



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:49 AM GMT

PDB ID : 2YH6  
Title : STRUCTURE OF THE N-TERMINAL DOMAIN OF BAMC FROM E. COLI  
Authors : Zeth, K.; Albrecht, R.  
Deposited on : 2011-04-27  
Resolution : 1.55 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

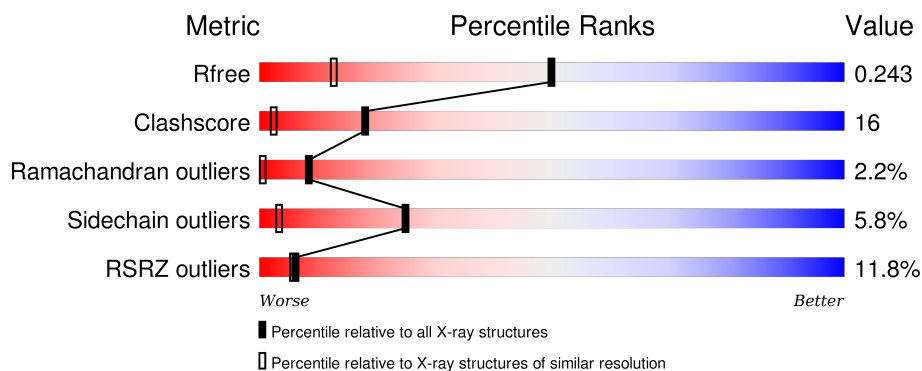
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.55 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))
$R_{free}$	91344	1665 (1.58-1.54)
Clashscore	102246	1014 (1.56-1.56)
Ramachandran outliers	100387	1704 (1.58-1.54)
Sidechain outliers	100360	1702 (1.58-1.54)
RSRZ outliers	91569	1668 (1.58-1.54)

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. 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	112	<div> <div>6%</div> <div>75%</div> <div>15%</div> <div>• • •</div> </div>
1	B	112	<div> <div>13%</div> <div>63%</div> <div>24%</div> <div>7%</div> <div>• •</div> </div>
1	C	112	<div> <div>17%</div> <div>63%</div> <div>28%</div> <div>• • •</div> </div>
1	D	112	<div> <div>9%</div> <div>71%</div> <div>19%</div> <div>7%</div> <div>• •</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	C	1188	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3572 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 LIPOPROTEIN 34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	108	Total	C	N	O	S	0	2	0
			863	536	149	175	3			
1	B	107	Total	C	N	O	S	0	1	0
			822	510	148	161	3			
1	C	109	Total	C	N	O	S	0	1	0
			854	530	151	170	3			
1	D	110	Total	C	N	O	S	0	2	0
			867	538	151	175	3			

- 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	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	A	1	Total	O	S	0	0
			5	4	1		
2	B	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		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	49	Total	O	0	0
			49	49		
3	B	22	Total	O	0	0
			22	22		
3	C	29	Total	O	0	0
			29	29		
3	D	36	Total	O	0	0
			36	36		

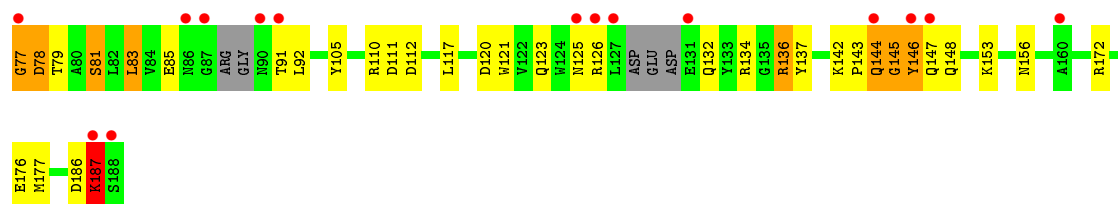
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

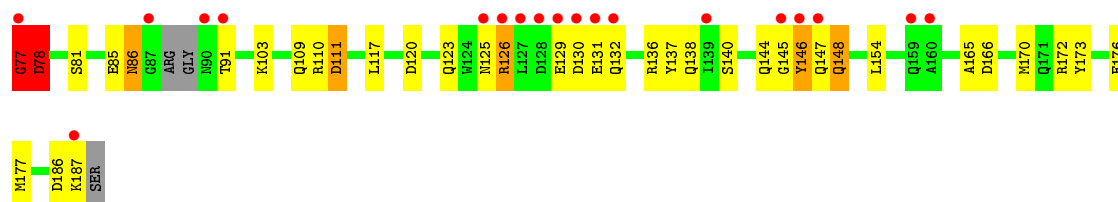
#### • Molecule 1: LIPOPROTEIN 34



#### • Molecule 1: LIPOPROTEIN 34



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#### • Molecule 1: LIPOPROTEIN 34



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.58Å 46.63Å 60.21Å 102.70° 92.86° 118.20°	Depositor
Resolution (Å)	30.00 – 1.55 39.78 – 1.50	Depositor EDS
% Data completeness (in resolution range)	95.8 (30.00-1.55) 67.2 (39.78-1.50)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.195 , 0.234 0.213 , 0.243	Depositor DCC
$R_{free}$ test set	2278 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.3	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 51.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 49692 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3572	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.48% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	1.37	3/881 (0.3%)	1.28	11/1197 (0.9%)
1	B	1.31	6/835 (0.7%)	1.32	14/1133 (1.2%)
1	C	1.36	6/869 (0.7%)	1.30	11/1180 (0.9%)
1	D	1.45	6/885 (0.7%)	1.33	13/1202 (1.1%)
All	All	1.37	21/3470 (0.6%)	1.31	49/4712 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	3
All	All	0	5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	77	GLY	N-CA	16.11	1.70	1.46
1	A	77	GLY	N-CA	14.54	1.67	1.46
1	C	77	GLY	C-O	-11.38	1.05	1.23
1	D	126	ARG	CB-CG	-8.40	1.29	1.52
1	D	103	LYS	CD-CE	-8.39	1.30	1.51
1	C	81	SER	CB-OG	-8.23	1.31	1.42
1	D	140	SER	CB-OG	-8.15	1.31	1.42
1	C	111	ASP	CB-CG	-7.93	1.35	1.51
1	B	81	SER	CB-OG	-7.92	1.31	1.42
1	C	77	GLY	N-CA	7.09	1.56	1.46
1	B	77	GLY	C-O	-6.83	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111	ASP	CB-CG	-6.83	1.37	1.51
1	C	176	GLU	CG-CD	-6.17	1.42	1.51
1	B	137	TYR	CG-CD1	5.83	1.46	1.39
1	A	104	ASN	CG-ND2	-5.53	1.19	1.32
1	C	173	TYR	CG-CD1	5.48	1.46	1.39
1	B	105	TYR	CD1-CE1	5.45	1.47	1.39
1	A	111	ASP	CB-CG	-5.36	1.40	1.51
1	D	111	ASP	CB-CG	-5.16	1.41	1.51
1	D	165	ALA	CA-CB	5.15	1.63	1.52
1	B	176	GLU	CG-CD	-5.06	1.44	1.51

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	78	ASP	CB-CG-OD1	13.33	130.30	118.30
1	A	136	ARG	NE-CZ-NH1	11.92	126.26	120.30
1	B	144	GLN	N-CA-C	-11.48	80.01	111.00
1	D	77	GLY	N-CA-C	11.18	141.04	113.10
1	A	77	GLY	N-CA-C	10.57	139.53	113.10
1	B	83	LEU	CA-CB-CG	-10.40	91.38	115.30
1	D	83	LEU	CA-CB-CG	-10.30	91.60	115.30
1	C	77	GLY	N-CA-C	9.97	138.03	113.10
1	B	110	ARG	NE-CZ-NH2	-8.73	115.93	120.30
1	C	177	MET	CG-SD-CE	-8.36	86.83	100.20
1	D	126	ARG	NE-CZ-NH1	-8.28	116.16	120.30
1	C	136	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	C	78	ASP	CB-CG-OD2	-7.93	111.16	118.30
1	B	136	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	A	136	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	C	120	ASP	CB-CG-OD1	7.32	124.88	118.30
1	A	172	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	C	145	GLY	N-CA-C	-7.06	95.45	113.10
1	A	78	ASP	N-CA-C	6.85	129.51	111.00
1	A	110	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	D	126	ARG	CB-CA-C	-6.63	97.15	110.40
1	A	111	ASP	CB-CG-OD2	6.43	124.09	118.30
1	C	172	ARG	NE-CZ-NH1	-6.43	117.08	120.30
1	B	177	MET	CG-SD-CE	-6.39	89.98	100.20
1	D	172	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	D	78	ASP	N-CA-C	6.21	127.77	111.00
1	D	172	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	B	176	GLU	OE1-CD-OE2	6.08	130.59	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	110	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	D	110	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	B	112	ASP	CB-CG-OD1	5.99	123.69	118.30
1	D	111	ASP	CB-CG-OD1	5.94	123.64	118.30
1	C	110	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	D	136	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	D	77	GLY	O-C-N	-5.78	113.45	122.70
1	A	145	GLY	C-N-CA	5.47	135.38	121.70
1	C	172	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	D	111	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	A	127	LEU	CB-CG-CD1	5.33	120.05	111.00
1	D	172	ARG	CG-CD-NE	-5.32	100.62	111.80
1	A	146	TYR	N-CA-CB	5.32	120.17	110.60
1	B	120	ASP	CB-CG-OD1	5.28	123.06	118.30
1	B	92	LEU	CB-CG-CD2	-5.24	102.09	111.00
1	B	172	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	B	146	TYR	N-CA-C	5.19	125.01	111.00
1	A	172	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	111	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	77	GLY	O-C-N	-5.05	114.61	122.70
1	B	145	GLY	N-CA-C	-5.03	100.52	113.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	GLY	Peptide
1	B	187	LYS	Peptide
1	C	111	ASP	Sidechain
1	C	144	GLN	Peptide
1	C	77	GLY	Peptide

## 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	863	0	845	29	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	822	0	799	31	1
1	C	854	0	830	31	2
1	D	867	0	850	32	0
2	A	15	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	49	0	0	5	0
3	B	22	0	0	0	0
3	C	29	0	0	7	0
3	D	36	0	0	1	0
All	All	3572	0	3324	106	2

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 16.

All (106) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:GLY:CA	1:A:77:GLY:N	1.67	1.57
1:D:77:GLY:N	1:D:77:GLY:CA	1.70	1.50
3:A:2007:HOH:O	1:B:77:GLY:N	1.64	1.27
1:C:186:ASP:HB3	3:C:2027:HOH:O	1.54	1.07
1:A:78:ASP:HB2	1:B:85:GLU:OE2	1.63	0.98
1:C:85:GLU:OE2	1:D:78:ASP:HB2	1.74	0.88
1:B:145:GLY:CA	1:B:147:GLN:H	1.87	0.87
1:A:153:LYS:HE3	3:A:2004:HOH:O	1.75	0.85
1:B:144:GLN:O	1:B:147:GLN:O	1.97	0.83
1:C:125:ASN:HA	1:C:132:GLN:HE21	1.47	0.79
1:B:145:GLY:HA2	1:B:147:GLN:H	1.48	0.77
1:C:77:GLY:HA3	1:D:83:LEU:O	1.84	0.77
1:C:146:TYR:N	1:C:146:TYR:HD1	1.82	0.77
1:B:145:GLY:HA3	1:B:147:GLN:N	2.00	0.77
1:B:123:GLN:HE21	1:B:132:GLN:CD	1.89	0.76
1:C:146:TYR:CD1	1:C:146:TYR:N	2.52	0.76
1:C:77:GLY:HA2	1:D:85:GLU:HG3	1.68	0.75
1:B:145:GLY:CA	1:B:147:GLN:N	2.51	0.72
1:C:78:ASP:HB3	1:D:85:GLU:OE2	1.92	0.70
1:B:134[B]:ARG:NH1	1:B:134[B]:ARG:HB3	2.09	0.68
1:A:85:GLU:OE2	1:B:78:ASP:HB2	1.96	0.66
1:C:117:LEU:HD12	1:C:117:LEU:C	2.16	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:LYS:NZ	3:C:2009:HOH:O	2.29	0.65
1:C:77:GLY:N	1:D:85:GLU:H	1.95	0.64
1:A:125:ASN:HA	1:A:132:GLN:HE21	1.63	0.64
1:C:125:ASN:HA	1:C:132:GLN:NE2	2.12	0.63
1:A:123:GLN:HE21	1:A:132:GLN:CD	2.01	0.63
1:A:111:ASP:HB2	3:A:2018:HOH:O	1.98	0.63
1:A:85:GLU:H	1:B:77:GLY:N	1.98	0.62
1:D:140:SER:OG	1:D:142:LYS:HE2	2.00	0.61
1:B:121:TRP:CE3	1:B:134[B]:ARG:HG3	2.36	0.61
1:A:147:GLN:OE1	1:A:147:GLN:HA	2.00	0.61
1:D:77:GLY:HA3	1:D:170:MET:CB	2.31	0.60
1:D:153:LYS:HE3	3:D:2002:HOH:O	2.01	0.60
1:D:146:TYR:O	1:D:147:GLN:OE1	2.20	0.60
1:A:145:GLY:HA3	1:A:146:TYR:CD2	2.37	0.59
1:A:151[B]:THR:HG23	3:A:2039:HOH:O	2.02	0.59
1:B:125:ASN:HA	1:B:132:GLN:HE21	1.68	0.59
1:C:146:TYR:HB2	1:C:147:GLN:OE1	2.03	0.58
1:D:123:GLN:HE21	1:D:132:GLN:CD	2.05	0.58
1:C:85:GLU:HA	1:C:147:GLN:HE21	1.69	0.58
1:A:77:GLY:HA2	1:A:171:GLN:CA	2.34	0.57
1:A:77:GLY:N	1:B:85:GLU:H	2.02	0.57
1:A:77:GLY:HA3	1:A:170:MET:CB	2.34	0.57
1:A:78:ASP:CB	1:B:85:GLU:OE2	2.47	0.56
1:A:145:GLY:HA3	1:A:146:TYR:HD2	1.68	0.56
1:B:125:ASN:HA	1:B:132:GLN:NE2	2.22	0.55
1:A:85:GLU:OE2	1:B:78:ASP:CB	2.55	0.54
1:D:123:GLN:HE21	1:D:132:GLN:CG	2.19	0.54
1:C:138:GLN:HG3	3:C:2012:HOH:O	2.07	0.54
1:D:123:GLN:HE21	1:D:132:GLN:HG2	1.72	0.54
1:A:172:ARG:HD2	1:B:186:ASP:OD2	2.09	0.53
1:D:77:GLY:HA2	1:D:171:GLN:CA	2.39	0.53
1:D:77:GLY:HA3	1:D:170:MET:HB3	1.89	0.52
1:B:123:GLN:HE21	1:B:132:GLN:CG	2.22	0.52
1:D:123:GLN:NE2	1:D:132:GLN:OE1	2.43	0.52
1:B:117:LEU:C	1:B:117:LEU:HD12	2.31	0.51
1:C:85:GLU:H	1:D:77:GLY:N	2.08	0.51
1:C:85:GLU:OE2	1:D:78:ASP:CB	2.55	0.51
1:A:123:GLN:NE2	1:A:132:GLN:OE1	2.44	0.51
1:A:145:GLY:CA	1:A:146:TYR:CD2	2.93	0.51
1:D:187:LYS:O	1:D:188:SER:HB2	2.11	0.50
1:A:77:GLY:HA3	1:A:170:MET:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:GLY:HA3	1:D:170:MET:HB2	1.94	0.50
1:C:78:ASP:CB	1:D:85:GLU:OE2	2.59	0.50
1:B:134[B]:ARG:NH1	1:B:134[B]:ARG:CB	2.74	0.50
1:B:134[B]:ARG:CB	1:B:134[B]:ARG:HH11	2.25	0.49
1:C:77:GLY:HA3	1:D:84:VAL:HA	1.95	0.49
1:D:77:GLY:HA2	1:D:171:GLN:N	2.28	0.49
1:C:103:LYS:CE	3:C:2009:HOH:O	2.60	0.48
1:D:136:ARG:HH11	1:D:156:ASN:ND2	2.12	0.48
1:C:78:ASP:HB2	3:C:2001:HOH:O	2.13	0.48
1:B:143:PRO:HA	1:B:148:GLN:HA	1.96	0.48
1:C:86:ASN:ND2	1:C:86:ASN:H	2.12	0.48
1:A:147:GLN:OE1	1:A:147:GLN:CA	2.62	0.48
1:C:166:ASP:O	1:C:170:MET:HG3	2.14	0.48
1:C:186:ASP:OD2	1:D:172:ARG:HD2	2.13	0.47
1:A:136:ARG:HH21	1:A:156:ASN:ND2	2.13	0.47
1:D:81:SER:OG	1:D:151[B]:THR:HG22	2.14	0.46
1:C:129:GLU:C	1:C:131:GLU:H	2.19	0.46
1:C:123:GLN:HE21	1:C:132:GLN:CD	2.19	0.46
1:C:103:LYS:HE3	3:C:2009:HOH:O	2.16	0.46
1:D:187:LYS:O	1:D:188:SER:CB	2.63	0.46
1:A:136:ARG:HH21	1:A:156:ASN:HD22	1.64	0.46
1:B:123:GLN:HE21	1:B:132:GLN:HG2	1.80	0.45
1:C:137:TYR:CE2	1:C:154:LEU:HD13	2.52	0.45
1:A:77:GLY:HA2	1:A:171:GLN:HA	1.99	0.45
1:D:136:ARG:HH11	1:D:156:ASN:HD22	1.66	0.44
1:A:81:SER:OG	1:A:151[B]:THR:HG22	2.17	0.44
1:D:117:LEU:C	1:D:117:LEU:HD12	2.39	0.43
3:A:2007:HOH:O	1:B:77:GLY:CA	2.42	0.43
1:B:147:GLN:HA	1:B:147:GLN:OE1	2.17	0.43
1:B:123:GLN:NE2	1:B:132:GLN:CD	2.66	0.43
1:A:77:GLY:HA2	1:A:171:GLN:N	2.33	0.43
1:B:134[B]:ARG:HB3	1:B:134[B]:ARG:CZ	2.49	0.42
1:D:77:GLY:HA2	1:D:171:GLN:HA	2.00	0.42
1:D:79:THR:CG2	1:D:151[A]:THR:HG23	2.49	0.42
1:A:140:SER:OG	1:A:151[B]:THR:OG1	2.38	0.42
1:B:136:ARG:HH11	1:B:156:ASN:ND2	2.18	0.41
1:C:148:GLN:NE2	3:C:2005:HOH:O	2.53	0.41
1:C:85:GLU:CA	1:C:147:GLN:HE21	2.33	0.41
1:B:142:LYS:HA	1:B:143:PRO:HD2	1.78	0.41
1:C:126:ARG:HD3	1:C:131:GLU:O	2.20	0.41
1:D:79:THR:HG23	1:D:151[A]:THR:CG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:THR:OG1	1:B:153:LYS:HG2	2.21	0.40
1:A:172:ARG:NH2	2:A:1189:SO4:O2	2.46	0.40

All (2) 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:146:TYR:OH	1:C:165:ALA:O[1_665]	2.08	0.12
1:B:187:LYS:NZ	1:C:187:LYS:NZ[1_554]	2.09	0.11

## 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	106/112 (95%)	100 (94%)	3 (3%)	3 (3%)	6	0
1	B	102/112 (91%)	97 (95%)	3 (3%)	2 (2%)	9	1
1	C	106/112 (95%)	100 (94%)	4 (4%)	2 (2%)	10	1
1	D	108/112 (96%)	104 (96%)	2 (2%)	2 (2%)	10	1
All	All	422/448 (94%)	401 (95%)	12 (3%)	9 (2%)	8	0

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	THR
1	B	91	THR
1	B	146	TYR
1	C	91	THR
1	D	91	THR
1	A	146	TYR
1	C	130	ASP

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Mol	Chain	Res	Type
1	A	78	ASP
1	D	78	ASP

### 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	95/95 (100%)	94 (99%)	1 (1%)	80	58
1	B	86/95 (90%)	81 (94%)	5 (6%)	25	3
1	C	91/95 (96%)	83 (91%)	8 (9%)	12	1
1	D	95/95 (100%)	87 (92%)	8 (8%)	14	1
All	All	367/380 (97%)	345 (94%)	22 (6%)	25	3

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	187	LYS
1	B	78	ASP
1	B	81	SER
1	B	83	LEU
1	B	126	ARG
1	B	187	LYS
1	C	78	ASP
1	C	86	ASN
1	C	109[A]	GLN
1	C	109[B]	GLN
1	C	126	ARG
1	C	140	SER
1	C	146	TYR
1	C	148	GLN
1	D	78	ASP
1	D	83	LEU
1	D	90	ASN
1	D	111	ASP
1	D	129	GLU

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Mol	Chain	Res	Type
1	D	142	LYS
1	D	147	GLN
1	D	187	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
1	A	132	GLN
1	A	156	ASN
1	B	115	GLN
1	B	123	GLN
1	B	132	GLN
1	B	156	ASN
1	C	86	ASN
1	C	123	GLN
1	C	132	GLN
1	C	148	GLN
1	C	156	ASN
1	D	115	GLN
1	D	123	GLN
1	D	132	GLN
1	D	144	GLN
1	D	156	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 carbohydrates in this entry.



## 5.6 Ligand geometry

6 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	1188	-	4,4,4	0.38	0	6,6,6	0.30	0
2	SO4	A	1189	-	4,4,4	0.50	0	6,6,6	0.27	0
2	SO4	A	1190	-	4,4,4	0.25	0	6,6,6	0.36	0
2	SO4	B	1189	-	4,4,4	0.22	0	6,6,6	0.29	0
2	SO4	C	1188	-	4,4,4	0.54	0	6,6,6	0.54	0
2	SO4	D	1189	-	4,4,4	0.20	0	6,6,6	0.12	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	1188	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1189	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1190	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1189	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1188	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1189	-	-	0/0/0/0	0/0/0/0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1189	SO4	1	0

## 5.7 Other polymers

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

### 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	108/112 (96%)	0.74	7 (6%) 22 22	5, 11, 27, 33	1 (0%)
1	B	107/112 (95%)	0.94	15 (14%) 4 3	6, 12, 28, 32	1 (0%)
1	C	109/112 (97%)	1.11	19 (17%) 2 2	5, 12, 29, 33	0
1	D	110/112 (98%)	0.70	10 (9%) 11 12	6, 12, 27, 33	0
All	All	434/448 (96%)	0.87	51 (11%) 6 6	5, 12, 28, 33	2 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	146	TYR	9.6
1	D	87	GLY	9.4
1	C	127	LEU	8.6
1	B	87	GLY	8.6
1	B	127	LEU	8.5
1	C	130	ASP	8.5
1	A	146	TYR	7.1
1	B	126	ARG	7.0
1	A	90	ASN	6.8
1	D	188	SER	5.8
1	C	126	ARG	5.4
1	D	90	ASN	5.0
1	B	90	ASN	4.8
1	C	128	ASP	4.6
1	B	146	TYR	4.2
1	B	91	THR	4.2
1	C	90	ASN	4.2
1	C	87	GLY	4.1
1	C	129	GLU	4.1
1	C	160	ALA	3.9
1	B	77	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	86	ASN	3.3
1	A	86	ASN	3.3
1	B	160	ALA	3.2
1	B	187	LYS	3.2
1	C	125	ASN	3.0
1	B	131	GLU	3.0
1	B	188	SER	2.9
1	C	131	GLU	2.8
1	D	85	GLU	2.8
1	C	77	GLY	2.7
1	B	125	ASN	2.7
1	A	145	GLY	2.6
1	B	147	GLN	2.6
1	C	91	THR	2.4
1	B	86	ASN	2.4
1	D	146	TYR	2.4
1	D	160	ALA	2.4
1	B	144	GLN	2.4
1	A	139	ILE	2.4
1	A	150	VAL	2.3
1	C	147	GLN	2.3
1	C	159	GLN	2.3
1	D	91	THR	2.3
1	C	139	ILE	2.3
1	D	147	GLN	2.2
1	A	160	ALA	2.2
1	C	132	GLN	2.2
1	C	145	GLY	2.1
1	C	187	LYS	2.1
1	D	83	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	C	1188	5/5	0.83	0.19	4.90	38,54,57,59	0
2	SO4	D	1189	5/5	0.94	0.10	0.50	78,78,78,78	0
2	SO4	B	1189	5/5	0.90	0.14	0.20	81,82,83,83	0
2	SO4	A	1188	5/5	0.98	0.11	0.15	31,32,33,36	0
2	SO4	A	1189	5/5	0.97	0.10	-0.34	33,34,36,38	0
2	SO4	A	1190	5/5	0.96	0.13	-	52,55,57,58	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.