1	1.00	0.05	15,15,15,15	1
3	CD	D	1166	1/1	1.00	0.04	15,15,15,15	1
3	CD	E	1168	1/1	1.00	0.05	14,14,14,14	1
3	CD	F	1168	1/1	1.00	0.06	15,15,15,15	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.