



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:16 am BST

PDB ID : 1V19  
Title : 2-KETO-3-DEOXYGLUCONATE KINASE FROM THERMUS THERMOPHILUS  
Authors : Tahirov, T.H.; Inagaki, E.  
Deposited on : 2004-04-12  
Resolution : 2.30 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

<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

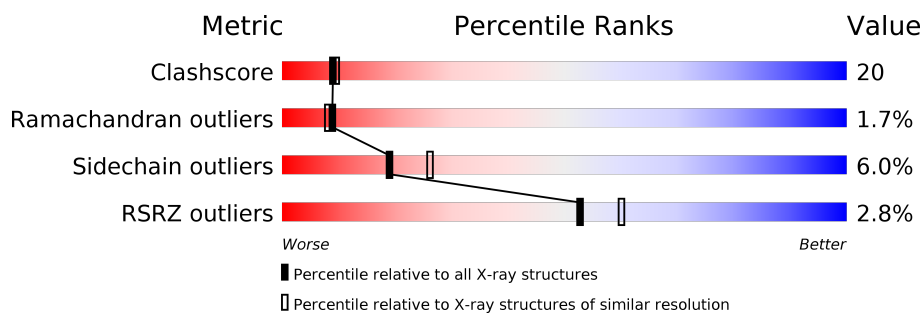
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 2.30 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))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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	309	 2% 63% 30% . .
1	B	309	 4% 61% 34% . .

## 2 Entry composition [i](#)

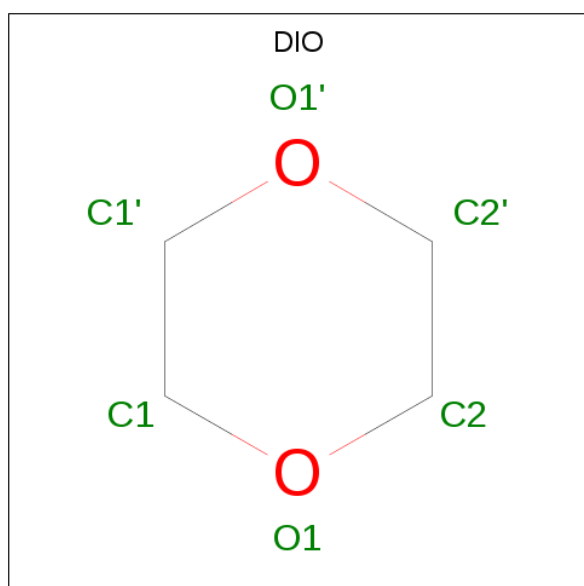
There are 3 unique types of molecules in this entry. The entry contains 4709 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2-KETO-3-DEOXYGLUCONATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	0	1
			2297	1465	410	419	3			
1	B	302	Total	C	N	O	S	0	0	1
			2297	1465	410	419	3			

- Molecule 2 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	4	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	57	Total	O	0	0
			57	57		

*Continued on next page...*

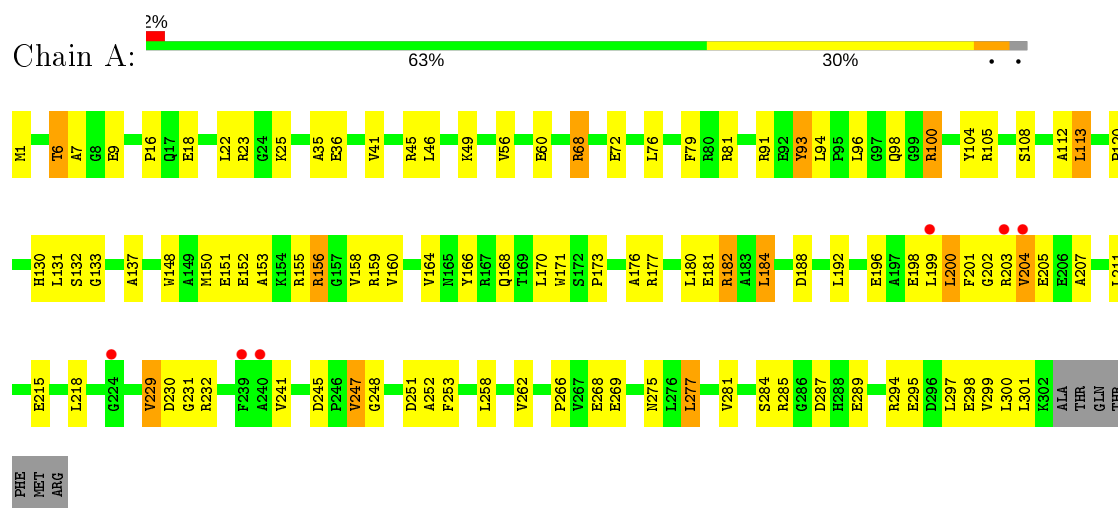
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	52	Total	O	0	0
			52	52		

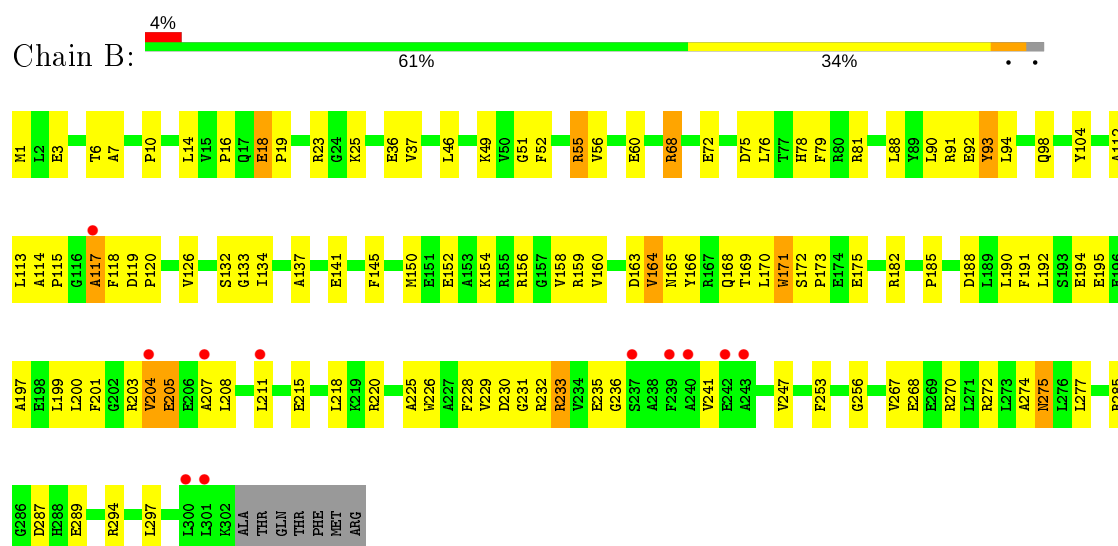
### 3 Residue-property plots

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: 2-KETO-3-DEOXYGLUCONATE KINASE



#### • Molecule 1: 2-KETO-3-DEOXYGLUCONATE KINASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.83Å 84.83Å 168.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.62 – 2.30 44.62 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.8 (44.62-2.30) 98.6 (44.62-2.25)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.22 (at 2.24Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.153 , 0.198 0.158 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.6	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 52.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.239 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4709	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DIO

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	0.40	0/2345	0.62	0/3179
1	B	0.38	0/2345	0.63	0/3179
All	All	0.39	0/4690	0.62	0/6358

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

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	2297	0	2298	85	0
1	B	2297	0	2298	104	0
2	A	6	0	8	2	0
3	A	57	0	0	6	0
3	B	52	0	0	10	0
All	All	4709	0	4604	186	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 20.

All (186) 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:267:VAL:HG22	1:B:270:ARG:NH2	1.88	0.89
1:B:55:ARG:HD3	3:B:2023:HOH:O	1.73	0.87
1:B:120:PRO:HB3	1:B:152:GLU:HG2	1.57	0.86
1:B:91:ARG:HD2	1:B:247:VAL:HG21	1.56	0.85
1:B:36:GLU:OE1	1:B:132:SER:HB3	1.76	0.85
1:B:285:ARG:HD2	3:B:2040:HOH:O	1.79	0.83
1:B:267:VAL:HG22	1:B:270:ARG:HH21	1.44	0.81
1:B:134:ILE:HG23	1:B:170:LEU:HD11	1.60	0.81
1:A:199:LEU:HD23	1:A:199:LEU:O	1.81	0.80
1:B:194:GLU:HG3	1:B:220:ARG:HG2	1.65	0.77
1:A:91:ARG:HD2	1:A:247:VAL:HG21	1.65	0.76
1:A:120:PRO:HB3	1:A:152:GLU:HG2	1.67	0.76
1:B:16:PRO:HB3	1:B:25:LYS:HG3	1.68	0.74
1:B:93:TYR:CZ	3:B:2026:HOH:O	2.40	0.74
1:B:152:GLU:HG3	1:B:156:ARG:NH2	2.03	0.73
1:B:3:GLU:HG3	1:B:49:LYS:HB2	1.70	0.73
1:A:68:ARG:HE	1:A:68:ARG:HA	1.54	0.73
1:B:199:LEU:HD23	1:B:199:LEU:O	1.89	0.72
1:B:46:LEU:HD11	1:B:277:LEU:HD21	1.70	0.72
1:A:120:PRO:HB3	1:A:152:GLU:CG	2.21	0.71
1:A:166:TYR:CE2	1:A:168:GLN:HG2	2.24	0.71
1:A:36:GLU:OE1	1:A:132:SER:HB3	1.92	0.69
1:B:46:LEU:HD22	1:B:297:LEU:HD11	1.75	0.69
1:B:166:TYR:CE2	1:B:168:GLN:HG2	2.27	0.69
1:B:56:VAL:HG23	1:B:81:ARG:HG2	1.76	0.68
1:B:94:LEU:HG	1:B:98:GLN:O	1.95	0.67
1:B:173:PRO:HB3	1:B:200:LEU:HD23	1.76	0.67
1:A:56:VAL:HG23	1:A:81:ARG:HG2	1.79	0.65
1:B:201:PHE:CZ	1:B:211:LEU:HD21	2.31	0.65
1:A:266:PRO:HD2	1:A:269:GLU:CD	2.16	0.65
1:A:297:LEU:O	1:A:301:LEU:HB2	1.96	0.65
1:A:184:LEU:HD13	1:A:184:LEU:O	1.97	0.64
1:A:16:PRO:HB3	1:A:25:LYS:HG3	1.78	0.64
1:A:152:GLU:HG3	1:A:156:ARG:NH2	2.13	0.63
1:B:10:PRO:HB3	1:B:37:VAL:HG21	1.78	0.63
1:B:68:ARG:HB2	3:B:2016:HOH:O	1.99	0.62
1:A:105:ARG:NH2	1:A:170:LEU:HD21	2.14	0.62
1:A:60:GLU:OE2	1:B:23:ARG:HB3	2.00	0.61
1:B:56:VAL:CG2	1:B:81:ARG:HG2	2.30	0.61
1:B:6:THR:OG1	1:B:36:GLU:HB3	2.00	0.61
1:A:6:THR:HG23	1:A:130:HIS:HB3	1.81	0.61
1:A:7:ALA:O	1:A:36:GLU:HG2	2.01	0.61

Continued on next page...



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:ASP:C	1:B:232:ARG:H	2.03	0.61
1:B:55:ARG:NH2	1:B:78:HIS:O	2.34	0.61
1:B:152:GLU:O	1:B:156:ARG:HD3	2.02	0.60
1:B:192:LEU:HD21	1:B:197:ALA:HB2	1.83	0.59
1:A:150:MET:HB2	1:A:160:VAL:HG21	1.83	0.59
1:A:35:ALA:HA	1:A:251:ASP:OD1	2.03	0.59
1:A:1:MET:O	1:A:49:LYS:HD3	2.03	0.58
1:B:14:LEU:HB2	1:B:90:LEU:HG	1.84	0.58
1:B:137:ALA:HB1	1:B:170:LEU:HB3	1.85	0.58
1:A:285:ARG:O	1:A:289:GLU:HB2	2.04	0.57
1:B:7:ALA:O	1:B:36:GLU:HG2	2.04	0.57
1:B:117:ALA:HB3	1:B:145:PHE:CE1	2.40	0.57
1:B:229:VAL:HG21	1:B:267:VAL:HG21	1.85	0.57
1:A:130:HIS:O	1:A:131:LEU:HD23	2.05	0.57
1:B:241:VAL:HG21	3:B:2044:HOH:O	2.05	0.56
1:B:91:ARG:CD	1:B:247:VAL:HG21	2.34	0.56
1:A:173:PRO:HB3	1:A:200:LEU:HD12	1.88	0.56
1:A:91:ARG:CD	1:A:247:VAL:HG21	2.34	0.56
1:B:37:VAL:HG23	3:B:2011:HOH:O	2.05	0.56
1:B:241:VAL:HG11	3:B:2044:HOH:O	2.06	0.55
1:A:252:ALA:HB2	1:A:281:VAL:HG21	1.88	0.55
1:A:230:ASP:C	1:A:232:ARG:H	2.09	0.55
1:B:93:TYR:CE1	3:B:2026:HOH:O	2.61	0.54
1:A:215:GLU:HG3	1:A:229:VAL:HG22	1.90	0.54
1:B:114:ALA:HB1	1:B:115:PRO:HD2	1.90	0.53
1:A:133:GLY:HA3	1:A:164:VAL:O	2.08	0.53
1:B:195:GLU:N	1:B:195:GLU:OE1	2.39	0.53
1:B:18:GLU:HB2	1:B:19:PRO:CD	2.38	0.53
1:A:285:ARG:HD3	3:A:2004:HOH:O	2.07	0.53
1:B:18:GLU:HB2	1:B:19:PRO:HD2	1.91	0.53
1:B:159:ARG:HA	1:B:188:ASP:OD1	2.08	0.53
1:A:104:TYR:HA	2:A:1302:DIO:H21	1.91	0.53
1:A:152:GLU:HG3	1:A:156:ARG:HH21	1.73	0.53
1:A:204:VAL:O	1:A:204:VAL:HG12	2.09	0.53
1:A:203:ARG:C	1:A:205:GLU:H	2.12	0.53
1:B:126:VAL:O	1:B:158:VAL:HG22	2.09	0.52
1:A:159:ARG:NH1	1:A:188:ASP:HB3	2.25	0.52
1:B:150:MET:HB2	1:B:160:VAL:HG21	1.92	0.52
1:A:201:PHE:CZ	1:A:211:LEU:HD21	2.46	0.51
1:A:151:GLU:HG2	1:A:155:ARG:HH21	1.75	0.51
1:B:164:VAL:CG2	1:B:190:LEU:HD11	2.41	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ARG:HB3	1:B:60:GLU:OE2	2.11	0.51
1:A:46:LEU:HD22	1:A:297:LEU:HD11	1.92	0.51
1:B:6:THR:HG23	1:B:52:PHE:HD1	1.76	0.51
1:A:176:ALA:O	1:A:180:LEU:HG	2.10	0.51
1:B:194:GLU:CG	1:B:220:ARG:HG2	2.39	0.51
1:B:159:ARG:HG2	1:B:188:ASP:OD1	2.11	0.51
1:B:203:ARG:C	1:B:205:GLU:H	2.15	0.51
1:B:204:VAL:O	1:B:204:VAL:HG12	2.11	0.51
1:B:164:VAL:HG23	1:B:190:LEU:HD11	1.92	0.50
1:B:19:PRO:HA	1:B:93:TYR:HD1	1.76	0.50
1:B:204:VAL:O	1:B:208:LEU:HG	2.11	0.50
1:B:232:ARG:NH2	1:B:268:GLU:OE1	2.41	0.50
2:A:1302:DIO:H1'1	1:B:104:TYR:HA	1.92	0.50
1:A:253:PHE:HE1	1:A:275:ASN:ND2	2.10	0.50
1:B:197:ALA:HB1	1:B:207:ALA:HB3	1.94	0.50
1:A:182:ARG:HH11	1:A:182:ARG:HG3	1.77	0.49
1:B:88:LEU:C	1:B:88:LEU:HD12	2.32	0.49
1:A:241:VAL:HG21	3:A:2046:HOH:O	2.13	0.49
1:B:120:PRO:HB2	1:B:156:ARG:CZ	2.43	0.49
1:A:182:ARG:NH1	1:A:182:ARG:HG3	2.27	0.49
1:B:16:PRO:HG2	3:B:2027:HOH:O	2.13	0.48
1:B:90:LEU:HD12	1:B:90:LEU:N	2.27	0.48
1:A:198:GLU:HG2	1:A:203:ARG:HA	1.95	0.48
1:B:267:VAL:HG23	3:B:2043:HOH:O	2.13	0.48
1:A:229:VAL:O	1:A:232:ARG:HB3	2.13	0.48
1:B:76:LEU:HB3	1:B:79:PHE:HB3	1.94	0.48
1:A:112:ALA:O	1:A:113:LEU:C	2.52	0.48
1:B:172:SER:OG	1:B:175:GLU:HG3	2.14	0.48
1:B:230:ASP:O	1:B:232:ARG:N	2.47	0.48
1:A:156:ARG:HG2	3:A:2036:HOH:O	2.14	0.47
1:B:256:GLY:CA	1:B:277:LEU:HD22	2.45	0.47
1:A:294:ARG:O	1:A:298:GLU:HG3	2.14	0.47
1:A:173:PRO:O	1:A:177:ARG:HB2	2.14	0.47
1:B:225:ALA:O	1:B:236:GLY:N	2.48	0.47
1:B:228:PHE:CE1	1:B:233:ARG:HG2	2.48	0.47
1:A:299:VAL:HG23	1:A:300:LEU:N	2.30	0.47
1:A:285:ARG:CD	3:A:2004:HOH:O	2.63	0.46
1:B:272:ARG:HG3	1:B:272:ARG:HH11	1.80	0.46
1:A:203:ARG:O	1:A:205:GLU:N	2.48	0.46
1:B:173:PRO:HA	1:B:200:LEU:CD2	2.45	0.46
1:A:68:ARG:CA	1:A:68:ARG:HE	2.27	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:GLU:O	1:B:92:GLU:HG3	2.15	0.46
1:B:137:ALA:HB3	1:B:170:LEU:HD13	1.97	0.46
1:A:230:ASP:O	1:A:232:ARG:N	2.48	0.46
1:A:56:VAL:CG2	1:A:81:ARG:HG2	2.44	0.46
1:B:220:ARG:HD2	1:B:226:TRP:CE3	2.51	0.46
1:B:1:MET:O	1:B:49:LYS:HD3	2.16	0.45
1:B:275:ASN:HD22	1:B:275:ASN:N	2.14	0.45
1:B:182:ARG:O	1:B:185:PRO:HD2	2.16	0.45
1:B:197:ALA:HB1	1:B:207:ALA:CB	2.46	0.45
1:A:94:LEU:HB2	1:A:98:GLN:O	2.17	0.45
1:B:173:PRO:HA	1:B:200:LEU:HD21	1.99	0.45
1:B:218:LEU:HD23	1:B:226:TRP:CE3	2.51	0.45
1:B:201:PHE:HB2	1:B:207:ALA:HB2	1.99	0.45
1:A:230:ASP:C	1:A:232:ARG:N	2.71	0.44
1:A:258:LEU:O	1:A:262:VAL:HG23	2.17	0.44
1:A:232:ARG:NH2	1:A:268:GLU:OE1	2.49	0.44
1:A:41:VAL:HG13	1:A:72:GLU:HG3	1.98	0.44
1:A:96:LEU:HB2	1:A:98:GLN:HE22	1.83	0.44
1:A:76:LEU:HB3	1:A:79:PHE:HB3	1.99	0.44
1:A:192:LEU:O	1:A:218:LEU:HA	2.18	0.44
1:B:137:ALA:HB2	1:B:171:TRP:CE2	2.52	0.44
1:A:201:PHE:HB2	1:A:207:ALA:HB2	1.99	0.44
1:B:78:HIS:CG	1:B:118:PHE:HB2	2.53	0.44
1:B:203:ARG:O	1:B:205:GLU:N	2.51	0.43
1:A:241:VAL:CG2	3:A:2046:HOH:O	2.65	0.43
1:B:51:GLY:HA2	1:B:75:ASP:HB3	1.99	0.43
1:A:156:ARG:HE	1:A:156:ARG:HB2	1.50	0.43
1:B:92:GLU:O	1:B:92:GLU:CG	2.67	0.43
1:B:137:ALA:HB1	1:B:170:LEU:CB	2.49	0.43
1:A:100:ARG:NH2	3:A:2028:HOH:O	2.49	0.43
1:A:245:ASP:HB3	1:A:284:SER:O	2.18	0.43
1:B:119:ASP:HA	1:B:120:PRO:HD2	1.87	0.43
1:B:233:ARG:HG2	1:B:233:ARG:HH11	1.83	0.43
1:A:153:ALA:HB1	1:A:158:VAL:HB	2.01	0.42
1:A:201:PHE:CE1	1:A:211:LEU:HD11	2.54	0.42
1:B:285:ARG:O	1:B:289:GLU:HB2	2.19	0.42
1:B:120:PRO:CB	1:B:152:GLU:HG2	2.40	0.42
1:A:137:ALA:HB1	1:A:170:LEU:CB	2.48	0.42
1:A:41:VAL:O	1:A:45:ARG:HG3	2.19	0.42
1:A:137:ALA:HB1	1:A:170:LEU:HB2	2.02	0.42
1:B:117:ALA:HB3	1:B:145:PHE:HE1	1.84	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:PHE:HA	1:B:274:ALA:O	2.19	0.42
1:A:248:GLY:HA3	1:A:287:ASP:O	2.20	0.42
1:B:215:GLU:OE1	1:B:270:ARG:NH1	2.52	0.42
1:B:230:ASP:C	1:B:232:ARG:N	2.70	0.42
1:A:22:LEU:HB3	1:B:60:GLU:HB3	2.01	0.41
1:A:9:GLU:OE2	1:A:108:SER:OG	2.26	0.41
1:A:46:LEU:HD11	1:A:277:LEU:HD11	2.01	0.41
1:A:295:GLU:HA	1:A:298:GLU:HG3	2.02	0.41
1:B:18:GLU:C	1:B:93:TYR:HE1	2.24	0.41
1:B:68:ARG:HD2	1:B:72:GLU:HG3	2.01	0.41
1:A:156:ARG:HB3	1:A:158:VAL:HG23	2.02	0.41
1:B:163:ASP:HA	1:B:191:PHE:HB2	2.03	0.41
1:A:173:PRO:HA	1:A:200:LEU:HD11	2.02	0.41
1:A:93:TYR:N	1:A:93:TYR:CD2	2.88	0.41
1:B:226:TRP:HD1	1:B:235:GLU:HA	1.86	0.41
1:B:197:ALA:O	1:B:201:PHE:HB2	2.21	0.41
1:A:229:VAL:HG12	1:A:230:ASP:OD2	2.20	0.40
1:A:202:GLY:C	1:A:203:ARG:HG3	2.41	0.40
1:B:133:GLY:HA3	1:B:164:VAL:O	2.21	0.40
1:A:120:PRO:HG3	1:A:148:TRP:CZ2	2.56	0.40
1:A:196:GLU:O	1:A:200:LEU:HB2	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	300/309 (97%)	284 (95%)	12 (4%)	4 (1%)	12	12
1	B	300/309 (97%)	278 (93%)	16 (5%)	6 (2%)	7	6
All	All	600/618 (97%)	562 (94%)	28 (5%)	10 (2%)	9	8

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	113	LEU
1	A	204	VAL
1	B	204	VAL
1	A	113	LEU
1	A	231	GLY
1	B	112	ALA
1	A	247	VAL
1	B	117	ALA
1	B	231	GLY
1	B	164	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	224/231 (97%)	211 (94%)	13 (6%)	20	27
1	B	224/231 (97%)	210 (94%)	14 (6%)	18	24
All	All	448/462 (97%)	421 (94%)	27 (6%)	19	26

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	18	GLU
1	A	68	ARG
1	A	93	TYR
1	A	100	ARG
1	A	156	ARG
1	A	171	TRP
1	A	181	GLU
1	A	182	ARG
1	A	184	LEU
1	A	200	LEU
1	A	229	VAL
1	A	277	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	18	GLU
1	B	55	ARG
1	B	68	ARG
1	B	93	TYR
1	B	141	GLU
1	B	154	LYS
1	B	165	ASN
1	B	169	THR
1	B	171	TRP
1	B	205	GLU
1	B	233	ARG
1	B	275	ASN
1	B	287	ASP
1	B	294	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	HIS
1	A	275	ASN
1	B	17	GLN
1	B	78	HIS
1	B	165	ASN
1	B	168	GLN
1	B	275	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	DIO	A	1302	-	6,6,6	0.77	0	6,6,6	0.55	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	DIO	A	1302	-	-	-	0/1/1/1

There are no bond length outliers.

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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1302	DIO	2	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	302/309 (97%)	-0.21	6 (1%) 65 71	21, 43, 90, 132	0
1	B	302/309 (97%)	-0.05	11 (3%) 42 49	22, 51, 101, 136	0
All	All	604/618 (97%)	-0.13	17 (2%) 53 60	21, 46, 97, 136	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	243	ALA	5.6
1	A	240	ALA	5.5
1	B	240	ALA	4.8
1	A	239	PHE	3.7
1	A	204	VAL	3.6
1	A	224	GLY	3.1
1	B	239	PHE	2.9
1	B	242	GLU	2.8
1	B	204	VAL	2.8
1	B	207	ALA	2.7
1	A	199	LEU	2.4
1	B	300	LEU	2.3
1	B	117	ALA	2.2
1	B	211	LEU	2.2
1	B	237	SER	2.1
1	B	301	LEU	2.1
1	A	203	ARG	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	DIO	A	1302	6/6	0.96	0.14	54,61,64,66	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.