



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 06:04 am BST

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

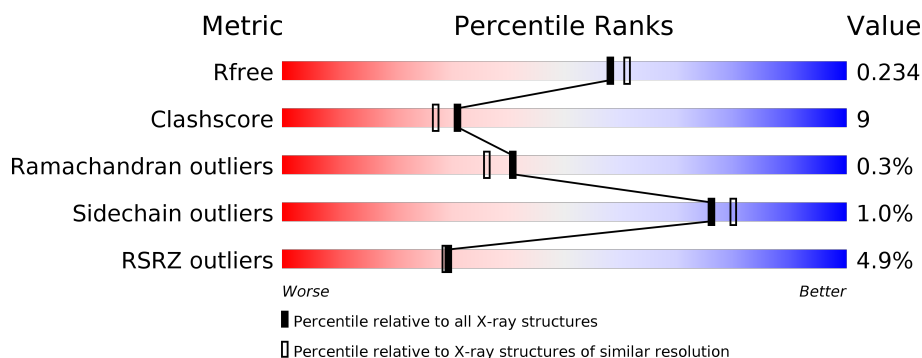
1 Overall quality at a glance

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}	130704	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (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 ≥ 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 $\leq 5\%$. 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> <div></div> <div>82%</div> <div>17%</div> </div> <div></div> </div>
1	B	310	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>18%</div> </div> <div></div> </div>
1	C	310	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>11%</div> </div> <div></div> </div>
1	D	310	<div> <div>11%</div> <div> <div></div> <div>80%</div> <div>18%</div> </div> <div></div> </div>

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: O₄S).



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

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

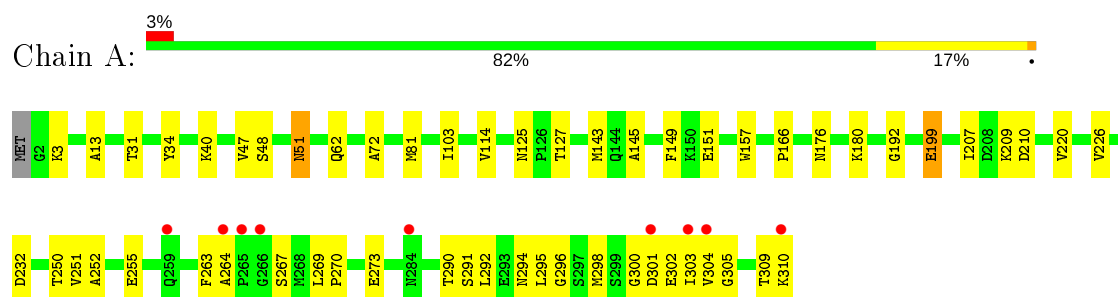
- Molecule 3 is water.

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		

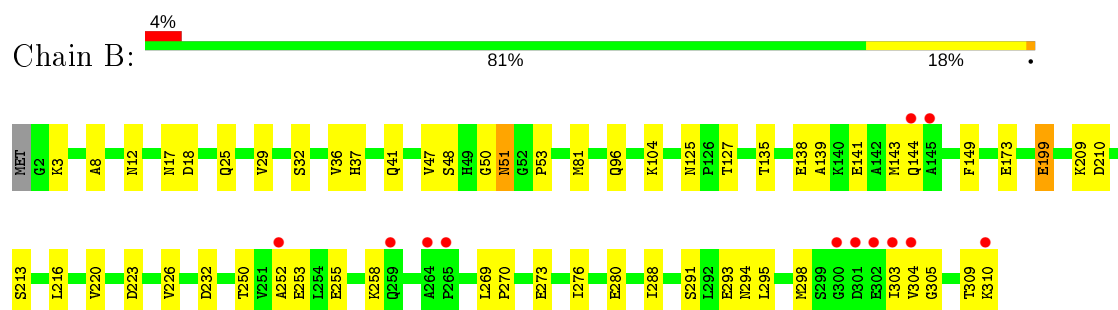
3 Residue-property plots [i](#)

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

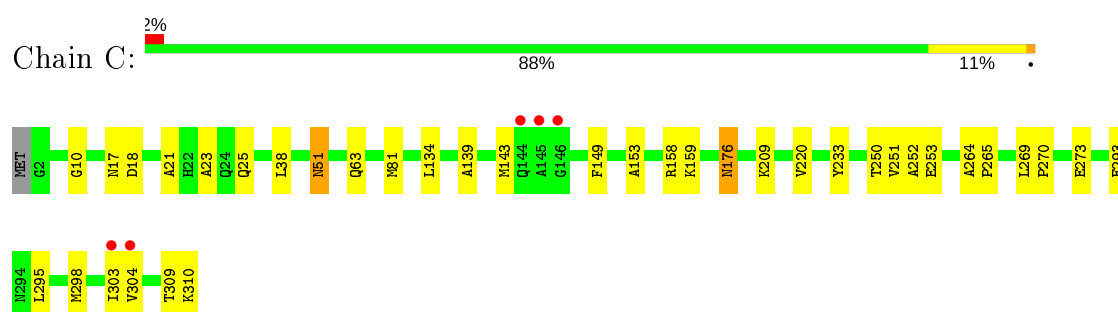
• Molecule 1: CARBAMATE KINASE 1



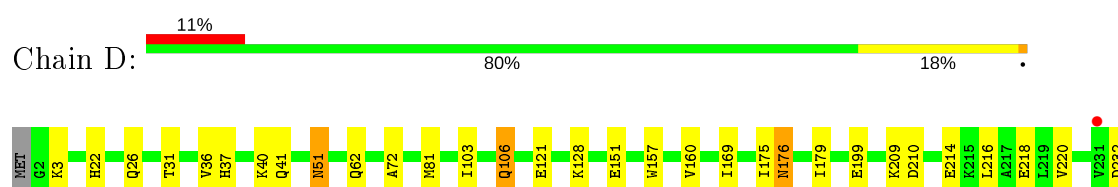
• Molecule 1: CARBAMATE KINASE 1



• 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, α , β , γ	80.89 Å 172.60 Å 98.63 Å 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
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.01 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.195 , 0.234 0.195 , 0.234	Depositor DCC
R_{free} test set	4450 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

¹ Intensities estimated from amplitudes.

² 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

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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

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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

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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

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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

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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 [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	307/310 (99%)	299 (97%)	6 (2%)	2 (1%)	22	15
1	B	307/310 (99%)	295 (96%)	12 (4%)	0	100	100
1	C	307/310 (99%)	296 (96%)	10 (3%)	1 (0%)	41	36
1	D	307/310 (99%)	297 (97%)	9 (3%)	1 (0%)	41	36
All	All	1228/1240 (99%)	1187 (97%)	37 (3%)	4 (0%)	41	36

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%)	81	85
1	B	248/249 (100%)	246 (99%)	2 (1%)	81	85
1	C	248/249 (100%)	246 (99%)	2 (1%)	81	85
1	D	248/249 (100%)	244 (98%)	4 (2%)	62	66
All	All	992/996 (100%)	982 (99%)	10 (1%)	76	80

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

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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	B	1312	-	4,4,4	1.86	2 (50%)	6,6,6	0.90	0
2	SO4	A	1314	-	4,4,4	1.88	2 (50%)	6,6,6	0.90	0
2	SO4	A	1313	-	4,4,4	1.87	2 (50%)	6,6,6	0.92	0
2	SO4	B	1311	-	4,4,4	1.83	2 (50%)	6,6,6	0.87	0
2	SO4	A	1311	-	4,4,4	1.83	2 (50%)	6,6,6	0.92	0
2	SO4	D	1311	-	4,4,4	1.84	2 (50%)	6,6,6	0.87	0
2	SO4	C	1312	-	4,4,4	1.88	2 (50%)	6,6,6	0.90	0
2	SO4	B	1314	-	4,4,4	1.87	2 (50%)	6,6,6	0.91	0
2	SO4	A	1312	-	4,4,4	1.89	2 (50%)	6,6,6	0.91	0
2	SO4	D	1314	-	4,4,4	1.87	2 (50%)	6,6,6	0.90	0
2	SO4	C	1311	-	4,4,4	1.85	2 (50%)	6,6,6	0.90	0
2	SO4	B	1313	-	4,4,4	1.83	2 (50%)	6,6,6	0.90	0
2	SO4	C	1313	-	4,4,4	1.83	2 (50%)	6,6,6	0.88	0
2	SO4	D	1313	-	4,4,4	1.86	2 (50%)	6,6,6	0.89	0
2	SO4	D	1312	-	4,4,4	1.89	2 (50%)	6,6,6	0.91	0

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1312	SO4	O1-S	3.15	1.63	1.46
2	A	1314	SO4	O1-S	3.13	1.63	1.46
2	A	1312	SO4	O1-S	3.13	1.62	1.46
2	C	1312	SO4	O1-S	3.10	1.62	1.46
2	B	1314	SO4	O1-S	3.09	1.62	1.46
2	B	1312	SO4	O1-S	3.08	1.62	1.46
2	D	1314	SO4	O1-S	3.07	1.62	1.46
2	D	1313	SO4	O1-S	3.07	1.62	1.46
2	A	1313	SO4	O1-S	3.07	1.62	1.46
2	B	1313	SO4	O1-S	3.03	1.62	1.46
2	B	1311	SO4	O1-S	2.99	1.62	1.46
2	D	1311	SO4	O1-S	2.99	1.62	1.46
2	C	1313	SO4	O1-S	2.98	1.62	1.46
2	C	1311	SO4	O1-S	2.93	1.61	1.46
2	A	1311	SO4	O1-S	2.92	1.61	1.46
2	C	1311	SO4	O3-S	-2.19	1.29	1.47
2	A	1311	SO4	O3-S	-2.16	1.30	1.47
2	D	1311	SO4	O3-S	-2.10	1.30	1.47
2	C	1312	SO4	O3-S	-2.09	1.30	1.47
2	A	1313	SO4	O3-S	-2.09	1.30	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1314	SO4	O3-S	-2.08	1.30	1.47
2	A	1312	SO4	O3-S	-2.06	1.30	1.47
2	D	1312	SO4	O3-S	-2.06	1.31	1.47
2	B	1311	SO4	O3-S	-2.06	1.31	1.47
2	B	1312	SO4	O3-S	-2.05	1.31	1.47
2	D	1313	SO4	O3-S	-2.05	1.31	1.47
2	B	1314	SO4	O3-S	-2.05	1.31	1.47
2	C	1313	SO4	O3-S	-2.04	1.31	1.47
2	A	1314	SO4	O3-S	-2.04	1.31	1.47
2	B	1313	SO4	O3-S	-2.00	1.31	1.47

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, 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	309/310 (99%)	0.21	9 (2%) 51 51	13, 24, 46, 60	0
1	B	309/310 (99%)	0.32	12 (3%) 39 39	14, 27, 50, 73	0
1	C	309/310 (99%)	0.05	5 (1%) 72 71	13, 22, 43, 65	0
1	D	309/310 (99%)	0.36	34 (11%) 5 5	13, 24, 65, 80	0
All	All	1236/1240 (99%)	0.24	60 (4%) 29 29	13, 24, 52, 80	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	303	ILE	9.0
1	D	241	PRO	6.8
1	A	303	ILE	5.4
1	D	301	ASP	5.2
1	D	239	GLY	5.2
1	D	238	TYR	5.1
1	B	145	ALA	5.0
1	D	300	GLY	4.8
1	D	243	GLU	4.8
1	B	301	ASP	4.7
1	C	145	ALA	4.7
1	A	264	ALA	4.6
1	D	304	VAL	4.2
1	D	266	GLY	4.2
1	D	235	CYS	4.2
1	D	234	VAL	3.8
1	D	242	ASP	3.6
1	D	261	GLY	3.6
1	D	231	VAL	3.5
1	B	310	LYS	3.5
1	D	265	PRO	3.4

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

6.5 Other polymers [i](#)

There are no such residues in this entry.