



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:32 PM UTC

PDB ID : 3CT4 / pdb_00003ct4
Title : Structure of Dha-kinase subunit DhaK from L. Lactis
Authors : Jeckelmann, J.M.; Zurbriggen, A.; Christen, S.; Baumann, U.; Erni, B.
Deposited on : 2008-04-11
Resolution : 2.50 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

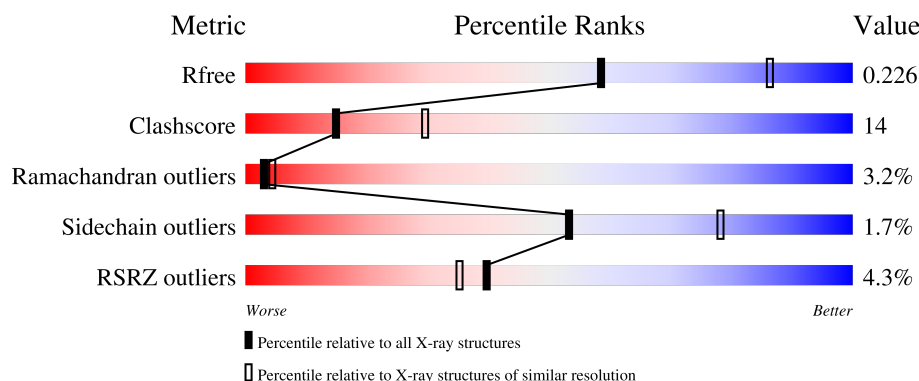
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

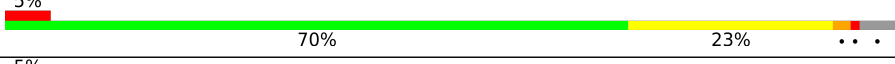
The reported resolution of this entry is 2.50 Å.

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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	332	
1	B	332	
1	C	332	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7703 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.

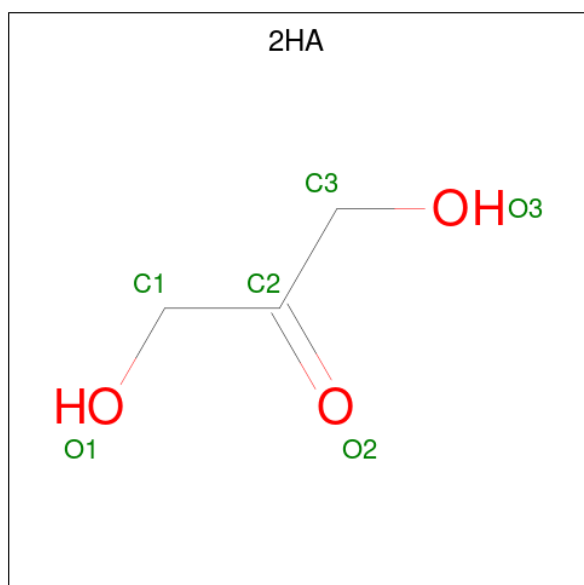
- Molecule 1 is a protein called PTS-dependent dihydroxyacetone kinase, dihydroxyacetone-binding subunit dhaK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2440	1549	395	482	14			
1	B	318	Total	C	N	O	S	0	0	0
			2440	1549	395	482	14			
1	C	318	Total	C	N	O	S	0	0	0
			2440	1549	395	482	14			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	GLU	LYS	SEE REMARK 999	UNP Q9CIV8
B	59	GLU	LYS	SEE REMARK 999	UNP Q9CIV8
C	59	GLU	LYS	SEE REMARK 999	UNP Q9CIV8

- Molecule 2 is Dihydroxyacetone (CCD ID: 2HA) (formula: $C_3H_6O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		

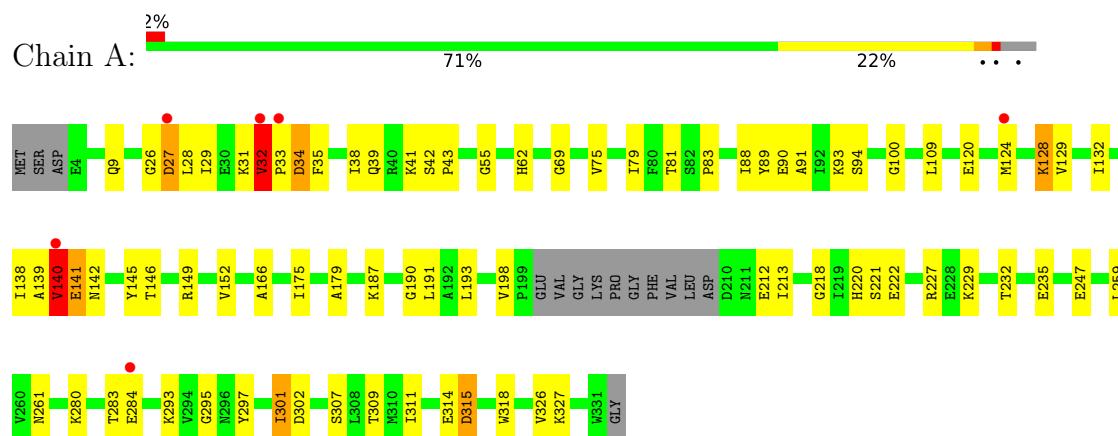
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	155	Total	O	0	0
			155	155		
3	B	77	Total	O	0	0
			77	77		
3	C	133	Total	O	0	0
			133	133		

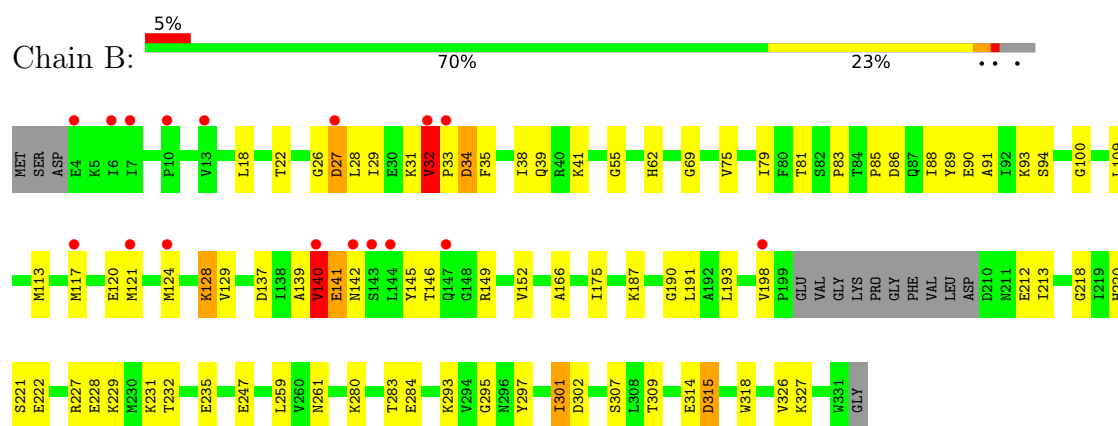
3 Residue-property plots

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.

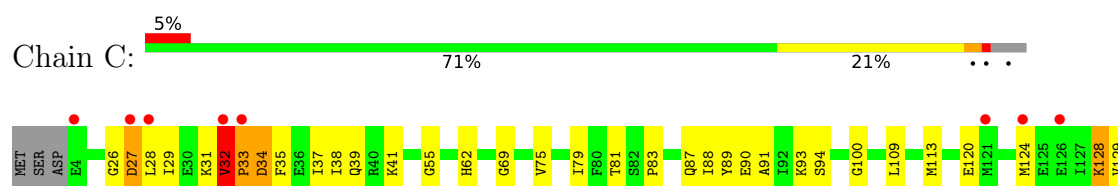
- Molecule 1: PTS-dependent dihydroxyacetone kinase, dihydroxyacetone-binding subunit dhaK

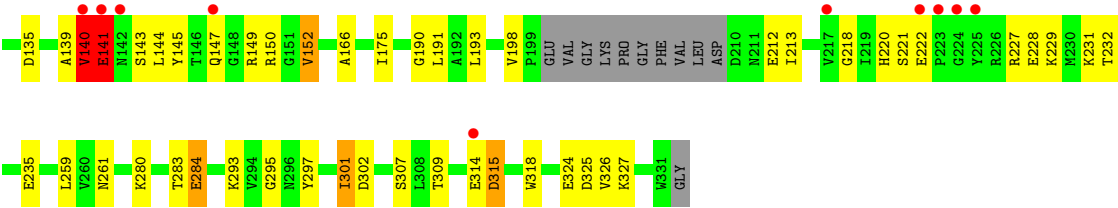


- Molecule 1: PTS-dependent dihydroxyacetone kinase, dihydroxyacetone-binding subunit dhaK



- Molecule 1: PTS-dependent dihydroxyacetone kinase, dihydroxyacetone-binding subunit dhaK





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	107.80Å 107.80Å 142.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.37 – 2.50 44.37 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (44.37-2.50) 98.7 (44.37-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 2.51Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.200 , 0.267 (Not available) , 0.226	Depositor DCC
R_{free} test set	1714 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7703	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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 50.60 % 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 6.3195e-05. 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: 2HA

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	0.39	0/2475	0.77	4/3336 (0.1%)
1	B	0.36	0/2475	0.76	3/3336 (0.1%)
1	C	0.39	0/2475	0.77	4/3336 (0.1%)
All	All	0.38	0/7425	0.77	11/10008 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	VAL	CA-C-N	9.22	131.36	119.84
1	A	32	VAL	C-N-CA	9.22	131.36	119.84
1	C	32	VAL	CA-C-N	9.16	131.29	119.84
1	C	32	VAL	C-N-CA	9.16	131.29	119.84
1	B	32	VAL	CA-C-N	9.14	131.26	119.84
1	B	32	VAL	C-N-CA	9.14	131.26	119.84
1	B	34	ASP	N-CA-C	-5.53	106.38	114.39
1	C	140	VAL	CB-CA-C	-5.47	102.32	111.29
1	C	34	ASP	N-CA-C	-5.31	106.69	114.39
1	A	140	VAL	N-CA-C	5.23	120.22	109.34
1	A	34	ASP	N-CA-C	-5.04	107.09	114.39

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	140	VAL	Peptide
1	C	140	VAL	Peptide

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	2440	0	2453	61	0
1	B	2440	0	2453	69	0
1	C	2440	0	2453	79	0
2	A	6	0	6	0	0
2	B	6	0	6	0	0
2	C	6	0	6	0	0
3	A	155	0	0	5	0
3	B	77	0	0	4	0
3	C	133	0	0	7	0
All	All	7703	0	7377	203	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 14.

All (203) 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:86:ASP:HB3	1:C:145:TYR:OH	1.76	0.84
1:B:75:VAL:HG23	1:B:83:PRO:HG2	1.60	0.84
1:A:75:VAL:HG23	1:A:83:PRO:HG2	1.61	0.83
1:C:75:VAL:HG23	1:C:83:PRO:HG2	1.61	0.82
1:C:314:GLU:HA	3:C:513:HOH:O	1.80	0.80
1:A:27:ASP:HA	3:A:471:HOH:O	1.80	0.78
1:A:32:VAL:O	1:A:34:ASP:N	2.16	0.78
1:C:32:VAL:O	1:C:34:ASP:N	2.15	0.78
1:B:32:VAL:O	1:B:34:ASP:N	2.16	0.77
1:A:31:LYS:HZ2	1:A:91:ALA:HA	1.51	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:LEU:HD22	1:C:213:ILE:HG22	1.68	0.76
1:A:193:LEU:HD22	1:A:213:ILE:HG22	1.68	0.75
1:C:31:LYS:HE2	1:C:39:GLN:OE1	1.86	0.75
1:C:27:ASP:HA	3:C:505:HOH:O	1.88	0.74
1:B:193:LEU:HD22	1:B:213:ILE:HG22	1.70	0.73
1:A:31:LYS:HE2	1:A:39:GLN:OE1	1.88	0.72
1:B:31:LYS:NZ	1:B:91:ALA:HA	2.06	0.71
1:A:280:LYS:O	1:A:283:THR:HG22	1.91	0.71
1:B:31:LYS:HE2	1:B:39:GLN:OE1	1.89	0.71
1:B:117:MET:HA	1:C:113:MET:HE1	1.73	0.71
1:C:280:LYS:O	1:C:283:THR:HG22	1.90	0.71
1:B:280:LYS:O	1:B:283:THR:HG22	1.91	0.70
1:C:31:LYS:NZ	1:C:91:ALA:HA	2.07	0.69
1:A:31:LYS:NZ	1:A:91:ALA:HA	2.07	0.69
1:A:29:ILE:HG23	1:A:41:LYS:HE3	1.75	0.68
1:C:29:ILE:CG2	1:C:41:LYS:HE3	2.24	0.68
1:A:29:ILE:CG2	1:A:41:LYS:HE3	2.23	0.68
1:C:29:ILE:HG23	1:C:41:LYS:HE3	1.75	0.67
1:C:31:LYS:HZ2	1:C:94:SER:HB3	1.61	0.66
1:B:29:ILE:HG23	1:B:41:LYS:HE3	1.77	0.66
1:B:29:ILE:CG2	1:B:41:LYS:HE3	2.26	0.65
1:B:79:ILE:HG21	1:B:198:VAL:HG13	1.79	0.65
1:C:79:ILE:HG21	1:C:198:VAL:HG13	1.80	0.64
1:B:120:GLU:OE2	1:C:147:GLN:NE2	2.27	0.64
3:B:385:HOH:O	1:C:144:LEU:HB3	1.99	0.63
1:B:121:MET:HB3	3:B:385:HOH:O	1.99	0.63
1:B:31:LYS:HZ2	1:B:94:SER:HB3	1.62	0.62
1:C:87:GLN:HG3	3:C:502:HOH:O	1.99	0.62
1:B:117:MET:HE3	1:C:109:LEU:HD23	1.82	0.60
1:A:79:ILE:HG21	1:A:198:VAL:HG13	1.83	0.60
1:A:232:THR:CG2	1:A:235:GLU:H	2.15	0.60
1:A:120:GLU:HG2	1:A:124:MET:HE3	1.84	0.59
1:A:31:LYS:NZ	1:A:94:SER:HB3	2.18	0.59
1:A:141:GLU:N	3:A:481:HOH:O	2.36	0.59
1:B:31:LYS:NZ	1:B:94:SER:HB3	2.17	0.59
1:B:31:LYS:HZ2	1:B:91:ALA:HA	1.67	0.59
1:C:31:LYS:NZ	1:C:94:SER:HB3	2.16	0.59
1:C:120:GLU:HG2	1:C:124:MET:HE3	1.84	0.58
1:B:31:LYS:O	1:B:32:VAL:C	2.46	0.58
1:A:212:GLU:HG2	1:A:229:LYS:HD3	1.84	0.57
1:B:212:GLU:HG2	1:B:229:LYS:HD3	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:LYS:O	1:C:32:VAL:C	2.46	0.57
1:C:139:ALA:O	1:C:140:VAL:HB	2.04	0.57
1:B:120:GLU:HG2	1:B:124:MET:HE3	1.85	0.57
1:C:31:LYS:HZ2	1:C:91:ALA:HA	1.70	0.57
1:C:212:GLU:HG2	1:C:229:LYS:HD3	1.87	0.56
1:A:31:LYS:O	1:A:32:VAL:C	2.49	0.56
1:A:69:GLY:HA3	1:A:326:VAL:HG12	1.87	0.56
1:C:314:GLU:O	1:C:315:ASP:HB2	2.05	0.55
1:C:232:THR:HG22	1:C:235:GLU:HG3	1.87	0.55
1:B:69:GLY:HA3	1:B:326:VAL:HG12	1.87	0.55
1:B:232:THR:CG2	1:B:235:GLU:H	2.19	0.55
1:C:232:THR:CG2	1:C:235:GLU:H	2.20	0.55
1:A:28:LEU:HD23	1:A:38:ILE:CG2	2.36	0.54
1:B:142:ASN:HA	1:B:146:THR:O	2.07	0.54
1:B:232:THR:HG23	1:B:235:GLU:H	1.73	0.54
1:B:314:GLU:O	1:B:315:ASP:HB2	2.06	0.54
1:C:28:LEU:HD23	1:C:38:ILE:CG2	2.38	0.54
1:A:232:THR:HG23	1:A:235:GLU:H	1.71	0.54
1:B:232:THR:HG22	1:B:235:GLU:HG3	1.88	0.54
1:C:232:THR:HG23	1:C:235:GLU:H	1.73	0.54
1:A:314:GLU:O	1:A:315:ASP:HB2	2.06	0.54
1:B:75:VAL:HG23	1:B:75:VAL:O	2.08	0.53
1:B:28:LEU:HD23	1:B:38:ILE:CG2	2.38	0.53
1:A:35:PHE:CZ	1:A:90:GLU:HG3	2.43	0.53
1:A:27:ASP:C	1:A:28:LEU:HD12	2.34	0.53
1:C:35:PHE:CZ	1:C:90:GLU:HG3	2.44	0.53
1:C:27:ASP:C	1:C:28:LEU:HD12	2.34	0.53
1:C:31:LYS:HZ1	1:C:91:ALA:HA	1.74	0.53
1:A:75:VAL:HG23	1:A:75:VAL:O	2.09	0.53
1:A:187:LYS:HE2	3:A:346:HOH:O	2.07	0.53
1:C:75:VAL:HG23	1:C:75:VAL:O	2.08	0.52
1:B:100:GLY:HA2	1:B:128:LYS:HD2	1.92	0.52
1:C:326:VAL:O	1:C:327:LYS:HD3	2.10	0.52
1:B:137:ASP:O	1:B:149:ARG:HB3	2.10	0.52
1:B:193:LEU:HD22	1:B:213:ILE:CG2	2.38	0.51
1:C:301:ILE:HG22	1:C:302:ASP:N	2.24	0.51
1:B:31:LYS:HZ1	1:B:91:ALA:HA	1.74	0.51
1:B:35:PHE:CZ	1:B:90:GLU:HG3	2.44	0.51
1:C:100:GLY:HA2	1:C:128:LYS:HD2	1.93	0.51
1:C:141:GLU:HB3	1:C:150:ARG:NH1	2.24	0.51
1:C:28:LEU:HD12	1:C:28:LEU:N	2.26	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:LEU:HD22	1:C:213:ILE:CG2	2.38	0.51
1:B:27:ASP:C	1:B:28:LEU:HD12	2.36	0.51
1:A:193:LEU:HD22	1:A:213:ILE:CG2	2.38	0.51
1:B:212:GLU:OE1	1:B:227:ARG:HD3	2.11	0.50
1:C:69:GLY:HA3	1:C:326:VAL:HG12	1.92	0.50
1:A:28:LEU:HD12	1:A:28:LEU:N	2.26	0.50
1:A:100:GLY:HA2	1:A:128:LYS:HD2	1.93	0.50
1:B:327:LYS:NZ	3:B:391:HOH:O	2.44	0.50
1:B:55:GLY:HA2	1:B:81:THR:O	2.11	0.50
1:B:145:TYR:O	1:B:146:THR:C	2.52	0.50
1:C:212:GLU:OE1	1:C:227:ARG:HD3	2.11	0.50
1:C:232:THR:HG22	1:C:235:GLU:CG	2.41	0.50
1:C:140:VAL:O	1:C:141:GLU:C	2.55	0.50
1:A:326:VAL:O	1:A:327:LYS:HD3	2.12	0.49
1:B:28:LEU:HD12	1:B:28:LEU:N	2.27	0.49
1:C:141:GLU:HG2	1:C:150:ARG:HD3	1.94	0.49
1:C:190:GLY:HA2	1:C:307:SER:HA	1.94	0.49
1:A:128:LYS:H	1:A:128:LYS:CD	2.25	0.49
1:B:191:LEU:C	1:B:191:LEU:HD12	2.38	0.49
1:B:301:ILE:HG22	1:B:302:ASP:N	2.28	0.49
1:B:232:THR:HG22	1:B:235:GLU:CG	2.42	0.49
1:A:191:LEU:C	1:A:191:LEU:HD12	2.38	0.49
1:A:187:LYS:HG3	1:A:247:GLU:HG2	1.95	0.48
1:C:128:LYS:H	1:C:128:LYS:CD	2.26	0.48
1:B:326:VAL:O	1:B:327:LYS:HD3	2.14	0.48
1:A:190:GLY:HA2	1:A:307:SER:HA	1.96	0.48
1:A:139:ALA:O	1:A:140:VAL:HB	2.14	0.48
1:B:187:LYS:HG3	1:B:247:GLU:HG2	1.95	0.48
1:A:212:GLU:OE1	1:A:227:ARG:HD3	2.15	0.47
1:B:190:GLY:HA2	1:B:307:SER:HA	1.96	0.47
1:C:140:VAL:CG1	1:C:141:GLU:N	2.76	0.47
1:A:9:GLN:HB2	3:A:345:HOH:O	2.13	0.47
1:B:213:ILE:C	1:B:213:ILE:HD12	2.39	0.47
1:A:109:LEU:HD22	1:A:145:TYR:HB3	1.97	0.47
1:C:191:LEU:HD12	1:C:191:LEU:C	2.39	0.47
1:B:109:LEU:O	1:B:113:MET:HG2	2.15	0.47
1:A:89:TYR:CZ	1:A:93:LYS:HD3	2.49	0.46
1:A:138:ILE:HG22	1:A:149:ARG:NH1	2.30	0.46
1:A:142:ASN:HA	1:A:146:THR:O	2.16	0.46
1:A:75:VAL:HG21	1:A:88:ILE:HG12	1.97	0.46
1:C:318:TRP:CD1	1:C:318:TRP:N	2.84	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ILE:HG22	3:A:478:HOH:O	2.15	0.46
1:A:31:LYS:HZ3	1:A:94:SER:HB3	1.81	0.46
1:A:293:LYS:HE3	1:A:297:TYR:CZ	2.51	0.46
1:B:259:LEU:HB3	1:B:309:THR:HB	1.98	0.46
1:C:33:PRO:HG3	3:C:504:HOH:O	2.16	0.46
1:B:128:LYS:CD	1:B:128:LYS:H	2.27	0.46
1:C:150:ARG:HD2	3:C:393:HOH:O	2.15	0.46
1:A:28:LEU:HD23	1:A:38:ILE:HG21	1.96	0.46
1:B:85:PRO:HB3	1:B:117:MET:HG2	1.97	0.46
1:A:232:THR:HG22	1:A:235:GLU:HG3	1.97	0.45
1:A:301:ILE:HG22	1:A:302:ASP:N	2.32	0.45
1:A:213:ILE:C	1:A:213:ILE:HD12	2.41	0.45
1:B:293:LYS:HE3	1:B:297:TYR:CZ	2.51	0.45
1:B:27:ASP:HA	3:B:395:HOH:O	2.15	0.45
1:B:139:ALA:O	1:B:140:VAL:HB	2.17	0.45
1:C:140:VAL:O	1:C:141:GLU:O	2.33	0.45
1:C:152:VAL:HB	3:C:490:HOH:O	2.15	0.45
1:C:315:ASP:HB2	3:C:433:HOH:O	2.17	0.45
1:A:55:GLY:HA2	1:A:81:THR:O	2.17	0.45
1:B:75:VAL:HG21	1:B:88:ILE:HG12	1.99	0.45
1:B:140:VAL:O	1:B:141:GLU:O	2.34	0.45
1:C:89:TYR:CZ	1:C:93:LYS:HD3	2.52	0.45
1:B:89:TYR:CZ	1:B:93:LYS:HD3	2.51	0.45
1:B:220:HIS:O	1:B:221:SER:HB2	2.17	0.45
1:C:218:GLY:HA3	1:C:222:GLU:HB2	2.00	0.44
1:A:90:GLU:OE1	1:A:93:LYS:HE3	2.17	0.44
1:B:28:LEU:HD23	1:B:38:ILE:HG21	1.98	0.44
1:B:218:GLY:HA3	1:B:222:GLU:HB2	2.00	0.44
1:A:232:THR:HG22	1:A:235:GLU:CG	2.48	0.44
1:C:75:VAL:HG21	1:C:88:ILE:HG12	2.00	0.44
1:A:42:SER:HA	1:A:43:PRO:HD3	1.92	0.44
1:A:218:GLY:HA3	1:A:222:GLU:HB2	2.00	0.44
1:C:28:LEU:HD23	1:C:38:ILE:HG21	1.98	0.44
1:B:18:LEU:O	1:B:22:THR:HG23	2.18	0.43
1:A:311:ILE:O	1:A:311:ILE:HG23	2.19	0.43
1:C:90:GLU:OE1	1:C:93:LYS:HE3	2.18	0.43
1:C:140:VAL:HG13	1:C:141:GLU:CA	2.49	0.43
1:A:261:ASN:HA	1:A:295:GLY:O	2.19	0.43
1:C:284:GLU:H	1:C:284:GLU:HG2	1.45	0.43
1:A:259:LEU:HB3	1:A:309:THR:HB	2.01	0.43
1:C:220:HIS:O	1:C:221:SER:HB2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:GLY:HA2	1:C:81:THR:O	2.19	0.42
1:A:220:HIS:O	1:A:221:SER:HB2	2.19	0.42
1:C:166:ALA:HA	1:C:175:ILE:HD11	2.02	0.42
1:A:132:ILE:HG12	1:A:179:ALA:HB1	2.01	0.42
1:B:117:MET:HE3	1:C:109:LEU:HB3	2.01	0.42
1:B:166:ALA:HA	1:B:175:ILE:HD11	2.02	0.42
1:B:261:ASN:HA	1:B:295:GLY:O	2.20	0.42
1:B:318:TRP:N	1:B:318:TRP:CD1	2.86	0.42
1:C:261:ASN:HA	1:C:295:GLY:O	2.20	0.41
1:C:293:LYS:HE3	1:C:297:TYR:CZ	2.55	0.41
1:C:140:VAL:HG13	1:C:141:GLU:N	2.35	0.41
1:C:229:LYS:HD3	1:C:229:LYS:HA	1.81	0.41
1:C:324:GLU:HG3	1:C:325:ASP:N	2.35	0.41
1:A:166:ALA:HA	1:A:175:ILE:HD11	2.02	0.41
1:B:18:LEU:HD22	1:B:38:ILE:HD11	2.01	0.41
1:B:117:MET:HG3	1:C:109:LEU:CD2	2.50	0.41
1:C:228:GLU:HG2	1:C:231:LYS:HD3	2.02	0.41
1:B:229:LYS:HD3	1:B:229:LYS:HA	1.80	0.41
1:C:141:GLU:HB3	1:C:150:ARG:CZ	2.50	0.41
1:C:141:GLU:HB2	1:C:143:SER:HB3	2.02	0.41
1:C:213:ILE:HD12	1:C:213:ILE:C	2.45	0.41
1:A:109:LEU:HD22	1:A:145:TYR:CB	2.51	0.41
1:C:259:LEU:HB3	1:C:309:THR:HB	2.02	0.41
1:B:90:GLU:OE1	1:B:93:LYS:HE3	2.22	0.41
1:C:31:LYS:HE3	1:C:37:ILE:HG21	2.03	0.40
1:A:318:TRP:CD1	1:A:318:TRP:N	2.88	0.40
1:B:228:GLU:HG2	1:B:231:LYS:HD3	2.02	0.40
1:C:135:ASP:HB2	1:C:149:ARG:HB2	2.03	0.40
1:C:31:LYS:HE3	1:C:37:ILE:CG2	2.51	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	314/332 (95%)	292 (93%)	12 (4%)	10 (3%)	3	4
1	B	314/332 (95%)	289 (92%)	15 (5%)	10 (3%)	3	4
1	C	314/332 (95%)	293 (93%)	11 (4%)	10 (3%)	3	4
All	All	942/996 (95%)	874 (93%)	38 (4%)	30 (3%)	3	4

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	ASP
1	A	33	PRO
1	A	140	VAL
1	A	141	GLU
1	B	27	ASP
1	B	33	PRO
1	B	140	VAL
1	B	141	GLU
1	C	27	ASP
1	C	33	PRO
1	C	140	VAL
1	A	26	GLY
1	A	62	HIS
1	A	315	ASP
1	B	26	GLY
1	B	62	HIS
1	B	315	ASP
1	C	26	GLY
1	C	62	HIS
1	C	141	GLU
1	C	315	ASP
1	A	32	VAL
1	B	32	VAL
1	B	301	ILE
1	C	32	VAL
1	A	301	ILE
1	C	301	ILE
1	A	152	VAL
1	B	152	VAL
1	C	152	VAL

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	262/273 (96%)	258 (98%)	4 (2%)	57	80
1	B	262/273 (96%)	258 (98%)	4 (2%)	57	80
1	C	262/273 (96%)	257 (98%)	5 (2%)	50	76
All	All	786/819 (96%)	773 (98%)	13 (2%)	53	78

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	VAL
1	A	128	LYS
1	A	129	VAL
1	A	284	GLU
1	B	32	VAL
1	B	128	LYS
1	B	129	VAL
1	B	284	GLU
1	C	32	VAL
1	C	128	LYS
1	C	129	VAL
1	C	141	GLU
1	C	284	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	317	GLN
1	B	9	GLN
1	B	317	GLN
1	C	9	GLN
1	C	271	GLN
1	C	296	ASN
1	C	317	GLN

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 ⓘ

3 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	2HA	C	333	-	5,5,5	5.13	1 (20%)	4,5,5	4.80	2 (50%)
2	2HA	A	333	-	5,5,5	5.21	1 (20%)	4,5,5	5.14	2 (50%)
2	2HA	B	333	-	5,5,5	5.20	1 (20%)	4,5,5	5.68	2 (50%)

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	2HA	C	333	-	-	2/4/4/4	-
2	2HA	A	333	-	-	2/4/4/4	-
2	2HA	B	333	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	333	2HA	O2-C2	11.54	1.42	1.21
2	B	333	2HA	O2-C2	11.53	1.42	1.21
2	C	333	2HA	O2-C2	11.37	1.41	1.21

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	333	2HA	O2-C2-C1	-8.00	108.14	120.91
2	B	333	2HA	O2-C2-C3	-7.63	108.73	120.91
2	A	333	2HA	O2-C2-C3	-7.41	109.08	120.91
2	A	333	2HA	O2-C2-C1	-6.64	110.30	120.91
2	C	333	2HA	O2-C2-C3	-6.62	110.33	120.91
2	C	333	2HA	O2-C2-C1	-6.51	110.51	120.91

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	333	2HA	O1-C1-C2-O2
2	A	333	2HA	O2-C2-C3-O3
2	B	333	2HA	O1-C1-C2-O2
2	B	333	2HA	O2-C2-C3-O3
2	C	333	2HA	O1-C1-C2-O2
2	C	333	2HA	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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	318/332 (95%)	-0.30	6 (1%) 66 62	15, 29, 66, 128	0
1	B	318/332 (95%)	0.17	17 (5%) 32 28	25, 40, 81, 133	0
1	C	318/332 (95%)	-0.13	18 (5%) 29 26	18, 31, 75, 129	0
All	All	954/996 (95%)	-0.08	41 (4%) 40 35	15, 33, 73, 133	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	140	VAL	6.8
1	C	222	GLU	5.8
1	A	32	VAL	4.8
1	C	223	PRO	4.6
1	B	140	VAL	4.6
1	C	140	VAL	4.3
1	C	32	VAL	4.2
1	C	225	TYR	4.0
1	B	33	PRO	3.9
1	B	143	SER	3.8
1	B	32	VAL	3.7
1	B	10	PRO	3.6
1	C	27	ASP	3.3
1	A	284	GLU	3.2
1	A	33	PRO	3.2
1	B	117	MET	3.1
1	B	147	GLN	3.1
1	C	124	MET	3.0
1	C	141	GLU	3.0
1	C	147	GLN	2.9
1	B	4	GLU	2.9
1	B	6	ILE	2.8
1	A	124	MET	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	224	GLY	2.7
1	C	33	PRO	2.7
1	B	142	ASN	2.6
1	B	198	VAL	2.6
1	B	124	MET	2.5
1	A	27	ASP	2.4
1	B	7	ILE	2.4
1	B	27	ASP	2.4
1	C	126	GLU	2.3
1	C	314	GLU	2.3
1	C	4	GLU	2.3
1	B	144	LEU	2.2
1	C	142	ASN	2.1
1	C	121	MET	2.1
1	C	217	VAL	2.1
1	C	28	LEU	2.1
1	B	121	MET	2.1
1	B	13	VAL	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(Å ²)	Q<0.9
2	2HA	B	333	6/6	0.96	0.06	16,29,34,47	0
2	2HA	C	333	6/6	0.98	0.04	14,22,25,42	0
2	2HA	A	333	6/6	0.99	0.04	13,18,21,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.