Full wwPDB X-ray Structure Validation Report (i)

Feb 17, 2024 – 10:40 PM EST

PDB ID	:	4BLM
Title	:	BETA-LACTAMASE OF BACILLUS LICHENIFORMIS 749(SLASH)C. REFINEMENT AT 2 ANGSTROMS RESOLUTION AND ANALYSIS OF HYDRATION
Authors	:	Knox, J.R.; Moews, P.C.
Deposited on	:	1991-05-28
Resolution	:	2.00 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

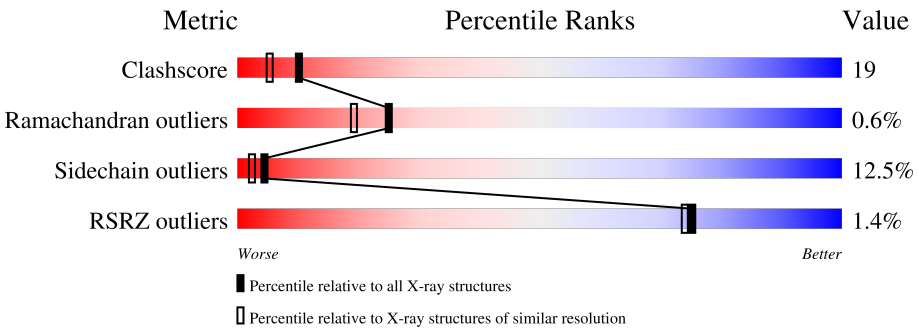
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 >=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 <=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	265	.% 64% 25% 6% • •
1	B	265	2% 62% 26% 7% • •

2 Entry composition (i)

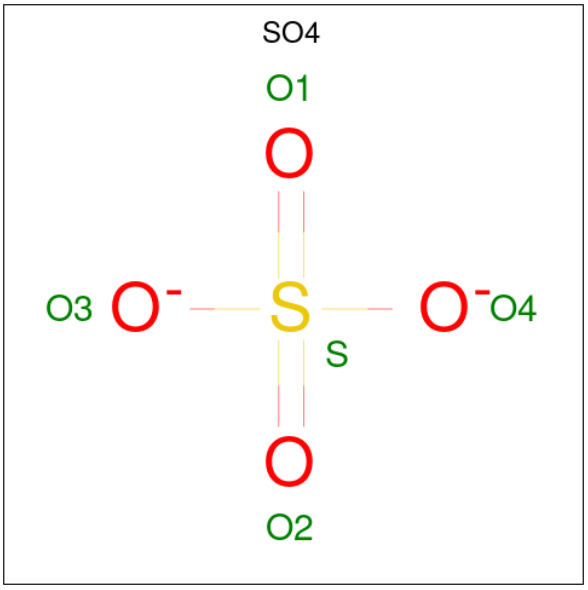
There are 3 unique types of molecules in this entry. The entry contains 4500 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BETA-LACTAMASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	256	2003	1256	346	398	3	0	0	0
1	B	256	2003	1256	346	398	3	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is water.

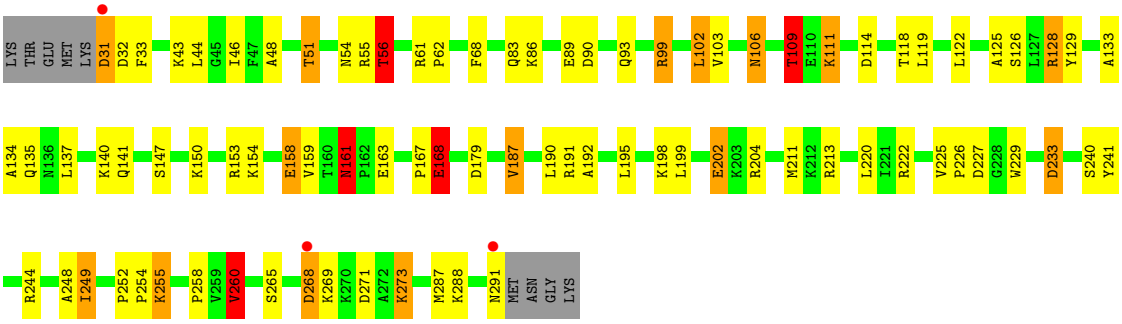
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	253	253	253	0	0
			Total	O		
3	B	231	231	231	0	0

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.

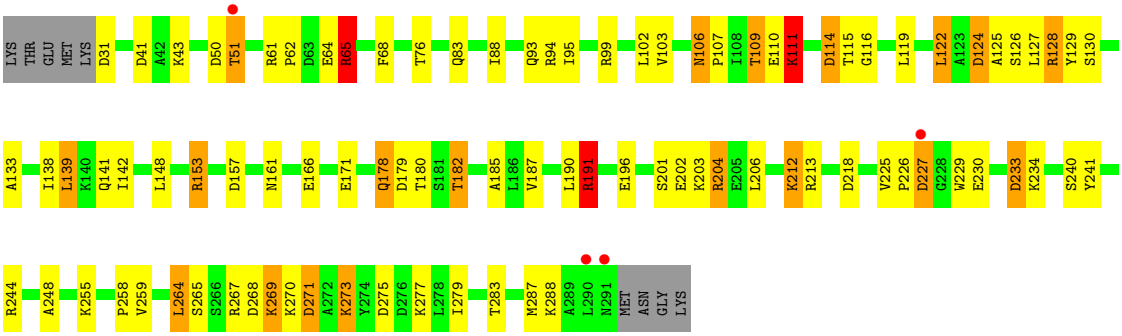
- Molecule 1: BETA-LACTAMASE

Chain A:



- Molecule 1: BETA-LACTAMASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.80Å 90.70Å 43.60Å 90.00° 104.50° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00 10.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.00) 89.3 (10.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.96 (at 2.01Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.161 , (Not available) 0.153 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	11.2	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 82.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4500	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.91% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.90	0/2033	1.65	34/2753 (1.2%)
1	B	0.87	0/2033	1.59	30/2753 (1.1%)
All	All	0.88	0/4066	1.62	64/5506 (1.2%)

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	B	0	2

There are no bond length outliers.

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	65	ARG	NE-CZ-NH1	-18.10	111.25	120.30
1	A	204	ARG	NE-CZ-NH2	-12.86	113.87	120.30
1	B	65	ARG	CD-NE-CZ	-11.48	107.53	123.60
1	A	222	ARG	NE-CZ-NH2	10.23	125.42	120.30
1	A	204	ARG	CD-NE-CZ	10.10	137.74	123.60
1	A	191	ARG	NE-CZ-NH1	-9.81	115.39	120.30
1	B	204	ARG	NE-CZ-NH1	9.78	125.19	120.30
1	B	128	ARG	NE-CZ-NH1	9.76	125.18	120.30
1	A	168	GLU	CA-CB-CG	9.75	134.85	113.40
1	A	114	ASP	CB-CG-OD1	9.48	126.84	118.30
1	A	191	ARG	NE-CZ-NH2	9.41	125.01	120.30
1	A	244	ARG	NE-CZ-NH1	9.11	124.85	120.30
1	A	233	ASP	CB-CG-OD2	8.29	125.76	118.30
1	A	56	THR	N-CA-CB	-8.06	94.98	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	182	THR	N-CA-CB	-7.86	95.37	110.30
1	B	65	ARG	NE-CZ-NH2	7.59	124.10	120.30
1	B	50	ASP	CB-CG-OD1	7.44	125.00	118.30
1	B	153	ARG	NE-CZ-NH2	-7.37	116.61	120.30
1	A	260	VAL	CB-CA-C	7.17	125.01	111.40
1	B	218	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	A	153	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	B	179	ASP	CB-CG-OD2	6.74	124.36	118.30
1	A	128	ARG	CD-NE-CZ	6.57	132.80	123.60
1	B	264	LEU	CA-CB-CG	6.46	130.17	115.30
1	A	158	GLU	OE1-CD-OE2	6.43	131.02	123.30
1	A	248	ALA	N-CA-CB	-6.32	101.25	110.10
1	B	233	ASP	CB-CG-OD1	-6.26	112.66	118.30
1	A	222	ARG	NE-CZ-NH1	-6.22	117.19	120.30
1	B	233	ASP	CB-CG-OD2	6.22	123.90	118.30
1	A	109	THR	N-CA-CB	-6.21	98.51	110.30
1	B	271	ASP	CB-CG-OD2	6.20	123.88	118.30
1	A	249	ILE	CB-CA-C	6.20	123.99	111.60
1	A	161	ASN	OD1-CG-ND2	6.07	135.85	121.90
1	B	124	ASP	CB-CG-OD2	6.05	123.74	118.30
1	A	168	GLU	CB-CG-CD	6.01	130.43	114.20
1	B	128	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	260	VAL	CA-CB-CG1	5.92	119.78	110.90
1	B	213	ARG	CD-NE-CZ	5.87	131.82	123.60
1	A	158	GLU	CB-CG-CD	-5.83	98.47	114.20
1	B	191	ARG	NE-CZ-NH1	-5.80	117.40	120.30
1	B	213	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	199	LEU	CA-CB-CG	5.66	128.32	115.30
1	B	182	THR	OG1-CB-CG2	5.62	122.93	110.00
1	B	83	GLN	CA-CB-CG	5.60	125.72	113.40
1	A	109	THR	OG1-CB-CG2	5.57	122.81	110.00
1	A	268	ASP	N-CA-CB	5.54	120.57	110.60
1	B	122	LEU	CA-CB-CG	5.53	128.02	115.30
1	A	202	GLU	CA-CB-CG	5.52	125.54	113.40
1	B	268	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	161	ASN	CA-CB-CG	-5.38	101.57	113.40
1	A	213	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	A	244	ARG	NH1-CZ-NH2	-5.30	113.56	119.40
1	A	199	LEU	CB-CG-CD1	5.30	120.01	111.00
1	A	153	ARG	CD-NE-CZ	5.29	131.01	123.60
1	B	65	ARG	CG-CD-NE	-5.28	100.71	111.80
1	B	111	LYS	CA-CB-CG	5.20	124.84	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	99	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	B	248	ALA	CB-CA-C	-5.17	102.34	110.10
1	B	259	VAL	CA-CB-CG1	5.09	118.54	110.90
1	A	161	ASN	N-CA-CB	-5.08	101.46	110.60
1	B	116	GLY	N-CA-C	-5.08	100.40	113.10
1	A	51	THR	OG1-CB-CG2	5.04	121.60	110.00
1	A	179	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	83	GLN	N-CA-CB	-5.02	101.57	110.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	244	ARG	Sidechain
1	B	65	ARG	Sidechain

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	2003	0	2016	63	0
1	B	2003	0	2016	88	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
3	A	253	0	0	24	0
3	B	231	0	0	36	1
All	All	4500	0	4032	152	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 19.

All (152) 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:269:LYS:NZ	1:A:271:ASP:HB2	1.64	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:THR:HG21	1:A:133:ALA:HB3	1.34	1.06
1:B:95:ILE:HD11	1:B:119:LEU:HG	1.39	1.05
1:A:106:ASN:HB3	1:A:109:THR:HG22	1.44	0.99
1:B:269:LYS:NZ	1:B:271:ASP:HB2	1.81	0.96
1:B:51:THR:HG23	1:B:258:PRO:O	1.66	0.96
1:B:109:THR:HG21	1:B:133:ALA:HB3	1.45	0.96
1:B:106:ASN:HB3	1:B:109:THR:HG22	1.50	0.93
1:A:269:LYS:HZ1	1:A:271:ASP:HB2	1.23	0.89
1:B:240:SER:HB2	3:B:1084:HOH:O	1.74	0.87
1:B:267:ARG:HD2	3:B:1044:HOH:O	1.73	0.87
1:B:128:ARG:N	3:B:1076:HOH:O	2.08	0.85
1:B:279:ILE:HG22	3:B:1006:HOH:O	1.79	0.83
1:A:122:LEU:HB2	3:A:1085:HOH:O	1.80	0.82
1:A:31:ASP:N	3:A:718:HOH:O	2.13	0.82
1:B:234:LYS:HE2	3:B:1021:HOH:O	1.80	0.82
1:A:106:ASN:HB3	1:A:109:THR:CG2	2.10	0.81
1:B:65:ARG:NH1	3:B:651:HOH:O	2.14	0.80
1:B:127:LEU:HA	3:B:1021:HOH:O	1.81	0.80
1:A:83:GLN:HG2	3:A:964:HOH:O	1.81	0.79
1:B:269:LYS:HZ1	1:B:271:ASP:HB2	1.47	0.78
1:A:93:GLN:NE2	3:A:807:HOH:O	2.14	0.77
1:A:269:LYS:HZ3	1:A:271:ASP:HB2	1.50	0.77
1:B:269:LYS:HZ2	1:B:271:ASP:HB2	1.50	0.77
1:A:129:TYR:N	3:A:996:HOH:O	2.03	0.75
1:B:51:THR:CG2	1:B:258:PRO:O	2.35	0.74
1:A:109:THR:HG21	1:A:133:ALA:CB	2.17	0.74
1:A:269:LYS:HE2	1:A:271:ASP:H	1.53	0.73
1:B:270:LYS:HG2	3:B:1084:HOH:O	1.90	0.71
1:A:126:SER:HB2	3:A:839:HOH:O	1.91	0.71
2:A:1:SO4:O2	3:A:749:HOH:O	2.08	0.70
1:A:126:SER:CB	3:A:839:HOH:O	2.39	0.70
1:B:124:ASP:O	3:B:1076:HOH:O	2.10	0.68
1:A:168:GLU:OE2	3:A:724:HOH:O	2.11	0.68
1:A:135:GLN:N	3:A:839:HOH:O	2.27	0.67
1:B:111:LYS:NZ	3:B:1056:HOH:O	2.29	0.66
1:B:106:ASN:HB3	1:B:109:THR:CG2	2.24	0.66
1:B:191:ARG:NH2	3:B:649:HOH:O	2.12	0.66
1:B:95:ILE:CD1	1:B:119:LEU:HG	2.19	0.66
1:A:54:ASN:ND2	3:A:914:HOH:O	2.27	0.65
1:A:125:ALA:O	3:A:996:HOH:O	2.14	0.65
1:B:65:ARG:CZ	3:B:651:HOH:O	2.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:LYS:HG3	3:A:1045:HOH:O	1.97	0.64
1:B:65:ARG:NH2	3:B:651:HOH:O	2.30	0.64
1:A:51:THR:OG1	1:A:258:PRO:O	2.12	0.64
1:B:43:LYS:HE3	1:B:64:GLU:HG2	1.81	0.63
1:A:106:ASN:CB	1:A:109:THR:HG22	2.25	0.62
1:B:65:ARG:NE	1:B:180:THR:OG1	2.29	0.62
1:B:161:ASN:ND2	3:B:1083:HOH:O	2.32	0.62
1:B:31:ASP:N	3:B:829:HOH:O	2.33	0.61
1:B:110:GLU:HG3	1:B:111:LYS:HD3	1.82	0.61
1:B:114:ASP:OD1	1:B:115:THR:HG23	2.01	0.61
1:A:128:ARG:N	3:A:996:HOH:O	2.34	0.60
1:B:191:ARG:NE	3:B:649:HOH:O	2.31	0.59
1:A:187:VAL:HB	1:A:260:VAL:HG22	1.84	0.59
1:B:124:ASP:OD1	3:B:668:HOH:O	2.17	0.59
1:A:287:MET:O	1:A:291:ASN:HB2	2.02	0.59
1:B:95:ILE:HD11	1:B:119:LEU:CG	2.25	0.59
1:B:212:LYS:HE2	3:B:693:HOH:O	2.02	0.58
1:B:283:THR:OG1	3:B:1006:HOH:O	2.17	0.58
1:B:204:ARG:HD3	3:B:917:HOH:O	2.03	0.58
1:A:254:PRO:HB2	1:A:255:LYS:HE2	1.86	0.58
1:B:109:THR:HG21	1:B:133:ALA:CB	2.28	0.57
1:B:114:ASP:OD1	1:B:114:ASP:C	2.43	0.57
1:A:161:ASN:HB2	3:A:727:HOH:O	2.04	0.57
1:B:102:LEU:CD2	1:B:109:THR:HG23	2.33	0.57
1:B:106:ASN:O	1:B:110:GLU:HG2	2.04	0.57
1:B:270:LYS:O	3:B:1084:HOH:O	2.17	0.57
1:B:61:ARG:N	1:B:62:PRO:CD	2.68	0.56
1:A:225:VAL:CG1	1:A:229:TRP:HB2	2.35	0.56
1:B:196:GLU:O	3:B:917:HOH:O	2.18	0.55
1:A:229:TRP:CH2	1:A:252:PRO:HB3	2.41	0.55
1:B:43:LYS:O	1:B:265:SER:HA	2.06	0.55
1:A:220:LEU:N	1:A:220:LEU:HD12	2.21	0.55
1:A:154:LYS:HD2	3:A:844:HOH:O	2.07	0.55
1:B:241:TYR:N	3:B:1084:HOH:O	2.36	0.54
1:B:94:ARG:NE	3:B:1055:HOH:O	2.38	0.54
1:A:161:ASN:CB	3:A:727:HOH:O	2.55	0.54
1:B:102:LEU:CD2	1:B:109:THR:CG2	2.86	0.54
1:B:102:LEU:HD21	1:B:109:THR:HG23	1.90	0.54
1:B:229:TRP:CD1	1:B:229:TRP:N	2.76	0.54
1:B:41:ASP:HB3	1:B:267:ARG:HH21	1.73	0.53
1:B:43:LYS:CE	1:B:64:GLU:HG2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:ALA:O	3:B:1076:HOH:O	2.19	0.53
1:A:83:GLN:NE2	3:A:873:HOH:O	2.41	0.53
1:A:269:LYS:CE	1:A:271:ASP:H	2.20	0.53
1:A:43:LYS:O	1:A:265:SER:HA	2.08	0.53
1:B:202:GLU:CD	1:B:202:GLU:H	2.11	0.52
1:B:270:LYS:HG2	3:B:887:HOH:O	2.10	0.52
1:B:212:LYS:HE3	1:B:230:GLU:OE2	2.08	0.52
1:B:225:VAL:CG1	1:B:229:TRP:HB2	2.41	0.51
1:B:88:ILE:HD12	1:B:206:LEU:HD11	1.92	0.51
1:A:61:ARG:N	1:A:62:PRO:CD	2.73	0.51
1:B:125:ALA:C	3:B:1076:HOH:O	2.49	0.51
1:A:192:ALA:HB1	1:A:198:LYS:HG2	1.94	0.50
1:B:119:LEU:HD21	1:B:141:GLN:HG3	1.94	0.50
1:B:234:LYS:CE	3:B:1021:HOH:O	2.48	0.49
1:B:61:ARG:HA	3:B:1069:HOH:O	2.13	0.49
1:B:227:ASP:HA	3:B:1059:HOH:O	2.12	0.49
1:A:241:TYR:HA	1:A:269:LYS:O	2.13	0.48
1:A:56:THR:HG21	3:A:868:HOH:O	2.14	0.48
1:B:114:ASP:OD1	1:B:115:THR:N	2.46	0.48
1:B:273:LYS:H	1:B:273:LYS:CD	2.27	0.48
1:B:273:LYS:H	1:B:273:LYS:CE	2.26	0.48
1:B:93:GLN:HG3	3:B:935:HOH:O	2.13	0.47
1:A:102:LEU:CD1	1:A:109:THR:HG23	2.44	0.47
1:B:61:ARG:N	1:B:62:PRO:HD3	2.30	0.47
1:A:33:PHE:CE1	1:A:46:ILE:HD13	2.50	0.47
1:A:102:LEU:HD11	1:A:109:THR:HG23	1.97	0.46
1:A:134:ALA:C	3:A:839:HOH:O	2.52	0.46
1:B:142:ILE:HD11	1:B:148:LEU:HB2	1.98	0.46
1:B:187:VAL:O	1:B:191:ARG:HB2	2.16	0.46
1:B:166:GLU:OE2	3:B:1023:HOH:O	2.20	0.46
1:A:111:LYS:HZ2	1:A:111:LYS:HG3	1.59	0.46
1:A:229:TRP:CZ3	1:A:252:PRO:HB3	2.51	0.46
1:A:252:PRO:HG2	1:A:255:LYS:O	2.15	0.46
1:A:89:GLU:H	1:A:89:GLU:CD	2.20	0.46
1:A:119:LEU:HD21	1:A:141:GLN:HG3	1.99	0.45
1:A:225:VAL:HG13	1:A:229:TRP:HB2	1.99	0.45
1:B:269:LYS:HZ1	1:B:271:ASP:CB	2.24	0.45
1:A:225:VAL:HA	1:A:226:PRO:HD3	1.84	0.44
1:B:88:ILE:HD11	1:B:203:LYS:HG2	1.99	0.44
1:A:255:LYS:H	1:A:255:LYS:HG2	1.57	0.43
1:B:126:SER:O	3:B:1021:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:ASP:OD1	1:B:277:LYS:HB2	2.17	0.43
1:A:273:LYS:H	1:A:273:LYS:CD	2.32	0.43
1:A:240:SER:O	1:A:241:TYR:HB2	2.19	0.43
1:A:119:LEU:HA	3:A:1085:HOH:O	2.19	0.43
1:B:178:GLN:CG	3:B:757:HOH:O	2.67	0.42
1:B:269:LYS:HD2	1:B:271:ASP:H	1.84	0.42
1:A:99:ARG:HA	1:A:102:LEU:HD22	2.00	0.42
1:B:65:ARG:HH11	1:B:65:ARG:HD2	1.28	0.42
1:A:55:ARG:NH1	3:A:797:HOH:O	2.50	0.42
1:B:283:THR:O	1:B:287:MET:HG2	2.20	0.42
1:B:129:TYR:N	3:B:1076:HOH:O	2.26	0.42
1:A:86:LYS:HB3	1:A:90:ASP:HB2	2.03	0.41
1:A:211:MET:HG2	3:A:639:HOH:O	2.20	0.41
1:B:161:ASN:HB2	3:B:1083:HOH:O	2.20	0.41
1:B:191:ARG:HH11	1:B:191:ARG:HD3	1.53	0.41
1:B:106:ASN:N	1:B:107:PRO:CD	2.84	0.41
1:B:139:LEU:HD23	1:B:139:LEU:HA	1.94	0.41
1:B:178:GLN:O	1:B:178:GLN:NE2	2.36	0.41
1:A:125:ALA:C	3:A:996:HOH:O	2.57	0.41
1:A:269:LYS:HZ1	1:A:271:ASP:CB	2.11	0.41
1:B:178:GLN:H	1:B:178:GLN:HG3	1.47	0.41
1:A:48:ALA:O	1:A:56:THR:HA	2.20	0.41
1:A:93:GLN:O	1:A:118:THR:HA	2.22	0.40
1:A:273:LYS:H	1:A:273:LYS:CE	2.33	0.40
1:B:76:THR:HG22	1:B:138:ILE:HG22	2.04	0.40
1:B:88:ILE:HD12	1:B:206:LEU:CD1	2.50	0.40
1:B:153:ARG:NH1	1:B:157:ASP:O	2.50	0.40
1:B:182:THR:OG1	1:B:185:ALA:CB	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)
3:B:674:HOH:O	3:B:859:HOH:O[1_556]	2.18	0.02

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	254/265 (96%)	248 (98%)	5 (2%)	1 (0%)	34	30
1	B	254/265 (96%)	245 (96%)	7 (3%)	2 (1%)	19	13
All	All	508/530 (96%)	493 (97%)	12 (2%)	3 (1%)	25	19

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	VAL
1	B	226	PRO
1	B	103	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	216/224 (96%)	185 (86%)	31 (14%)	3	1
1	B	216/224 (96%)	193 (89%)	23 (11%)	6	3
All	All	432/448 (96%)	378 (88%)	54 (12%)	4	2

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ASP
1	A	32	ASP
1	A	44	LEU

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Mol	Chain	Res	Type
1	A	56	THR
1	A	68	PHE
1	A	99	ARG
1	A	102	LEU
1	A	106	ASN
1	A	109	THR
1	A	111	LYS
1	A	137	LEU
1	A	147	SER
1	A	150	LYS
1	A	158	GLU
1	A	159	VAL
1	A	161	ASN
1	A	163	GLU
1	A	167	PRO
1	A	168	GLU
1	A	187	VAL
1	A	190	LEU
1	A	195	LEU
1	A	202	GLU
1	A	227	ASP
1	A	233	ASP
1	A	249	ILE
1	A	255	LYS
1	A	260	VAL
1	A	268	ASP
1	A	273	LYS
1	A	288	LYS
1	B	51	THR
1	B	65	ARG
1	B	68	PHE
1	B	106	ASN
1	B	109	THR
1	B	111	LYS
1	B	114	ASP
1	B	122	LEU
1	B	130	SER
1	B	139	LEU
1	B	171	GLU
1	B	178	GLN
1	B	190	LEU
1	B	191	ARG

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Mol	Chain	Res	Type
1	B	201	SER
1	B	212	LYS
1	B	227	ASP
1	B	233	ASP
1	B	255	LYS
1	B	264	LEU
1	B	269	LYS
1	B	273	LYS
1	B	288	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	83	GLN
1	A	161	ASN
1	A	170	ASN
1	B	92	ASN
1	B	214	ASN

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)

2 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	B	1	-	4,4,4	0.61	0	6,6,6	0.24	0
2	SO4	A	1	-	4,4,4	0.68	0	6,6,6	0.32	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	1	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, 95th 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^2)	Q<0.9
1	A	256/265 (96%)	-0.72	3 (1%)	79	78	2, 10, 27, 45	0
1	B	256/265 (96%)	-0.62	4 (1%)	72	70	3, 11, 34, 57	0
All	All	512/530 (96%)	-0.67	7 (1%)	75	74	2, 11, 30, 57	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	291	ASN	5.5
1	B	290	LEU	2.8
1	A	31	ASP	2.6
1	A	291	ASN	2.3
1	B	227	ASP	2.3
1	A	268	ASP	2.1
1	B	51	THR	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, 95th 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^2)	Q<0.9
2	SO4	B	1	5/5	0.95	0.14	52,52,54,54	2
2	SO4	A	1	5/5	0.98	0.09	31,33,35,35	3

6.5 Other polymers (i)

There are no such residues in this entry.