



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 09:05 pm GMT

PDB ID : 2WE4  
Title : Carbamate kinase from *Enterococcus faecalis* bound to a sulfate ion and two water molecules, which mimic the substrate carbamyl phosphate  
Authors : Ramon-Maiques, S.; Marina, A.; Gil-Ortiz, F.; Rubio, V.  
Deposited on : 2009-03-27  
Resolution : 2.02 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

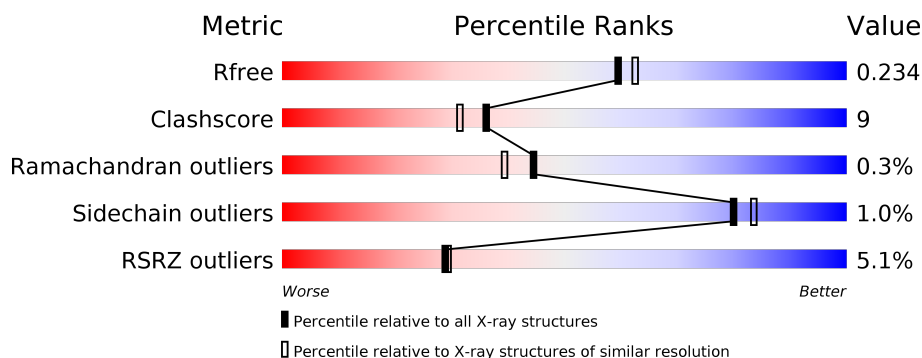
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.02 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))
$R_{free}$	100719	8396 (2.04-2.00)
Clashscore	112137	9678 (2.04-2.00)
Ramachandran outliers	110173	9566 (2.04-2.00)
Sidechain outliers	110143	9565 (2.04-2.00)
RSRZ outliers	101464	8490 (2.04-2.00)

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 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>3%</div> <div>82% 17% .</div> </div>
1	B	310	<div> <div>5%</div> <div>81% 18% .</div> </div>
1	C	310	<div> <div>2%</div> <div>88% 11% .</div> </div>
1	D	310	<div> <div>11%</div> <div>80% 18% .</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	1312	-	-	-	X
2	SO4	D	1312	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10190 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 CARBAMATE KINASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2302	1451	390	452	9			
1	B	309	Total	C	N	O	S	0	0	0
			2302	1451	390	452	9			
1	C	309	Total	C	N	O	S	0	0	0
			2302	1451	390	452	9			
1	D	309	Total	C	N	O	S	0	0	0
			2302	1451	390	452	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	A	1	Total	O	S	0	0
			5	4	1		

*Continued on next page...*

*Continued from previous page...*

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		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	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	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

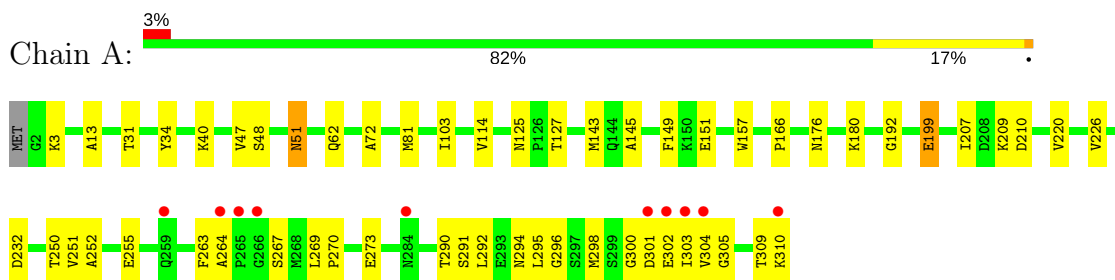
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	252	Total	O	0	0
			252	252		
3	B	200	Total	O	0	0
			200	200		
3	C	254	Total	O	0	0
			254	254		
3	D	201	Total	O	0	0
			201	201		

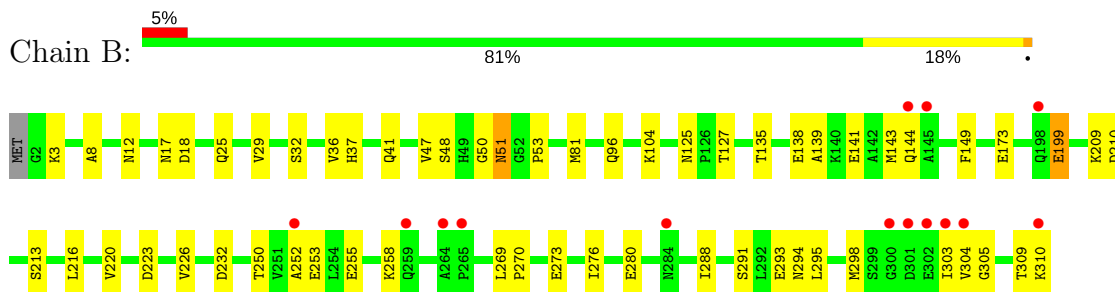
### 3 Residue-property plots

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

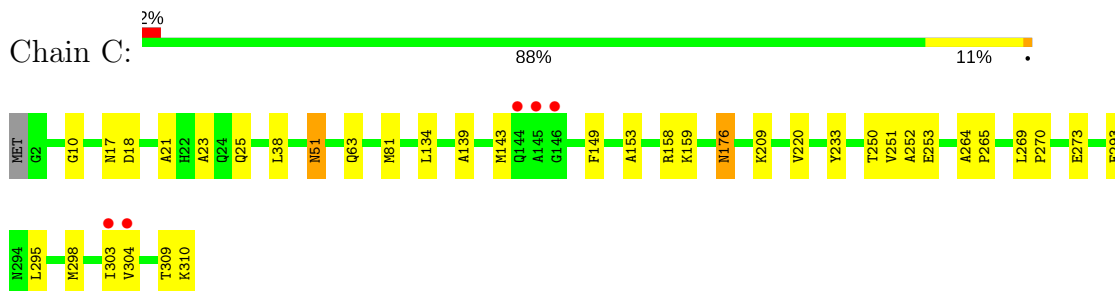
#### • Molecule 1: CARBAMATE KINASE 1



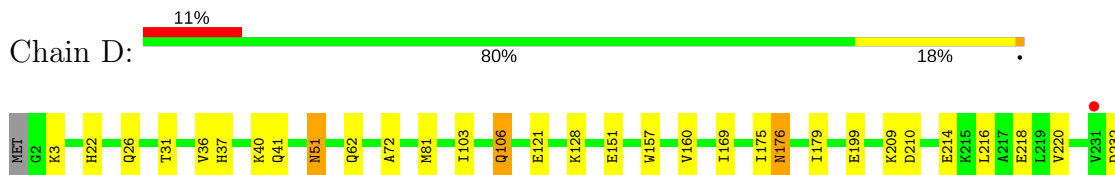
#### • Molecule 1: CARBAMATE KINASE 1

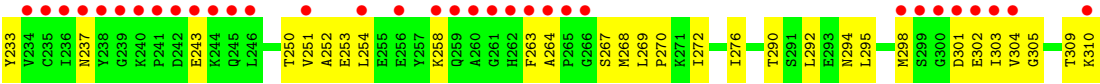


#### • Molecule 1: CARBAMATE KINASE 1



#### • Molecule 1: CARBAMATE KINASE 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.89Å 172.60Å 98.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.02 49.70 – 2.02	Depositor EDS
% Data completeness (in resolution range)	96.1 (20.00-2.02) 96.2 (49.70-2.02)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 2.01Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.195 , 0.234 0.195 , 0.234	Depositor DCC
$R_{free}$ test set	4439 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.2	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 52.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10190	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	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 23.45 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.6544e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.29	0/2337	0.57	0/3171
1	B	0.28	0/2337	0.53	0/3171
1	C	0.29	0/2337	0.56	0/3171
1	D	0.28	0/2337	0.55	0/3171
All	All	0.29	0/9348	0.55	0/12684

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	2302	0	2337	43	0
1	B	2302	0	2337	48	0
1	C	2302	0	2337	32	0
1	D	2302	0	2337	50	0
2	A	20	0	0	0	0
2	B	20	0	0	1	0
2	C	15	0	0	0	0
2	D	20	0	0	0	0
3	A	252	0	0	4	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	200	0	0	2	0
3	C	254	0	0	3	0
3	D	201	0	0	0	0
All	All	10190	0	9348	169	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 9.

All (169) 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:D:176:ASN:HD21	1:D:220:VAL:HA	1.21	1.04
1:A:31:THR:HG23	1:A:292:LEU:HD21	1.39	1.01
1:D:251:VAL:HB	1:D:310:LYS:HD3	1.45	0.99
1:A:252:ALA:HB2	1:A:310:LYS:HE3	1.49	0.94
1:B:252:ALA:HB2	1:B:310:LYS:HE3	1.51	0.90
1:C:251:VAL:HB	1:C:310:LYS:HD3	1.55	0.88
1:C:252:ALA:HB2	1:C:310:LYS:HE3	1.56	0.88
1:B:298:MET:HE2	1:B:303:ILE:HA	1.57	0.87
1:C:298:MET:HE3	1:C:303:ILE:HD12	1.58	0.86
1:B:104:LYS:HE2	1:B:104:LYS:HA	1.60	0.83
1:D:31:THR:HG23	1:D:292:LEU:HD21	1.66	0.78
1:D:252:ALA:HB2	1:D:310:LYS:HE3	1.66	0.75
1:B:309:THR:O	1:B:310:LYS:HB3	1.85	0.75
1:B:81:MET:HE2	1:D:81:MET:HB3	1.67	0.75
1:D:176:ASN:ND2	1:D:220:VAL:HA	2.01	0.73
1:C:309:THR:O	1:C:310:LYS:HB2	1.89	0.73
1:D:106:GLN:HA	1:D:106:GLN:HE21	1.54	0.72
1:D:199:GLU:H	1:D:199:GLU:CD	1.93	0.71
1:B:173:GLU:HG2	3:B:2124:HOH:O	1.92	0.70
1:A:309:THR:O	1:A:310:LYS:HB3	1.92	0.70
1:D:309:THR:O	1:D:310:LYS:HB2	1.91	0.69
1:B:294:ASN:HD21	1:B:304:VAL:HG12	1.61	0.66
1:B:139:ALA:O	1:B:143:MET:HG3	1.96	0.66
1:C:269:LEU:HB3	1:C:270:PRO:HD3	1.79	0.65
1:B:3:LYS:HG3	1:B:223:ASP:HB2	1.80	0.64
1:D:36:VAL:O	1:D:40:LYS:HG3	1.98	0.63
1:B:96:GLN:HG3	3:B:2084:HOH:O	1.98	0.63
1:D:269:LEU:HB3	1:D:270:PRO:HD3	1.81	0.63
1:C:139:ALA:O	1:C:143:MET:HG3	2.00	0.62
1:D:309:THR:O	1:D:310:LYS:CB	2.48	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:THR:HB	1:A:310:LYS:HD2	1.81	0.62
1:B:255:GLU:OE1	1:B:258:LYS:HE2	1.99	0.62
1:C:309:THR:O	1:C:310:LYS:CB	2.49	0.60
1:D:40:LYS:HG2	1:D:103:ILE:HD11	1.84	0.60
1:C:250:THR:HB	1:C:310:LYS:HD2	1.83	0.60
1:B:17:ASN:CG	1:B:18:ASP:H	2.03	0.60
1:B:294:ASN:HD21	1:B:304:VAL:CG1	2.15	0.60
1:D:237:ASN:HB2	1:D:243:GLU:HA	1.84	0.60
1:C:17:ASN:CG	1:C:18:ASP:H	2.06	0.58
1:D:272:ILE:O	1:D:276:ILE:HG12	2.04	0.58
1:A:31:THR:CG2	1:A:292:LEU:HD21	2.24	0.58
1:B:17:ASN:ND2	1:B:18:ASP:H	2.01	0.58
1:B:199:GLU:H	1:B:199:GLU:CD	2.08	0.57
1:A:176:ASN:O	1:A:180:LYS:HG3	2.04	0.57
1:C:252:ALA:CB	1:C:310:LYS:HE3	2.33	0.57
1:B:269:LEU:O	1:B:273:GLU:HG2	2.05	0.57
1:A:232:ASP:O	1:A:305:GLY:HA2	2.05	0.56
1:A:199:GLU:CD	1:A:199:GLU:H	2.08	0.56
1:D:232:ASP:CG	1:D:294:ASN:HD21	2.08	0.56
1:D:290:THR:HB	1:D:305:GLY:HA3	1.88	0.56
1:B:141:GLU:HA	1:B:144:GLN:HE21	1.71	0.56
1:C:298:MET:HE2	1:C:303:ILE:HB	1.87	0.56
1:A:269:LEU:HB3	1:A:270:PRO:HD3	1.87	0.56
1:D:298:MET:HG3	1:D:302:GLU:O	2.06	0.55
1:C:21:ALA:O	1:C:25:GLN:HG3	2.07	0.55
1:B:226:VAL:HG11	1:B:295:LEU:HD11	1.89	0.55
1:A:81:MET:HB3	1:C:81:MET:HE2	1.88	0.55
1:A:232:ASP:HA	1:A:294:ASN:ND2	2.22	0.54
1:D:36:VAL:HG12	1:D:40:LYS:HE3	1.90	0.53
1:B:252:ALA:CB	1:B:310:LYS:HE3	2.33	0.53
1:A:145:ALA:HB2	3:A:2139:HOH:O	2.07	0.53
1:A:13:ALA:HB2	3:A:2007:HOH:O	2.09	0.52
1:C:251:VAL:CB	1:C:310:LYS:HD3	2.35	0.52
1:A:304:VAL:HA	3:A:2205:HOH:O	2.10	0.52
1:C:38:LEU:HD11	1:C:295:LEU:HD22	1.92	0.51
1:D:295:LEU:HD23	1:D:303:ILE:CD1	2.41	0.51
1:A:232:ASP:HA	1:A:294:ASN:HD21	1.76	0.50
1:A:269:LEU:O	1:A:273:GLU:HG3	2.11	0.50
1:A:51:ASN:N	1:A:51:ASN:HD22	2.10	0.50
1:B:252:ALA:H	1:B:310:LYS:HD3	1.77	0.49
1:D:199:GLU:CD	1:D:199:GLU:N	2.64	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:MET:O	1:D:272:ILE:HG12	2.13	0.49
1:B:81:MET:HB3	1:D:81:MET:HE2	1.94	0.49
1:A:252:ALA:H	1:A:310:LYS:HD3	1.77	0.48
1:A:81:MET:HE2	1:C:81:MET:HB3	1.94	0.48
1:B:269:LEU:HB3	1:B:270:PRO:HD3	1.95	0.48
1:C:176:ASN:HD21	1:C:220:VAL:HA	1.78	0.48
1:A:250:THR:HB	1:A:310:LYS:CD	2.42	0.48
1:D:209:LYS:HG3	1:D:210:ASP:N	2.29	0.48
1:D:250:THR:HB	1:D:310:LYS:HD2	1.95	0.48
1:B:32:SER:O	1:B:36:VAL:HG23	2.13	0.48
1:C:293:GLU:CD	1:C:293:GLU:H	2.16	0.48
1:B:291:SER:OG	1:B:294:ASN:HB2	2.14	0.48
1:D:3:LYS:HE3	1:D:301:ASP:OD2	2.14	0.48
1:A:294:ASN:OD1	1:A:304:VAL:HB	2.13	0.47
1:B:232:ASP:O	1:B:305:GLY:HA2	2.15	0.47
1:B:309:THR:O	1:B:310:LYS:CB	2.61	0.47
1:D:258:LYS:HE3	1:D:269:LEU:HD11	1.96	0.47
1:B:12:ASN:HA	1:B:53:PRO:HG2	1.97	0.47
1:A:252:ALA:CB	1:A:310:LYS:HE3	2.32	0.47
1:B:216:LEU:O	1:B:220:VAL:HG22	2.15	0.47
1:B:47:VAL:HG12	1:B:48:SER:N	2.30	0.47
1:D:254:LEU:HD12	1:D:276:ILE:HD11	1.97	0.47
1:D:264:ALA:HB3	1:D:267:SER:OG	2.15	0.47
1:D:251:VAL:HG13	1:D:276:ILE:HG23	1.96	0.47
1:A:151:GLU:HB2	1:A:157:TRP:CE2	2.50	0.46
1:A:209:LYS:HG3	1:A:210:ASP:N	2.29	0.46
1:D:151:GLU:HB2	1:D:157:TRP:CE2	2.50	0.46
1:A:34:TYR:HD1	1:A:296:GLY:HA3	1.79	0.46
1:D:37:HIS:O	1:D:41:GLN:HG2	2.16	0.46
1:B:135:THR:OG1	1:B:138:GLU:HG3	2.15	0.46
1:C:134:LEU:HD12	1:C:149:PHE:CE2	2.51	0.46
1:A:166:PRO:HG3	1:A:207:ILE:HG21	1.97	0.46
1:C:18:ASP:HB3	1:C:23:ALA:CB	2.46	0.45
1:B:209:LYS:HG3	1:B:210:ASP:N	2.32	0.45
1:D:232:ASP:O	1:D:305:GLY:HA2	2.17	0.45
1:C:298:MET:CE	1:C:303:ILE:HB	2.45	0.45
1:D:250:THR:OG1	1:D:253:GLU:HG3	2.17	0.45
1:B:8:ALA:HB2	1:B:213:SER:OG	2.17	0.45
1:B:50:GLY:HA3	2:B:1311:SO4:O2	2.17	0.45
1:D:292:LEU:HD12	1:D:295:LEU:HD12	1.98	0.45
1:B:276:ILE:O	1:B:280:GLU:HG3	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:LYS:HE2	1:B:104:LYS:CA	2.41	0.45
1:D:295:LEU:HD23	1:D:303:ILE:HD11	1.99	0.44
1:B:51:ASN:ND2	1:B:51:ASN:C	2.70	0.44
1:B:25:GLN:O	1:B:29:VAL:HG23	2.17	0.44
1:D:51:ASN:N	1:D:51:ASN:HD22	2.14	0.44
1:C:51:ASN:N	1:C:51:ASN:HD22	2.15	0.44
1:B:288:ILE:HD13	1:B:303:ILE:HG21	2.00	0.44
1:A:3:LYS:HE3	1:A:301:ASP:OD1	2.18	0.44
1:A:62:GLN:HB3	1:A:72:ALA:HB1	2.00	0.44
1:C:159:LYS:NZ	3:C:2133:HOH:O	2.50	0.44
1:D:176:ASN:ND2	1:D:220:VAL:HG12	2.33	0.44
1:D:22:HIS:O	1:D:26:GLN:HG3	2.18	0.44
1:D:298:MET:CE	1:D:303:ILE:HB	2.48	0.44
1:B:293:GLU:CD	1:B:293:GLU:H	2.21	0.43
1:B:3:LYS:HG3	1:B:223:ASP:CB	2.45	0.43
1:C:298:MET:HG3	1:C:303:ILE:HB	2.00	0.43
1:A:143:MET:HE3	1:A:149:PHE:H	1.83	0.43
1:C:250:THR:OG1	1:C:253:GLU:HG3	2.18	0.43
1:D:51:ASN:ND2	1:D:51:ASN:C	2.72	0.43
1:A:302:GLU:HA	1:A:302:GLU:OE1	2.19	0.43
1:C:17:ASN:CG	1:C:18:ASP:N	2.72	0.42
1:D:175:ILE:O	1:D:179:ILE:HG13	2.19	0.42
1:D:298:MET:HE2	1:D:303:ILE:HB	2.01	0.42
1:B:37:HIS:O	1:B:41:GLN:HG2	2.18	0.42
1:A:40:LYS:HG2	1:A:103:ILE:HD11	2.01	0.42
1:A:264:ALA:HB3	1:A:267:SER:OG	2.20	0.42
1:A:298:MET:HG3	1:A:303:ILE:HG22	2.01	0.42
1:A:47:VAL:HG12	1:A:48:SER:N	2.35	0.42
1:B:250:THR:OG1	1:B:253:GLU:HG3	2.20	0.42
1:B:294:ASN:ND2	1:B:304:VAL:HB	2.34	0.42
1:B:298:MET:HE1	1:B:303:ILE:HG23	2.02	0.42
1:D:233:TYR:OH	1:D:304:VAL:HG13	2.19	0.42
1:A:226:VAL:HG11	1:A:295:LEU:HD11	2.01	0.41
1:A:290:THR:OG1	1:A:291:SER:N	2.53	0.41
1:A:251:VAL:O	1:A:255:GLU:HG2	2.19	0.41
1:C:264:ALA:HA	1:C:265:PRO:HD3	1.91	0.41
1:D:252:ALA:H	1:D:310:LYS:CD	2.33	0.41
1:A:114:VAL:CG2	1:A:192:GLY:HA3	2.50	0.41
1:A:34:TYR:CD1	1:A:296:GLY:HA3	2.55	0.41
1:B:51:ASN:N	1:B:51:ASN:HD22	2.17	0.41
1:C:10:GLY:HA2	1:C:209:LYS:HE3	2.02	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:ILE:HD12	1:D:216:LEU:HA	2.02	0.41
1:A:176:ASN:HD21	1:A:220:VAL:HA	1.85	0.41
1:B:298:MET:CE	1:B:303:ILE:HG23	2.50	0.41
1:C:269:LEU:O	1:C:273:GLU:HG3	2.21	0.41
1:C:233:TYR:OH	1:C:304:VAL:HG13	2.21	0.41
1:A:125:ASN:O	1:A:127:THR:HG23	2.21	0.41
1:D:62:GLN:HB3	1:D:72:ALA:HB1	2.03	0.41
1:B:143:MET:CE	1:B:149:PHE:H	2.34	0.41
1:C:158:ARG:HB2	3:C:2131:HOH:O	2.19	0.41
1:D:254:LEU:CD1	1:D:276:ILE:HD11	2.51	0.41
1:D:128:LYS:O	1:D:160:VAL:HA	2.21	0.40
1:A:298:MET:CE	1:A:303:ILE:HG22	2.51	0.40
1:C:63:GLN:HG3	3:C:2054:HOH:O	2.21	0.40
1:D:214:GLU:O	1:D:218:GLU:HG3	2.22	0.40
1:A:145:ALA:HB3	3:A:2136:HOH:O	2.22	0.40
1:B:125:ASN:O	1:B:127:THR:HG23	2.20	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	307/310 (99%)	299 (97%)	6 (2%)	2 (1%)	25	17
1	B	307/310 (99%)	295 (96%)	12 (4%)	0	100	100
1	C	307/310 (99%)	296 (96%)	10 (3%)	1 (0%)	44	39
1	D	307/310 (99%)	297 (97%)	9 (3%)	1 (0%)	44	39
All	All	1228/1240 (99%)	1187 (97%)	37 (3%)	4 (0%)	44	39

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	153	ALA
1	D	263	PHE
1	A	263	PHE
1	A	300	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	248/249 (100%)	246 (99%)	2 (1%)	85	88
1	B	248/249 (100%)	246 (99%)	2 (1%)	85	88
1	C	248/249 (100%)	246 (99%)	2 (1%)	85	88
1	D	248/249 (100%)	244 (98%)	4 (2%)	68	70
All	All	992/996 (100%)	982 (99%)	10 (1%)	80	83

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	199	GLU
1	B	51	ASN
1	B	199	GLU
1	C	51	ASN
1	C	176	ASN
1	D	51	ASN
1	D	106	GLN
1	D	121	GLU
1	D	176	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	170	HIS
1	A	245	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	17	ASN
1	B	51	ASN
1	B	95	ASN
1	B	106	GLN
1	B	144	GLN
1	B	248	ASN
1	B	294	ASN
1	C	12	ASN
1	C	51	ASN
1	C	57	ASN
1	C	170	HIS
1	C	176	ASN
1	C	248	ASN
1	D	51	ASN
1	D	106	GLN
1	D	176	ASN
1	D	294	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

15 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	1311	-	4,4,4	1.82	2 (50%)	6,6,6	0.89	0
2	SO4	A	1312	-	4,4,4	1.87	1 (25%)	6,6,6	0.88	0
2	SO4	A	1313	-	4,4,4	1.85	1 (25%)	6,6,6	0.89	0
2	SO4	A	1314	-	4,4,4	1.87	1 (25%)	6,6,6	0.87	0
2	SO4	B	1311	-	4,4,4	1.82	1 (25%)	6,6,6	0.84	0
2	SO4	B	1312	-	4,4,4	1.85	1 (25%)	6,6,6	0.87	0
2	SO4	B	1313	-	4,4,4	1.82	1 (25%)	6,6,6	0.87	0
2	SO4	B	1314	-	4,4,4	1.85	1 (25%)	6,6,6	0.88	0
2	SO4	C	1311	-	4,4,4	1.83	2 (50%)	6,6,6	0.87	0
2	SO4	C	1312	-	4,4,4	1.87	1 (25%)	6,6,6	0.87	0
2	SO4	C	1313	-	4,4,4	1.81	1 (25%)	6,6,6	0.85	0
2	SO4	D	1311	-	4,4,4	1.83	1 (25%)	6,6,6	0.84	0
2	SO4	D	1312	-	4,4,4	1.88	1 (25%)	6,6,6	0.88	0
2	SO4	D	1313	-	4,4,4	1.84	1 (25%)	6,6,6	0.86	0
2	SO4	D	1314	-	4,4,4	1.85	1 (25%)	6,6,6	0.87	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	1311	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1312	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1313	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1314	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1311	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1312	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1313	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1314	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1311	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1312	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1313	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1311	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1312	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1313	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1314	-	-	0/0/0/0	0/0/0/0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1311	SO4	O3-S	-2.04	1.29	1.47
2	A	1311	SO4	O3-S	-2.02	1.30	1.47
2	A	1311	SO4	O1-S	2.99	1.61	1.45
2	C	1311	SO4	O1-S	3.00	1.61	1.45
2	C	1313	SO4	O1-S	3.05	1.62	1.45
2	D	1311	SO4	O1-S	3.06	1.62	1.45
2	B	1311	SO4	O1-S	3.06	1.62	1.45
2	B	1313	SO4	O1-S	3.10	1.62	1.45
2	A	1313	SO4	O1-S	3.13	1.62	1.45
2	D	1313	SO4	O1-S	3.13	1.62	1.45
2	D	1314	SO4	O1-S	3.14	1.62	1.45
2	B	1312	SO4	O1-S	3.14	1.62	1.45
2	B	1314	SO4	O1-S	3.16	1.62	1.45
2	C	1312	SO4	O1-S	3.17	1.62	1.45
2	A	1312	SO4	O1-S	3.19	1.62	1.45
2	A	1314	SO4	O1-S	3.20	1.63	1.45
2	D	1312	SO4	O1-S	3.22	1.63	1.45

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	B	1311	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

### 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	309/310 (99%)	0.21	10 (3%) 48 49	13, 24, 46, 60	0
1	B	309/310 (99%)	0.33	14 (4%) 34 34	14, 27, 50, 73	0
1	C	309/310 (99%)	0.06	5 (1%) 72 72	13, 22, 43, 65	0
1	D	309/310 (99%)	0.36	34 (11%) 6 6	13, 24, 65, 80	0
All	All	1236/1240 (99%)	0.24	63 (5%) 29 29	13, 24, 52, 80	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	303	ILE	9.0
1	D	241	PRO	6.7
1	A	303	ILE	5.5
1	D	239	GLY	5.3
1	D	301	ASP	5.3
1	B	145	ALA	5.1
1	D	238	TYR	5.1
1	D	243	GLU	4.8
1	D	300	GLY	4.7
1	B	301	ASP	4.7
1	C	145	ALA	4.7
1	A	264	ALA	4.6
1	D	235	CYS	4.2
1	D	266	GLY	4.2
1	D	304	VAL	4.2
1	D	234	VAL	3.8
1	D	242	ASP	3.7
1	D	231	VAL	3.6
1	B	310	LYS	3.5
1	D	261	GLY	3.5
1	D	265	PRO	3.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	264	ALA	3.4
1	D	260	ALA	3.3
1	B	265	PRO	3.2
1	D	262	HIS	3.2
1	A	310	LYS	3.2
1	A	265	PRO	3.2
1	B	304	VAL	3.1
1	A	304	VAL	3.1
1	B	302	GLU	3.1
1	D	240	LYS	3.0
1	D	298	MET	3.0
1	A	284	ASN	3.0
1	B	252	ALA	2.9
1	C	303	ILE	2.8
1	B	264	ALA	2.8
1	C	304	VAL	2.8
1	D	236	ILE	2.7
1	D	251	VAL	2.7
1	D	259	GLN	2.7
1	A	301	ASP	2.7
1	D	244	LYS	2.7
1	C	144	GLN	2.6
1	D	258	LYS	2.6
1	B	259	GLN	2.6
1	D	237	ASN	2.6
1	D	263	PHE	2.5
1	A	266	GLY	2.5
1	D	254	LEU	2.4
1	B	144	GLN	2.4
1	C	146	GLY	2.4
1	D	256	GLU	2.3
1	D	310	LYS	2.3
1	D	246	LEU	2.3
1	D	302	GLU	2.3
1	B	300	GLY	2.2
1	D	245	GLN	2.2
1	A	259	GLN	2.2
1	D	303	ILE	2.1
1	D	299	SER	2.0
1	A	302	GLU	2.0
1	B	284	ASN	2.0
1	B	198	GLN	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(Å <sup>2</sup> )	Q<0.9
2	SO4	C	1312	5/5	0.80	0.26	3.04	86,87,87,87	0
2	SO4	D	1312	5/5	0.90	0.19	2.74	62,62,62,63	0
2	SO4	A	1312	5/5	0.92	0.14	0.54	66,67,67,68	0
2	SO4	B	1313	5/5	0.99	0.16	0.22	39,40,40,41	0
2	SO4	B	1311	5/5	0.99	0.12	0.04	26,27,29,31	0
2	SO4	D	1311	5/5	0.99	0.11	-0.07	19,23,24,26	0
2	SO4	A	1311	5/5	0.99	0.13	-0.12	22,23,24,24	0
2	SO4	A	1313	5/5	0.97	0.12	-0.71	34,35,37,40	0
2	SO4	C	1311	5/5	0.99	0.11	-0.79	21,24,26,27	0
2	SO4	C	1313	5/5	1.00	0.09	-1.07	21,23,23,24	0
2	SO4	D	1314	5/5	0.94	0.25	-1.29	72,73,73,73	0
2	SO4	A	1314	5/5	0.95	0.14	-	55,56,57,57	0
2	SO4	B	1312	5/5	0.94	0.14	-	80,80,80,80	0
2	SO4	D	1313	5/5	0.97	0.13	-	49,49,50,51	0
2	SO4	B	1314	5/5	0.94	0.16	-	69,70,70,70	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.