



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:23 AM UTC

PDB ID : 2WE4 / pdb_00002we4
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

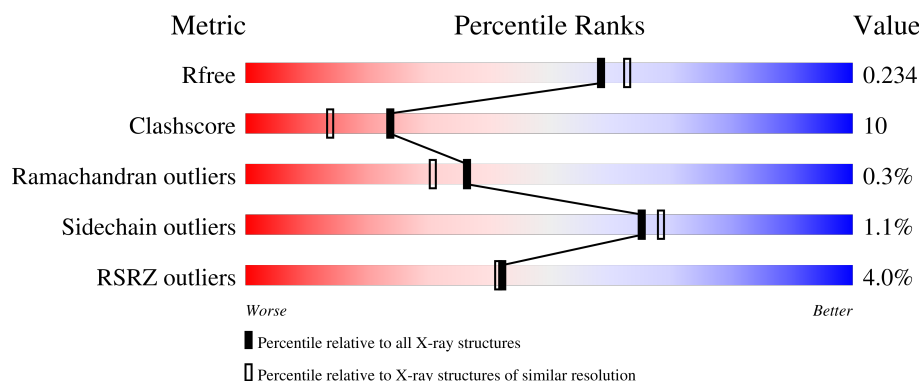
1 Overall quality at a glance

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}	180053	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	3% 79% 19% .
1	B	310	5% 79% 20% .
1	C	310	2% 85% 14% .
1	D	310	6% 79% 19% .

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 (CCD ID: 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		

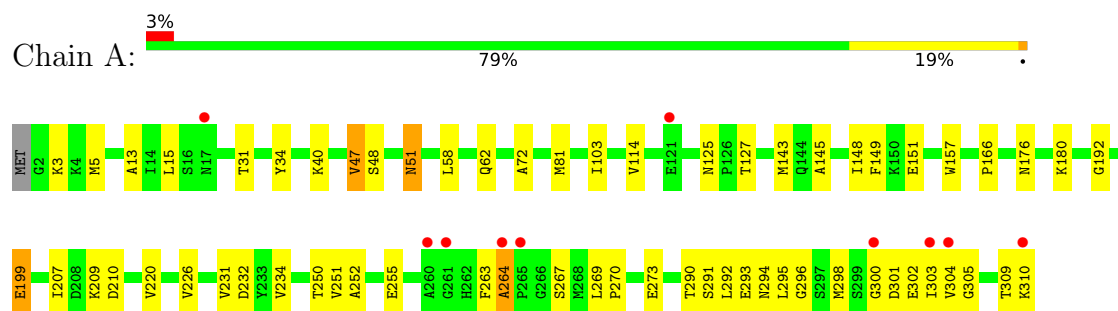
- Molecule 3 is water.

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		

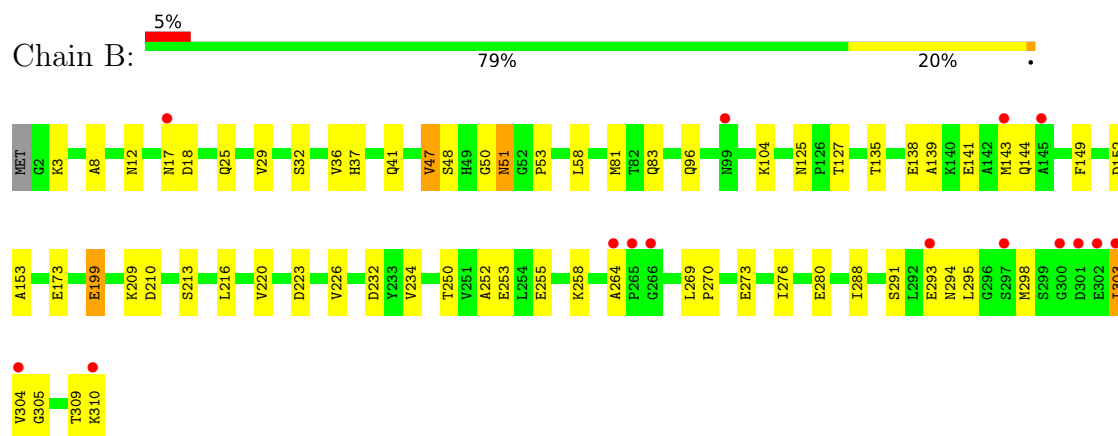
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

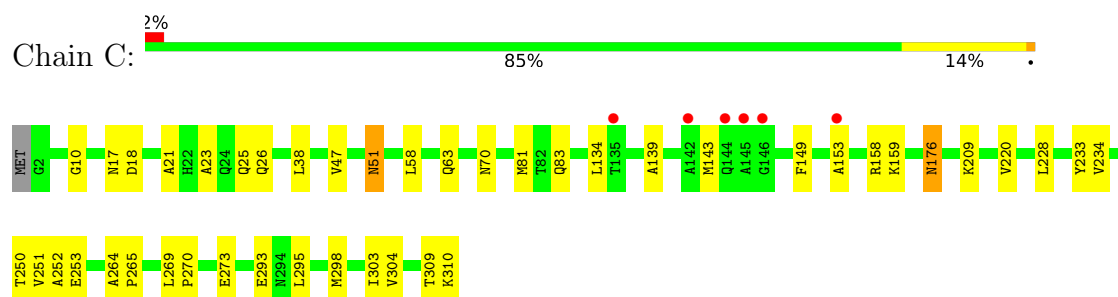
• Molecule 1: CARBAMATE KINASE 1



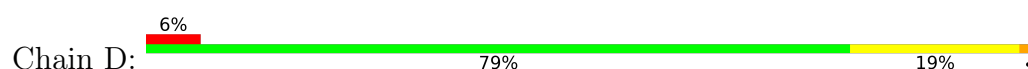
• Molecule 1: CARBAMATE KINASE 1

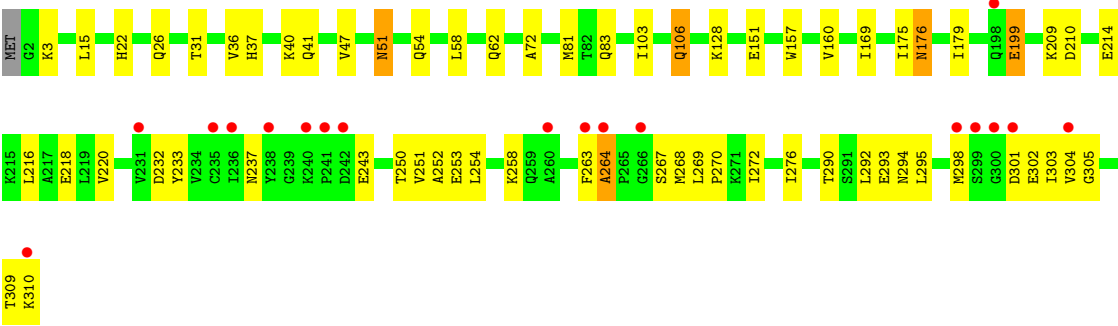


• Molecule 1: CARBAMATE KINASE 1



• 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	80.89Å 172.60Å 98.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.02 20.00 – 2.02	Depositor EDS
% Data completeness (in resolution range)	96.1 (20.00-2.02) 96.7 (20.00-2.02)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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	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)	0.36 , 47.1	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	0.95	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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	0.36	0/2337	0.91	5/3171 (0.2%)
1	B	0.34	0/2337	0.85	6/3171 (0.2%)
1	C	0.37	0/2337	0.88	6/3171 (0.2%)
1	D	0.35	0/2337	0.86	5/3171 (0.2%)
All	All	0.36	0/9348	0.88	22/12684 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	VAL	N-CA-C	7.56	120.68	108.97
1	C	234	VAL	N-CA-C	-7.45	99.99	109.30
1	A	231	VAL	N-CA-C	6.78	118.59	108.96
1	A	47	VAL	N-CA-C	6.74	119.14	108.89
1	B	234	VAL	N-CA-C	-6.42	101.27	109.30
1	C	47	VAL	N-CA-C	6.20	118.32	108.89
1	A	264	ALA	CA-C-N	6.12	125.61	119.24
1	A	264	ALA	C-N-CA	6.12	125.61	119.24
1	B	264	ALA	CA-C-N	6.11	126.55	119.47
1	B	264	ALA	C-N-CA	6.11	126.55	119.47
1	A	234	VAL	N-CA-C	-6.06	101.73	109.30
1	B	303	ILE	N-CA-C	6.05	112.69	106.21
1	D	47	VAL	N-CA-C	5.90	117.86	108.89
1	C	83	GLN	N-CA-C	-5.82	105.07	111.82
1	C	228	LEU	N-CA-C	5.26	118.64	110.17
1	D	83	GLN	N-CA-C	-5.25	105.73	111.82
1	B	83	GLN	N-CA-C	-5.18	105.81	111.82
1	C	70	ASN	CA-C-N	5.17	125.07	119.85
1	C	70	ASN	C-N-CA	5.17	125.07	119.85
1	D	54	GLN	N-CA-C	5.16	116.59	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	264	ALA	CA-C-N	5.05	125.08	119.32
1	D	264	ALA	C-N-CA	5.05	125.08	119.32

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	51	0
1	B	2302	0	2337	55	0
1	C	2302	0	2337	35	0
1	D	2302	0	2337	56	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
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	189	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 10.

All (189) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:ALA:HB2	1:C:310:LYS:HE3	1.56	0.88
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:A:81:MET:HE2	1:C:81:MET:HE2	1.60	0.81
1:B:81:MET:HE2	1:D:81:MET:HE2	1.62	0.80
1:B:298:MET:HE2	1:B:303:ILE:HA	1.62	0.79
1:B:58:LEU:HD13	1:D:81:MET:HE1	1.65	0.78
1:D:31:THR:HG23	1:D:292:LEU:HD21	1.66	0.78
1:B:143:MET:HE3	1:B:149:PHE:H	1.49	0.77
1:D:199:GLU:H	1:D:199:GLU:CD	1.93	0.76
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: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:HE21	1:D:106:GLN:HA	1.54	0.72
1:A:298:MET:HE2	1:A:303:ILE:HG22	1.72	0.72
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:A:81:MET:HE1	1:C:58:LEU:HD13	1.73	0.69
1:D:309:THR:O	1:D:310:LYS:HB2	1.91	0.69
1:B:81:MET:HE1	1:D:58:LEU:HD13	1.75	0.69
1:A:58:LEU:HD13	1:C:81:MET:HE1	1.77	0.67
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:17:ASN:CG	1:B:18:ASP:H	2.03	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:17:ASN:CG	1:C:18:ASP:H	2.06	0.62
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
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:B:199:GLU:H	1:B:199:GLU:CD	2.08	0.62
1:D:232:ASP:CG	1:D:294:ASN:HD21	2.08	0.61
1:A:199:GLU:H	1:A:199:GLU:CD	2.08	0.61
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:143:MET:HE3	1:A:149:PHE:H	1.69	0.58
1:A:298:MET:HE2	1:A:303:ILE:CG2	2.34	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:D:298:MET:HE3	1:D:303:ILE:HB	1.87	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: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: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:D:199:GLU:CD	1:D:199:GLU:N	2.64	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:C:298:MET:HE2	1:C:303:ILE:HB	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:C:293:GLU:H	1:C:293:GLU:CD	2.16	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:51:ASN:HD22	1:A:51:ASN:N	2.10	0.50
1:A:269:LEU:O	1:A:273:GLU:HG3	2.11	0.50
1:B:252:ALA:H	1:B:310:LYS:HD3	1.77	0.49
1:D:268:MET:O	1:D:272:ILE:HG12	2.13	0.49
1:A:252:ALA:H	1:A:310:LYS:HD3	1.77	0.48
1:B:269:LEU:HB3	1:B:270:PRO:HD3	1.95	0.48
1:B:293:GLU:H	1:B:293:GLU:CD	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:143:MET:HE3	1:A:148:ILE:HA	1.94	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:17:ASN:CG	1:B:18:ASP:N	2.72	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:C:17:ASN:CG	1:C:18:ASP:N	2.72	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:47:VAL:HG12	1:B:48:SER:N	2.30	0.47
1:B:216:LEU:O	1:B:220:VAL:HG22	2.15	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:B:81:MET:HE1	1:D:58:LEU:CD1	2.44	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:B:51:ASN:ND2	1:B:51:ASN:C	2.70	0.46
1:C:298:MET:CE	1:C:303:ILE:HB	2.45	0.46
1:D:51:ASN:C	1:D:51:ASN:ND2	2.72	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:B:81:MET:HE2	1:D:81:MET:HB3	1.98	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:GLN:O	1:B:29:VAL:HG23	2.17	0.44
1:D:51:ASN:HD22	1:D:51:ASN:N	2.14	0.44
1:C:51:ASN:HD22	1:C:51:ASN:N	2.15	0.44
1:B:288:ILE:HD13	1:B:303:ILE:HG21	2.00	0.44
1:D:15:LEU:C	1:D:15:LEU:HD23	2.43	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:22:HIS:O	1:D:26:GLN:HG3	2.18	0.44
1:D:176:ASN:ND2	1:D:220:VAL:HG12	2.33	0.44
1:D:298:MET:CE	1:D:303:ILE:HB	2.48	0.44
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:5:MET:HE2	1:A:226:VAL:HG21	2.00	0.43
1:A:15:LEU:C	1:A:15:LEU:HD23	2.44	0.43
1:C:250:THR:OG1	1:C:253:GLU:HG3	2.18	0.43
1:A:302:GLU:OE1	1:A:302:GLU:HA	2.19	0.43
1:C:51:ASN:HD22	1:C:51:ASN:C	2.27	0.43
1:D:51:ASN:C	1:D:51:ASN:HD22	2.27	0.42
1:D:175:ILE:O	1:D:179:ILE:HG13	2.19	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:293:GLU:H	1:A:293:GLU:CD	2.27	0.42
1:A:47:VAL:HG12	1:A:48:SER:N	2.35	0.42
1:A:298:MET:HG3	1:A:303:ILE:HG22	2.01	0.42
1:B:152:ASP:O	1:B:153:ALA:C	2.62	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:A:51:ASN:C	1:A:51:ASN:ND2	2.78	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:D:293:GLU:H	1:D:293:GLU:CD	2.27	0.41
1:A:34:TYR:CD1	1:A:296:GLY:HA3	2.55	0.41
1:A:114:VAL:CG2	1:A:192:GLY:HA3	2.50	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:B:51:ASN:C	1:B:51:ASN:HD22	2.27	0.41
1:C:51:ASN:C	1:C:51:ASN:ND2	2.75	0.41
1:D:169:ILE:HD12	1:D:216:LEU:HA	2.02	0.41
1:A:5:MET:HE1	1:A:298:MET:HE1	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:A:125:ASN:O	1:A:127:THR:HG23	2.21	0.41
1:B:298:MET:HE2	1:B:303:ILE:CA	2.42	0.41
1:C:233:TYR:OH	1:C:304:VAL:HG13	2.21	0.41
1:C:269:LEU:O	1:C:273:GLU:HG3	2.21	0.41
1:D:62:GLN:HB3	1:D:72:ALA:HB1	2.03	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:B:298:MET:HE2	1:B:303:ILE:HG12	2.02	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%)	18	10
1	B	307/310 (99%)	295 (96%)	12 (4%)	0	100	100
1	C	307/310 (99%)	296 (96%)	10 (3%)	1 (0%)	36	31
1	D	307/310 (99%)	297 (97%)	9 (3%)	1 (0%)	36	31
All	All	1228/1240 (99%)	1187 (97%)	37 (3%)	4 (0%)	36	31

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%)	73	75
1	B	248/249 (100%)	246 (99%)	2 (1%)	73	75
1	C	248/249 (100%)	245 (99%)	3 (1%)	63	65
1	D	248/249 (100%)	244 (98%)	4 (2%)	55	56
All	All	992/996 (100%)	981 (99%)	11 (1%)	65	68

All (11) 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	26	GLN
1	C	51	ASN
1	C	176	ASN
1	D	51	ASN
1	D	106	GLN
1	D	176	ASN
1	D	199	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	92	ASN
1	A	113	GLN
1	A	170	HIS
1	A	245	GLN
1	A	282	GLN
1	B	51	ASN
1	B	113	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	92	ASN
1	C	113	GLN
1	C	170	HIS
1	C	176	ASN
1	C	282	GLN
1	C	294	ASN
1	D	51	ASN
1	D	92	ASN
1	D	95	ASN
1	D	106	GLN
1	D	176	ASN
1	D	277	GLN
1	D	294	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	1313	-	4,4,4	1.85	2 (50%)	6,6,6	0.84	0
2	SO4	A	1312	-	4,4,4	1.86	2 (50%)	6,6,6	0.84	0
2	SO4	B	1314	-	4,4,4	1.84	2 (50%)	6,6,6	0.84	0
2	SO4	D	1314	-	4,4,4	1.85	2 (50%)	6,6,6	0.83	0
2	SO4	A	1314	-	4,4,4	1.86	2 (50%)	6,6,6	0.83	0
2	SO4	B	1312	-	4,4,4	1.84	2 (50%)	6,6,6	0.83	0
2	SO4	D	1313	-	4,4,4	1.84	2 (50%)	6,6,6	0.82	0
2	SO4	A	1311	-	4,4,4	1.82	2 (50%)	6,6,6	0.85	0
2	SO4	D	1311	-	4,4,4	1.82	2 (50%)	6,6,6	0.80	0
2	SO4	D	1312	-	4,4,4	1.87	2 (50%)	6,6,6	0.84	0
2	SO4	B	1311	-	4,4,4	1.82	2 (50%)	6,6,6	0.80	0
2	SO4	C	1313	-	4,4,4	1.81	2 (50%)	6,6,6	0.81	0
2	SO4	C	1312	-	4,4,4	1.86	2 (50%)	6,6,6	0.83	0
2	SO4	C	1311	-	4,4,4	1.83	2 (50%)	6,6,6	0.83	0
2	SO4	B	1313	-	4,4,4	1.81	2 (50%)	6,6,6	0.83	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	3.07	1.63	1.44
2	A	1314	SO4	O1-S	3.05	1.63	1.44
2	A	1312	SO4	O1-S	3.05	1.62	1.44
2	C	1312	SO4	O1-S	3.03	1.62	1.44
2	B	1314	SO4	O1-S	3.02	1.62	1.44
2	B	1312	SO4	O1-S	3.00	1.62	1.44
2	D	1314	SO4	O1-S	3.00	1.62	1.44
2	D	1313	SO4	O1-S	2.99	1.62	1.44
2	A	1313	SO4	O1-S	2.99	1.62	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1313	SO4	O1-S	2.96	1.62	1.44
2	B	1311	SO4	O1-S	2.92	1.62	1.44
2	D	1311	SO4	O1-S	2.92	1.62	1.44
2	C	1313	SO4	O1-S	2.92	1.62	1.44
2	C	1311	SO4	O1-S	2.87	1.61	1.44
2	A	1311	SO4	O1-S	2.86	1.61	1.44
2	C	1311	SO4	O3-S	-2.22	1.29	1.48
2	A	1311	SO4	O3-S	-2.19	1.30	1.48
2	D	1311	SO4	O3-S	-2.13	1.30	1.48
2	C	1312	SO4	O3-S	-2.12	1.30	1.48
2	A	1313	SO4	O3-S	-2.12	1.30	1.48
2	D	1314	SO4	O3-S	-2.11	1.30	1.48
2	A	1312	SO4	O3-S	-2.09	1.30	1.48
2	D	1312	SO4	O3-S	-2.09	1.31	1.48
2	B	1311	SO4	O3-S	-2.09	1.31	1.48
2	B	1312	SO4	O3-S	-2.08	1.31	1.48
2	D	1313	SO4	O3-S	-2.08	1.31	1.48
2	B	1314	SO4	O3-S	-2.08	1.31	1.48
2	C	1313	SO4	O3-S	-2.07	1.31	1.48
2	A	1314	SO4	O3-S	-2.07	1.31	1.48
2	B	1313	SO4	O3-S	-2.03	1.31	1.48

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%)	-0.08	10 (3%) 50 49	13, 24, 46, 60	0
1	B	309/310 (99%)	0.05	15 (4%) 35 34	14, 27, 50, 73	0
1	C	309/310 (99%)	-0.19	6 (1%) 66 66	13, 22, 43, 65	0
1	D	309/310 (99%)	0.04	18 (5%) 29 28	13, 24, 65, 80	0
All	All	1236/1240 (99%)	-0.04	49 (3%) 42 41	13, 24, 52, 80	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	303	ILE	6.3
1	A	264	ALA	4.9
1	B	304	VAL	4.7
1	D	266	GLY	4.5
1	A	303	ILE	4.3
1	D	260	ALA	4.0
1	C	145	ALA	3.4
1	C	146	GLY	3.2
1	D	238	TYR	3.1
1	D	242	ASP	3.1
1	A	304	VAL	3.0
1	D	301	ASP	3.0
1	B	300	GLY	3.0
1	D	300	GLY	2.9
1	D	304	VAL	2.8
1	B	310	LYS	2.7
1	D	241	PRO	2.7
1	A	260	ALA	2.6
1	B	99	ASN	2.6
1	B	264	ALA	2.6
1	D	310	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	235	CYS	2.6
1	B	145	ALA	2.6
1	B	265	PRO	2.4
1	D	299	SER	2.4
1	A	310	LYS	2.4
1	A	265	PRO	2.3
1	C	135	THR	2.3
1	C	144	GLN	2.3
1	D	198	GLN	2.3
1	C	142	ALA	2.3
1	A	17	ASN	2.2
1	D	240	LYS	2.2
1	B	293	GLU	2.2
1	B	302	GLU	2.2
1	D	264	ALA	2.2
1	D	263	PHE	2.1
1	C	153	ALA	2.1
1	B	266	GLY	2.1
1	B	17	ASN	2.1
1	B	301	ASP	2.1
1	B	297	SER	2.1
1	A	121	GLU	2.1
1	A	261	GLY	2.1
1	A	300	GLY	2.1
1	D	298	MET	2.0
1	D	236	ILE	2.0
1	D	231	VAL	2.0
1	B	143	MET	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	SO4	C	1312	5/5	0.79	0.18	86,87,87,87	0
2	SO4	A	1312	5/5	0.84	0.14	66,67,67,68	0
2	SO4	D	1312	5/5	0.87	0.17	62,62,62,63	0
2	SO4	D	1314	5/5	0.87	0.11	72,73,73,73	0
2	SO4	B	1312	5/5	0.90	0.09	80,80,80,80	0
2	SO4	B	1314	5/5	0.91	0.09	69,70,70,70	0
2	SO4	A	1314	5/5	0.93	0.08	55,56,57,57	0
2	SO4	D	1313	5/5	0.94	0.09	49,49,50,51	0
2	SO4	A	1313	5/5	0.96	0.08	34,35,37,40	0
2	SO4	B	1311	5/5	0.98	0.05	26,27,29,31	0
2	SO4	C	1311	5/5	0.98	0.05	21,24,26,27	0
2	SO4	B	1313	5/5	0.98	0.08	39,40,40,41	0
2	SO4	A	1311	5/5	0.99	0.05	22,23,24,24	0
2	SO4	C	1313	5/5	0.99	0.03	21,23,23,24	0
2	SO4	D	1311	5/5	0.99	0.05	19,23,24,26	0

6.5 Other polymers

There are no such residues in this entry.