



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2023 – 05:09 pm GMT

PDB ID : 2Y4P
Title : Dimeric structure of DAPK-1 catalytic domain
Authors : de Diego, I.; Lehmann, F.; Wilmanns, M.
Deposited on : 2011-01-07
Resolution : 2.65 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
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
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

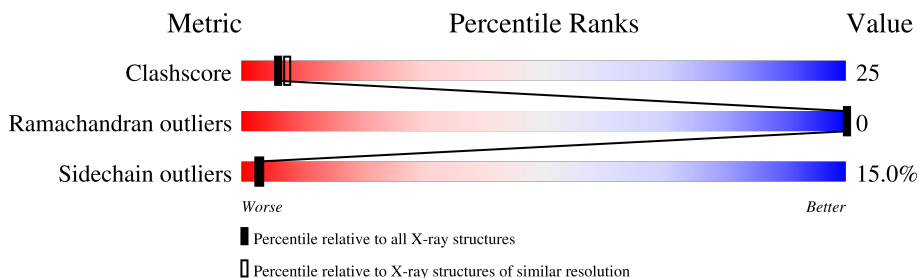
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)

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 $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	285	60% 23% 5% 12%
1	B	285	37% 21% 7% 35%
1	C	285	56% 30% 7% 7%
1	D	285	36% 25% 8% 32%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7346 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 DEATH-ASSOCIATED PROTEIN KINASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	251	Total 2024	C 1306	N 330	O 384	S 4	0	0	0
1	B	184	Total 1475	C 958	N 235	O 279	S 3	0	0	0
1	C	264	Total 2122	C 1361	N 353	O 404	S 4	0	0	0
1	D	194	Total 1550	C 1004	N 248	O 295	S 3	0	0	0

- Molecule 2 is water.

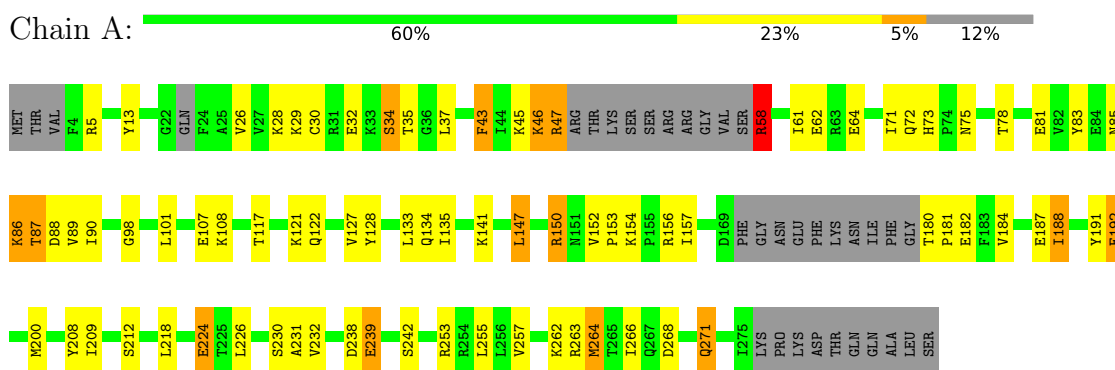
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	51	Total 51	O 51	0	0
2	B	23	Total 23	O 23	0	0
2	C	58	Total 58	O 58	0	0
2	D	43	Total 43	O 43	0	0

3 Residue-property plots i

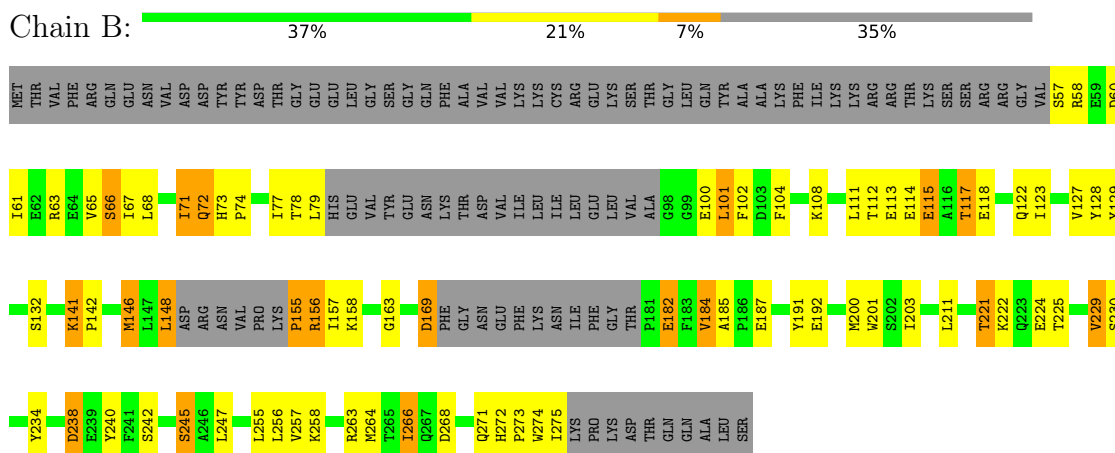
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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 failed to run properly.

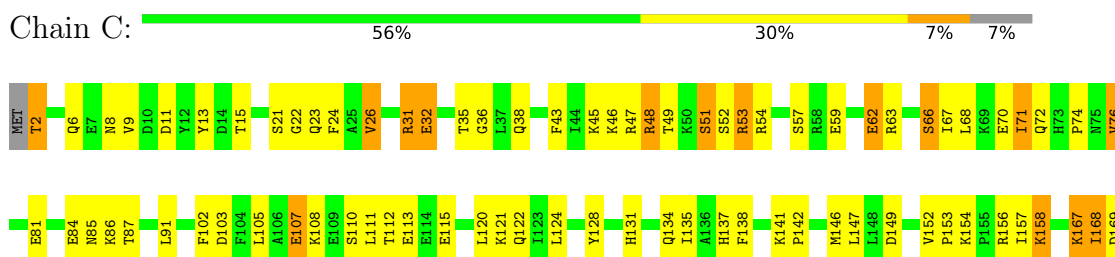
- Molecule 1: DEATH-ASSOCIATED PROTEIN KINASE 1

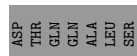


- Molecule 1: DEATH-ASSOCIATED PROTEIN KINASE 1

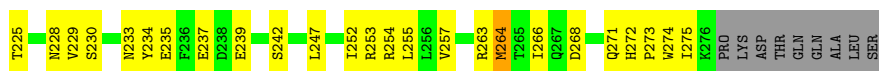
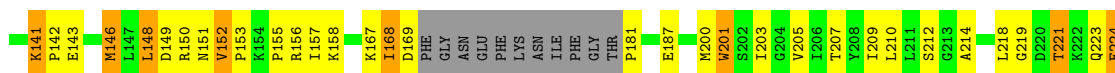
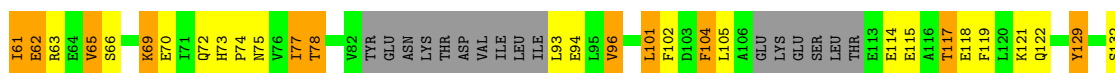
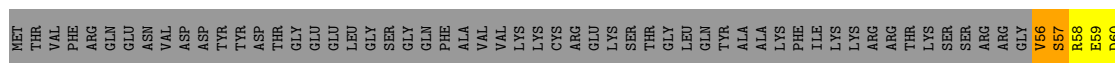
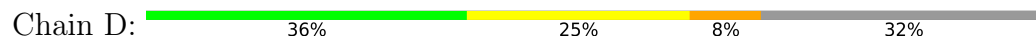


- Molecule 1: DEATH-ASSOCIATED PROTEIN KINASE 1





- Molecule 1: DEATH-ASSOCIATED PROTEIN KINASE 1



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.94Å 73.70Å 120.28Å 90.00° 101.24° 90.00°	Depositor
Resolution (Å)	117.97 – 2.65	Depositor
% Data completeness (in resolution range)	98.0 (117.97-2.65)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 2.65Å)	Xtrriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.252 , 0.312	Depositor
Wilson B-factor (Å ²)	38.7	Xtrriage
Anisotropy	0.734	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7346	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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 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	1.77	8/2063 (0.4%)	0.89	1/2788 (0.0%)
1	B	1.69	8/1505 (0.5%)	0.85	0/2036
1	C	1.54	8/2162 (0.4%)	0.92	3/2921 (0.1%)
1	D	1.67	6/1582 (0.4%)	0.82	0/2144
All	All	1.67	30/7312 (0.4%)	0.88	4/9889 (0.0%)

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	C	0	3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	275	ILE	C-N	-18.18	0.92	1.34
1	C	91	LEU	CA-C	-9.90	1.27	1.52
1	C	66	SER	N-CA	-9.21	1.27	1.46
1	C	76	VAL	N-CA	-8.43	1.29	1.46
1	B	234	TYR	CD2-CE2	-5.94	1.30	1.39
1	B	234	TYR	CD1-CE1	-5.90	1.30	1.39
1	A	208	TYR	CD1-CE1	-5.89	1.30	1.39
1	C	128	TYR	CD1-CE1	-5.88	1.30	1.39
1	D	234	TYR	CD2-CE2	-5.74	1.30	1.39
1	B	128	TYR	CD1-CE1	-5.69	1.30	1.39
1	A	184	VAL	CB-CG1	-5.66	1.41	1.52
1	D	234	TYR	CD1-CE1	-5.66	1.30	1.39
1	D	129	TYR	CD2-CE2	-5.64	1.30	1.39
1	A	208	TYR	CD2-CE2	-5.57	1.30	1.39
1	B	240	TYR	CD1-CE1	-5.57	1.30	1.39
1	B	240	TYR	CE1-CZ	-5.45	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	32	GLU	CG-CD	-5.44	1.43	1.51
1	A	128	TYR	CD2-CE2	-5.39	1.31	1.39
1	A	128	TYR	CD1-CE1	-5.35	1.31	1.39
1	B	229	VAL	CB-CG2	-5.33	1.41	1.52
1	C	128	TYR	CD2-CE2	-5.28	1.31	1.39
1	D	129	TYR	CD1-CE1	-5.27	1.31	1.39
1	A	30	CYS	CB-SG	-5.19	1.73	1.81
1	C	184	VAL	CB-CG1	-5.15	1.42	1.52
1	A	128	TYR	CE1-CZ	-5.12	1.31	1.38
1	B	184	VAL	CB-CG1	-5.09	1.42	1.52
1	A	127	VAL	CB-CG2	-5.08	1.42	1.52
1	D	201	TRP	CB-CG	-5.06	1.41	1.50
1	B	182	GLU	CG-CD	-5.05	1.44	1.51
1	D	205	VAL	CB-CG2	-5.05	1.42	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	91	LEU	CA-C-O	-11.88	95.14	120.10
1	C	91	LEU	CA-C-N	7.01	132.62	117.20
1	A	58	ARG	NE-CZ-NH1	-5.85	117.38	120.30
1	C	91	LEU	O-C-N	5.15	130.94	122.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	275	ILE	Mainchain
1	C	66	SER	Mainchain
1	C	76	VAL	Mainchain

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	2024	0	2009	72	1
1	B	1475	0	1461	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2122	0	2105	90	1
1	D	1550	0	1524	108	1
2	A	51	0	0	4	0
2	B	23	0	0	4	0
2	C	58	0	0	12	0
2	D	43	0	0	13	0
All	All	7346	0	7099	352	2

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 25.

All (352) 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:C:180:THR:HG23	1:C:181:PRO:CD	1.35	1.55
1:D:181:PRO:HD2	2:D:2020:HOH:O	1.23	1.34
1:D:78:THR:HG23	1:D:94:GLU:OE2	1.29	1.32
1:D:70:GLU:OE2	1:D:167:LYS:NZ	1.61	1.30
1:A:180:THR:CG2	1:A:181:PRO:HD3	1.64	1.26
1:A:180:THR:HG23	1:A:181:PRO:CD	1.67	1.25
1:B:112:THR:N	1:B:115:GLU:OE2	1.67	1.25
1:C:22:GLY:C	2:C:2007:HOH:O	1.76	1.24
1:C:13:TYR:OH	1:C:81:GLU:OE1	1.56	1.22
1:D:223:GLN:HB3	2:D:2029:HOH:O	1.09	1.21
1:C:180:THR:CG2	1:C:181:PRO:HD3	1.70	1.19
1:C:102:PHE:HB2	2:C:2020:HOH:O	1.41	1.18
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.24	1.16
1:C:2:THR:N	1:C:62:GLU:OE2	1.79	1.14
1:D:129:TYR:O	1:D:132:SER:OG	1.62	1.14
1:D:62:GLU:HB2	2:D:2001:HOH:O	1.47	1.14
1:B:78:THR:CG2	2:B:2004:HOH:O	1.92	1.14
1:C:180:THR:CG2	1:C:181:PRO:CD	2.21	1.13
1:A:152:VAL:HG13	1:A:153:PRO:CD	1.77	1.13
1:D:62:GLU:CB	2:D:2001:HOH:O	1.97	1.13
1:D:56:VAL:HB	1:D:61:ILE:HD11	1.30	1.12
1:D:209:ILE:O	1:D:212:SER:O	1.65	1.11
1:A:152:VAL:CG1	1:A:153:PRO:HD2	1.80	1.09
1:C:31:ARG:HH11	1:C:31:ARG:CG	1.62	1.09
1:C:180:THR:HG23	1:C:181:PRO:HD3	1.13	1.08
1:D:58:ARG:HA	1:D:61:ILE:HD13	1.33	1.07
1:A:13:TYR:OH	1:A:81:GLU:OE1	1.70	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:GLU:OE1	1:B:245:SER:OG	1.71	1.06
1:D:78:THR:CG2	1:D:94:GLU:OE2	2.03	1.06
1:D:61:ILE:N	1:D:61:ILE:HD12	1.68	1.05
1:A:180:THR:CG2	1:A:181:PRO:CD	2.27	1.05
1:B:112:THR:HB	1:B:115:GLU:HG3	1.39	1.04
1:C:180:THR:HG23	1:C:181:PRO:HD2	1.08	1.04
1:B:57:SER:O	1:B:61:ILE:HD13	1.59	1.03
1:A:152:VAL:CG1	1:A:153:PRO:CD	2.35	1.03
1:D:58:ARG:O	2:D:2001:HOH:O	1.74	1.03
1:B:221:THR:OG1	1:B:224:GLU:HB2	1.61	1.00
1:B:200:MET:HE2	1:B:203:ILE:HD12	1.40	0.98
1:D:117:THR:O	1:D:121:LYS:HG3	1.63	0.98
1:B:112:THR:HG22	1:B:114:GLU:H	1.28	0.96
1:C:31:ARG:NH1	1:C:31:ARG:HG2	1.44	0.96
1:B:78:THR:HG21	2:B:2004:HOH:O	1.54	0.95
1:C:192:GLU:HG2	1:C:192:GLU:O	1.67	0.95
1:A:192:GLU:O	1:A:192:GLU:HG2	1.64	0.94
1:C:31:ARG:HH11	1:C:31:ARG:HG2	0.81	0.94
1:D:61:ILE:CD1	1:D:61:ILE:H	1.80	0.94
1:A:209:ILE:O	1:A:212:SER:O	1.87	0.92
1:C:149:ASP:OD2	1:C:152:VAL:HG23	1.68	0.92
1:D:61:ILE:N	1:D:61:ILE:CD1	2.34	0.91
1:D:61:ILE:HD12	1:D:61:ILE:H	1.35	0.91
1:D:152:VAL:HG22	1:D:153:PRO:HD2	1.53	0.90
1:A:58:ARG:CD	1:A:58:ARG:N	2.29	0.90
1:B:112:THR:HG22	1:B:114:GLU:N	1.86	0.89
1:C:180:THR:CG2	1:C:181:PRO:HD2	1.95	0.89
1:D:254:ARG:NH1	2:D:2039:HOH:O	2.05	0.88
1:C:22:GLY:CA	2:C:2007:HOH:O	2.13	0.88
1:C:31:ARG:CG	1:C:31:ARG:NH1	2.29	0.88
1:A:58:ARG:N	1:A:58:ARG:HD3	1.87	0.88
1:C:180:THR:CB	1:C:181:PRO:HD3	2.04	0.87
1:D:104:PHE:CE1	1:D:105:LEU:HD21	2.10	0.86
1:B:200:MET:CE	1:B:203:ILE:HD12	2.05	0.86
1:C:135:ILE:HG13	1:C:167:LYS:HE2	1.56	0.85
1:D:59:GLU:O	2:D:2001:HOH:O	1.93	0.85
1:D:104:PHE:O	1:D:104:PHE:CD1	2.30	0.85
1:B:112:THR:HB	1:B:115:GLU:CG	2.07	0.84
1:C:275:ILE:O	2:C:2058:HOH:O	1.96	0.84
1:D:56:VAL:HB	1:D:61:ILE:CD1	2.08	0.83
1:D:73:HIS:HE1	1:D:75:ASN:HD22	1.21	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:PRO:C	1:B:156:ARG:HD3	1.99	0.83
1:A:64:GLU:OE2	2:A:2009:HOH:O	1.96	0.82
1:A:122:GLN:HE22	1:A:156:ARG:HA	1.45	0.82
1:C:23:GLN:N	2:C:2007:HOH:O	1.99	0.82
1:D:104:PHE:CD1	1:D:105:LEU:CD2	2.63	0.82
1:A:232:VAL:HG12	1:A:232:VAL:O	1.79	0.81
1:C:8:ASN:O	1:C:11:ASP:HB2	1.81	0.80
1:D:62:GLU:N	2:D:2001:HOH:O	2.12	0.80
1:A:180:THR:HG23	1:A:181:PRO:HD3	0.83	0.80
1:C:70:GLU:OE1	2:C:2017:HOH:O	2.00	0.79
1:C:192:GLU:CD	1:C:192:GLU:H	1.84	0.79
1:C:31:ARG:HD3	1:C:38:GLN:HG3	1.64	0.79
1:C:192:GLU:O	1:C:192:GLU:CG	2.30	0.78
1:B:78:THR:HG22	2:B:2004:HOH:O	1.68	0.77
1:C:53:ARG:HD2	1:C:54:ARG:H	1.47	0.77
1:D:58:ARG:CA	1:D:61:ILE:HD13	2.14	0.77
1:D:104:PHE:O	1:D:104:PHE:CG	2.37	0.77
1:A:46:LYS:HD3	1:A:89:VAL:HG23	1.67	0.76
1:B:192:GLU:O	1:B:192:GLU:HG2	1.84	0.76
1:D:181:PRO:CD	2:D:2020:HOH:O	1.99	0.76
1:D:73:HIS:CE1	1:D:75:ASN:HD22	2.02	0.75
1:D:221:THR:OG1	1:D:224:GLU:OE1	2.05	0.74
1:A:257:VAL:O	1:A:263:ARG:NH1	2.20	0.74
1:B:60:ASP:OD1	1:B:63:ARG:NH1	2.20	0.74
1:D:74:PRO:O	1:D:158:LYS:HE2	1.86	0.74
1:D:257:VAL:O	1:D:263:ARG:NH1	2.20	0.73
1:D:104:PHE:CE1	1:D:105:LEU:CD2	2.70	0.73
1:A:180:THR:CG2	1:A:181:PRO:HD2	2.19	0.72
1:D:104:PHE:O	1:D:105:LEU:HD23	1.89	0.72
1:C:22:GLY:HA3	2:C:2007:HOH:O	1.79	0.72
1:A:192:GLU:O	1:A:192:GLU:CG	2.37	0.72
1:C:26:VAL:HG23	1:C:43:PHE:HB2	1.72	0.72
1:B:257:VAL:O	1:B:263:ARG:NH1	2.23	0.71
1:D:104:PHE:CD1	1:D:105:LEU:HD23	2.24	0.71
1:A:264:MET:HG2	1:A:268:ASP:HB2	1.73	0.71
1:B:113:GLU:CD	1:B:245:SER:OG	2.29	0.71
1:A:180:THR:HG22	1:A:181:PRO:HD2	1.73	0.70
1:A:152:VAL:HG12	1:A:153:PRO:CD	2.20	0.70
1:B:156:ARG:HD3	1:B:156:ARG:N	2.05	0.70
1:B:266:ILE:O	1:B:266:ILE:HG13	1.91	0.70
1:A:152:VAL:HG12	1:A:153:PRO:HD2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:THR:HG22	1:A:181:PRO:CD	2.20	0.69
1:A:152:VAL:HG13	1:A:153:PRO:HD3	1.74	0.69
1:D:104:PHE:CD1	1:D:105:LEU:HD21	2.25	0.69
1:A:200:MET:HE1	1:A:266:ILE:HD13	1.75	0.69
1:B:77:ILE:HA	1:B:158:LYS:HD3	1.75	0.68
1:D:117:THR:HG23	1:D:121:LYS:HE2	1.76	0.68
1:D:78:THR:HG23	1:D:94:GLU:CD	2.13	0.67
1:D:56:VAL:O	1:D:61:ILE:HD11	1.93	0.67
1:D:61:ILE:O	1:D:65:VAL:HG23	1.94	0.67
1:C:152:VAL:HG13	1:C:153:PRO:HD2	1.76	0.67
1:A:187:GLU:OE2	2:A:2034:HOH:O	2.13	0.66
1:B:112:THR:CB	1:B:115:GLU:OE2	2.43	0.66
1:D:96:VAL:HG12	1:D:148:LEU:HA	1.77	0.66
1:C:180:THR:OG1	1:C:181:PRO:HD3	1.95	0.65
1:B:57:SER:O	1:B:61:ILE:CD1	2.41	0.65
1:B:112:THR:HB	1:B:115:GLU:OE2	1.96	0.65
1:D:104:PHE:HE1	1:D:105:LEU:HD21	1.56	0.65
1:C:180:THR:CB	1:C:181:PRO:CD	2.64	0.65
1:B:257:VAL:HB	1:B:263:ARG:HG2	1.78	0.65
1:D:122:GLN:HE22	1:D:156:ARG:HA	1.62	0.65
1:A:152:VAL:HG12	1:A:153:PRO:N	2.12	0.64
1:D:77:ILE:HD13	1:D:93:LEU:HD22	1.78	0.64
1:B:112:THR:CG2	1:B:114:GLU:H	2.06	0.64
1:C:209:ILE:O	1:C:212:SER:O	2.14	0.64
1:C:237:GLU:HG2	2:C:2049:HOH:O	1.97	0.64
1:C:24:PHE:N	2:C:2007:HOH:O	2.32	0.63
1:D:122:GLN:NE2	1:D:157:ILE:H	1.97	0.63
1:B:57:SER:OG	1:B:58:ARG:N	2.29	0.63
1:A:87:THR:HG22	1:A:88:ASP:CG	2.18	0.62
1:A:133:LEU:HB2	1:A:135:ILE:HD12	1.81	0.62
1:D:65:VAL:O	1:D:69:LYS:HD3	1.99	0.62
1:D:275:ILE:O	1:D:275:ILE:HG22	2.00	0.62
1:C:63:ARG:O	1:C:67:ILE:HG13	2.00	0.62
1:C:48:ARG:NH1	2:C:2009:HOH:O	2.32	0.62
1:B:146:MET:O	1:B:157:ILE:HA	2.00	0.62
1:B:200:MET:HE2	1:B:200:MET:HA	1.82	0.61
1:D:104:PHE:CD1	1:D:104:PHE:C	2.73	0.61
1:B:264:MET:CG	1:B:268:ASP:HB2	2.30	0.61
1:D:149:ASP:OD1	1:D:151:ASN:N	2.31	0.61
1:A:117:THR:CG2	1:A:117:THR:O	2.49	0.61
1:B:148:LEU:HD21	1:B:158:LYS:HE2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:ARG:HD2	1:C:54:ARG:N	2.14	0.61
1:A:263:ARG:NH2	1:B:187:GLU:OE2	2.34	0.61
1:C:103:ASP:O	1:C:107:GLU:OE1	2.17	0.60
1:D:101:LEU:HD23	1:D:102:PHE:CD1	2.37	0.60
1:C:48:ARG:NH1	2:C:2010:HOH:O	2.33	0.60
1:D:56:VAL:CB	1:D:61:ILE:HD11	2.19	0.60
1:A:191:TYR:HH	1:B:191:TYR:HH	1.49	0.60
1:D:117:THR:CG2	1:D:121:LYS:HE2	2.31	0.60
1:C:200:MET:HE1	1:C:266:ILE:HD13	1.84	0.59
1:B:112:THR:HB	1:B:115:GLU:CD	2.22	0.59
1:B:258:LYS:NZ	1:C:238:ASP:OD1	2.35	0.59
1:C:43:PHE:N	1:C:43:PHE:CD1	2.71	0.59
1:A:117:THR:O	1:A:117:THR:HG22	2.03	0.59
1:B:112:THR:HG21	1:B:114:GLU:HB3	1.85	0.58
1:C:168:ILE:HG22	1:C:168:ILE:O	2.03	0.58
1:A:73:HIS:HE1	1:A:75:ASN:HD22	1.52	0.58
1:B:273:PRO:C	1:B:275:ILE:H	2.07	0.58
1:B:101:LEU:HD23	1:B:102:PHE:CE1	2.39	0.58
1:C:264:MET:HG2	1:C:268:ASP:HB2	1.84	0.58
1:D:62:GLU:CA	2:D:2001:HOH:O	2.36	0.58
1:D:253:ARG:NH2	2:D:2038:HOH:O	2.32	0.58
1:A:43:PHE:CD1	1:A:43:PHE:N	2.73	0.57
1:A:152:VAL:CG1	1:A:153:PRO:N	2.63	0.57
1:D:59:GLU:C	2:D:2001:HOH:O	2.38	0.57
1:D:61:ILE:HD13	1:D:61:ILE:H	1.68	0.57
1:B:264:MET:HG2	1:B:268:ASP:HB2	1.87	0.57
1:B:273:PRO:C	1:B:275:ILE:N	2.57	0.57
1:D:200:MET:CE	1:D:203:ILE:HD12	2.35	0.56
1:A:200:MET:CE	1:A:266:ILE:HD13	2.36	0.56
1:B:112:THR:CA	1:B:115:GLU:OE2	2.50	0.56
1:C:31:ARG:CD	1:C:38:GLN:HG3	2.35	0.56
1:C:257:VAL:HB	1:C:263:ARG:HG2	1.87	0.56
1:A:253:ARG:NH2	2:A:2047:HOH:O	2.31	0.55
1:D:57:SER:O	1:D:60:ASP:HB2	2.06	0.55
1:A:58:ARG:N	1:A:58:ARG:HD2	2.21	0.55
1:D:104:PHE:HD1	1:D:105:LEU:CD2	2.17	0.55
1:D:264:MET:CG	1:D:268:ASP:HB3	2.37	0.55
1:B:157:ILE:HG13	1:B:157:ILE:O	2.07	0.54
1:A:47:ARG:HG3	1:A:47:ARG:O	2.06	0.54
1:B:113:GLU:O	1:B:117:THR:HB	2.07	0.54
1:C:32:GLU:O	1:C:36:GLY:N	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:THR:N	1:C:115:GLU:OE1	2.37	0.54
1:D:56:VAL:C	1:D:61:ILE:HD11	2.28	0.54
1:A:85:ASN:OD1	1:A:87:THR:N	2.40	0.53
1:C:152:VAL:CG1	1:C:153:PRO:HD2	2.38	0.53
1:D:266:ILE:HG22	2:D:2013:HOH:O	2.07	0.53
1:B:63:ARG:NH2	1:B:163:GLY:O	2.42	0.52
1:A:218:LEU:HD13	1:B:182:GLU:CD	2.30	0.52
1:A:238:ASP:OD1	1:A:239:GLU:N	2.43	0.52
1:A:257:VAL:HB	1:A:263:ARG:HG2	1.92	0.52
1:C:32:GLU:HB3	1:C:35:THR:OG1	2.10	0.52
1:A:85:ASN:OD1	1:A:85:ASN:C	2.47	0.52
1:C:105:LEU:CD2	1:C:111:LEU:HD11	2.39	0.52
1:C:47:ARG:HD3	1:C:54:ARG:O	2.10	0.52
1:B:61:ILE:HD12	1:B:61:ILE:N	2.25	0.52
1:A:58:ARG:N	1:A:61:ILE:HD12	2.25	0.52
1:A:134:GLN:NE2	2:A:2025:HOH:O	2.42	0.51
1:C:85:ASN:OD1	1:C:85:ASN:C	2.46	0.51
1:B:72:GLN:N	1:B:129:TYR:OH	2.33	0.51
1:C:137:HIS:O	1:C:138:PHE:HB2	2.10	0.51
1:B:225:THR:O	1:B:229:VAL:HG23	2.11	0.51
1:C:121:LYS:HE2	2:C:2058:HOH:O	2.10	0.51
1:B:113:GLU:OE2	1:B:245:SER:OG	2.29	0.51
1:C:184:VAL:CG1	1:C:188:ILE:HB	2.41	0.50
1:B:184:VAL:HG12	1:B:185:ALA:N	2.26	0.50
1:A:264:MET:HG2	1:A:268:ASP:CB	2.41	0.50
1:C:49:THR:O	1:C:52:SER:HB2	2.11	0.50
1:C:134:GLN:HB2	1:C:167:LYS:NZ	2.26	0.50
1:D:247:LEU:HB3	1:D:274:TRP:HB2	1.92	0.50
1:C:184:VAL:CG1	1:C:188:ILE:CG2	2.89	0.50
1:A:192:GLU:CD	1:A:192:GLU:H	2.15	0.50
1:B:65:VAL:O	1:B:66:SER:C	2.48	0.50
1:D:168:ILE:O	1:D:169:ASP:OD1	2.30	0.50
1:B:112:THR:CG2	1:B:113:GLU:N	2.75	0.49
1:B:112:THR:CG2	1:B:114:GLU:HB3	2.42	0.49
1:B:61:ILE:CD1	1:B:61:ILE:N	2.76	0.49
1:B:264:MET:HG3	1:B:268:ASP:HB2	1.94	0.49
1:B:129:TYR:O	1:B:132:SER:OG	2.20	0.49
1:B:201:TRP:C	1:B:201:TRP:CD1	2.86	0.49
1:B:141:LYS:CB	1:B:142:PRO:HD2	2.43	0.49
1:B:73:HIS:CG	1:B:74:PRO:HD2	2.47	0.48
1:B:104:PHE:CD1	1:B:104:PHE:C	2.86	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:VAL:HG13	1:C:153:PRO:CD	2.43	0.48
1:D:257:VAL:HB	1:D:263:ARG:HG2	1.94	0.48
1:C:152:VAL:CG1	1:C:153:PRO:CD	2.92	0.48
1:D:115:GLU:HA	1:D:118:GLU:OE1	2.13	0.48
1:D:209:ILE:HG12	1:D:214:ALA:O	2.13	0.48
1:C:152:VAL:HG12	1:C:153:PRO:N	2.27	0.48
1:B:68:LEU:HB3	1:B:79:LEU:HB2	1.95	0.48
1:A:180:THR:N	1:A:181:PRO:HD2	2.28	0.48
1:B:156:ARG:N	1:B:156:ARG:CD	2.69	0.48
1:C:184:VAL:HG11	1:C:188:ILE:CG2	2.42	0.48
1:C:192:GLU:CD	1:C:192:GLU:N	2.61	0.48
1:A:32:GLU:HB3	1:A:35:THR:OG1	2.13	0.48
1:C:122:GLN:HE22	1:C:156:ARG:HA	1.78	0.48
1:D:275:ILE:O	1:D:275:ILE:CG2	2.61	0.48
1:B:112:THR:HG22	1:B:113:GLU:N	2.29	0.47
1:C:105:LEU:HD21	1:C:111:LEU:HD11	1.96	0.47
1:B:123:ILE:HG13	1:B:157:ILE:HD13	1.96	0.47
1:B:169:ASP:O	2:B:2009:HOH:O	2.20	0.47
1:D:104:PHE:HD2	1:D:150:ARG:HG2	1.78	0.47
1:B:155:PRO:C	1:B:156:ARG:CD	2.76	0.47
1:B:141:LYS:HB2	1:B:142:PRO:HD2	1.96	0.47
1:B:272:HIS:CG	1:B:273:PRO:HD2	2.49	0.47
1:C:53:ARG:CD	1:C:54:ARG:N	2.78	0.47
1:C:120:LEU:O	1:C:124:LEU:HG	2.15	0.47
1:B:122:GLN:HE22	1:B:156:ARG:HA	1.80	0.46
1:D:56:VAL:O	1:D:57:SER:C	2.52	0.46
1:B:141:LYS:CB	1:B:142:PRO:CD	2.93	0.46
1:D:264:MET:HG2	1:D:268:ASP:CB	2.45	0.46
1:B:101:LEU:HD23	1:B:102:PHE:CD1	2.51	0.46
1:B:200:MET:CE	1:B:200:MET:HA	2.45	0.46
1:A:98:GLY:HA2	1:A:150:ARG:NH1	2.30	0.46
1:C:147:LEU:HD23	1:C:147:LEU:HA	1.77	0.46
1:A:73:HIS:CE1	1:A:75:ASN:HD22	2.32	0.46
1:A:117:THR:O	1:A:121:LYS:HG3	2.16	0.46
1:A:232:VAL:O	1:A:232:VAL:CG1	2.52	0.46
1:D:235:GLU:HG3	1:D:237:GLU:HG3	1.97	0.46
1:A:238:ASP:O	1:A:242:SER:HB2	2.16	0.45
1:B:238:ASP:O	1:B:242:SER:HB2	2.17	0.45
1:C:184:VAL:HG13	1:C:188:ILE:HB	1.98	0.45
1:D:201:TRP:CD1	1:D:201:TRP:C	2.89	0.45
1:B:77:ILE:HG12	1:B:78:THR:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:TYR:C	1:D:132:SER:OG	2.47	0.45
1:B:200:MET:CE	1:B:203:ILE:CD1	2.88	0.45
1:C:8:ASN:OD1	1:C:9:VAL:N	2.48	0.45
1:C:111:LEU:HA	1:C:115:GLU:OE1	2.16	0.45
1:C:209:ILE:O	1:C:209:ILE:HG22	2.16	0.45
1:D:141:LYS:HB2	1:D:142:PRO:HD2	1.97	0.45
1:C:8:ASN:OD1	1:C:8:ASN:C	2.55	0.45
1:C:131:HIS:CD2	1:C:196:LEU:HD22	2.52	0.45
1:D:119:PHE:CD1	1:D:119:PHE:N	2.85	0.45
1:D:122:GLN:HE22	1:D:157:ILE:H	1.65	0.45
1:C:182:GLU:HG3	1:D:218:LEU:HD13	1.98	0.44
1:D:96:VAL:CG1	1:D:148:LEU:HA	2.46	0.44
1:D:146:MET:O	1:D:157:ILE:HA	2.17	0.44
1:A:86:LYS:HD2	1:A:86:LYS:HA	1.75	0.44
1:B:127:VAL:HG12	1:B:266:ILE:HD13	1.98	0.44
1:C:107:GLU:C	1:C:108:LYS:HG3	2.38	0.44
1:D:56:VAL:O	1:D:61:ILE:CD1	2.62	0.44
1:C:47:ARG:HD2	1:C:52:SER:O	2.18	0.44
1:D:143:GLU:O	1:D:146:MET:CE	2.65	0.44
1:A:101:LEU:HA	1:A:147:LEU:HD22	1.98	0.44
1:A:224:GLU:HA	1:C:227:ALA:HB1	2.00	0.44
1:D:58:ARG:O	1:D:59:GLU:C	2.54	0.44
1:A:238:ASP:OD1	1:A:238:ASP:C	2.55	0.44
1:C:184:VAL:HG11	1:C:188:ILE:HG22	2.00	0.44
1:D:104:PHE:CE1	1:D:105:LEU:HD23	2.49	0.44
1:D:200:MET:CE	1:D:200:MET:HA	2.46	0.43
1:D:152:VAL:HG12	1:D:155:PRO:HA	2.00	0.43
1:C:74:PRO:O	1:C:158:LYS:CE	2.66	0.43
1:B:71:ILE:HA	1:B:129:TYR:OH	2.18	0.43
1:D:101:LEU:HD23	1:D:102:PHE:HD1	1.81	0.43
1:D:272:HIS:HA	1:D:273:PRO:HD3	1.86	0.43
1:B:192:GLU:OE1	1:B:192:GLU:N	2.51	0.43
1:A:255:LEU:O	1:A:263:ARG:HD3	2.19	0.43
1:B:115:GLU:HG3	1:B:115:GLU:H	1.62	0.43
1:D:73:HIS:CG	1:D:74:PRO:HD2	2.54	0.43
1:B:148:LEU:CD2	1:B:158:LYS:HG3	2.49	0.42
1:C:141:LYS:HB2	1:C:142:PRO:HD2	2.01	0.42
1:A:262:LYS:HA	1:A:262:LYS:HD3	1.84	0.42
1:D:207:THR:HG22	1:D:252:ILE:HD11	2.01	0.42
1:C:208:TYR:CD1	1:C:216:PRO:HD3	2.54	0.42
1:C:53:ARG:CD	1:C:54:ARG:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:SER:O	1:D:61:ILE:CD1	2.68	0.42
1:D:70:GLU:CD	1:D:167:LYS:NZ	2.59	0.42
1:D:200:MET:CE	1:D:203:ILE:CD1	2.98	0.42
1:D:264:MET:HG3	1:D:268:ASP:HB3	2.01	0.42
1:D:228:ASN:OD1	1:D:233:ASN:ND2	2.39	0.42
1:A:122:GLN:NE2	1:A:156:ARG:HA	2.25	0.42
1:D:225:THR:O	1:D:229:VAL:HG23	2.20	0.42
1:A:231:ALA:HB2	1:C:233:ASN:HB2	2.02	0.42
1:D:77:ILE:CD1	1:D:93:LEU:HD22	2.45	0.42
1:D:200:MET:HE3	1:D:203:ILE:HD12	2.02	0.42
1:B:68:LEU:HD23	1:B:68:LEU:HA	1.80	0.42
1:D:141:LYS:HB2	1:D:142:PRO:CD	2.49	0.41
1:B:117:THR:HG22	1:B:118:GLU:N	2.35	0.41
1:C:46:LYS:NZ	1:C:84:GLU:OE2	2.46	0.41
1:D:255:LEU:HD23	1:D:255:LEU:HA	1.80	0.41
1:A:37:LEU:HD23	1:A:37:LEU:HA	1.59	0.41
1:A:46:LYS:CD	1:A:89:VAL:HG23	2.45	0.41
1:B:256:LEU:HD23	1:B:256:LEU:HA	1.74	0.41
1:B:273:PRO:O	1:B:275:ILE:N	2.53	0.41
1:A:83:TYR:HB2	1:A:90:ILE:HB	2.02	0.41
1:C:68:LEU:HD23	1:C:71:ILE:HD11	2.02	0.41
1:D:223:GLN:CD	1:D:223:GLN:H	2.24	0.41
1:D:101:LEU:CD2	1:D:102:PHE:CD1	3.04	0.41
1:D:101:LEU:CD1	1:D:119:PHE:CD2	3.03	0.41
1:A:45:LYS:HD3	1:A:45:LYS:HA	1.79	0.41
1:B:148:LEU:HD13	1:B:148:LEU:HA	1.87	0.41
1:B:247:LEU:HB3	1:B:274:TRP:HB2	2.02	0.41
1:B:255:LEU:HA	1:B:255:LEU:HD23	1.80	0.40
1:A:187:GLU:HG2	1:A:188:ILE:H	1.86	0.40
1:D:264:MET:HG2	1:D:268:ASP:HB3	2.02	0.40
1:B:148:LEU:HD21	1:B:158:LYS:HG3	2.02	0.40
1:C:152:VAL:CG1	1:C:153:PRO:N	2.83	0.40
1:D:69:LYS:HZ2	1:D:69:LYS:HG2	1.76	0.40
1:D:73:HIS:CE1	1:D:75:ASN:ND2	2.82	0.40
1:D:152:VAL:CG1	1:D:155:PRO:HA	2.51	0.40
1:A:152:VAL:HG12	1:A:154:LYS:H	1.87	0.40
1:B:211:LEU:HD23	1:B:211:LEU:HA	1.87	0.40
1:C:74:PRO:O	1:C:158:LYS:HE2	2.22	0.40

All (2) 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)
1:C:51:SER:OG	1:D:219:GLY:O[2_646]	1.37	0.83
1:A:34:SER:O	1:A:271:GLN:NE2[2_647]	1.40	0.80

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	243/285 (85%)	240 (99%)	3 (1%)	0	100	100
1	B	176/285 (62%)	171 (97%)	5 (3%)	0	100	100
1	C	258/285 (90%)	252 (98%)	6 (2%)	0	100	100
1	D	186/285 (65%)	179 (96%)	7 (4%)	0	100	100
All	All	863/1140 (76%)	842 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	219/254 (86%)	189 (86%)	30 (14%)	3	4
1	B	161/254 (63%)	138 (86%)	23 (14%)	3	3
1	C	231/254 (91%)	197 (85%)	34 (15%)	3	3
1	D	169/254 (66%)	139 (82%)	30 (18%)	2	1
All	All	780/1016 (77%)	663 (85%)	117 (15%)	3	3

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	26	VAL
1	A	28	LYS
1	A	29	LYS
1	A	34	SER
1	A	43	PHE
1	A	46	LYS
1	A	47	ARG
1	A	58	ARG
1	A	62	GLU
1	A	71	ILE
1	A	72	GLN
1	A	78	THR
1	A	86	LYS
1	A	87	THR
1	A	107	GLU
1	A	108	LYS
1	A	141	LYS
1	A	147	LEU
1	A	150	ARG
1	A	157	ILE
1	A	182	GLU
1	A	188	ILE
1	A	192	GLU
1	A	224	GLU
1	A	226	LEU
1	A	230	SER
1	A	239	GLU
1	A	264	MET
1	A	271	GLN
1	B	66	SER
1	B	67	ILE
1	B	71	ILE
1	B	72	GLN
1	B	100	GLU
1	B	101	LEU
1	B	108	LYS
1	B	111	LEU
1	B	115	GLU
1	B	117	THR
1	B	141	LYS
1	B	146	MET

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Mol	Chain	Res	Type
1	B	148	LEU
1	B	155	PRO
1	B	156	ARG
1	B	169	ASP
1	B	221	THR
1	B	222	LYS
1	B	230	SER
1	B	238	ASP
1	B	245	SER
1	B	266	ILE
1	B	271	GLN
1	C	2	THR
1	C	6	GLN
1	C	15	THR
1	C	21	SER
1	C	26	VAL
1	C	31	ARG
1	C	45	LYS
1	C	48	ARG
1	C	51	SER
1	C	53	ARG
1	C	57	SER
1	C	59	GLU
1	C	62	GLU
1	C	71	ILE
1	C	72	GLN
1	C	86	LYS
1	C	87	THR
1	C	107	GLU
1	C	110	SER
1	C	113	GLU
1	C	146	MET
1	C	154	LYS
1	C	157	ILE
1	C	158	LYS
1	C	167	LYS
1	C	168	ILE
1	C	169	ASP
1	C	180	THR
1	C	192	GLU
1	C	226	LEU
1	C	230	SER

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Mol	Chain	Res	Type
1	C	242	SER
1	C	264	MET
1	C	271	GLN
1	D	56	VAL
1	D	57	SER
1	D	61	ILE
1	D	62	GLU
1	D	63	ARG
1	D	65	VAL
1	D	66	SER
1	D	69	LYS
1	D	72	GLN
1	D	77	ILE
1	D	78	THR
1	D	96	VAL
1	D	101	LEU
1	D	104	PHE
1	D	114	GLU
1	D	117	THR
1	D	141	LYS
1	D	146	MET
1	D	148	LEU
1	D	152	VAL
1	D	168	ILE
1	D	187	GLU
1	D	210	LEU
1	D	221	THR
1	D	224	GLU
1	D	230	SER
1	D	239	GLU
1	D	242	SER
1	D	264	MET
1	D	271	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	72	GLN
1	A	75	ASN
1	A	122	GLN
1	A	144	ASN

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Mol	Chain	Res	Type
1	A	190	ASN
1	B	122	GLN
1	B	131	HIS
1	B	144	ASN
1	B	190	ASN
1	C	6	GLN
1	C	72	GLN
1	C	75	ASN
1	C	122	GLN
1	C	144	ASN
1	C	190	ASN
1	D	73	HIS
1	D	122	GLN
1	D	144	ASN

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	275:ILE	C	276:LYS	N	0.92

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.