



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 3, 2023 – 10:37 AM EDT

PDB ID : 3S40
Title : The crystal structure of a diacylglycerol kinases from Bacillus anthracis str. Sterne
Authors : Tan, K.; Zhang, R.; Xu, X.; Cui, H.; Peterson, S.; Savchenko, A.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2011-05-18
Resolution : 2.10 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

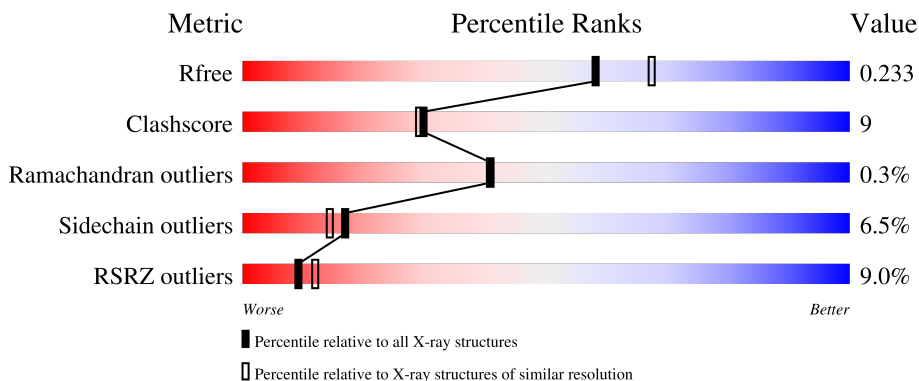
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	304	 3% 73% 16% • 11%
1	B	304	 9% 73% 20% • •
1	C	304	 8% 78% 14% • 6%
1	D	304	 13% 63% 21% • 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8929 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 diacylglycerol kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	272	2099	1351	339	402	5	2	0	0	0
1	B	293	2252	1448	364	433	5	2	0	0	0
1	C	287	2215	1422	360	426	5	2	0	0	0
1	D	264	2034	1314	328	385	5	2	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q81KC6
A	0	HIS	-	expression tag	UNP Q81KC6
A	301	GLY	-	expression tag	UNP Q81KC6
A	302	SER	-	expression tag	UNP Q81KC6
B	-1	GLY	-	expression tag	UNP Q81KC6
B	0	HIS	-	expression tag	UNP Q81KC6
B	301	GLY	-	expression tag	UNP Q81KC6
B	302	SER	-	expression tag	UNP Q81KC6
C	-1	GLY	-	expression tag	UNP Q81KC6
C	0	HIS	-	expression tag	UNP Q81KC6
C	301	GLY	-	expression tag	UNP Q81KC6
C	302	SER	-	expression tag	UNP Q81KC6
D	-1	GLY	-	expression tag	UNP Q81KC6
D	0	HIS	-	expression tag	UNP Q81KC6
D	301	GLY	-	expression tag	UNP Q81KC6
D	302	SER	-	expression tag	UNP Q81KC6

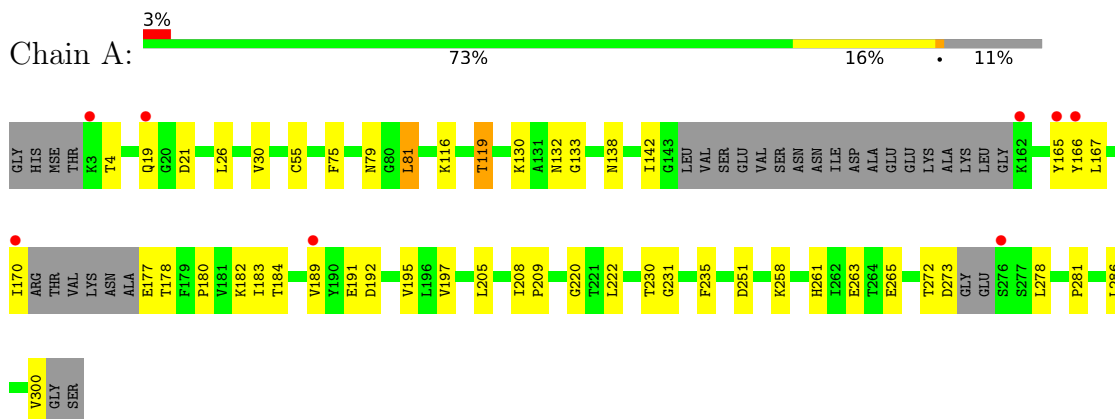
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	89	Total O 89 89	0	0
2	B	86	Total O 86 86	0	0
2	C	73	Total O 73 73	0	0
2	D	81	Total O 81 81	0	0

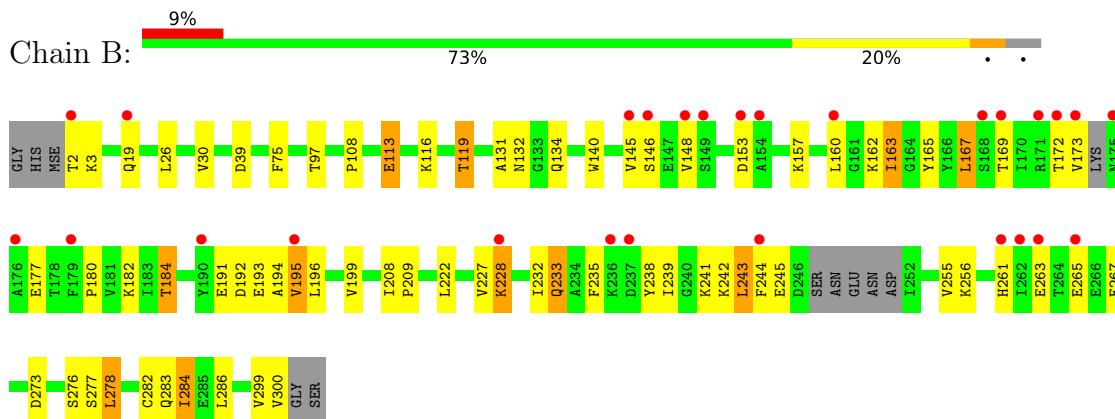
3 Residue-property plots [i](#)

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.

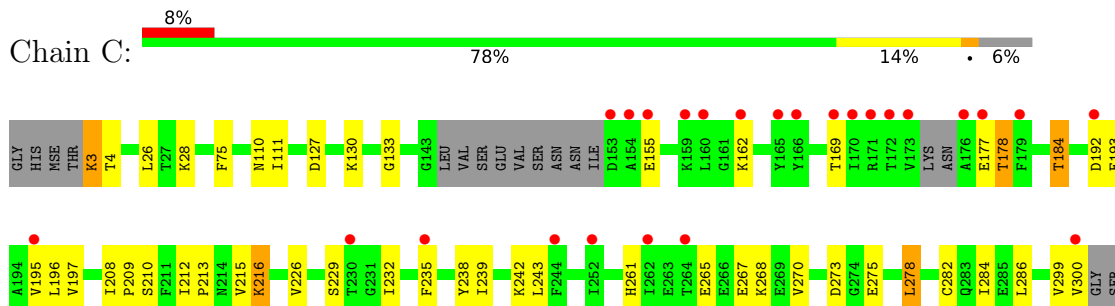
- Molecule 1: diacylglycerol kinase



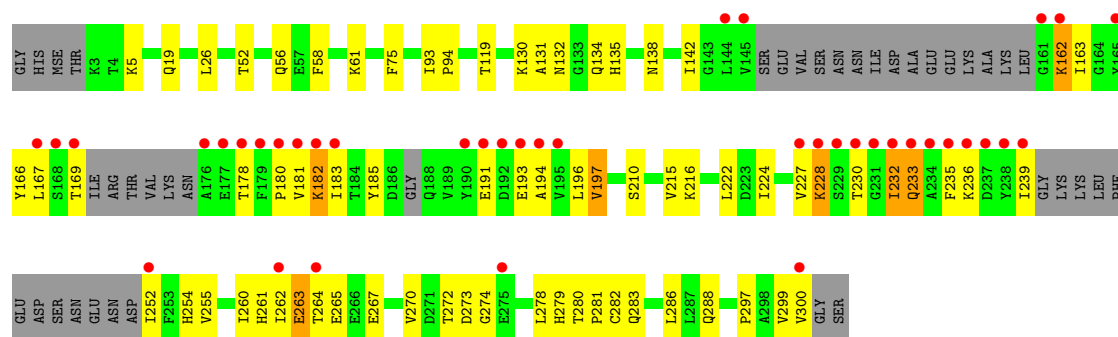
- Molecule 1: diacylglycerol kinase



- Molecule 1: diacylglycerol kinase



- Molecule 1: diacylglycerol kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.61Å 130.76Å 72.79Å 90.00° 115.04° 90.00°	Depositor
Resolution (Å)	43.23 – 2.10 46.43 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.6 (43.23-2.10) 99.5 (46.43-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.10Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.175 , 0.238 0.177 , 0.233	Depositor DCC
R_{free} test set	3170 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtrriage
Anisotropy	0.261	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8929	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.57% of the height of the origin peak. No significant pseudotranslation is detected.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.41	0/2141	0.55	0/2901
1	B	0.39	0/2295	0.54	0/3110
1	C	0.36	0/2258	0.53	0/3057
1	D	0.37	0/2074	0.55	0/2810
All	All	0.38	0/8768	0.54	0/11878

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	2099	0	2078	35	0
1	B	2252	0	2251	53	0
1	C	2215	0	2208	27	0
1	D	2034	0	2034	56	0
2	A	89	0	0	2	0
2	B	86	0	0	1	0
2	C	73	0	0	1	0
2	D	81	0	0	6	0
All	All	8929	0	8571	162	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 (162) 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:283:GLN:HG2	1:D:281:PRO:HG2	1.52	0.91
1:D:263:GLU:OE2	1:D:281:PRO:HB3	1.73	0.89
1:B:184:THR:HG23	1:B:261:HIS:HB3	1.57	0.87
1:A:182:LYS:HG3	1:A:191:GLU:HG3	1.60	0.84
1:C:178:THR:HG23	1:C:193:GLU:OE2	1.80	0.82
1:C:275:GLU:H	1:C:275:GLU:CD	1.86	0.79
1:A:180:PRO:HG2	1:A:265:GLU:HB2	1.66	0.78
1:B:196:LEU:HB3	1:B:227:VAL:CG2	2.17	0.75
1:A:166:TYR:O	1:A:170:ILE:HG13	1.86	0.75
1:B:157:LYS:HE2	1:B:162:LYS:HE2	1.70	0.74
1:B:196:LEU:HB3	1:B:227:VAL:HG22	1.70	0.73
1:C:195:VAL:HG23	1:C:229:SER:HA	1.71	0.73
1:A:167:LEU:HA	1:A:170:ILE:HD12	1.70	0.72
1:B:134:GLN:HG2	1:B:278:LEU:HD21	1.72	0.72
1:C:195:VAL:HG21	1:C:232:ILE:HD11	1.73	0.70
1:D:180:PRO:HA	1:D:193:GLU:HA	1.74	0.70
1:D:183:ILE:HG23	1:D:262:ILE:HG12	1.74	0.70
1:B:180:PRO:HG2	1:B:265:GLU:HG2	1.74	0.69
1:D:299:VAL:HG23	1:D:300:VAL:HG12	1.74	0.68
1:A:116:LYS:O	1:A:119:THR:HB	1.94	0.67
1:B:233:GLN:NE2	1:B:233:GLN:H	1.92	0.67
1:A:184:THR:HG22	1:A:189:VAL:HG12	1.77	0.66
1:A:182:LYS:HG3	1:A:191:GLU:CG	2.24	0.66
1:B:132:ASN:HD21	1:B:282:CYS:HA	1.59	0.66
1:B:283:GLN:CG	1:D:281:PRO:HG2	2.24	0.65
1:C:184:THR:HG23	2:C:331:HOH:O	1.96	0.64
1:B:182:LYS:HG3	1:B:191:GLU:HG2	1.80	0.63
1:B:180:PRO:HG2	1:B:265:GLU:CG	2.29	0.62
1:B:194:ALA:HA	1:B:228:LYS:HA	1.79	0.62
1:D:227:VAL:HG12	1:D:252:ILE:HG12	1.79	0.62
1:B:261:HIS:NE2	1:D:261:HIS:HE1	1.97	0.62
1:C:3:LYS:HD2	1:C:4:THR:N	2.14	0.62
1:B:148:VAL:HG13	1:B:153:ASP:HB2	1.83	0.61
1:A:167:LEU:HD23	1:A:170:ILE:HD12	1.81	0.60
1:D:182:LYS:HD2	1:D:263:GLU:HB2	1.83	0.60
1:D:19:GLN:HA	1:D:19:GLN:OE1	2.01	0.60
1:D:130:LYS:HG3	1:D:135:HIS:CD2	2.36	0.59
1:C:197:VAL:HG22	1:C:226:VAL:HG22	1.85	0.59
1:C:75:PHE:CD1	1:C:273:ASP:HB2	2.38	0.59
1:A:55:CYS:HB3	1:A:81:LEU:HD13	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:VAL:CG2	1:C:229:SER:HA	2.33	0.59
1:B:116:LYS:O	1:B:119:THR:HB	2.04	0.58
1:D:131:ALA:O	1:D:134:GLN:HB3	2.04	0.58
1:A:184:THR:OG1	1:A:261:HIS:HB3	2.03	0.57
1:C:270:VAL:HB	1:C:278:LEU:HD13	1.86	0.57
1:D:194:ALA:HA	1:D:228:LYS:HA	1.87	0.57
1:D:196:LEU:HB3	1:D:227:VAL:HG22	1.86	0.57
1:A:21:ASP:HA	2:A:303:HOH:O	2.04	0.57
1:D:264:THR:HA	2:D:375:HOH:O	2.05	0.56
1:C:235:PHE:CE1	1:C:239:ILE:HD11	2.40	0.56
1:D:58:PHE:HA	1:D:61:LYS:HG3	1.86	0.56
1:D:185:TYR:CE2	1:D:255:VAL:HG21	2.40	0.56
1:D:142:ILE:HG12	1:D:197:VAL:HG13	1.86	0.56
1:B:131:ALA:HB2	1:B:284:ILE:HD13	1.86	0.56
1:B:261:HIS:NE2	1:D:261:HIS:CE1	2.74	0.56
1:B:208:ILE:HG23	1:B:209:PRO:HD2	1.89	0.55
1:C:208:ILE:HB	1:C:209:PRO:HD2	1.89	0.55
1:B:184:THR:CG2	1:B:261:HIS:HB3	2.34	0.55
1:A:167:LEU:HA	1:A:170:ILE:CD1	2.36	0.55
1:B:235:PHE:O	1:B:238:TYR:HB3	2.08	0.54
1:C:127:ASP:HB3	1:C:286:LEU:HD21	1.90	0.54
1:D:299:VAL:O	1:D:300:VAL:HB	2.07	0.54
1:D:300:VAL:HG13	1:D:300:VAL:O	2.08	0.54
1:D:288:GLN:HG2	2:D:327:HOH:O	2.08	0.53
1:D:278:LEU:HD12	1:D:279:HIS:H	1.74	0.53
1:B:132:ASN:ND2	1:B:282:CYS:HA	2.23	0.52
1:D:233:GLN:HA	1:D:236:LYS:NZ	2.24	0.52
1:A:177:GLU:HG3	1:A:178:THR:N	2.24	0.52
1:D:52:THR:O	1:D:56:GLN:HG3	2.10	0.52
1:C:235:PHE:O	1:C:239:ILE:HG12	2.10	0.52
1:B:191:GLU:O	1:B:192:ASP:HB2	2.09	0.52
1:D:224:ILE:HD11	1:D:260:ILE:HD13	1.91	0.51
1:B:238:TYR:CZ	1:B:244:PHE:HD1	2.28	0.51
1:B:169:THR:O	1:B:172:THR:HG22	2.11	0.51
1:A:130:LYS:HD3	1:A:133:GLY:HA2	1.92	0.50
1:B:238:TYR:CZ	1:B:244:PHE:CD1	3.00	0.50
1:C:268:LYS:HB3	1:C:268:LYS:NZ	2.26	0.50
1:D:228:LYS:HE2	1:D:252:ILE:N	2.27	0.50
1:A:130:LYS:NZ	1:C:133:GLY:HA3	2.27	0.49
1:D:166:TYR:HD2	1:D:167:LEU:HD12	1.78	0.49
1:D:232:ILE:HG23	1:D:233:GLN:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:ILE:CG1	1:D:197:VAL:HG13	2.42	0.49
1:B:108:PRO:HB2	1:B:113:GLU:HB3	1.94	0.49
1:B:195:VAL:HG13	1:B:227:VAL:HG23	1.95	0.49
1:B:2:THR:HG22	1:B:3:LYS:N	2.28	0.48
1:D:224:ILE:HD11	1:D:260:ILE:CD1	2.43	0.48
1:A:170:ILE:HD13	1:A:235:PHE:HE2	1.79	0.48
1:D:215:VAL:O	1:D:216:LYS:HD2	2.14	0.48
1:A:231:GLY:CA	1:A:251:ASP:HB3	2.44	0.48
1:B:182:LYS:HD2	1:B:263:GLU:OE1	2.13	0.48
1:B:242:LYS:HA	1:B:244:PHE:CZ	2.49	0.48
1:B:172:THR:HG23	1:B:173:VAL:N	2.29	0.48
1:A:177:GLU:HG3	1:A:178:THR:HG23	1.96	0.48
1:C:300:VAL:HG13	1:C:300:VAL:O	2.14	0.48
1:A:261:HIS:NE2	1:C:261:HIS:HE1	2.11	0.47
1:D:254:HIS:CD2	1:D:255:VAL:N	2.82	0.47
1:D:280:THR:HB	1:D:281:PRO:HA	1.95	0.47
1:D:232:ILE:C	1:D:232:ILE:HD13	2.35	0.47
1:D:233:GLN:HA	1:D:236:LYS:HZ1	1.78	0.47
1:B:169:THR:O	1:B:169:THR:HG22	2.15	0.47
1:D:162:LYS:N	1:D:162:LYS:HD2	2.29	0.47
1:C:28:LYS:HD2	1:C:111:ILE:HD11	1.96	0.47
1:D:169:THR:C	2:D:315:HOH:O	2.53	0.46
1:D:227:VAL:HG11	1:D:235:PHE:CD1	2.50	0.46
1:A:263:GLU:HG3	2:A:390:HOH:O	2.15	0.46
1:B:140:TRP:HB3	1:B:199:VAL:HB	1.98	0.46
1:D:232:ILE:HD13	1:D:232:ILE:O	2.16	0.46
1:A:132:ASN:HB2	1:A:278:LEU:HD22	1.98	0.46
1:D:235:PHE:O	1:D:239:ILE:HG12	2.15	0.45
1:B:235:PHE:O	1:B:239:ILE:HG12	2.17	0.45
1:A:231:GLY:HA2	1:A:251:ASP:HB3	1.99	0.45
1:C:238:TYR:CD1	1:C:239:ILE:HD13	2.51	0.45
1:C:130:LYS:O	1:C:284:ILE:HA	2.16	0.45
1:B:75:PHE:CD1	1:B:273:ASP:HB2	2.52	0.45
1:B:180:PRO:CG	1:B:265:GLU:HG3	2.47	0.45
1:D:181:VAL:HA	2:D:375:HOH:O	2.17	0.44
1:D:75:PHE:CD1	1:D:273:ASP:HB2	2.52	0.44
1:B:255:VAL:HG22	1:B:256:LYS:N	2.32	0.44
1:D:181:VAL:HG22	1:D:182:LYS:N	2.32	0.44
1:B:146:SER:HG	1:B:165:TYR:HD2	1.65	0.44
1:D:163:ILE:O	1:D:167:LEU:HD13	2.17	0.44
1:D:299:VAL:O	1:D:300:VAL:CB	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:PHE:CE1	1:A:79:ASN:ND2	2.86	0.43
1:C:215:VAL:O	1:C:216:LYS:HD2	2.18	0.43
1:A:272:THR:O	1:A:273:ASP:C	2.57	0.43
1:A:281:PRO:HG2	1:C:261:HIS:CG	2.53	0.43
1:B:180:PRO:HA	1:B:193:GLU:HA	2.00	0.43
1:B:299:VAL:HG23	1:B:300:VAL:HG12	2.01	0.43
1:C:210:SER:O	1:C:242:LYS:HE2	2.19	0.43
1:D:93:ILE:HA	1:D:94:PRO:HD3	1.84	0.43
1:A:220:GLY:O	1:A:258:LYS:HE2	2.19	0.42
1:B:228:LYS:HE2	2:B:386:HOH:O	2.19	0.42
1:A:208:ILE:HB	1:A:209:PRO:HD2	2.01	0.42
1:D:132:ASN:C	1:D:134:GLN:H	2.23	0.42
1:B:276:SER:OG	1:B:277:SER:N	2.52	0.42
1:D:272:THR:HG23	1:D:274:GLY:H	1.83	0.42
1:A:30:VAL:CG1	1:B:30:VAL:HG11	2.50	0.42
1:D:264:THR:HG22	2:D:375:HOH:O	2.19	0.42
1:D:261:HIS:HD2	1:D:283:GLN:OE1	2.03	0.42
1:B:131:ALA:CB	1:B:284:ILE:HD13	2.49	0.42
1:B:97:THR:HG21	1:B:160:LEU:HD23	2.02	0.42
1:D:138:ASN:HB2	1:D:273:ASP:OD1	2.20	0.42
1:D:142:ILE:CG2	1:D:270:VAL:HG22	2.49	0.42
1:D:261:HIS:HA	1:D:282:CYS:O	2.20	0.41
1:C:212:ILE:HA	1:C:213:PRO:HD3	1.88	0.41
1:A:142:ILE:HG12	1:A:197:VAL:HB	2.02	0.41
1:B:39:ASP:C	1:B:39:ASP:OD1	2.59	0.41
1:B:243:LEU:HD23	1:B:243:LEU:HA	1.81	0.41
1:A:142:ILE:CG1	1:A:197:VAL:HB	2.50	0.41
1:A:167:LEU:O	1:A:170:ILE:HB	2.21	0.41
1:B:163:ILE:HD13	1:B:163:ILE:O	2.21	0.41
1:A:177:GLU:HG3	1:A:178:THR:H	1.85	0.41
1:A:183:ILE:O	1:A:189:VAL:HA	2.21	0.41
1:D:222:LEU:HG	1:D:286:LEU:HD12	2.03	0.41
1:B:180:PRO:CG	1:B:265:GLU:CG	2.99	0.41
1:A:30:VAL:HG11	1:B:30:VAL:CG1	2.51	0.40
1:A:222:LEU:HD21	1:A:286:LEU:HD13	2.02	0.40
1:B:167:LEU:HD12	1:B:167:LEU:HA	1.86	0.40
1:B:222:LEU:HG	1:B:286:LEU:HD12	2.04	0.40
1:C:208:ILE:HB	1:C:209:PRO:CD	2.51	0.40
1:C:110:ASN:OD1	1:C:110:ASN:C	2.60	0.40
1:D:297:PRO:HD2	2:D:350:HOH:O	2.21	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	264/304 (87%)	253 (96%)	11 (4%)	0	100	100
1	B	287/304 (94%)	280 (98%)	7 (2%)	0	100	100
1	C	281/304 (92%)	272 (97%)	8 (3%)	1 (0%)	34	32
1	D	254/304 (84%)	243 (96%)	9 (4%)	2 (1%)	19	15
All	All	1086/1216 (89%)	1048 (96%)	35 (3%)	3 (0%)	41	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	265	GLU
1	C	267	GLU
1	D	267	GLU

5.3.2 Protein sidechains [i](#)

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	230/254 (91%)	218 (95%)	12 (5%)	23	21
1	B	247/254 (97%)	228 (92%)	19 (8%)	13	9
1	C	242/254 (95%)	226 (93%)	16 (7%)	16	14
1	D	223/254 (88%)	209 (94%)	14 (6%)	18	15
All	All	942/1016 (93%)	881 (94%)	61 (6%)	17	14

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	19	GLN
1	A	26	LEU
1	A	81	LEU
1	A	119	THR
1	A	138	ASN
1	A	165	TYR
1	A	192	ASP
1	A	195	VAL
1	A	205	LEU
1	A	230	THR
1	A	300	VAL
1	B	19	GLN
1	B	26	LEU
1	B	113	GLU
1	B	119	THR
1	B	145	VAL
1	B	163	ILE
1	B	167	LEU
1	B	177	GLU
1	B	184	THR
1	B	195	VAL
1	B	228	LYS
1	B	232	ILE
1	B	233	GLN
1	B	241	LYS
1	B	243	LEU
1	B	245	GLU
1	B	267	GLU
1	B	278	LEU
1	B	284	ILE
1	C	3	LYS
1	C	26	LEU
1	C	155	GLU
1	C	162	LYS
1	C	169	THR
1	C	177	GLU
1	C	178	THR
1	C	184	THR
1	C	192	ASP
1	C	196	LEU
1	C	216	LYS
1	C	243	LEU

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Mol	Chain	Res	Type
1	C	265	GLU
1	C	278	LEU
1	C	282	CYS
1	C	299	VAL
1	D	5	LYS
1	D	26	LEU
1	D	119	THR
1	D	162	LYS
1	D	178	THR
1	D	182	LYS
1	D	191	GLU
1	D	197	VAL
1	D	210	SER
1	D	228	LYS
1	D	230	THR
1	D	232	ILE
1	D	233	GLN
1	D	263	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	134	GLN
1	B	23	HIS
1	B	188	GLN
1	C	23	HIS
1	C	134	GLN
1	C	261	HIS
1	D	134	GLN
1	D	233	GLN
1	D	254	HIS
1	D	261	HIS

5.3.3 RNA

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	270/304 (88%)	0.09	8 (2%) 50 56	16, 36, 92, 120	0
1	B	291/304 (95%)	0.22	27 (9%) 8 11	17, 38, 99, 125	0
1	C	285/304 (93%)	0.24	25 (8%) 10 12	18, 40, 95, 166	0
1	D	262/304 (86%)	0.64	40 (15%) 2 3	19, 40, 120, 170	0
All	All	1108/1216 (91%)	0.29	100 (9%) 9 12	16, 39, 101, 170	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	153	ASP	7.4
1	D	233	GLN	7.0
1	D	232	ILE	6.6
1	D	168	SER	6.1
1	D	144	LEU	6.0
1	D	190	TYR	5.9
1	C	170	ILE	5.7
1	D	234	ALA	5.6
1	D	237	ASP	5.0
1	C	171	ARG	4.9
1	D	231	GLY	4.7
1	C	173	VAL	4.6
1	D	169	THR	4.5
1	D	235	PHE	4.5
1	D	229	SER	4.5
1	D	230	THR	4.3
1	C	166	TYR	4.1
1	D	193	GLU	4.1
1	C	160	LEU	3.9
1	B	179	PHE	3.9
1	C	179	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	165	TYR	3.8
1	C	230	THR	3.8
1	D	145	VAL	3.7
1	B	265	GLU	3.6
1	B	146	SER	3.6
1	D	165	TYR	3.6
1	B	2	THR	3.6
1	C	162	LYS	3.5
1	B	228	LYS	3.5
1	D	195	VAL	3.3
1	D	179	PHE	3.3
1	D	181	VAL	3.2
1	D	177	GLU	3.2
1	D	176	ALA	3.2
1	D	180	PRO	3.0
1	A	19	GLN	3.0
1	D	238	TYR	3.0
1	B	19	GLN	3.0
1	C	159	LYS	3.0
1	A	170	ILE	2.9
1	D	228	LYS	2.9
1	C	169	THR	2.9
1	C	244	PHE	2.9
1	A	3	LYS	2.9
1	B	263	GLU	2.9
1	D	192	ASP	2.8
1	C	252	ILE	2.8
1	D	161	GLY	2.8
1	C	154	ALA	2.7
1	D	183	ILE	2.7
1	D	262	ILE	2.7
1	C	172	THR	2.7
1	D	178	THR	2.6
1	B	149	SER	2.6
1	C	155	GLU	2.6
1	D	239	ILE	2.6
1	B	168	SER	2.6
1	D	275	GLU	2.6
1	A	276	SER	2.5
1	B	172	THR	2.5
1	A	165	TYR	2.5
1	D	227	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	176	ALA	2.5
1	C	192	ASP	2.5
1	C	262	ILE	2.5
1	D	194	ALA	2.5
1	B	236	LYS	2.4
1	B	262	ILE	2.4
1	B	171	ARG	2.4
1	B	237	ASP	2.4
1	C	176	ALA	2.4
1	B	169	THR	2.4
1	D	264	THR	2.4
1	B	173	VAL	2.4
1	D	252	ILE	2.4
1	A	166	TYR	2.4
1	B	195	VAL	2.3
1	D	182	LYS	2.3
1	B	160	LEU	2.3
1	B	145	VAL	2.3
1	A	162	LYS	2.2
1	D	300	VAL	2.2
1	D	191	GLU	2.2
1	B	175	ASN	2.2
1	C	264	THR	2.2
1	C	177	GLU	2.2
1	B	261	HIS	2.2
1	C	300	VAL	2.1
1	B	190	TYR	2.1
1	B	154	ALA	2.1
1	D	236	LYS	2.1
1	D	167	LEU	2.1
1	A	189	VAL	2.1
1	B	153	ASP	2.1
1	C	235	PHE	2.1
1	C	195	VAL	2.0
1	D	162	LYS	2.0
1	B	244	PHE	2.0
1	B	148	VAL	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 monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.