



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:31 PM GMT

PDB ID : 1B7B  
Title : Carbamate kinase from *Enterococcus faecalis*  
Authors : Marina, A.; Alzari, P.M.; Bravo, J.; Uriarte, M.; Barcelona, B.; Fita, I.; Rubio, V.  
Deposited on : 1999-01-20  
Resolution : 2.80 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

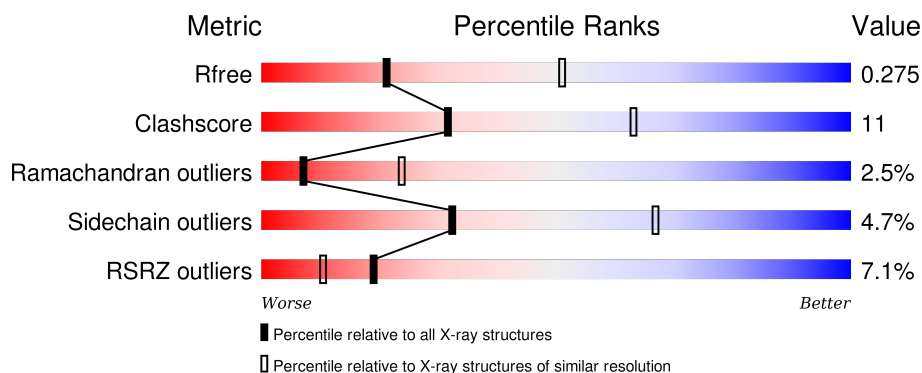
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	310	<div> <div>4%</div> <div>75%</div> <div>21%</div> <div>..</div> </div>
1	B	310	<div> <div>12%</div> <div>74%</div> <div>22%</div> <div>..</div> </div>
1	C	310	<div> <div>3%</div> <div>76%</div> <div>19%</div> <div>..</div> </div>
1	D	310	<div> <div>10%</div> <div>73%</div> <div>23%</div> <div>..</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9512 atoms, of which 280 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 CARBAMATE KINASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	307	Total	C	H	N	O	S	0	0	0
			2356	1441	70	387	449	9			
1	B	307	Total	C	H	N	O	S	0	0	0
			2356	1441	70	387	449	9			
1	C	307	Total	C	H	N	O	S	0	0	0
			2356	1441	70	387	449	9			
1	D	307	Total	C	H	N	O	S	0	0	0
			2356	1441	70	387	449	9			

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



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		

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

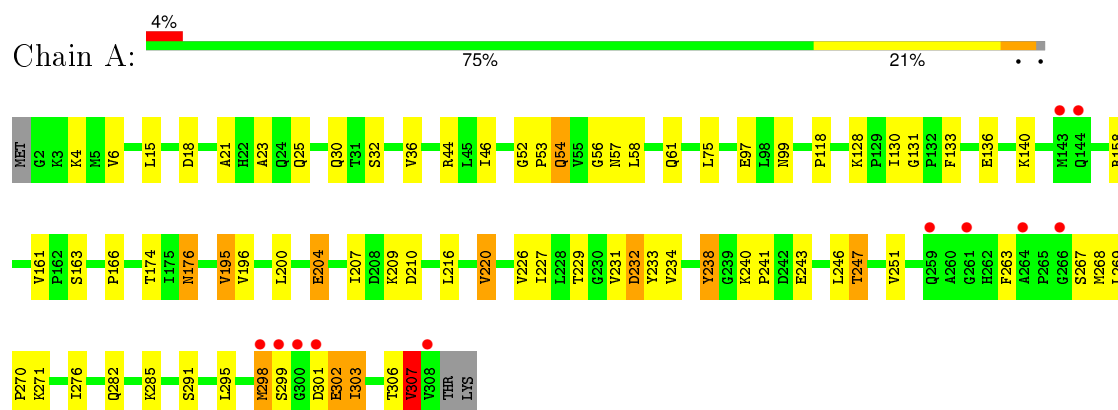
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	0
			16	16		
3	B	17	Total	O	0	0
			17	17		
3	C	18	Total	O	0	0
			18	18		
3	D	17	Total	O	0	0
			17	17		

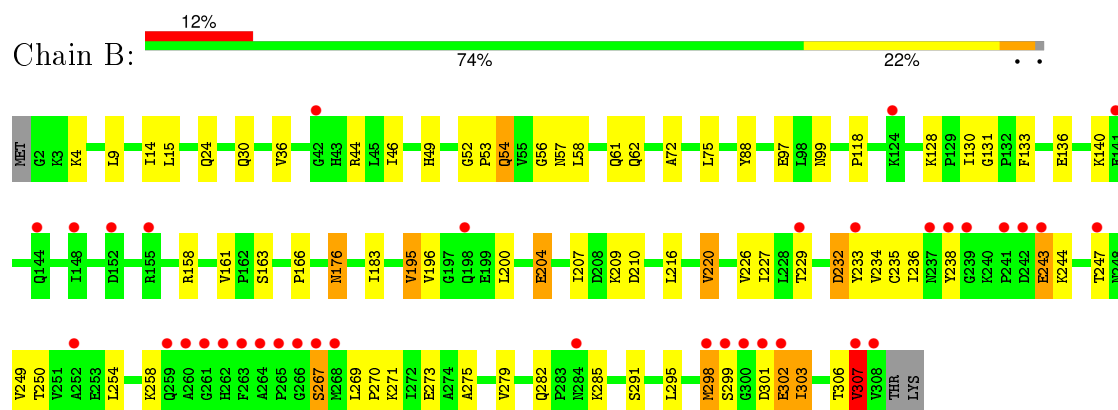
### 3 Residue-property plots

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.

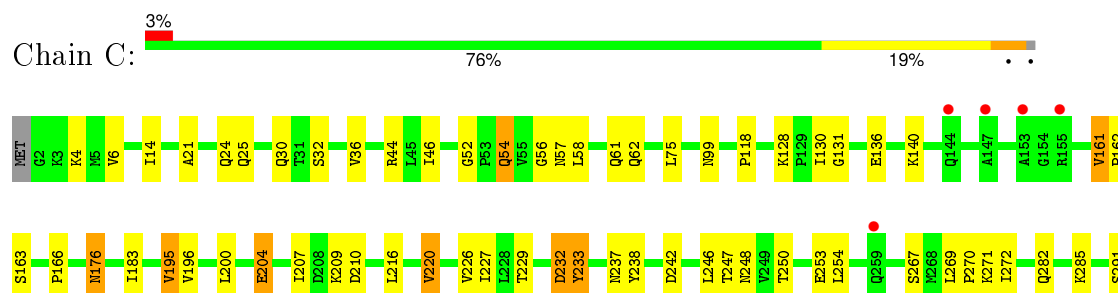
#### • Molecule 1: CARBAMATE KINASE

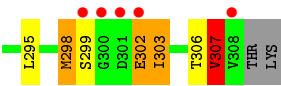


#### • Molecule 1: CARBAMATE KINASE

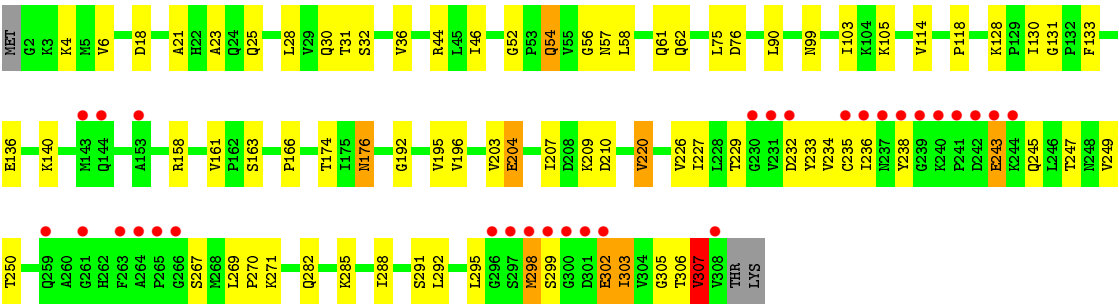


#### • Molecule 1: CARBAMATE KINASE





● Molecule 1: CARBAMATE KINASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.86Å 172.92Å 98.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 14.91 – 2.80	Depositor EDS
% Data completeness (in resolution range)	89.5 (15.00-2.80) 82.0 (14.91-2.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.224 , 0.283 0.222 , 0.275	Depositor DCC
$R_{free}$ test set	2893 reflections (10.20%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.6	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 50.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>1</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 28366 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	9512	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.17 % 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 1.9298e-03.*

<sup>1</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	0.30	0/2321	0.57	0/3151
1	B	0.30	0/2321	0.57	0/3151
1	C	0.30	0/2321	0.58	0/3151
1	D	0.30	0/2321	0.57	0/3151
All	All	0.30	0/9284	0.57	0/12604

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	2286	70	2317	51	0
1	B	2286	70	2317	52	0
1	C	2286	70	2317	43	0
1	D	2286	70	2317	54	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	17	0	0	0	0
3	C	18	0	0	0	0
3	D	17	0	0	0	0
All	All	9232	280	9268	198	0

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 11.

All (198) 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:B:232:ASP:HB2	1:B:302:GLU:HG3	1.50	0.91
1:C:232:ASP:HB2	1:C:302:GLU:HG3	1.69	0.74
1:C:75:LEU:HB3	1:C:204:GLU:HG3	1.70	0.74
1:A:75:LEU:HB3	1:A:204:GLU:HG3	1.70	0.73
1:B:235:CYS:SG	1:B:243:GLU:HG3	2.29	0.73
1:D:75:LEU:HB3	1:D:204:GLU:HG3	1.73	0.70
1:A:234:VAL:HG23	1:A:303:ILE:HG13	1.74	0.70
1:B:234:VAL:HG23	1:B:303:ILE:HG13	1.73	0.70
1:A:246:LEU:HB2	1:A:303:ILE:HD12	1.74	0.69
1:B:75:LEU:HB3	1:B:204:GLU:HG3	1.75	0.68
1:D:269:LEU:HB3	1:D:270:PRO:HD3	1.77	0.67
1:B:234:VAL:H	1:B:303:ILE:HD11	1.61	0.64
1:A:128:LYS:HB2	1:A:163:SER:OG	1.97	0.64
1:C:269:LEU:HB3	1:C:270:PRO:HD3	1.79	0.64
1:B:269:LEU:HB3	1:B:270:PRO:HD3	1.80	0.64
1:D:128:LYS:HB2	1:D:163:SER:OG	1.98	0.64
1:A:75:LEU:CB	1:A:204:GLU:HG3	2.28	0.63
1:C:128:LYS:HB2	1:C:163:SER:OG	1.99	0.63
1:A:233:TYR:CD1	1:A:302:GLU:HB3	2.34	0.62
1:A:269:LEU:HB3	1:A:270:PRO:HD3	1.79	0.62
1:A:267:SER:O	1:A:270:PRO:HD2	1.99	0.61
1:B:249:VAL:HG21	1:B:254:LEU:HD21	1.82	0.61
1:B:128:LYS:HB2	1:B:163:SER:OG	2.00	0.61
1:B:4:LYS:HA	1:B:44:ARG:HB2	1.83	0.60
1:A:232:ASP:HB2	1:A:302:GLU:HG3	1.83	0.60
1:A:233:TYR:HA	1:A:303:ILE:HG12	1.83	0.59
1:B:136:GLU:HG2	1:B:140:LYS:HE3	1.83	0.59
1:D:267:SER:O	1:D:271:LYS:HG2	2.02	0.59
1:B:58:LEU:HA	1:B:61:GLN:HE21	1.66	0.59
1:B:46:ILE:HD13	1:B:220:VAL:HG11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:ILE:CG2	1:C:271:LYS:HD2	2.32	0.59
1:D:54:GLN:H	1:D:54:GLN:NE2	2.01	0.59
1:D:176:ASN:HD21	1:D:220:VAL:HA	1.65	0.59
1:C:250:THR:HB	1:C:253:GLU:HG3	1.84	0.59
1:C:246:LEU:HB2	1:C:303:ILE:HD12	1.85	0.58
1:A:136:GLU:HG2	1:A:140:LYS:HE3	1.85	0.58
1:C:233:TYR:CD1	1:C:302:GLU:HB3	2.39	0.58
1:A:226:VAL:HG11	1:A:295:LEU:HD11	1.85	0.58
1:C:247:THR:O	1:C:303:ILE:HA	2.03	0.57
1:D:4:LYS:HA	1:D:44:ARG:HB2	1.85	0.57
1:D:250:THR:HA	1:D:306:THR:O	2.05	0.56
1:D:136:GLU:HG2	1:D:140:LYS:HE3	1.88	0.56
1:C:226:VAL:HG11	1:C:295:LEU:HD11	1.85	0.56
1:A:130:ILE:HD12	1:A:161:VAL:HB	1.87	0.56
1:D:176:ASN:ND2	1:D:220:VAL:HA	2.21	0.56
1:D:227:ILE:CG2	1:D:271:LYS:HD2	2.36	0.55
1:B:233:TYR:CD1	1:B:302:GLU:HB3	2.41	0.55
1:C:267:SER:O	1:C:270:PRO:HD2	2.06	0.55
1:B:226:VAL:HG11	1:B:295:LEU:HD11	1.88	0.55
1:C:118:PRO:HD3	1:C:196:VAL:HG13	1.89	0.54
1:C:306:THR:O	1:C:307:VAL:HG13	2.07	0.54
1:A:18:ASP:HB3	1:A:23:ALA:CB	2.38	0.54
1:C:46:ILE:HD13	1:C:220:VAL:HG11	1.89	0.54
1:A:227:ILE:CG2	1:A:271:LYS:HD2	2.38	0.53
1:D:46:ILE:HD13	1:D:220:VAL:HG11	1.90	0.53
1:C:58:LEU:HA	1:C:61:GLN:HE21	1.74	0.53
1:D:235:CYS:SG	1:D:245:GLN:HG2	2.48	0.53
1:D:232:ASP:O	1:D:233:TYR:HB2	2.08	0.53
1:B:209:LYS:HG3	1:B:210:ASP:N	2.24	0.53
1:B:227:ILE:CG2	1:B:271:LYS:HD2	2.40	0.52
1:D:118:PRO:HD3	1:D:196:VAL:HG13	1.92	0.52
1:D:58:LEU:HA	1:D:61:GLN:HE21	1.74	0.52
1:C:75:LEU:CB	1:C:204:GLU:HG3	2.37	0.52
1:B:54:GLN:H	1:B:54:GLN:NE2	2.07	0.52
1:A:58:LEU:HA	1:A:61:GLN:HE21	1.75	0.52
1:A:54:GLN:H	1:A:54:GLN:NE2	2.07	0.52
1:D:226:VAL:HG11	1:D:295:LEU:HD11	1.91	0.52
1:C:232:ASP:O	1:C:233:TYR:HB2	2.10	0.52
1:A:166:PRO:HG3	1:A:207:ILE:HG21	1.91	0.52
1:B:232:ASP:O	1:B:233:TYR:HB2	2.09	0.51
1:B:166:PRO:HG3	1:B:207:ILE:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ASN:HD21	1:A:220:VAL:HA	1.75	0.51
1:C:229:THR:O	1:C:291:SER:HA	2.10	0.51
1:A:4:LYS:HA	1:A:44:ARG:HB2	1.91	0.51
1:A:32:SER:O	1:A:36:VAL:HG23	2.11	0.51
1:D:76:ASP:HB3	1:D:203:VAL:O	2.11	0.51
1:C:237:ASN:CB	1:C:242:ASP:HB2	2.41	0.51
1:D:75:LEU:CB	1:D:204:GLU:HG3	2.38	0.50
1:D:267:SER:O	1:D:270:PRO:HD2	2.11	0.50
1:D:234:VAL:HG23	1:D:303:ILE:HG13	1.92	0.50
1:A:306:THR:O	1:A:307:VAL:HG13	2.12	0.50
1:B:56:GLY:HA3	1:B:131:GLY:CA	2.42	0.50
1:B:75:LEU:CB	1:B:204:GLU:HG3	2.41	0.50
1:A:46:ILE:HD13	1:A:220:VAL:HG11	1.94	0.50
1:D:166:PRO:HG3	1:D:207:ILE:HG21	1.94	0.50
1:A:216:LEU:O	1:A:220:VAL:HB	2.12	0.49
1:B:229:THR:O	1:B:291:SER:HA	2.12	0.49
1:B:195:VAL:HG11	1:B:200:LEU:HD22	1.94	0.49
1:B:130:ILE:HD12	1:B:161:VAL:HB	1.94	0.49
1:A:267:SER:O	1:A:271:LYS:HG2	2.12	0.49
1:B:306:THR:O	1:B:307:VAL:HG13	2.12	0.49
1:D:114:VAL:HG23	1:D:192:GLY:HA3	1.95	0.49
1:A:251:VAL:HG13	1:A:276:ILE:HG23	1.94	0.49
1:C:166:PRO:HG3	1:C:207:ILE:HG21	1.94	0.49
1:B:118:PRO:HD3	1:B:196:VAL:HG13	1.95	0.49
1:C:136:GLU:HG2	1:C:140:LYS:HE3	1.94	0.49
1:D:247:THR:O	1:D:303:ILE:HA	2.13	0.49
1:B:258:LYS:NZ	1:B:273:GLU:HG2	2.27	0.49
1:C:14:ILE:HG22	1:C:24:GLN:HE21	1.77	0.49
1:B:250:THR:HA	1:B:306:THR:O	2.12	0.49
1:D:18:ASP:HB3	1:D:23:ALA:CB	2.43	0.49
1:B:233:TYR:HA	1:B:303:ILE:HG12	1.94	0.48
1:A:234:VAL:H	1:A:303:ILE:HD11	1.78	0.48
1:A:246:LEU:HB2	1:A:303:ILE:CD1	2.44	0.48
1:A:118:PRO:HD3	1:A:196:VAL:HG13	1.96	0.48
1:A:133:PHE:CE2	1:A:158:ARG:HD2	2.49	0.48
1:A:232:ASP:O	1:A:233:TYR:HB2	2.14	0.48
1:D:130:ILE:HD12	1:D:161:VAL:HB	1.95	0.47
1:C:130:ILE:HD12	1:C:161:VAL:HB	1.96	0.47
1:C:282:GLN:HB2	1:C:285:LYS:HG3	1.95	0.47
1:C:54:GLN:H	1:C:54:GLN:NE2	2.13	0.47
1:B:62:GLN:HB3	1:B:72:ALA:HB1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:ASN:HD21	1:B:220:VAL:HA	1.79	0.47
1:D:236:ILE:O	1:D:243:GLU:HA	2.13	0.47
1:D:233:TYR:CD1	1:D:302:GLU:HB3	2.50	0.47
1:D:57:ASN:O	1:D:61:GLN:HG3	2.14	0.47
1:A:57:ASN:O	1:A:61:GLN:HG3	2.14	0.47
1:D:58:LEU:O	1:D:62:GLN:HG2	2.15	0.47
1:D:232:ASP:HB2	1:D:302:GLU:HG3	1.97	0.46
1:A:176:ASN:ND2	1:A:220:VAL:HA	2.30	0.46
1:A:15:LEU:HD13	1:A:53:PRO:HB2	1.98	0.46
1:C:21:ALA:O	1:C:25:GLN:HG3	2.15	0.46
1:D:229:THR:O	1:D:291:SER:HA	2.15	0.46
1:B:58:LEU:O	1:B:62:GLN:HG2	2.15	0.46
1:C:195:VAL:HG11	1:C:200:LEU:HD22	1.98	0.46
1:A:195:VAL:HG11	1:A:200:LEU:HD22	1.98	0.46
1:B:57:ASN:O	1:B:61:GLN:HG3	2.15	0.46
1:D:56:GLY:HA3	1:D:131:GLY:CA	2.46	0.45
1:D:118:PRO:HB3	1:D:196:VAL:HG11	1.98	0.45
1:B:195:VAL:HG22	1:B:200:LEU:O	2.16	0.45
1:D:282:GLN:HB2	1:D:285:LYS:HG3	1.97	0.45
1:B:216:LEU:O	1:B:220:VAL:HB	2.16	0.45
1:B:282:GLN:HB2	1:B:285:LYS:HG3	1.99	0.45
1:C:209:LYS:HG3	1:C:210:ASP:N	2.30	0.45
1:B:236:ILE:HD11	1:B:244:LYS:HD3	1.98	0.45
1:C:216:LEU:O	1:C:220:VAL:HB	2.16	0.45
1:B:14:ILE:HG22	1:B:24:GLN:HE21	1.82	0.45
1:C:233:TYR:HA	1:C:303:ILE:HG12	1.98	0.45
1:A:229:THR:O	1:A:291:SER:HA	2.17	0.45
1:A:282:GLN:HB2	1:A:285:LYS:CG	2.47	0.45
1:C:57:ASN:O	1:C:61:GLN:HG3	2.17	0.45
1:D:28:LEU:HD22	1:D:90:LEU:HD13	1.98	0.45
1:B:267:SER:O	1:B:271:LYS:HG2	2.16	0.45
1:D:306:THR:O	1:D:307:VAL:HG13	2.17	0.45
1:B:267:SER:O	1:B:270:PRO:HD2	2.17	0.44
1:B:133:PHE:CE2	1:B:158:ARG:HD2	2.52	0.44
1:B:176:ASN:ND2	1:B:220:VAL:HA	2.31	0.44
1:B:295:LEU:HD23	1:B:301:ASP:OD2	2.18	0.44
1:C:176:ASN:HD21	1:C:220:VAL:HA	1.82	0.44
1:A:282:GLN:HB2	1:A:285:LYS:HG3	1.99	0.44
1:C:4:LYS:HA	1:C:44:ARG:HB2	2.00	0.44
1:C:58:LEU:O	1:C:62:GLN:HG2	2.17	0.44
1:C:254:LEU:HD13	1:C:272:ILE:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:PRO:HB3	1:C:196:VAL:HG11	2.00	0.44
1:A:56:GLY:HA3	1:A:131:GLY:CA	2.47	0.44
1:A:295:LEU:HD23	1:A:301:ASP:OD2	2.18	0.43
1:D:31:THR:HG22	1:D:292:LEU:HD23	2.00	0.43
1:A:247:THR:O	1:A:303:ILE:HA	2.18	0.43
1:C:56:GLY:HA3	1:C:131:GLY:CA	2.48	0.43
1:A:238:TYR:O	1:A:243:GLU:HB2	2.19	0.43
1:C:6:VAL:HA	1:C:46:ILE:O	2.17	0.43
1:D:235:CYS:HB3	1:D:243:GLU:HG3	2.01	0.43
1:D:32:SER:O	1:D:36:VAL:HG23	2.18	0.43
1:A:240:LYS:HB3	1:A:241:PRO:HD2	1.99	0.43
1:D:209:LYS:HG3	1:D:210:ASP:N	2.34	0.43
1:B:279:VAL:HG11	1:B:306:THR:HA	2.01	0.43
1:B:118:PRO:HB3	1:B:196:VAL:HG11	2.00	0.43
1:D:249:VAL:HG23	1:D:305:GLY:HA2	2.01	0.43
1:A:263:PHE:HB3	1:A:268:MET:HB3	2.01	0.42
1:A:209:LYS:HG3	1:A:210:ASP:N	2.33	0.42
1:B:282:GLN:HB2	1:B:285:LYS:CG	2.49	0.42
1:B:15:LEU:HD13	1:B:53:PRO:HB2	2.01	0.42
1:A:174:THR:HG23	1:C:183:ILE:HD13	2.00	0.42
1:D:133:PHE:CE2	1:D:158:ARG:HD2	2.55	0.42
1:C:282:GLN:HB2	1:C:285:LYS:CG	2.49	0.42
1:D:103:ILE:HG22	1:D:105:LYS:HG2	2.01	0.42
1:B:136:GLU:O	1:B:140:LYS:HG3	2.20	0.42
1:B:183:ILE:HD13	1:D:174:THR:HG23	2.02	0.42
1:B:36:VAL:HG21	1:B:97:GLU:HB3	2.02	0.41
1:A:36:VAL:HG21	1:A:97:GLU:HB3	2.01	0.41
1:D:136:GLU:O	1:D:140:LYS:HG3	2.21	0.41
1:B:275:ALA:O	1:B:279:VAL:HG23	2.21	0.41
1:D:233:TYR:HA	1:D:303:ILE:HG12	2.02	0.41
1:C:161:VAL:HG13	1:C:162:PRO:HD2	2.02	0.41
1:C:267:SER:O	1:C:271:LYS:HG2	2.21	0.41
1:A:229:THR:HG22	1:A:231:VAL:H	1.86	0.41
1:A:232:ASP:CB	1:A:302:GLU:HG3	2.51	0.41
1:D:6:VAL:HA	1:D:46:ILE:O	2.20	0.41
1:D:233:TYR:CE1	1:D:302:GLU:HB3	2.55	0.40
1:D:114:VAL:CG2	1:D:192:GLY:HA3	2.50	0.40
1:A:6:VAL:HA	1:A:46:ILE:O	2.21	0.40
1:B:9:LEU:O	1:B:49:HIS:HA	2.21	0.40
1:A:21:ALA:O	1:A:25:GLN:HG3	2.22	0.40
1:D:234:VAL:H	1:D:303:ILE:HD11	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:288:ILE:HA	1:D:303:ILE:O	2.21	0.40
1:D:28:LEU:HA	1:D:31:THR:OG1	2.22	0.40
1:C:32:SER:O	1:C:36:VAL:HG23	2.21	0.40
1:D:21:ALA:O	1:D:25:GLN:HG3	2.21	0.40

There are no symmetry-related clashes.

## 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	305/310 (98%)	282 (92%)	16 (5%)	7 (2%)	8	26
1	B	305/310 (98%)	282 (92%)	14 (5%)	9 (3%)	5	18
1	C	305/310 (98%)	284 (93%)	14 (5%)	7 (2%)	8	26
1	D	305/310 (98%)	278 (91%)	20 (7%)	7 (2%)	8	26
All	All	1220/1240 (98%)	1126 (92%)	64 (5%)	30 (2%)	7	24

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	238	TYR
1	A	299	SER
1	A	303	ILE
1	B	247	THR
1	B	299	SER
1	B	303	ILE
1	C	299	SER
1	C	303	ILE
1	D	238	TYR
1	D	299	SER
1	D	303	ILE

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Mol	Chain	Res	Type
1	A	247	THR
1	A	307	VAL
1	B	267	SER
1	B	307	VAL
1	C	238	TYR
1	D	243	GLU
1	D	307	VAL
1	B	298	MET
1	C	307	VAL
1	A	298	MET
1	B	243	GLU
1	C	298	MET
1	D	52	GLY
1	B	52	GLY
1	C	233	TYR
1	D	298	MET
1	B	238	TYR
1	C	52	GLY
1	A	52	GLY

### 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	246/249 (99%)	235 (96%)	11 (4%)	34	68
1	B	246/249 (99%)	234 (95%)	12 (5%)	31	65
1	C	246/249 (99%)	233 (95%)	13 (5%)	28	61
1	D	246/249 (99%)	236 (96%)	10 (4%)	37	72
All	All	984/996 (99%)	938 (95%)	46 (5%)	32	67

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	54	GLN

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Mol	Chain	Res	Type
1	A	99	ASN
1	A	176	ASN
1	A	195	VAL
1	A	204	GLU
1	A	220	VAL
1	A	232	ASP
1	A	298	MET
1	A	302	GLU
1	A	307	VAL
1	B	30	GLN
1	B	54	GLN
1	B	88	TYR
1	B	99	ASN
1	B	176	ASN
1	B	195	VAL
1	B	204	GLU
1	B	220	VAL
1	B	232	ASP
1	B	298	MET
1	B	302	GLU
1	B	307	VAL
1	C	30	GLN
1	C	54	GLN
1	C	99	ASN
1	C	161	VAL
1	C	176	ASN
1	C	195	VAL
1	C	204	GLU
1	C	220	VAL
1	C	232	ASP
1	C	248	ASN
1	C	298	MET
1	C	302	GLU
1	C	307	VAL
1	D	30	GLN
1	D	54	GLN
1	D	99	ASN
1	D	176	ASN
1	D	195	VAL
1	D	204	GLU
1	D	220	VAL
1	D	298	MET

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Mol	Chain	Res	Type
1	D	302	GLU
1	D	307	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	54	GLN
1	A	61	GLN
1	A	63	GLN
1	A	96	GLN
1	A	176	ASN
1	B	24	GLN
1	B	54	GLN
1	B	61	GLN
1	B	63	GLN
1	B	170	HIS
1	B	176	ASN
1	B	248	ASN
1	C	24	GLN
1	C	54	GLN
1	C	61	GLN
1	C	63	GLN
1	C	176	ASN
1	D	24	GLN
1	D	54	GLN
1	D	61	GLN
1	D	63	GLN
1	D	176	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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	1375	-	4,4,4	1.49	1 (25%)	6,6,6	0.56	0
2	SO4	B	2375	-	4,4,4	1.58	1 (25%)	6,6,6	0.45	0
2	SO4	C	3375	-	4,4,4	1.49	1 (25%)	6,6,6	0.60	0
2	SO4	D	4375	-	4,4,4	1.58	1 (25%)	6,6,6	0.49	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	1375	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2375	-	-	0/0/0/0	0/0/0/0
2	SO4	C	3375	-	-	0/0/0/0	0/0/0/0
2	SO4	D	4375	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3375	SO4	O3-S	2.14	1.55	1.47
2	A	1375	SO4	O3-S	2.23	1.55	1.47
2	B	2375	SO4	O3-S	2.27	1.55	1.47
2	D	4375	SO4	O3-S	2.35	1.55	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	307/310 (99%)	-0.17	11 (3%) 46 34	5, 29, 68, 94	0
1	B	307/310 (99%)	0.29	36 (11%) 6 3	11, 37, 86, 96	0
1	C	307/310 (99%)	-0.32	10 (3%) 50 38	4, 26, 63, 88	0
1	D	307/310 (99%)	0.26	30 (9%) 10 5	7, 31, 93, 100	0
All	All	1228/1240 (99%)	0.01	87 (7%) 19 10	4, 31, 82, 100	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	261	GLY	10.8
1	A	308	VAL	9.3
1	A	300	GLY	9.1
1	A	299	SER	7.3
1	D	230	GLY	7.2
1	D	300	GLY	7.0
1	B	299	SER	6.9
1	D	241	PRO	6.9
1	C	308	VAL	6.7
1	D	266	GLY	6.6
1	B	308	VAL	6.1
1	D	299	SER	6.1
1	D	308	VAL	6.1
1	D	238	TYR	5.6
1	B	265	PRO	5.4
1	B	298	MET	5.2
1	D	236	ILE	5.1
1	D	244	LYS	5.1
1	D	239	GLY	5.0
1	D	263	PHE	5.0
1	B	301	ASP	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	144	GLN	4.7
1	D	298	MET	4.6
1	D	232	ASP	4.6
1	D	144	GLN	4.5
1	D	237	ASN	4.5
1	D	231	VAL	4.5
1	B	266	GLY	4.4
1	D	264	ALA	4.3
1	B	259	GLN	4.2
1	B	300	GLY	4.2
1	B	261	GLY	4.1
1	D	259	GLN	4.1
1	B	238	TYR	4.1
1	D	297	SER	4.0
1	D	243	GLU	3.9
1	D	143	MET	3.9
1	B	144	GLN	3.9
1	A	298	MET	3.8
1	B	42	GLY	3.7
1	D	301	ASP	3.7
1	B	239	GLY	3.6
1	C	153	ALA	3.6
1	B	237	ASN	3.6
1	D	240	LYS	3.5
1	C	299	SER	3.5
1	D	265	PRO	3.4
1	A	261	GLY	3.4
1	B	242	ASP	3.3
1	A	144	GLN	3.3
1	C	302	GLU	3.2
1	B	262	HIS	3.1
1	B	155	ARG	2.9
1	B	263	PHE	2.9
1	B	264	ALA	2.9
1	A	266	GLY	2.9
1	B	241	PRO	2.8
1	B	307	VAL	2.8
1	B	267	SER	2.8
1	B	284	ASN	2.8
1	D	153	ALA	2.8
1	B	260	ALA	2.8
1	B	302	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	242	ASP	2.7
1	B	252	ALA	2.7
1	C	301	ASP	2.7
1	A	143	MET	2.6
1	B	233	TYR	2.6
1	A	259	GLN	2.5
1	A	301	ASP	2.5
1	B	268	MET	2.5
1	B	198	GLN	2.4
1	B	229	THR	2.3
1	B	243	GLU	2.3
1	D	235	CYS	2.3
1	D	302	GLU	2.3
1	C	259	GLN	2.2
1	A	264	ALA	2.2
1	B	247	THR	2.2
1	B	124	LYS	2.2
1	D	296	GLY	2.2
1	C	147	ALA	2.1
1	C	300	GLY	2.1
1	B	148	ILE	2.0
1	C	155	ARG	2.0
1	B	141	GLU	2.0
1	B	152	ASP	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 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( $\text{\AA}^2$ )	Q<0.9
2	SO4	D	4375	5/5	0.98	0.12	-0.45	43,44,47,47	0
2	SO4	C	3375	5/5	0.98	0.13	-0.71	19,23,27,31	0
2	SO4	A	1375	5/5	0.99	0.08	-1.09	13,14,20,24	0
2	SO4	B	2375	5/5	0.98	0.10	-1.11	33,37,40,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.