



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:37 PM GMT

PDB ID : 1K57  
Title : OXA 10 class D beta-lactamase at pH 6.0  
Authors : Golemi, D.; Maveyraud, L.; Vakulenko, S.; Samama, J.P.; Mobashery, S.  
Deposited on : 2001-10-10  
Resolution : 1.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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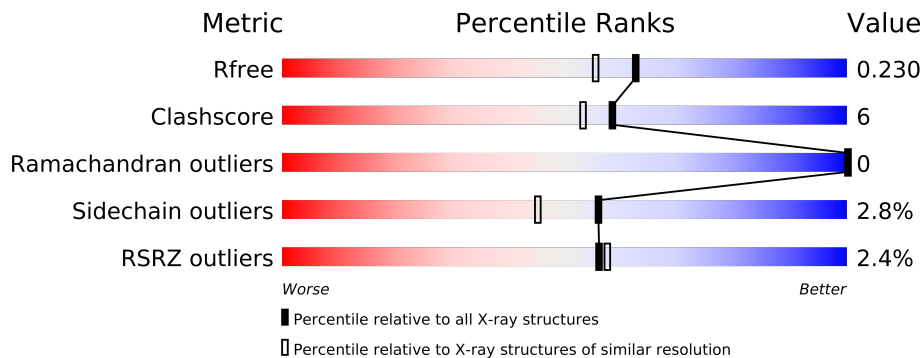
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.90 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))
$R_{free}$	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	246	
1	B	246	
2	C	246	
2	D	246	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	SO4	A	1002	-	X
3	SO4	A	1008	-	X
3	SO4	B	1006	-	X
3	SO4	B	1007	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	SO4	B	1011	-	X
3	SO4	C	1009	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8304 atoms, of which 0 are hydrogen and 0 are deuterium.

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 OXA-10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	1	0
			1936	1239	324	366	7			
1	B	245	Total	C	N	O	S	0	1	0
			1946	1244	326	369	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	70	KCX	LYS	MODIFIED RESIDUE	UNP P14489
B	70	KCX	LYS	MODIFIED RESIDUE	UNP P14489

- Molecule 2 is a protein called BETA LACTAMASE OXA-10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	241	Total	C	N	O	S	0	0	0
			1893	1214	314	359	6			
2	D	240	Total	C	N	O	S	0	1	0
			1888	1209	313	360	6			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	118	Total	O	0	0
			118	118		

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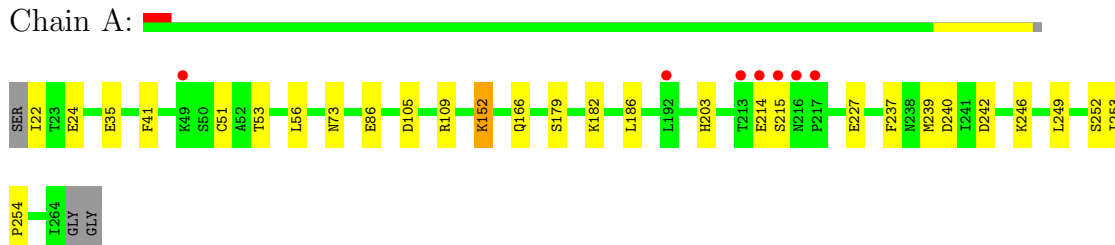
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	154	Total 154	O 154	0	0
4	C	127	Total 127	O 127	0	0
4	D	187	Total 187	O 187	0	0

### 3 Residue-property plots

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.

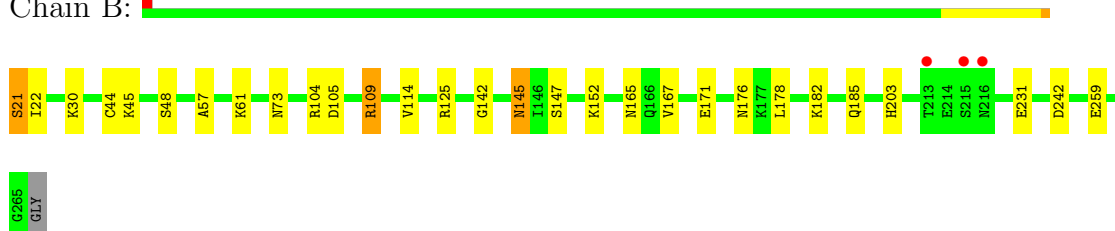
- Molecule 1: BETA LACTAMASE OXA-10

Chain A:



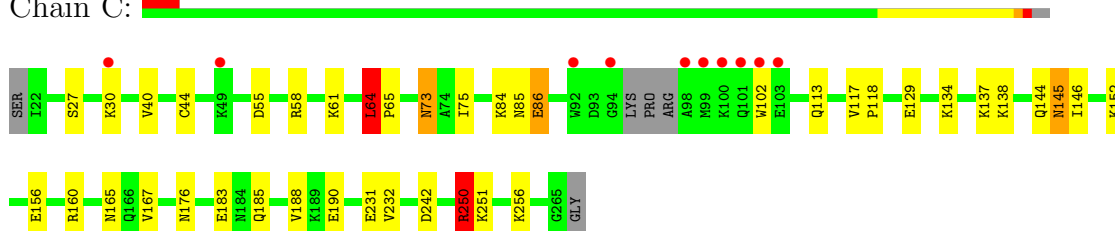
- Molecule 1: BETA LACTAMASE OXA-10

Chain B:



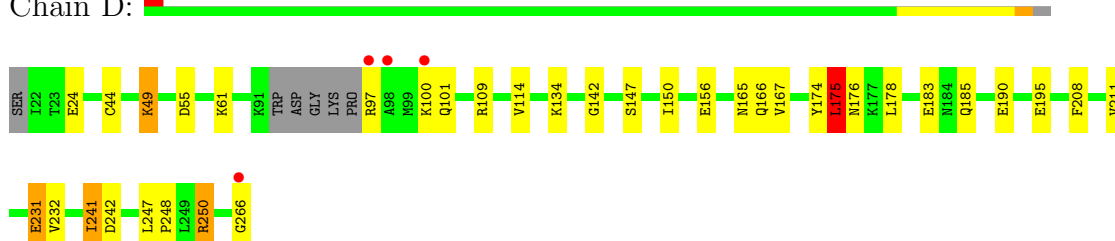
- Molecule 2: BETA LACTAMASE OXA-10

Chain C:



- Molecule 2: BETA LACTAMASE OXA-10

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.75Å 82.52Å 101.79Å 90.00° 95.50° 90.00°	Depositor
Resolution (Å)	33.77 – 1.90 33.77 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.6 (33.77-1.90) 97.6 (33.77-1.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 1.89Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.179 , 0.222 0.191 , 0.230	Depositor DCC
$R_{free}$ test set	1693 reflections (2.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.2	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 39.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 84561 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8304	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	1.00	2/1964 (0.1%)	0.95	4/2653 (0.2%)
1	B	1.11	2/1974 (0.1%)	0.96	5/2666 (0.2%)
2	C	1.08	2/1932 (0.1%)	1.05	8/2611 (0.3%)
2	D	1.13	5/1925 (0.3%)	0.98	4/2599 (0.2%)
All	All	1.08	11/7795 (0.1%)	0.99	21/10529 (0.2%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	250	ARG	CG-CD	-7.40	1.33	1.51
2	D	231	GLU	CD-OE1	6.44	1.32	1.25
1	A	239	MET	SD-CE	-6.33	1.42	1.77
2	C	86	GLU	CD-OE1	6.30	1.32	1.25
2	C	256	LYS	CD-CE	5.99	1.66	1.51
2	D	24	GLU	CD-OE1	5.66	1.31	1.25
2	D	114	VAL	CB-CG2	-5.63	1.41	1.52
1	A	86	GLU	CD-OE2	5.41	1.31	1.25
1	B	259	GLU	CD-OE2	5.29	1.31	1.25
1	B	114	VAL	CB-CG2	-5.21	1.42	1.52
2	D	147	SER	CB-OG	-5.16	1.35	1.42

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	250	ARG	NE-CZ-NH2	-13.20	113.70	120.30
2	C	250	ARG	NE-CZ-NH1	13.10	126.85	120.30
2	C	55	ASP	CB-CG-OD2	8.30	125.77	118.30
2	D	175	LEU	CB-CG-CD1	8.01	124.62	111.00
1	B	242	ASP	CB-CG-OD2	7.85	125.36	118.30
1	A	242	ASP	CB-CG-OD2	7.56	125.11	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	ASP	CB-CG-OD2	7.17	124.75	118.30
2	C	242	ASP	CB-CG-OD2	6.79	124.41	118.30
2	D	242	ASP	CB-CG-OD2	5.94	123.64	118.30
2	D	55	ASP	CB-CG-OD2	5.79	123.51	118.30
2	D	109	ARG	NE-CZ-NH1	5.77	123.19	120.30
2	C	250	ARG	CD-NE-CZ	5.71	131.59	123.60
2	C	256	LYS	CD-CE-NZ	5.70	124.81	111.70
1	B	109	ARG	NE-CZ-NH2	-5.57	117.52	120.30
2	C	64	LEU	CB-CG-CD1	5.50	120.34	111.00
1	A	109	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	B	125	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	B	104	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	A	240	ASP	CB-CG-OD1	5.38	123.14	118.30
1	B	105	ASP	CB-CG-OD2	5.24	123.02	118.30
2	C	64	LEU	CA-CB-CG	5.08	126.98	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1936	0	1928	15	0
1	B	1946	0	1936	27	0
2	C	1893	0	1878	29	0
2	D	1888	0	1878	32	0
3	A	15	0	0	0	0
3	B	20	0	0	0	0
3	C	10	0	0	1	0
3	D	10	0	0	0	0
4	A	118	0	0	3	0
4	B	154	0	0	5	0
4	C	127	0	0	1	0
4	D	187	0	0	6	0
All	All	8304	0	7620	95	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (95) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:195:GLU:HG3	4:D:1196:HOH:O	1.54	1.06
1:B:182:LYS:HD3	2:D:183:GLU:OE2	1.64	0.98
2:C:84:LYS:HD3	2:C:85:ASN:ND2	1.86	0.89
2:C:134:LYS:HE2	2:C:138:LYS:HE3	1.56	0.85
1:B:22:ILE:N	4:B:1159:HOH:O	2.12	0.82
1:B:21:SER:C	4:B:1159:HOH:O	2.19	0.81
1:B:182:LYS:HD3	2:D:183:GLU:CD	2.01	0.81
2:C:84:LYS:HD3	2:C:85:ASN:HD22	1.47	0.77
2:D:211:VAL:HA	2:D:241[A]:ILE:CD1	2.13	0.77
1:B:182:LYS:CD	2:D:183:GLU:OE2	2.40	0.70
2:C:64:LEU:HD13	2:C:160:ARG:NH2	2.07	0.70
1:B:30:LYS:N	1:B:30:LYS:HD3	2.09	0.66
2:D:266:GLY:HA2	4:D:1170:HOH:O	1.95	0.66
1:B:203:HIS:HD2	4:B:1091:HOH:O	1.80	0.64
2:D:211:VAL:HG22	2:D:241[A]:ILE:HD11	1.78	0.64
1:B:21:SER:HB3	4:B:1121:HOH:O	1.98	0.64
1:B:30:LYS:N	1:B:30:LYS:CD	2.60	0.64
1:A:246:LYS:HE2	4:A:1100:HOH:O	1.99	0.61
1:A:203:HIS:HD2	4:A:1019:HOH:O	1.82	0.61
2:C:134:LYS:CE	2:C:138:LYS:HE3	2.28	0.59
2:D:61:LYS:HE2	4:D:1182:HOH:O	2.03	0.59
2:D:100:LYS:N	2:D:101:GLN:OE1	2.36	0.59
2:D:211:VAL:HA	2:D:241[A]:ILE:HD12	1.83	0.59
2:C:84:LYS:CD	2:C:85:ASN:HD22	2.15	0.58
2:C:250:ARG:NH2	3:C:1004:SO4:O2	2.36	0.58
2:D:101:GLN:CD	2:D:101:GLN:H	2.07	0.58
2:D:208:PHE:HE1	2:D:241[A]:ILE:HG21	1.67	0.57
2:D:49:LYS:HA	2:D:49:LYS:HE2	1.86	0.57
1:B:145:ASN:HD22	1:B:147:SER:H	1.52	0.56
2:C:129:GLU:HG3	2:C:146:ILE:HD11	1.90	0.54
2:C:27:SER:O	2:C:30:LYS:HG2	2.07	0.54
2:D:247:LEU:N	2:D:248:PRO:CD	2.71	0.54
2:C:145:ASN:C	2:C:145:ASN:HD22	2.11	0.53
1:A:186:LEU:HD21	2:C:86:GLU:OE2	2.07	0.53
2:D:241[A]:ILE:HD13	2:D:241[A]:ILE:C	2.30	0.52
2:D:44:CYS:SG	2:D:167:VAL:HG11	2.51	0.51
2:C:61:LYS:HD3	4:C:1134:HOH:O	2.11	0.50
2:C:44:CYS:SG	2:C:167:VAL:HG11	2.51	0.50
2:D:97:ARG:N	4:D:1191:HOH:O	2.44	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:134:LYS:HE2	2:C:138:LYS:CE	2.35	0.49
2:C:250:ARG:HG2	2:C:251:LYS:N	2.25	0.49
2:C:176:ASN:HA	2:C:185:GLN:NE2	2.27	0.49
2:D:150:ILE:HG13	2:D:150:ILE:O	2.11	0.49
1:A:203:HIS:HE1	2:C:190:GLU:OE1	1.95	0.49
2:D:97:ARG:CB	4:D:1139:HOH:O	2.61	0.49
2:D:208:PHE:CE1	2:D:241[A]:ILE:HG21	2.46	0.49
1:B:145:ASN:HD22	1:B:145:ASN:C	2.16	0.49
1:B:145:ASN:ND2	1:B:147:SER:H	2.11	0.49
2:D:178:LEU:H	2:D:185:GLN:HE22	1.60	0.48
1:B:182:LYS:CE	2:D:183:GLU:OE2	2.62	0.48
1:A:182:LYS:HE2	2:C:183:GLU:HG3	1.96	0.48
2:D:100:LYS:HA	2:D:100:LYS:HD2	1.62	0.47
2:C:64:LEU:HD13	2:C:160:ARG:HH21	1.79	0.47
2:C:117:VAL:N	2:C:118:PRO:CD	2.78	0.47
2:C:137:LYS:HA	2:C:144:GLN:NE2	2.30	0.47
2:D:174:TYR:HD2	2:D:175:LEU:HD13	1.80	0.46
1:A:227:GLU:OE1	4:A:1124:HOH:O	2.21	0.46
1:B:21:SER:N	4:B:1159:HOH:O	2.49	0.46
1:A:22:ILE:HD11	1:A:53:THR:CG2	2.46	0.46
1:A:237:PHE:CD1	1:A:237:PHE:C	2.89	0.46
1:B:176:ASN:ND2	1:B:182:LYS:HE3	2.32	0.45
1:B:48:SER:OG	1:B:171:GLU:OE1	2.18	0.45
2:D:174:TYR:CD2	2:D:175:LEU:HD13	2.52	0.45
1:A:152:LYS:HB3	1:A:152:LYS:HE3	1.68	0.45
1:A:249:LEU:HA	1:A:252:SER:OG	2.17	0.44
1:B:142:GLY:H	1:B:165:ASN:HD21	1.64	0.44
2:C:40:VAL:HB	2:C:58:ARG:HD3	2.00	0.44
1:B:44:CYS:SG	1:B:167:VAL:HG11	2.58	0.44
1:B:22:ILE:O	1:B:22:ILE:HG23	2.17	0.43
1:A:41:PHE:HD2	1:A:237:PHE:HB2	1.83	0.43
2:C:134:LYS:CD	2:C:138:LYS:HE3	2.49	0.43
1:A:253:ILE:HB	1:A:254:PRO:HD3	2.00	0.42
1:B:45:LYS:HE3	1:B:231:GLU:HG2	2.01	0.42
1:B:176:ASN:HA	1:B:185:GLN:NE2	2.34	0.42
2:C:113:GLN:HB3	2:C:113:GLN:HE21	1.65	0.42
1:A:22:ILE:HA	1:A:51:CYS:O	2.19	0.42
1:B:203:HIS:HE1	2:D:190:GLU:OE1	2.02	0.42
1:A:35:GLU:HG3	1:A:249:LEU:HD22	2.02	0.42
1:B:57:ALA:O	1:B:61:LYS:HG3	2.20	0.42
1:B:178:LEU:H	1:B:185:GLN:HE22	1.66	0.42
1:A:24:GLU:HB2	1:A:56:LEU:HG	2.00	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:152:LYS:HB3	1:B:152:LYS:HE2	1.73	0.41
1:B:30:LYS:HD3	1:B:30:LYS:H	1.82	0.41
1:B:109:ARG:HH21	1:B:109:ARG:HD2	1.59	0.41
2:C:75:ILE:HG12	2:C:188:VAL:HG21	2.01	0.41
2:D:231:GLU:HG3	2:D:232:VAL:N	2.35	0.41
2:D:142:GLY:H	2:D:165:ASN:ND2	2.19	0.41
2:C:73:ASN:HD22	2:C:73:ASN:HA	1.68	0.41
2:D:241[A]:ILE:HD13	2:D:241[A]:ILE:O	2.21	0.41
2:C:84:LYS:O	2:C:84:LYS:HG2	2.20	0.40
2:C:231:GLU:HG3	2:C:232:VAL:N	2.36	0.40
2:D:176:ASN:HA	2:D:185:GLN:NE2	2.36	0.40
2:D:211:VAL:HA	2:D:241[A]:ILE:HD13	1.99	0.40
2:D:156:GLU:OE1	4:D:1151:HOH:O	2.21	0.40
2:C:102:TRP:CD1	2:C:102:TRP:N	2.88	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	241/246 (98%)	234 (97%)	7 (3%)	0	100	100
1	B	243/246 (99%)	238 (98%)	5 (2%)	0	100	100
2	C	237/246 (96%)	231 (98%)	6 (2%)	0	100	100
2	D	237/246 (96%)	231 (98%)	6 (2%)	0	100	100
All	All	958/984 (97%)	934 (98%)	24 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	203 (97%)	6 (3%)	55	44
1	B	210/209 (100%)	207 (99%)	3 (1%)	78	75
2	C	204/210 (97%)	196 (96%)	8 (4%)	43	30
2	D	204/210 (97%)	197 (97%)	7 (3%)	49	36
All	All	827/838 (99%)	803 (97%)	24 (3%)	56	44

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	ASN
1	A	152	LYS
1	A	166	GLN
1	A	179	SER
1	A	214	GLU
1	A	215	SER
1	B	21	SER
1	B	73	ASN
1	B	145	ASN
2	C	64	LEU
2	C	65	PRO
2	C	73	ASN
2	C	145	ASN
2	C	152	LYS
2	C	156	GLU
2	C	165	ASN
2	C	250	ARG
2	D	49	LYS
2	D	134	LYS
2	D	166	GLN
2	D	175	LEU
2	D	241[A]	ILE
2	D	241[B]	ILE
2	D	250	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	ASN

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Mol	Chain	Res	Type
1	A	165	ASN
1	A	166	GLN
1	A	203	HIS
1	B	73	ASN
1	B	122	GLN
1	B	145	ASN
1	B	165	ASN
1	B	185	GLN
1	B	203	HIS
2	C	73	ASN
2	C	113	GLN
2	C	121	GLN
2	C	144	GLN
2	C	145	ASN
2	C	185	GLN
2	D	113	GLN
2	D	121	GLN
2	D	165	ASN
2	D	166	GLN
2	D	185	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	KCX	A	70	1	11,11,12	6.32	4 (36%)	10,12,14	2.18	4 (40%)
1	KCX	B	70	1	11,11,12	5.81	2 (18%)	10,12,14	3.42	4 (40%)

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
1	KCX	A	70	1	-	0/8/10/12	0/0/0/0
1	KCX	B	70	1	-	0/8/10/12	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	70	KCX	O-C	19.76	1.25	1.11
1	B	70	KCX	O-C	18.07	1.23	1.11
1	B	70	KCX	CX-NZ	5.75	1.38	1.32
1	A	70	KCX	CX-NZ	4.65	1.37	1.32
1	A	70	KCX	CB-CA	3.38	1.56	1.53
1	A	70	KCX	CA-C	2.25	1.52	1.48

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	70	KCX	OQ2-CX-NZ	7.25	125.35	116.33
1	B	70	KCX	OQ2-CX-OQ1	-7.11	113.30	122.17
1	A	70	KCX	OQ2-CX-NZ	3.79	121.05	116.33
1	A	70	KCX	C-CA-N	-3.51	110.32	113.83
1	A	70	KCX	OQ2-CX-OQ1	-3.51	117.79	122.17
1	B	70	KCX	CE-NZ-CX	2.36	126.30	121.99
1	A	70	KCX	OQ1-CX-NZ	-2.28	121.15	124.94
1	B	70	KCX	OQ1-CX-NZ	-2.17	121.32	124.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

11 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	$\# Z  > 2$
3	SO4	A	1001	-	4,4,4	0.85	0	6,6,6	0.27	0
3	SO4	A	1002	-	4,4,4	0.28	0	6,6,6	1.27	1 (16%)
3	SO4	A	1008	-	4,4,4	0.28	0	6,6,6	1.04	1 (16%)
3	SO4	B	1003	-	4,4,4	1.11	0	6,6,6	1.15	1 (16%)
3	SO4	B	1006	-	4,4,4	0.48	0	6,6,6	0.85	0
3	SO4	B	1007	-	4,4,4	0.16	0	6,6,6	0.38	0
3	SO4	B	1011	-	4,4,4	0.22	0	6,6,6	1.10	0
3	SO4	C	1004	-	4,4,4	0.28	0	6,6,6	0.36	0
3	SO4	C	1009	-	4,4,4	0.38	0	6,6,6	0.24	0
3	SO4	D	1005	-	4,4,4	0.25	0	6,6,6	0.66	0
3	SO4	D	1010	-	4,4,4	0.71	0	6,6,6	0.78	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
3	SO4	A	1001	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1002	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1008	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1003	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1006	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1007	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1011	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1004	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1009	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1005	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1010	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	SO4	O2-S-O1	-3.03	99.51	109.53
3	B	1003	SO4	O2-S-O1	-2.41	101.56	109.53
3	A	1008	SO4	O2-S-O1	2.22	116.88	109.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	243/246 (98%)	0.06	7 (2%) 49 50	14, 23, 39, 52	0
1	B	245/246 (99%)	-0.03	3 (1%) 75 78	11, 19, 30, 40	0
2	C	241/246 (97%)	-0.00	10 (4%) 35 36	13, 22, 39, 51	0
2	D	240/246 (97%)	-0.11	4 (1%) 67 69	9, 18, 33, 45	0
All	All	969/984 (98%)	-0.02	24 (2%) 56 56	9, 20, 37, 52	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	216	ASN	4.2
2	C	49	LYS	3.3
1	A	214	GLU	3.3
2	C	101	GLN	3.2
2	C	99	MET	3.0
2	C	92	TRP	2.9
1	B	215	SER	2.8
2	C	30	LYS	2.8
2	C	100	LYS	2.8
1	A	215	SER	2.7
1	B	216	ASN	2.7
2	D	266	GLY	2.7
2	C	98	ALA	2.6
1	A	213	THR	2.4
2	D	98	ALA	2.4
2	C	94	GLY	2.3
1	A	217	PRO	2.3
1	A	192	LEU	2.3
1	A	49	LYS	2.2
2	C	103	GLU	2.2
2	C	102	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	100	LYS	2.1
1	B	213	THR	2.1
2	D	97	ARG	2.0

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

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	KCX	B	70	12/13	0.14	0.96	10,12,24,26	0
1	KCX	A	70	12/13	0.11	0.19	13,15,25,27	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	B	1007	5/5	0.33	25.53	61,64,65,65	0
3	SO4	A	1002	5/5	0.22	8.36	35,40,42,46	0
3	SO4	B	1006	5/5	0.18	3.15	42,42,48,49	0
3	SO4	A	1008	5/5	0.22	2.99	40,40,41,41	0
3	SO4	C	1009	5/5	0.20	2.70	30,33,33,35	0
3	SO4	B	1011	5/5	0.20	2.14	29,34,35,36	0
3	SO4	C	1004	5/5	0.13	1.78	38,39,43,45	0
3	SO4	D	1005	5/5	0.11	1.34	30,31,34,41	0
3	SO4	D	1010	5/5	0.12	0.32	24,25,25,26	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	B	1003	5/5	0.09	-0.80	25,29,32,33	0
3	SO4	A	1001	5/5	0.07	-1.12	26,30,30,33	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.