Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 12:44 AM EDT

PDB ID	:	1U0R
Title	:	Crystal structure of Mycobacterium tuberculosis NAD kinase
Authors	:	Garavaglia, S.; Raffaelli, N.; Finaurini, L.; Magni, G.; Rizzi, M.; TB Structural Genomics Consortium (TBSGC)
Deposited on	:	2004-07-14
Resolution	:	2.80 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 (i) 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 (i)) were used in the production of this report:

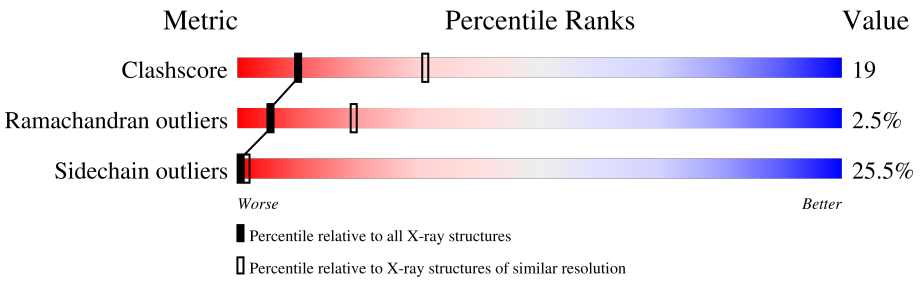
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	307	55% 27% 8% • 8%
1	B	307	42% 34% 8% • 16%
1	C	307	57% 26% 9% • 7%
1	D	307	48% 35% 13% • •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8778 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 Inorganic polyphosphate/ATP-NAD kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	281	2121	1336	384	395	6	0	0	0
1	B	258	1941	1225	352	358	6	0	0	0
1	C	285	2156	1353	394	403	6	0	0	0
1	D	301	2257	1417	412	420	8	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	81	81	81	0	0
2	B	56	56	56	0	0
2	C	90	90	90	0	0
2	D	76	76	76	0	0

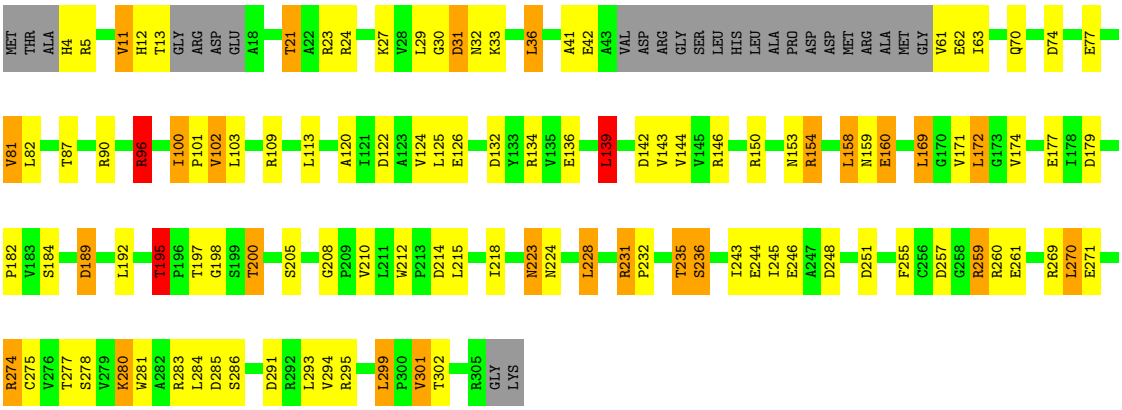
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

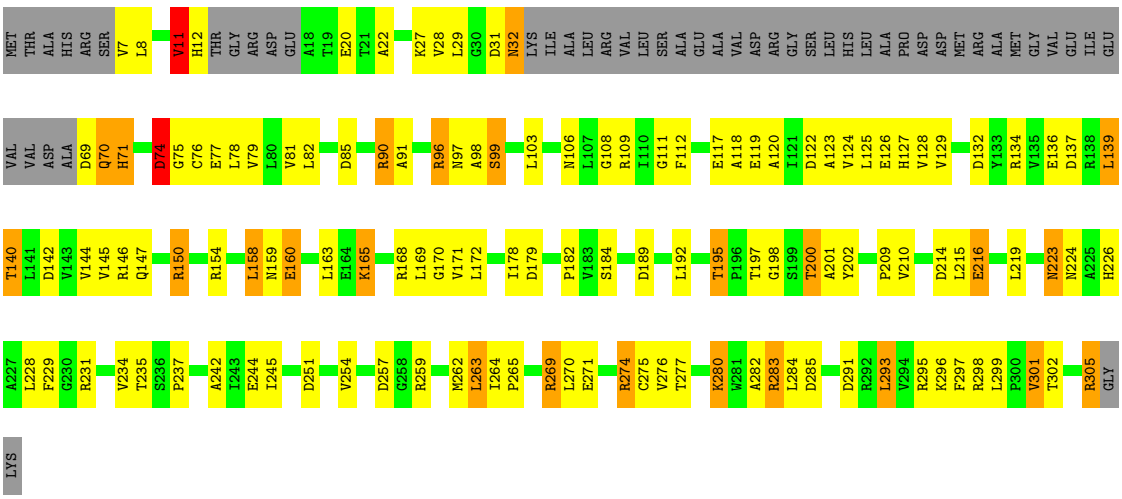
• Molecule 1: Inorganic polyphosphate/ATP-NAD kinase

Chain A: 55% 27% 8% • 8%



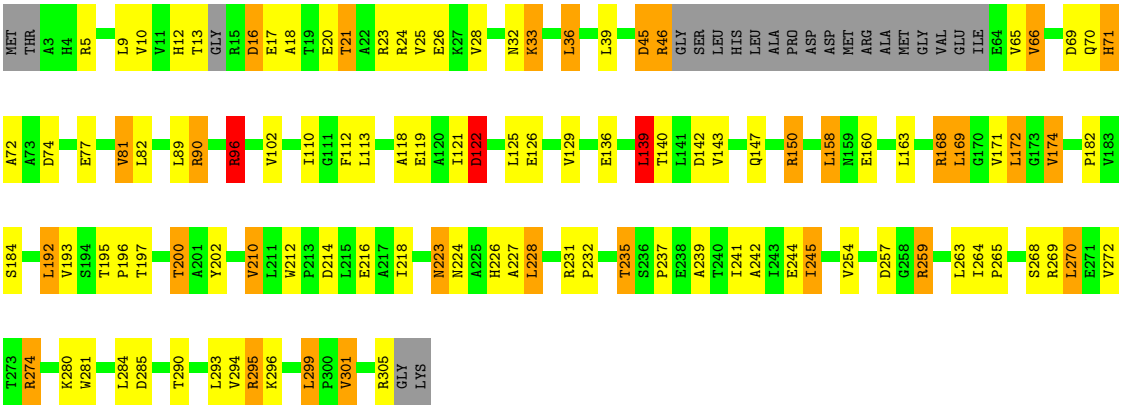
• Molecule 1: Inorganic polyphosphate/ATP-NAD kinase

Chain B: 42% 34% 8% • 16%



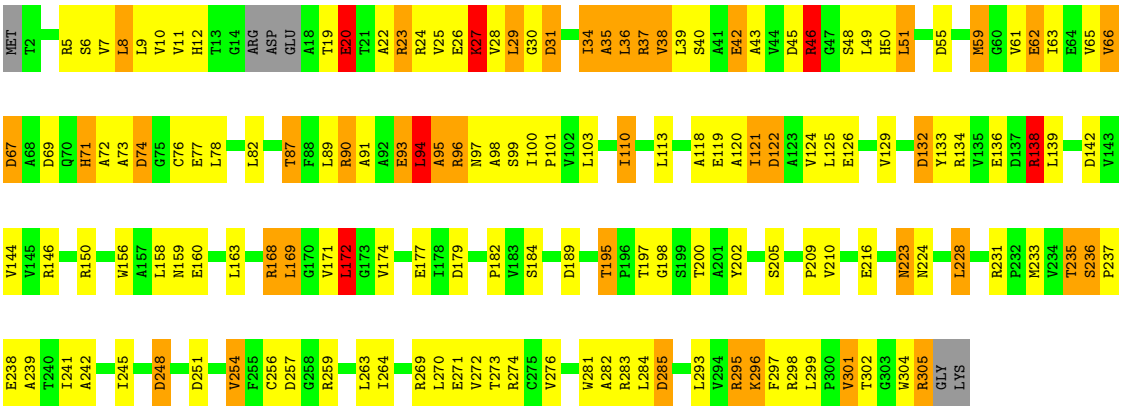
• Molecule 1: Inorganic polyphosphate/ATP-NAD kinase

Chain C:



- Molecule 1: Inorganic polyphosphate/ATP-NAD kinase

Chain D:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	118.51Å 118.51Å 222.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80	Depositor
% Data completeness (in resolution range)	99.2 (50.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.223 , 0.286	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8778	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

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	0.89	1/2154 (0.0%)	1.08	19/2931 (0.6%)
1	B	0.77	0/1973	1.04	14/2685 (0.5%)
1	C	0.88	1/2189 (0.0%)	1.06	10/2977 (0.3%)
1	D	0.84	0/2293	1.07	14/3119 (0.4%)
All	All	0.85	2/8609 (0.0%)	1.06	57/11712 (0.5%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	13	THR	CB-OG1	5.13	1.53	1.43
1	C	74	ASP	CB-CG	5.08	1.62	1.51

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	74	ASP	CB-CG-OD2	8.91	126.32	118.30
1	A	257	ASP	CB-CG-OD2	8.10	125.59	118.30
1	B	214	ASP	CB-CG-OD2	7.88	125.39	118.30
1	B	257	ASP	CB-CG-OD2	7.40	124.96	118.30
1	A	142	ASP	CB-CG-OD2	7.21	124.79	118.30
1	D	169	LEU	CA-CB-CG	7.09	131.61	115.30
1	D	251	ASP	CB-CG-OD2	6.84	124.45	118.30
1	B	291	ASP	CB-CG-OD2	6.83	124.45	118.30
1	A	96	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	D	45	ASP	CB-CG-OD2	6.72	124.35	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	228	LEU	CA-CB-CG	6.68	130.66	115.30
1	A	102	VAL	CB-CA-C	-6.67	98.73	111.40
1	C	169	LEU	CA-CB-CG	6.59	130.47	115.30
1	A	214	ASP	CB-CG-OD2	6.54	124.19	118.30
1	C	69	ASP	CB-CG-OD2	6.54	124.19	118.30
1	D	138	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	C	263	LEU	CA-CB-CG	6.39	129.99	115.30
1	A	139	LEU	CA-CB-CG	6.33	129.87	115.30
1	A	260	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	D	172	LEU	CA-CB-CG	6.18	129.52	115.30
1	B	142	ASP	CB-CG-OD2	5.93	123.64	118.30
1	D	67	ASP	CB-CG-OD2	5.87	123.58	118.30
1	D	285	ASP	CB-CG-OD2	5.82	123.54	118.30
1	D	179	ASP	CB-CG-OD2	5.78	123.50	118.30
1	B	139	LEU	CA-CB-CG	5.77	128.56	115.30
1	C	139	LEU	CA-CB-CG	5.64	128.28	115.30
1	D	55	ASP	CB-CG-OD2	5.64	123.38	118.30
1	C	96	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	D	263	LEU	CA-CB-CG	5.64	128.26	115.30
1	B	274	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	B	69	ASP	CB-CG-OD2	5.57	123.31	118.30
1	D	248	ASP	CB-CG-OD2	5.55	123.30	118.30
1	D	31	ASP	CB-CG-OD2	5.51	123.26	118.30
1	B	189	ASP	CB-CG-OD2	5.49	123.24	118.30
1	B	285	ASP	CB-CG-OD2	5.43	123.18	118.30
1	A	215	LEU	CB-CG-CD2	-5.41	101.80	111.00
1	A	31	ASP	CB-CG-OD2	5.40	123.16	118.30
1	D	90	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	179	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	251	ASP	CB-CG-OD2	5.36	123.12	118.30
1	C	214	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	132	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	195	THR	N-CA-CB	-5.29	100.25	110.30
1	D	189	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	74	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	132	ASP	CB-CG-OD2	5.25	123.03	118.30
1	C	142	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	291	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	45	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	145	VAL	N-CA-C	-5.14	97.11	111.00
1	A	275	CYS	CA-CB-SG	-5.14	104.74	114.00
1	A	248	ASP	CB-CG-OD2	5.14	122.92	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	122	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	31	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	189	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	285	ASP	CB-CG-OD2	5.04	122.84	118.30
1	B	179	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	11	VAL	Peptide

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	2121	0	2150	65	0
1	B	1941	0	1958	83	0
1	C	2156	0	2178	73	0
1	D	2257	0	2277	126	0
2	A	81	0	0	7	1
2	B	56	0	0	4	0
2	C	90	0	0	8	0
2	D	76	0	0	10	1
All	All	8778	0	8563	324	1

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 19.

All (324) 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:12:HIS:CE1	2:D:379:HOH:O	1.80	1.28
1:C:72:ALA:HB3	2:C:321:HOH:O	1.49	1.12
1:A:158:LEU:O	1:A:195:THR:HG21	1.57	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:GLY:HA3	1:D:61:VAL:HG12	1.42	1.00
1:D:6:SER:HA	1:D:35:ALA:HB2	1.45	0.98
1:B:11:VAL:HG23	1:B:12:HIS:HB3	1.47	0.95
1:C:195:THR:HG22	1:C:197:THR:H	1.29	0.95
1:D:61:VAL:O	1:D:63:ILE:N	2.01	0.94
1:B:7:VAL:N	1:B:76:CYS:SG	2.41	0.94
1:B:305:ARG:HH11	1:B:305:ARG:HG3	1.33	0.91
1:B:96:ARG:HG2	1:B:96:ARG:HH11	1.36	0.90
1:B:158:LEU:O	1:B:195:THR:HG21	1.72	0.89
1:A:96:ARG:HG2	1:A:96:ARG:HH11	1.37	0.87
1:D:6:SER:HA	1:D:35:ALA:CB	2.05	0.86
1:C:113:LEU:HD22	1:C:281:TRP:HH2	1.41	0.85
1:D:94:LEU:O	1:D:96:ARG:N	2.10	0.84
1:D:90:ARG:O	1:D:93:GLU:CB	2.26	0.83
1:B:244:GLU:OE1	1:C:305:ARG:HB2	1.79	0.82
1:C:5:ARG:HD2	1:C:77:GLU:OE1	1.79	0.82
1:C:223:ASN:C	1:C:223:ASN:HD22	1.83	0.82
1:A:195:THR:HG22	1:A:198:GLY:H	1.44	0.80
1:A:223:ASN:HD21	1:B:224:ASN:HD21	1.30	0.80
1:C:66:VAL:HG21	2:C:354:HOH:O	1.83	0.79
1:D:48:SER:HB2	1:D:51:LEU:HG	1.65	0.79
1:D:97:ASN:HB3	2:D:341:HOH:O	1.83	0.79
1:A:5:ARG:HD2	1:A:77:GLU:OE1	1.84	0.78
1:B:96:ARG:HH11	1:B:96:ARG:CG	1.97	0.78
1:A:81:VAL:HG23	1:A:103:LEU:O	1.85	0.76
1:D:7:VAL:H	1:D:35:ALA:HB3	1.51	0.75
1:D:90:ARG:O	1:D:93:GLU:HB2	1.86	0.75
1:B:305:ARG:HG3	1:B:305:ARG:NH1	2.02	0.74
1:D:12:HIS:ND1	2:D:379:HOH:O	1.96	0.73
1:D:71:HIS:O	1:D:73:ALA:N	2.20	0.73
1:A:96:ARG:HH11	1:A:96:ARG:CG	2.00	0.73
1:C:224:ASN:HD21	1:D:223:ASN:HD21	1.35	0.73
1:A:154:ARG:HD3	2:A:364:HOH:O	1.90	0.71
1:C:172:LEU:HD13	1:C:174:VAL:HG23	1.72	0.71
2:B:362:HOH:O	1:C:231:ARG:HD3	1.89	0.71
1:C:305:ARG:NE	2:C:339:HOH:O	2.23	0.70
1:D:90:ARG:O	1:D:93:GLU:HB3	1.90	0.70
1:A:160:GLU:HG2	2:A:335:HOH:O	1.91	0.70
1:B:301:VAL:CG2	1:C:182:PRO:HB2	2.22	0.69
1:B:90:ARG:CZ	2:B:348:HOH:O	2.39	0.69
1:D:89:LEU:HD23	1:D:158:LEU:HD23	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ASP:O	1:B:76:CYS:N	2.27	0.68
1:C:195:THR:HG22	1:C:197:THR:N	2.06	0.68
1:B:182:PRO:HB2	1:C:301:VAL:HG22	1.76	0.68
1:D:296:LYS:NZ	2:D:311:HOH:O	2.27	0.68
1:C:110:ILE:HD11	2:C:313:HOH:O	1.94	0.67
1:C:26:GLU:HG3	1:C:36:LEU:HD12	1.75	0.67
1:D:254:VAL:HG13	1:D:264:ILE:HD11	1.76	0.67
1:D:23:ARG:HB2	1:D:23:ARG:HH11	1.59	0.67
1:D:30:GLY:HA3	1:D:61:VAL:CG1	2.22	0.66
1:C:96:ARG:HG2	1:C:96:ARG:HH11	1.60	0.65
1:B:90:ARG:HG2	1:B:259:ARG:CZ	2.27	0.65
1:B:112:PHE:CE2	1:B:296:LYS:HG3	2.31	0.64
1:C:112:PHE:CD2	1:C:200:THR:HG21	2.34	0.63
1:A:61:VAL:N	2:A:382:HOH:O	2.32	0.63
1:A:153:ASN:ND2	2:A:388:HOH:O	2.33	0.62
1:B:301:VAL:HG22	1:C:182:PRO:HB2	1.82	0.62
1:B:99:SER:HB2	1:B:280:LYS:NZ	2.14	0.62
1:D:223:ASN:C	1:D:223:ASN:HD22	2.03	0.62
1:A:269:ARG:NH1	1:A:271:GLU:OE2	2.33	0.62
1:A:159:ASN:C	1:A:160:GLU:HG3	2.19	0.61
1:C:139:LEU:HD13	1:C:274:ARG:HD3	1.81	0.61
1:B:163:LEU:HD11	1:B:245:ILE:HD11	1.81	0.61
1:D:48:SER:CB	1:D:51:LEU:HG	2.30	0.61
1:D:73:ALA:O	1:D:74:ASP:OD1	2.18	0.61
1:D:172:LEU:HD21	1:D:245:ILE:HD12	1.82	0.61
1:A:218:ILE:HB	1:A:235:THR:HG22	1.83	0.61
1:C:21:THR:HG22	1:C:121:ILE:HD13	1.81	0.61
1:A:195:THR:HG22	1:A:198:GLY:N	2.14	0.61
1:B:11:VAL:HG23	1:B:12:HIS:CB	2.28	0.61
1:B:20:GLU:C	1:B:22:ALA:H	2.03	0.60
1:D:78:LEU:HD12	1:D:101:PRO:HB2	1.82	0.60
1:D:254:VAL:HG13	1:D:264:ILE:CD1	2.30	0.60
1:C:96:ARG:HH11	1:C:96:ARG:CG	2.14	0.60
1:C:218:ILE:HB	1:C:235:THR:HG22	1.83	0.60
1:D:223:ASN:HD22	1:D:224:ASN:N	1.99	0.60
1:D:5:ARG:NH1	1:D:77:GLU:OE2	2.28	0.60
1:D:61:VAL:O	1:D:61:VAL:HG23	2.02	0.60
1:D:235:THR:CG2	1:D:239:ALA:HB3	2.31	0.60
1:B:269:ARG:HD3	1:B:271:GLU:OE2	2.01	0.60
1:A:200:THR:HG23	2:A:356:HOH:O	2.02	0.59
1:A:235:THR:HG23	1:A:236:SER:O	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:HIS:HE1	2:D:379:HOH:O	1.40	0.59
1:A:12:HIS:HA	1:A:41:ALA:HB3	1.84	0.59
1:D:38:VAL:HG12	1:D:42:GLU:HB3	1.84	0.59
1:D:24:ARG:O	1:D:28:VAL:HG23	2.03	0.59
1:D:110:ILE:HD13	1:D:295:ARG:HD3	1.85	0.58
1:D:254:VAL:HG13	1:D:264:ILE:CG1	2.32	0.58
1:B:223:ASN:C	1:B:223:ASN:HD22	2.07	0.58
1:A:172:LEU:HD13	1:A:174:VAL:HG23	1.84	0.58
1:D:43:ALA:HA	1:D:48:SER:OG	2.02	0.58
1:D:61:VAL:C	1:D:63:ILE:N	2.55	0.58
1:D:160:GLU:HG2	2:D:333:HOH:O	2.02	0.58
1:C:193:VAL:HG11	1:C:272:VAL:HG11	1.85	0.58
1:C:110:ILE:HA	2:C:375:HOH:O	2.03	0.58
1:C:224:ASN:HD21	1:D:223:ASN:ND2	2.01	0.57
1:D:242:ALA:HA	1:D:270:LEU:O	2.04	0.57
1:B:305:ARG:HH11	1:B:305:ARG:CG	2.11	0.57
1:B:182:PRO:HB2	1:C:301:VAL:CG2	2.34	0.57
1:D:25:VAL:O	1:D:29:LEU:HB2	2.04	0.57
1:B:28:VAL:O	1:B:32:ASN:ND2	2.37	0.57
1:D:7:VAL:H	1:D:35:ALA:CB	2.18	0.56
1:D:36:LEU:HB3	1:D:63:ILE:HG23	1.87	0.56
1:D:120:ALA:HB2	2:D:364:HOH:O	2.05	0.56
1:D:163:LEU:HD11	1:D:245:ILE:HD11	1.87	0.56
1:D:38:VAL:HG12	1:D:42:GLU:HG2	1.88	0.55
1:D:90:ARG:NH1	2:D:379:HOH:O	2.28	0.55
1:C:9:LEU:HD11	1:C:82:LEU:HG	1.89	0.55
1:B:293:LEU:HD22	1:B:297:PHE:CD1	2.42	0.55
1:C:228:LEU:HD21	1:D:297:PHE:O	2.07	0.55
1:C:242:ALA:HA	1:C:270:LEU:O	2.07	0.55
1:D:202:TYR:O	1:D:205:SER:HB2	2.06	0.55
1:B:7:VAL:CA	1:B:76:CYS:SG	2.95	0.55
1:D:158:LEU:O	1:D:195:THR:HG21	2.08	0.54
1:A:144:VAL:HG23	1:A:271:GLU:HB2	1.89	0.54
1:A:154:ARG:HG2	1:A:154:ARG:HH11	1.71	0.54
1:C:294:VAL:HA	1:C:299:LEU:HB2	1.88	0.54
1:D:216:GLU:O	1:D:237:PRO:HG3	2.07	0.54
1:A:223:ASN:C	1:A:223:ASN:HD22	2.10	0.54
1:C:16:ASP:C	1:C:18:ALA:H	2.11	0.54
1:A:120:ALA:O	1:A:124:VAL:HG23	2.08	0.53
1:D:254:VAL:HG13	1:D:264:ILE:HG13	1.89	0.53
1:A:96:ARG:HG2	1:A:96:ARG:NH1	2.14	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:VAL:HG22	1:C:125:LEU:HD21	1.90	0.53
1:D:39:LEU:HD23	1:D:42:GLU:OE2	2.09	0.53
1:D:61:VAL:HG23	1:D:63:ILE:HB	1.89	0.53
1:B:118:ALA:C	1:B:120:ALA:H	2.11	0.53
1:B:293:LEU:HD22	1:B:297:PHE:HD1	1.73	0.53
1:C:16:ASP:HB3	1:C:18:ALA:H	1.73	0.53
1:D:90:ARG:NH2	2:D:379:HOH:O	2.33	0.53
1:C:192:LEU:HD11	1:C:202:TYR:CD2	2.44	0.53
1:C:71:HIS:CD2	1:C:72:ALA:H	2.27	0.52
1:B:20:GLU:C	1:B:22:ALA:N	2.62	0.52
1:C:125:LEU:O	1:C:129:VAL:HG23	2.09	0.52
1:B:136:GLU:HG2	1:B:283:ARG:HG3	1.91	0.52
1:B:125:LEU:O	1:B:129:VAL:HG23	2.10	0.52
1:B:144:VAL:HG22	1:B:271:GLU:HB2	1.91	0.52
1:D:177:GLU:OE1	1:D:269:ARG:NH2	2.42	0.52
1:C:90:ARG:NH1	2:C:309:HOH:O	2.41	0.52
1:C:163:LEU:HD21	1:C:245:ILE:HD11	1.90	0.52
1:B:106:ASN:HD21	1:B:111:GLY:H	1.58	0.52
1:B:165:LYS:HD2	1:B:170:GLY:O	2.09	0.52
1:D:235:THR:HG23	1:D:239:ALA:HB3	1.92	0.52
1:A:223:ASN:ND2	1:B:224:ASN:HD21	2.02	0.52
1:C:32:ASN:O	1:C:33:LYS:HB2	2.09	0.52
1:B:242:ALA:HA	1:B:270:LEU:O	2.10	0.51
1:D:6:SER:O	1:D:76:CYS:HB3	2.10	0.51
1:D:87:THR:HG23	1:D:90:ARG:NH2	2.25	0.51
1:B:96:ARG:HG2	1:B:96:ARG:NH1	2.16	0.51
1:A:21:THR:HG23	2:A:365:HOH:O	2.08	0.51
1:A:11:VAL:HG13	1:A:82:LEU:HB2	1.93	0.51
1:A:224:ASN:HD21	1:B:223:ASN:ND2	2.08	0.51
1:C:216:GLU:O	1:C:237:PRO:HG3	2.11	0.51
1:D:93:GLU:HA	1:D:156:TRP:HZ2	1.76	0.51
1:A:294:VAL:HA	1:A:299:LEU:HB2	1.91	0.51
1:D:118:ALA:C	1:D:120:ALA:H	2.13	0.50
1:D:8:LEU:HD13	1:D:37:ARG:HB3	1.92	0.50
1:A:208:GLY:O	1:D:231:ARG:NH1	2.40	0.50
1:B:74:ASP:C	1:B:76:CYS:H	2.12	0.50
1:B:229:PHE:HB2	1:D:228:LEU:HG	1.93	0.50
1:C:223:ASN:HD22	1:C:224:ASN:N	2.08	0.50
1:D:144:VAL:HG22	1:D:271:GLU:HB2	1.92	0.50
1:B:254:VAL:HG22	1:B:262:MET:HB2	1.93	0.50
1:D:20:GLU:C	1:D:22:ALA:N	2.64	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:PRO:HB2	1:D:209:PRO:HB3	1.94	0.49
1:B:305:ARG:HB3	1:C:244:GLU:OE1	2.12	0.49
1:A:283:ARG:O	1:A:284:LEU:HD12	2.11	0.49
1:B:123:ALA:O	1:B:127:HIS:HD2	1.95	0.49
1:B:192:LEU:HD11	1:B:202:TYR:CD2	2.47	0.49
1:D:37:ARG:NH1	1:D:74:ASP:HB3	2.27	0.49
1:B:140:THR:HG22	1:B:275:CYS:CB	2.42	0.49
1:C:235:THR:HG21	1:C:241:ILE:HD11	1.92	0.49
1:D:120:ALA:O	1:D:122:ASP:N	2.45	0.49
1:B:118:ALA:O	1:B:120:ALA:N	2.44	0.49
1:C:265:PRO:O	1:C:268:SER:OG	2.24	0.49
1:A:113:LEU:HD22	1:A:281:TRP:HH2	1.78	0.49
1:C:121:ILE:HG23	1:C:122:ASP:H	1.77	0.48
1:B:301:VAL:HG21	1:C:182:PRO:HG2	1.95	0.48
1:D:7:VAL:N	1:D:35:ALA:HB3	2.25	0.48
1:B:90:ARG:HG2	1:B:259:ARG:NH2	2.28	0.48
1:C:168:ARG:HE	1:C:168:ARG:HB3	1.42	0.48
1:C:139:LEU:HD12	1:C:140:THR:N	2.28	0.48
1:D:132:ASP:OD1	1:D:132:ASP:C	2.50	0.48
1:C:254:VAL:HG21	1:C:270:LEU:HD11	1.95	0.48
1:A:301:VAL:HG22	1:D:182:PRO:HB2	1.96	0.48
1:D:91:ALA:HA	1:D:94:LEU:HD12	1.96	0.48
1:D:94:LEU:C	1:D:96:ARG:H	2.16	0.48
1:A:101:PRO:HA	1:A:280:LYS:HB2	1.96	0.47
1:A:182:PRO:HB2	1:D:301:VAL:HG22	1.96	0.47
1:C:113:LEU:HD22	1:C:281:TRP:CH2	2.33	0.47
1:D:23:ARG:O	1:D:27:LYS:N	2.40	0.47
1:B:99:SER:HB2	1:B:280:LYS:HZ3	1.80	0.47
1:C:290:THR:O	1:C:294:VAL:HG23	2.14	0.47
1:D:121:ILE:O	1:D:121:ILE:HG13	2.15	0.47
1:B:98:ALA:O	1:B:99:SER:C	2.53	0.47
1:B:195:THR:HG22	1:B:198:GLY:H	1.78	0.47
1:B:301:VAL:HG13	2:B:335:HOH:O	2.14	0.47
1:D:195:THR:HG22	1:D:197:THR:N	2.29	0.47
1:B:78:LEU:HG	1:B:79:VAL:N	2.29	0.47
1:B:168:ARG:HD2	1:B:168:ARG:HA	1.56	0.46
1:A:139:LEU:C	1:A:139:LEU:HD12	2.35	0.46
1:B:70:GLN:O	1:B:71:HIS:HB2	2.15	0.46
1:C:254:VAL:HB	1:C:264:ILE:HD11	1.96	0.46
1:D:8:LEU:HD12	1:D:9:LEU:O	2.15	0.46
1:D:95:ALA:O	1:D:99:SER:N	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:LEU:HA	1:D:281:TRP:HH2	1.80	0.46
1:B:283:ARG:O	1:B:284:LEU:HD12	2.16	0.46
1:D:168:ARG:HD2	1:D:168:ARG:HA	1.62	0.46
1:A:212:TRP:CZ3	1:D:233:MET:HB3	2.50	0.46
1:D:43:ALA:HB1	1:D:51:LEU:HD21	1.96	0.46
1:A:255:PHE:CE2	1:A:261:GLU:HG3	2.51	0.46
1:D:223:ASN:C	1:D:223:ASN:ND2	2.69	0.46
1:D:43:ALA:O	1:D:51:LEU:HD21	2.15	0.45
1:C:223:ASN:C	1:C:223:ASN:ND2	2.55	0.45
1:D:59:MET:HB3	1:D:61:VAL:HG22	1.98	0.45
1:B:81:VAL:HG21	1:B:91:ALA:CB	2.46	0.45
1:D:9:LEU:HG	1:D:10:VAL:N	2.30	0.45
1:D:98:ALA:O	1:D:100:ILE:HG23	2.16	0.45
1:A:100:ILE:HB	1:A:101:PRO:CD	2.47	0.45
1:A:218:ILE:HB	1:A:235:THR:CG2	2.46	0.45
1:C:136:GLU:HB3	2:C:363:HOH:O	2.16	0.45
1:B:96:ARG:CG	1:B:96:ARG:NH1	2.65	0.45
1:B:263:LEU:O	1:B:265:PRO:HD3	2.17	0.45
1:C:89:LEU:HD23	1:C:158:LEU:HD21	1.98	0.45
1:D:256:CYS:O	1:D:257:ASP:HB2	2.16	0.45
1:D:5:ARG:O	1:D:35:ALA:HB2	2.16	0.45
1:B:219:LEU:HD13	1:B:234:VAL:HG22	1.99	0.45
1:A:223:ASN:C	1:A:223:ASN:ND2	2.70	0.45
1:D:235:THR:HG23	1:D:239:ALA:CB	2.47	0.45
1:A:169:LEU:O	1:A:169:LEU:HD23	2.17	0.44
1:C:28:VAL:HG11	1:C:125:LEU:HB3	1.99	0.44
1:C:210:VAL:HG22	1:C:212:TRP:CZ3	2.52	0.44
1:D:61:VAL:O	1:D:63:ILE:HB	2.17	0.44
1:D:304:TRP:CG	1:D:305:ARG:N	2.86	0.44
1:A:245:ILE:O	1:A:246:GLU:C	2.56	0.44
1:D:11:VAL:HG22	1:D:12:HIS:N	2.32	0.44
1:A:62:GLU:C	1:A:63:ILE:HG13	2.36	0.44
1:A:231:ARG:HA	1:A:232:PRO:HD3	1.90	0.44
1:B:150:ARG:NH1	1:B:150:ARG:HB3	2.32	0.44
1:D:96:ARG:HD3	1:D:156:TRP:CD2	2.53	0.44
1:D:254:VAL:CG1	1:D:264:ILE:HG13	2.48	0.44
1:B:195:THR:CG2	1:B:197:THR:H	2.31	0.44
1:B:223:ASN:C	1:B:223:ASN:ND2	2.70	0.44
1:C:10:VAL:HB	1:C:81:VAL:HG13	2.00	0.44
1:C:226:HIS:O	1:C:227:ALA:HB2	2.18	0.44
1:A:96:ARG:CG	1:A:96:ARG:NH1	2.68	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:LEU:HD23	1:A:125:LEU:HA	1.83	0.44
1:C:12:HIS:O	1:C:13:THR:HB	2.17	0.44
1:D:46:ARG:C	1:D:48:SER:N	2.71	0.44
1:D:195:THR:HG22	1:D:198:GLY:H	1.83	0.44
1:A:159:ASN:HB3	1:A:160:GLU:HG3	2.00	0.43
1:B:112:PHE:CZ	1:B:296:LYS:HG3	2.52	0.43
1:D:120:ALA:C	1:D:122:ASP:N	2.71	0.43
1:D:103:LEU:HB2	1:D:282:ALA:HB3	2.01	0.43
1:D:296:LYS:HE2	2:D:329:HOH:O	2.19	0.43
1:A:195:THR:CG2	1:A:198:GLY:H	2.23	0.43
1:C:235:THR:CG2	1:C:239:ALA:HB3	2.48	0.43
1:C:150:ARG:HE	1:C:150:ARG:HB3	1.70	0.43
1:D:120:ALA:C	1:D:122:ASP:H	2.21	0.43
1:A:30:GLY:C	1:A:32:ASN:H	2.22	0.43
1:B:198:GLY:C	1:B:200:THR:H	2.20	0.43
1:B:254:VAL:HG13	1:B:264:ILE:HD11	2.00	0.43
1:C:46:ARG:NH1	2:C:332:HOH:O	2.52	0.43
1:D:146:ARG:NH1	1:D:146:ARG:HG3	2.33	0.43
1:B:90:ARG:NH1	2:B:348:HOH:O	2.50	0.43
1:D:19:THR:C	1:D:20:GLU:HG3	2.39	0.43
1:D:23:ARG:HA	1:D:26:GLU:HB2	2.01	0.43
1:D:25:VAL:HA	1:D:125:LEU:HD11	2.00	0.43
1:A:143:VAL:HA	1:A:271:GLU:O	2.19	0.43
1:B:140:THR:HG22	1:B:275:CYS:HB3	2.01	0.43
1:B:159:ASN:HB3	1:B:160:GLU:HG3	2.01	0.43
1:C:195:THR:HG23	1:C:196:PRO:HD2	2.01	0.43
1:B:209:PRO:HB3	1:C:232:PRO:HB2	2.00	0.42
1:D:254:VAL:HG11	1:D:270:LEU:HD11	2.01	0.42
1:B:103:LEU:HD13	1:B:282:ALA:CB	2.50	0.42
1:D:61:VAL:CG2	1:D:63:ILE:HB	2.49	0.42
1:A:21:THR:CG2	2:A:365:HOH:O	2.67	0.42
1:B:103:LEU:HD13	1:B:282:ALA:HB3	2.00	0.42
1:D:43:ALA:HA	1:D:48:SER:HG	1.84	0.42
1:C:235:THR:HG23	1:C:239:ALA:HB3	2.02	0.42
1:D:146:ARG:HG3	1:D:146:ARG:HH11	1.84	0.42
1:D:94:LEU:H	1:D:94:LEU:HG	1.59	0.42
1:A:224:ASN:HD21	1:B:223:ASN:HD21	1.67	0.42
1:D:35:ALA:O	1:D:63:ILE:HA	2.20	0.42
1:D:125:LEU:O	1:D:129:VAL:HG23	2.19	0.42
1:C:257:ASP:O	1:C:259:ARG:HG2	2.20	0.41
1:D:78:LEU:HD13	1:D:133:TYR:CZ	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:ALA:O	1:C:121:ILE:HG22	2.20	0.41
1:D:121:ILE:HA	1:D:124:VAL:HB	2.01	0.41
1:A:198:GLY:C	1:A:200:THR:H	2.23	0.41
1:A:299:LEU:HD12	1:A:299:LEU:HA	1.84	0.41
1:B:74:ASP:HB2	1:B:98:ALA:HB3	2.03	0.41
1:C:192:LEU:HD11	1:C:202:TYR:HD2	1.85	0.41
1:A:189:ASP:OD2	1:B:202:TYR:OH	2.35	0.41
1:A:205:SER:OG	1:B:226:HIS:HD2	2.03	0.41
1:A:274:ARG:O	1:A:274:ARG:HG3	2.20	0.41
1:D:25:VAL:HG22	1:D:125:LEU:HD11	2.02	0.41
1:D:38:VAL:HG12	1:D:42:GLU:CB	2.50	0.41
1:D:46:ARG:H	1:D:46:ARG:HG2	1.58	0.41
1:A:195:THR:CG2	1:A:197:THR:HB	2.50	0.41
1:D:235:THR:HG22	1:D:236:SER:O	2.21	0.41
1:D:5:ARG:O	1:D:34:ILE:O	2.38	0.41
1:D:121:ILE:O	1:D:125:LEU:HB2	2.21	0.41
1:A:23:ARG:O	1:A:27:LYS:HG3	2.20	0.41
1:A:36:LEU:HD23	1:A:36:LEU:HA	1.84	0.41
1:A:177:GLU:OE2	1:A:269:ARG:NH2	2.54	0.41
1:B:229:PHE:CE1	1:B:231:ARG:HB2	2.55	0.41
1:C:16:ASP:C	1:C:18:ALA:N	2.73	0.41
1:C:71:HIS:HD2	1:C:72:ALA:H	1.69	0.41
1:D:7:VAL:O	1:D:7:VAL:HG12	2.20	0.41
1:D:43:ALA:HB3	1:D:66:VAL:HG13	2.03	0.41
1:A:270:LEU:HD23	1:A:270:LEU:HA	1.85	0.40
1:B:7:VAL:HG12	1:B:8:LEU:O	2.21	0.40
1:D:138:ARG:HH11	1:D:138:ARG:CG	2.35	0.40
1:B:124:VAL:O	1:B:128:VAL:HG23	2.20	0.40
1:B:195:THR:HG22	1:B:197:THR:H	1.87	0.40
1:C:110:ILE:HG23	1:C:295:ARG:HH11	1.86	0.40
1:D:90:ARG:HH11	1:D:90:ARG:HG3	1.86	0.40
1:A:158:LEU:HD11	1:A:281:TRP:HZ2	1.86	0.40
1:B:81:VAL:CG2	1:B:91:ALA:CB	3.00	0.40
1:B:216:GLU:O	1:B:237:PRO:HG3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:316:HOH:O	2:D:320:HOH:O[4_555]	2.14	0.06

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	275/307 (90%)	261 (95%)	12 (4%)	2 (1%)	22 53
1	B	252/307 (82%)	225 (89%)	19 (8%)	8 (3%)	4 13
1	C	279/307 (91%)	253 (91%)	24 (9%)	2 (1%)	22 53
1	D	297/307 (97%)	256 (86%)	25 (8%)	16 (5%)	2 5
All	All	1103/1228 (90%)	995 (90%)	80 (7%)	28 (2%)	5 19

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	75	GLY
1	B	119	GLU
1	D	20	GLU
1	D	62	GLU
1	D	72	ALA
1	D	74	ASP
1	D	95	ALA
1	A	31	ASP
1	B	71	HIS
1	B	99	SER
1	C	65	VAL
1	D	34	ILE
1	D	46	ARG
1	D	67	ASP
1	D	93	GLU
1	D	94	LEU
1	D	119	GLU
1	A	259	ARG
1	B	165	LYS
1	B	74	ASP
1	B	108	GLY
1	C	119	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	27	LYS
1	D	36	LEU
1	D	71	HIS
1	B	201	ALA
1	D	35	ALA
1	D	66	VAL

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	223/242 (92%)	169 (76%)	54 (24%)	0 2
1	B	202/242 (84%)	148 (73%)	54 (27%)	0 1
1	C	226/242 (93%)	175 (77%)	51 (23%)	1 2
1	D	235/242 (97%)	168 (72%)	67 (28%)	0 1
All	All	886/968 (92%)	660 (74%)	226 (26%)	0 1

All (226) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	HIS
1	A	11	VAL
1	A	21	THR
1	A	24	ARG
1	A	29	LEU
1	A	33	LYS
1	A	36	LEU
1	A	42	GLU
1	A	70	GLN
1	A	74	ASP
1	A	81	VAL
1	A	87	THR
1	A	90	ARG
1	A	96	ARG
1	A	100	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	102	VAL
1	A	109	ARG
1	A	122	ASP
1	A	126	GLU
1	A	134	ARG
1	A	136	GLU
1	A	139	LEU
1	A	146	ARG
1	A	150	ARG
1	A	154	ARG
1	A	158	LEU
1	A	160	GLU
1	A	169	LEU
1	A	171	VAL
1	A	172	LEU
1	A	184	SER
1	A	192	LEU
1	A	195	THR
1	A	200	THR
1	A	210	VAL
1	A	223	ASN
1	A	228	LEU
1	A	231	ARG
1	A	235	THR
1	A	236	SER
1	A	243	ILE
1	A	244	GLU
1	A	259	ARG
1	A	270	LEU
1	A	274	ARG
1	A	277	THR
1	A	278	SER
1	A	280	LYS
1	A	286	SER
1	A	293	LEU
1	A	295	ARG
1	A	299	LEU
1	A	301	VAL
1	A	302	THR
1	B	11	VAL
1	B	27	LYS
1	B	29	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	32	ASN
1	B	70	GLN
1	B	74	ASP
1	B	77	GLU
1	B	82	LEU
1	B	85	ASP
1	B	90	ARG
1	B	96	ARG
1	B	97	ASN
1	B	109	ARG
1	B	117	GLU
1	B	122	ASP
1	B	126	GLU
1	B	134	ARG
1	B	137	ASP
1	B	139	LEU
1	B	140	THR
1	B	146	ARG
1	B	147	GLN
1	B	150	ARG
1	B	154	ARG
1	B	158	LEU
1	B	160	GLU
1	B	169	LEU
1	B	171	VAL
1	B	172	LEU
1	B	178	ILE
1	B	184	SER
1	B	195	THR
1	B	200	THR
1	B	210	VAL
1	B	215	LEU
1	B	216	GLU
1	B	223	ASN
1	B	228	LEU
1	B	235	THR
1	B	251	ASP
1	B	263	LEU
1	B	269	ARG
1	B	274	ARG
1	B	276	VAL
1	B	277	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	280	LYS
1	B	283	ARG
1	B	293	LEU
1	B	295	ARG
1	B	298	ARG
1	B	299	LEU
1	B	301	VAL
1	B	302	THR
1	B	305	ARG
1	C	16	ASP
1	C	17	GLU
1	C	20	GLU
1	C	21	THR
1	C	23	ARG
1	C	24	ARG
1	C	33	LYS
1	C	36	LEU
1	C	39	LEU
1	C	45	ASP
1	C	46	ARG
1	C	66	VAL
1	C	70	GLN
1	C	71	HIS
1	C	81	VAL
1	C	90	ARG
1	C	96	ARG
1	C	102	VAL
1	C	122	ASP
1	C	126	GLU
1	C	139	LEU
1	C	143	VAL
1	C	147	GLN
1	C	150	ARG
1	C	158	LEU
1	C	160	GLU
1	C	168	ARG
1	C	169	LEU
1	C	171	VAL
1	C	172	LEU
1	C	174	VAL
1	C	184	SER
1	C	192	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	200	THR
1	C	210	VAL
1	C	223	ASN
1	C	228	LEU
1	C	235	THR
1	C	245	ILE
1	C	259	ARG
1	C	269	ARG
1	C	270	LEU
1	C	274	ARG
1	C	280	LYS
1	C	284	LEU
1	C	285	ASP
1	C	293	LEU
1	C	295	ARG
1	C	296	LYS
1	C	299	LEU
1	C	301	VAL
1	D	8	LEU
1	D	20	GLU
1	D	23	ARG
1	D	27	LYS
1	D	29	LEU
1	D	31	ASP
1	D	37	ARG
1	D	38	VAL
1	D	40	SER
1	D	42	GLU
1	D	46	ARG
1	D	49	LEU
1	D	50	HIS
1	D	51	LEU
1	D	59	MET
1	D	62	GLU
1	D	65	VAL
1	D	69	ASP
1	D	82	LEU
1	D	87	THR
1	D	94	LEU
1	D	96	ARG
1	D	110	ILE
1	D	121	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	122	ASP
1	D	126	GLU
1	D	132	ASP
1	D	134	ARG
1	D	136	GLU
1	D	138	ARG
1	D	139	LEU
1	D	142	ASP
1	D	150	ARG
1	D	159	ASN
1	D	168	ARG
1	D	169	LEU
1	D	171	VAL
1	D	172	LEU
1	D	174	VAL
1	D	184	SER
1	D	195	THR
1	D	200	THR
1	D	210	VAL
1	D	223	ASN
1	D	228	LEU
1	D	235	THR
1	D	236	SER
1	D	238	GLU
1	D	241	ILE
1	D	248	ASP
1	D	254	VAL
1	D	259	ARG
1	D	272	VAL
1	D	273	THR
1	D	274	ARG
1	D	276	VAL
1	D	283	ARG
1	D	284	LEU
1	D	285	ASP
1	D	293	LEU
1	D	295	ARG
1	D	296	LYS
1	D	298	ARG
1	D	299	LEU
1	D	301	VAL
1	D	302	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	305	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	223	ASN
1	A	250	HIS
1	B	32	ASN
1	B	106	ASN
1	B	127	HIS
1	B	223	ASN
1	B	226	HIS
1	C	71	HIS
1	C	223	ASN
1	D	106	ASN
1	D	223	ASN
1	D	250	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no 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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.