



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:43 PM UTC

PDB ID : 1OKV / pdb_00001okv
Title : Cyclin A binding groove inhibitor H-Arg-Arg-Leu-Ile-Phe-NH₂
Authors : Kontopidis, G.; Andrews, M.; McInnes, C.; Cowan, A.; Powers, H.; Innes, L.; Plater, A.; Griffiths, G.; Paterson, D.; Zheleva, D.; Lane, D.; Green, S.; Walkinshaw, M.; Fischer, P.
Deposited on : 2003-07-30
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

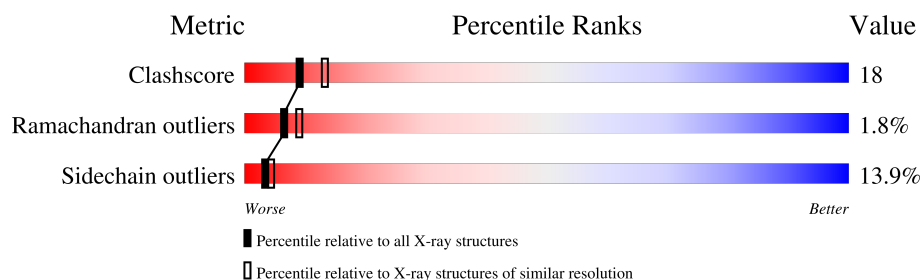
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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 was not executed.

Mol	Chain	Length	Quality of chain
1	A	298	
1	C	298	
2	B	260	
2	D	260	
3	E	6	
3	F	6	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9787 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 CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	1
			2370	1541	403	418	8			
1	C	296	Total	C	N	O	S	0	0	0
			2377	1547	402	420	8			

- Molecule 2 is a protein called CYCLIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	0	0
			2082	1349	339	383	11			
2	D	260	Total	C	N	O	S	0	0	0
			2101	1359	342	389	11			

- Molecule 3 is a protein called H-ARG-ARG-LEU-ILE-PHE-NH₂.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	6	Total	C	N	O	0	0	1
			50	33	12	5			
3	F	6	Total	C	N	O	0	0	1
			50	33	12	5			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	210	Total	O	0	0
			210	210		
4	B	152	Total	O	0	0
			152	152		
4	C	221	Total	O	0	0
			221	221		
4	D	159	Total	O	0	0
			159	159		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	7	Total	O	0	0
			7	7		
4	F	8	Total	O	0	0
			8	8		

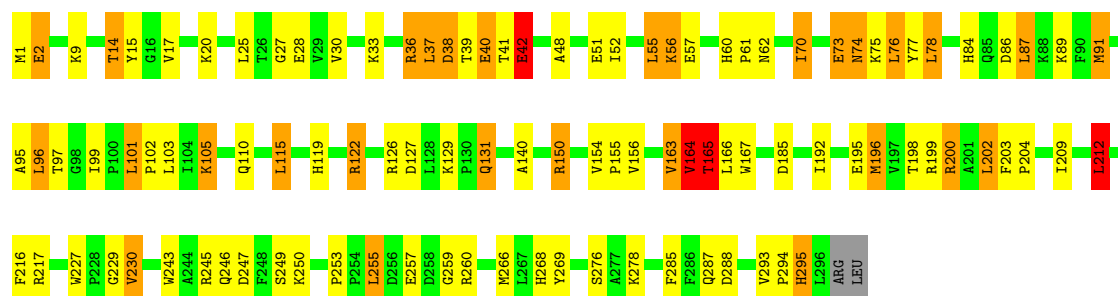
3 Residue-property plots

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

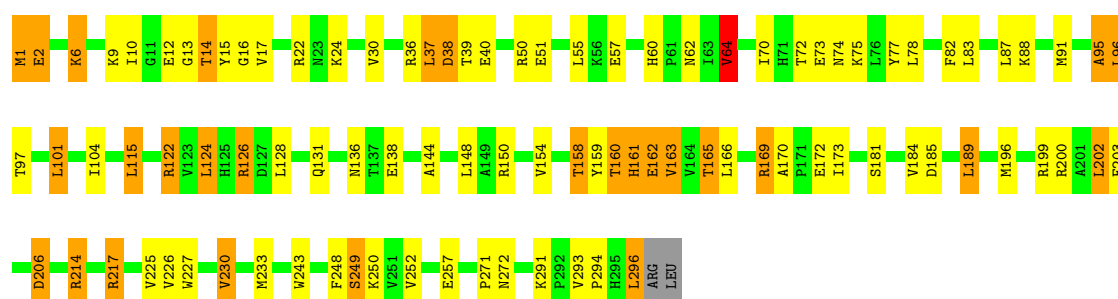
• Molecule 1: CELL DIVISION PROTEIN KINASE 2

Chain A: 



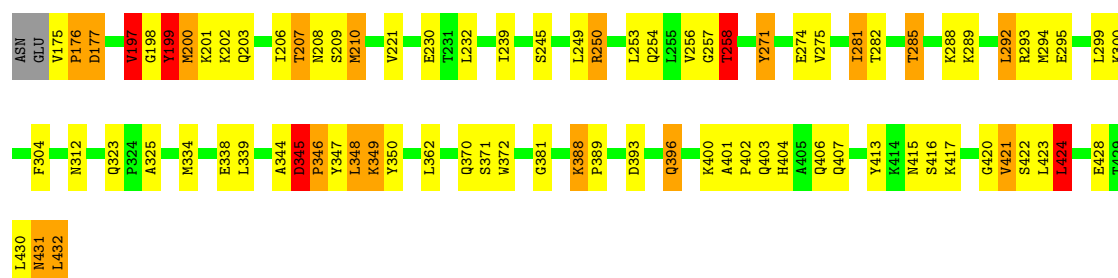
• Molecule 1: CELL DIVISION PROTEIN KINASE 2

Chain C: 



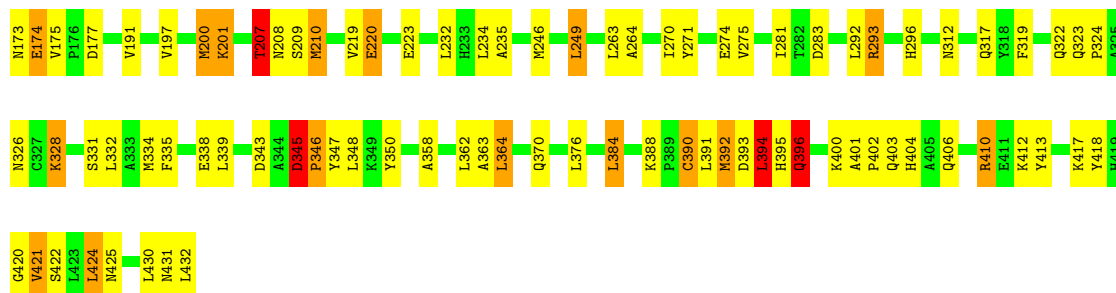
• Molecule 2: CYCLIN A2

Chain B: 

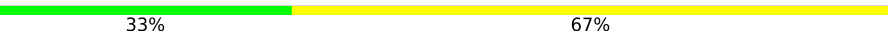


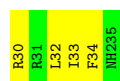
- Molecule 2: CYCLIN A2

Chain D:  67% 25% 6% •

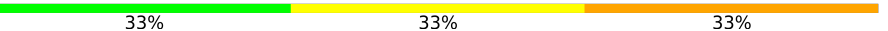


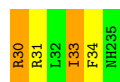
- Molecule 3: H-ARG-ARG-LEU-ILE-PHE-NH2

Chain E:  33% 67%



- Molecule 3: H-ARG-ARG-LEU-ILE-PHE-NH2

Chain F:  33% 33% 33%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.19Å 113.88Å 155.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.00 – 2.40	Depositor
% Data completeness (in resolution range)	96.8 (17.00-2.40)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.197 , 0.278	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9787	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NH2

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	1.03	4/2432 (0.2%)	1.24	15/3302 (0.5%)
1	C	1.00	2/2438 (0.1%)	1.21	3/3308 (0.1%)
2	B	0.93	1/2132 (0.0%)	1.23	10/2894 (0.3%)
2	D	1.02	1/2151 (0.0%)	1.25	13/2920 (0.4%)
3	E	0.74	0/49	1.46	0/63
3	F	0.92	0/49	1.21	0/63
All	All	0.99	8/9251 (0.1%)	1.23	41/12550 (0.3%)

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
2	D	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	210	MET	SD-CE	-16.97	1.37	1.79
1	C	1	MET	SD-CE	-10.52	1.53	1.79
1	A	196	MET	SD-CE	-10.03	1.54	1.79
1	A	295	HIS	C-N	-8.03	1.22	1.33
1	A	266	MET	SD-CE	-6.36	1.63	1.79
1	C	233	MET	SD-CE	-5.84	1.65	1.79
2	B	200	MET	SD-CE	-5.75	1.65	1.79
1	A	269	TYR	C-O	-5.10	1.18	1.24

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	VAL	N-CA-C	11.34	121.31	110.42
1	A	84	HIS	N-CA-C	8.41	122.64	112.38
2	B	177	ASP	N-CA-C	-7.94	103.60	113.28
2	B	347	TYR	N-CA-C	7.73	121.81	112.38
2	D	345	ASP	O-C-N	7.68	130.16	121.32
1	C	64	VAL	CB-CA-C	-6.90	100.12	111.51
1	A	253	PRO	N-CA-C	6.74	118.93	110.70
1	C	95	ALA	N-CA-C	-6.35	101.71	110.35
1	A	42	GLU	N-CA-C	6.32	121.27	113.50
2	D	345	ASP	CA-C-O	-6.24	111.61	120.16
2	D	201	LYS	N-CA-C	-6.18	106.06	113.97
2	D	394	LEU	N-CA-C	-6.13	97.75	110.80
2	D	207	THR	N-CA-CB	-6.10	101.08	111.69
2	D	390	CYS	N-CA-C	-6.07	104.75	111.36
1	A	212	LEU	N-CA-C	-6.03	104.62	111.07
1	A	97	THR	N-CA-C	-5.90	106.12	113.55
2	D	345	ASP	CA-C-N	5.83	127.12	119.84
2	D	345	ASP	C-N-CA	5.83	127.12	119.84
2	B	197	VAL	N-CA-CB	5.76	117.29	110.55
1	A	165	THR	OG1-CB-CG2	-5.71	97.88	109.30
1	C	181	SER	N-CA-C	-5.69	100.48	108.96
2	B	381	GLY	N-CA-C	-5.68	107.40	115.30
1	A	99	ILE	N-CA-C	-5.63	102.83	108.96
1	A	163	VAL	N-CA-CB	-5.55	104.69	112.35
2	B	258	THR	N-CA-C	-5.49	105.38	111.36
2	B	203	GLN	CB-CA-C	5.43	117.73	110.13
2	D	396	GLN	N-CA-C	-5.36	105.33	111.07
2	D	220	GLU	CB-CA-C	-5.32	102.46	110.92
1	A	166	LEU	N-CA-C	5.32	117.49	111.11
1	A	163	VAL	CB-CA-C	-5.28	105.12	110.88
2	D	363	ALA	N-CA-C	-5.23	105.48	111.07
1	A	156	VAL	N-CA-C	5.20	115.85	107.73
2	B	274	GLU	N-CA-C	-5.19	103.30	110.35
1	A	28	GLU	N-CA-C	5.18	117.55	110.24
1	A	91	MET	CG-SD-CE	-5.14	89.60	100.90
1	A	165	THR	N-CA-CB	5.13	119.17	110.49
2	B	413	TYR	N-CA-C	5.11	119.23	113.15
2	D	275	VAL	CB-CA-C	-5.09	105.27	112.14
2	B	221	VAL	N-CA-C	-5.07	105.44	110.62
2	B	271	TYR	CB-CA-C	5.04	116.86	110.16
2	D	328	LYS	N-CA-C	-5.00	105.93	112.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	345	ASP	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	2370	0	2415	102	0
1	C	2377	0	2424	97	0
2	B	2082	0	2103	67	0
2	D	2101	0	2119	84	0
3	E	50	0	56	5	0
3	F	50	0	56	5	0
4	A	210	0	0	17	1
4	B	152	0	0	13	0
4	C	221	0	0	22	1
4	D	159	0	0	13	0
4	E	7	0	0	0	0
4	F	8	0	0	2	0
All	All	9787	0	9173	333	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 18.

All (333) 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)
2:D:343:ASP:HB3	2:D:345:ASP:OD2	1.33	1.23
1:C:159:TYR:CD1	2:D:270:ILE:HG23	1.79	1.17
1:C:159:TYR:CE1	2:D:270:ILE:HG23	1.86	1.11
1:A:38:ASP:OD2	1:A:42:GLU:N	1.82	1.10
1:A:36:ARG:O	1:A:37:LEU:HD23	1.53	1.08
2:B:345:ASP:HB2	2:B:346:PRO:HD3	1.32	1.07
2:D:345:ASP:HB2	2:D:346:PRO:HD3	1.36	1.03
1:C:159:TYR:CD1	2:D:270:ILE:CG2	2.42	1.03
1:A:36:ARG:O	1:A:37:LEU:CD2	2.10	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:LYS:HD2	1:C:6:LYS:H	1.34	0.93
2:B:432:LEU:C	2:B:432:LEU:HD23	1.96	0.90
2:D:296:HIS:CD2	4:D:2094:HOH:O	2.25	0.89
1:C:159:TYR:HD1	2:D:270:ILE:CG2	1.86	0.89
1:C:159:TYR:CE1	2:D:270:ILE:CG2	2.58	0.87
2:D:322:GLN:NE2	2:D:326:ASN:H	1.74	0.86
1:C:51:GLU:O	1:C:55:LEU:HB2	1.77	0.85
1:C:206:ASP:HA	4:C:2151:HOH:O	1.77	0.85
2:D:343:ASP:CB	2:D:345:ASP:OD2	2.22	0.85
1:A:154:VAL:HB	4:B:2070:HOH:O	1.76	0.84
2:D:220:GLU:OE2	3:F:30:ARG:NH1	2.10	0.83
2:B:421:VAL:O	2:B:424:LEU:HD22	1.79	0.82
2:B:345:ASP:HB2	2:B:346:PRO:CD	2.09	0.82
1:A:95:ALA:O	1:A:96:LEU:HB2	1.79	0.81
1:A:73:GLU:HG2	1:C:2:GLU:HG2	1.64	0.80
1:C:162:GLU:HA	4:C:2125:HOH:O	1.81	0.80
1:A:131:GLN:HG2	4:A:2102:HOH:O	1.81	0.79
1:C:214:ARG:NH1	4:C:2155:HOH:O	2.16	0.79
2:B:424:LEU:HD13	2:B:424:LEU:H	1.48	0.79
1:A:15:TYR:HD2	1:A:33:LYS:HD3	1.47	0.79
1:C:95:ALA:O	1:C:96:LEU:HB3	1.83	0.79
1:C:202:LEU:HD13	1:C:203:PHE:CE2	2.18	0.79
2:D:418:TYR:O	2:D:421:VAL:HG23	1.82	0.78
1:C:202:LEU:HD13	1:C:203:PHE:CZ	2.20	0.77
1:A:227:TRP:O	1:A:230:VAL:HG22	1.84	0.77
2:D:283:ASP:OD2	3:F:30:ARG:HA	1.85	0.76
1:A:57:GLU:OE1	1:A:122:ARG:NH2	2.19	0.76
3:F:33:ILE:O	4:F:2005:HOH:O	2.03	0.76
1:C:38:ASP:HB3	4:C:2039:HOH:O	1.87	0.75
1:C:227:TRP:O	1:C:230:VAL:HG23	1.87	0.75
1:C:172:GLU:CG	1:C:271:PRO:HG3	2.18	0.74
2:D:338:GLU:OE1	2:D:412:LYS:NZ	2.20	0.74
1:C:172:GLU:HG2	1:C:271:PRO:CG	2.17	0.74
1:A:60:HIS:HD2	1:A:62:ASN:H	1.34	0.74
1:A:126:ARG:O	1:A:164:VAL:HG21	1.88	0.73
1:C:163:VAL:HG23	1:C:163:VAL:O	1.88	0.73
1:C:172:GLU:HG2	1:C:271:PRO:HG3	1.69	0.73
2:D:322:GLN:HE22	2:D:326:ASN:H	1.34	0.73
2:D:345:ASP:HB2	2:D:346:PRO:CD	2.17	0.72
2:B:250:ARG:HG2	2:B:250:ARG:HH11	1.54	0.72
1:A:56:LYS:HD2	4:B:2088:HOH:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:432:LEU:C	2:B:432:LEU:CD2	2.62	0.71
1:C:214:ARG:HG2	1:C:214:ARG:HH11	1.54	0.70
2:D:209:SER:HB2	4:D:2056:HOH:O	1.92	0.70
1:C:124:LEU:CD1	1:C:126:ARG:HG3	2.20	0.70
1:C:206:ASP:OD2	1:C:206:ASP:N	2.25	0.70
2:B:206:ILE:HA	2:B:210:MET:SD	2.31	0.70
1:C:163:VAL:O	1:C:163:VAL:CG2	2.39	0.70
2:D:432:LEU:O	4:D:2159:HOH:O	2.09	0.69
1:C:72:THR:OG1	1:C:75:LYS:HG2	1.93	0.69
1:A:15:TYR:CD2	1:A:33:LYS:HD3	2.27	0.69
1:A:36:ARG:C	1:A:37:LEU:HD22	2.18	0.68
1:A:150:ARG:NH2	4:A:2113:HOH:O	2.26	0.68
2:B:201:LYS:HE3	2:B:202:LYS:HD2	1.74	0.68
2:D:223:GLU:CD	2:D:412:LYS:HD2	2.18	0.68
1:A:42:GLU:OE2	2:B:275:VAL:HG23	1.94	0.68
1:A:95:ALA:O	1:A:96:LEU:CB	2.42	0.67
2:B:175:VAL:HG23	4:B:2019:HOH:O	1.95	0.67
1:A:294:PRO:C	4:A:2206:HOH:O	2.37	0.67
2:D:388:LYS:O	2:D:392:MET:HG2	1.94	0.67
1:A:36:ARG:C	1:A:37:LEU:CD2	2.68	0.67
1:C:128:LEU:HD13	1:C:189:LEU:HD13	1.76	0.67
2:B:404:HIS:HD2	2:B:406:GLN:H	1.41	0.66
1:C:39:THR:C	1:C:40:GLU:CA	2.69	0.66
2:B:207:THR:HG22	2:B:210:MET:HG2	1.77	0.66
2:D:418:TYR:O	2:D:421:VAL:CG2	2.44	0.66
1:C:200:ARG:CZ	4:C:2148:HOH:O	2.44	0.66
2:B:198:GLY:O	2:B:201:LYS:HG2	1.96	0.65
1:A:36:ARG:O	1:A:37:LEU:HD22	1.95	0.65
1:C:214:ARG:HH11	1:C:214:ARG:CG	2.09	0.65
2:D:346:PRO:HD2	2:D:347:TYR:H	1.62	0.65
1:C:166:LEU:HD23	1:C:169:ARG:HH21	1.61	0.65
1:A:48:ALA:O	1:A:52:ILE:HG13	1.97	0.65
2:B:423:LEU:O	2:B:424:LEU:O	2.15	0.64
1:C:101:LEU:HG	4:C:2081:HOH:O	1.96	0.64
2:D:210:MET:HE3	3:F:34:PHE:HB3	1.78	0.64
1:C:126:ARG:NH1	4:C:2103:HOH:O	2.31	0.63
1:A:38:ASP:OD2	1:A:41:THR:CA	2.46	0.63
1:C:131:GLN:NE2	4:C:2105:HOH:O	2.32	0.63
2:D:345:ASP:CB	2:D:346:PRO:HD3	2.21	0.63
1:A:154:VAL:HG13	1:A:155:PRO:HD2	1.79	0.63
2:B:346:PRO:O	2:B:349:LYS:HG3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:345:ASP:O	4:B:2108:HOH:O	2.16	0.62
1:A:75:LYS:HD2	1:A:77:TYR:OH	1.99	0.62
2:D:384:LEU:HD12	2:D:384:LEU:O	2.00	0.62
1:A:38:ASP:OD2	1:A:41:THR:C	2.41	0.62
1:C:6:LYS:H	1:C:6:LYS:CD	2.05	0.62
2:B:423:LEU:O	2:B:424:LEU:C	2.42	0.61
1:C:50:ARG:HD3	1:C:150:ARG:HD2	1.82	0.61
1:C:75:LYS:HG3	1:C:77:TYR:CE1	2.36	0.61
1:A:33:LYS:HE3	4:A:2040:HOH:O	2.00	0.61
1:A:73:GLU:CG	1:C:2:GLU:HG2	2.29	0.61
1:A:164:VAL:O	1:A:165:THR:HG22	2.01	0.60
1:A:60:HIS:CD2	1:A:62:ASN:H	2.17	0.60
1:C:40:GLU:HB3	4:C:2039:HOH:O	2.00	0.60
1:C:37:LEU:O	1:C:39:THR:N	2.34	0.60
1:A:51:GLU:O	1:A:55:LEU:HB2	2.02	0.60
2:B:230:GLU:OE1	2:B:312:ASN:ND2	2.32	0.60
1:C:1:MET:CE	1:C:70:ILE:HD12	2.30	0.60
1:C:37:LEU:O	1:C:38:ASP:C	2.44	0.60
1:C:50:ARG:NH2	4:C:2050:HOH:O	2.35	0.60
1:A:150:ARG:HG3	1:A:150:ARG:HH11	1.66	0.60
1:A:212:LEU:HD22	1:A:216:PHE:CZ	2.37	0.60
1:A:91:MET:HE3	1:A:196:MET:HA	1.83	0.59
1:A:276:SER:HB3	2:B:175:VAL:HG11	1.84	0.59
2:B:281:ILE:O	3:E:30:ARG:N	2.35	0.59
1:A:1:MET:HE2	1:A:70:ILE:HD12	1.84	0.59
1:A:202:LEU:HD13	1:A:203:PHE:CE2	2.37	0.59
2:D:396:GLN:HG3	2:D:400:LYS:HD2	1.84	0.59
1:A:105:LYS:NZ	4:A:2093:HOH:O	2.25	0.59
2:D:319:PHE:O	2:D:322:GLN:HB2	2.02	0.59
1:C:101:LEU:HD22	1:C:104:ILE:HD12	1.85	0.58
1:C:173:ILE:HD11	1:C:184:VAL:HG11	1.85	0.58
1:C:227:TRP:O	1:C:230:VAL:CG2	2.51	0.58
2:D:401:ALA:HB1	2:D:410:ARG:HD2	1.84	0.58
1:C:227:TRP:CG	1:C:230:VAL:HG22	2.38	0.58
1:A:200:ARG:NH2	4:A:2151:HOH:O	2.36	0.58
2:B:197:VAL:N	4:B:2031:HOH:O	2.36	0.58
2:D:430:LEU:HD21	4:D:2137:HOH:O	2.01	0.58
1:A:38:ASP:OD2	1:A:41:THR:N	2.37	0.58
1:A:150:ARG:NH1	4:A:2112:HOH:O	2.22	0.57
1:A:105:LYS:HE3	1:A:285:PHE:O	2.05	0.57
1:A:227:TRP:CE3	1:A:230:VAL:HG13	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:HIS:N	4:A:2206:HOH:O	2.38	0.57
2:D:432:LEU:C	4:D:2159:HOH:O	2.48	0.56
1:C:165:THR:HG21	4:C:2105:HOH:O	2.04	0.56
1:C:126:ARG:NH2	1:C:148:LEU:O	2.33	0.56
1:A:91:MET:HE1	1:A:195:GLU:HG2	1.86	0.56
1:A:150:ARG:HG3	1:A:150:ARG:NH1	2.19	0.56
1:A:202:LEU:HD13	1:A:203:PHE:CZ	2.40	0.56
1:C:95:ALA:O	1:C:96:LEU:CB	2.53	0.55
1:A:20:LYS:NZ	4:A:2024:HOH:O	2.38	0.55
1:A:38:ASP:CG	1:A:41:THR:H	2.14	0.55
1:C:172:GLU:HG2	1:C:271:PRO:HG2	1.87	0.55
1:C:248:PHE:O	1:C:250:LYS:N	2.39	0.55
1:A:73:GLU:HG2	1:C:2:GLU:CG	2.36	0.55
1:C:101:LEU:CG	4:C:2081:HOH:O	2.54	0.55
1:A:227:TRP:CD2	1:A:230:VAL:HG13	2.42	0.55
1:C:101:LEU:HD12	4:C:2041:HOH:O	2.06	0.55
2:B:206:ILE:HD13	2:B:253:LEU:HD13	1.88	0.54
2:B:254:GLN:HG3	3:E:32:LEU:HD12	1.90	0.54
1:C:248:PHE:O	1:C:249:SER:C	2.51	0.54
1:A:73:GLU:CD	1:C:2:GLU:HG2	2.32	0.54
1:A:78:LEU:HD23	1:A:78:LEU:N	2.23	0.54
2:D:346:PRO:CD	2:D:347:TYR:H	2.20	0.54
1:A:27:GLY:HA3	2:D:249:LEU:HD22	1.89	0.53
1:C:60:HIS:CD2	1:C:62:ASN:H	2.26	0.53
2:D:338:GLU:CD	2:D:412:LYS:NZ	2.66	0.53
1:C:227:TRP:HB3	1:C:230:VAL:HG21	1.90	0.53
2:B:420:GLY:O	2:B:422:SER:N	2.42	0.53
2:B:254:GLN:O	2:B:258:THR:HB	2.09	0.53
1:A:1:MET:CE	1:A:70:ILE:HD12	2.39	0.53
1:C:16:GLY:HA3	4:C:2017:HOH:O	2.09	0.53
1:A:212:LEU:HD22	1:A:216:PHE:CE1	2.45	0.52
1:A:105:LYS:HD2	1:A:285:PHE:CZ	2.45	0.52
2:B:210:MET:CE	3:E:34:PHE:HB3	2.39	0.52
3:F:31:ARG:NH2	4:F:2003:HOH:O	2.43	0.52
1:A:167:TRP:CD1	1:A:204:PRO:HA	2.44	0.52
1:A:246:GLN:HB3	4:A:2179:HOH:O	2.09	0.52
2:D:270:ILE:HG22	2:D:271:TYR:CE2	2.45	0.52
1:A:129:LYS:HE3	1:A:131:GLN:HG3	1.90	0.52
1:C:75:LYS:HG3	1:C:77:TYR:HE1	1.75	0.52
2:B:175:VAL:O	2:B:177:ASP:N	2.42	0.52
2:D:430:LEU:CD2	4:D:2137:HOH:O	2.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:TYR:OH	4:C:2070:HOH:O	2.09	0.51
1:A:115:LEU:HD13	1:A:119:HIS:CE1	2.45	0.51
2:D:394:LEU:O	2:D:396:GLN:N	2.44	0.51
2:B:207:THR:H	2:B:210:MET:HG3	1.75	0.51
2:B:404:HIS:CD2	2:B:406:GLN:H	2.27	0.51
2:B:325:ALA:HB2	4:B:2097:HOH:O	2.09	0.51
2:D:338:GLU:OE2	2:D:412:LYS:NZ	2.44	0.51
2:D:332:LEU:HB2	2:D:421:VAL:HG11	1.92	0.51
2:B:420:GLY:O	2:B:421:VAL:C	2.54	0.51
1:C:115:LEU:HD11	1:C:185:ASP:HB3	1.93	0.51
2:D:401:ALA:N	2:D:402:PRO:CD	2.74	0.51
2:B:282:THR:O	2:B:285:THR:HG22	2.11	0.51
1:C:73:GLU:OE2	2:D:293:ARG:NH2	2.43	0.50
2:D:404:HIS:HD2	2:D:406:GLN:HB2	1.77	0.50
2:D:335:PHE:HB2	2:D:413:TYR:CD2	2.47	0.50
2:B:432:LEU:HD21	4:B:2125:HOH:O	2.11	0.50
2:D:393:ASP:C	2:D:394:LEU:O	2.51	0.50
1:C:158:THR:HG21	4:C:2129:HOH:O	2.11	0.50
2:D:270:ILE:HG22	2:D:271:TYR:CD2	2.47	0.50
2:B:282:THR:HB	2:B:285:THR:HG23	1.92	0.49
2:B:388:LYS:HG3	4:B:2125:HOH:O	2.12	0.49
2:D:413:TYR:C	2:D:422:SER:OG	2.55	0.49
1:A:38:ASP:OD2	1:A:41:THR:HB	2.12	0.49
1:A:154:VAL:CG1	1:A:155:PRO:HD2	2.43	0.49
1:C:9:LYS:HD2	1:C:17:VAL:HG13	1.94	0.49
1:A:247:ASP:OD2	1:A:249:SER:HB3	2.13	0.49
1:C:160:THR:O	1:C:161:HIS:HB2	2.12	0.49
2:B:371:SER:O	2:B:372:TRP:C	2.56	0.48
2:B:176:PRO:HB3	4:B:2023:HOH:O	2.13	0.48
2:D:191:VAL:O	2:D:191:VAL:CG1	2.61	0.48
2:D:322:GLN:HG2	4:D:2105:HOH:O	2.13	0.48
2:D:358:ALA:HA	2:D:391:LEU:HD13	1.95	0.48
1:C:124:LEU:HD13	1:C:126:ARG:HG3	1.96	0.48
1:A:60:HIS:CG	1:A:61:PRO:HD2	2.49	0.48
2:B:396:GLN:HG3	4:B:2128:HOH:O	2.13	0.48
1:C:82:PHE:C	1:C:83:LEU:HG	2.38	0.48
4:A:2036:HOH:O	2:D:246:MET:HE2	2.12	0.48
2:D:391:LEU:HD23	2:D:432:LEU:HD11	1.96	0.48
2:B:207:THR:O	2:B:210:MET:HG3	2.14	0.48
1:A:51:GLU:HG3	1:A:55:LEU:HD22	1.96	0.48
1:A:105:LYS:HD2	1:A:285:PHE:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:ARG:HH12	1:C:159:TYR:HE2	1.58	0.48
1:C:159:TYR:HE1	2:D:270:ILE:CG2	2.18	0.48
1:C:91:MET:HE3	1:C:196:MET:HG2	1.95	0.47
1:C:227:TRP:HB3	1:C:230:VAL:CG2	2.44	0.47
1:A:129:LYS:HA	1:A:192:ILE:HD11	1.95	0.47
2:D:191:VAL:O	2:D:191:VAL:HG12	2.14	0.47
2:D:345:ASP:CB	2:D:346:PRO:CD	2.86	0.47
2:D:404:HIS:HD2	2:D:406:GLN:H	1.62	0.47
2:B:338:GLU:O	2:B:339:LEU:C	2.55	0.47
1:C:60:HIS:HD2	1:C:62:ASN:H	1.62	0.47
2:D:392:MET:HG3	4:D:2134:HOH:O	2.14	0.47
1:C:249:SER:HB2	4:C:2173:HOH:O	2.14	0.47
1:C:166:LEU:HD23	1:C:169:ARG:NH2	2.28	0.47
1:C:200:ARG:NH1	4:C:2148:HOH:O	2.48	0.47
1:C:126:ARG:CZ	4:C:2103:HOH:O	2.62	0.46
1:C:248:PHE:C	1:C:250:LYS:N	2.71	0.46
1:A:41:THR:O	2:B:275:VAL:HG21	2.15	0.46
1:C:13:GLY:O	1:C:14:THR:C	2.58	0.46
1:A:101:LEU:HB2	4:A:2045:HOH:O	2.16	0.46
2:D:173:ASN:N	4:D:2022:HOH:O	2.48	0.46
1:A:39:THR:HG21	1:A:74:ASN:HB3	1.98	0.46
2:D:177:ASP:C	2:D:177:ASP:OD1	2.58	0.46
2:B:201:LYS:HE3	2:B:202:LYS:CD	2.45	0.46
1:C:217:ARG:HG2	1:C:243:TRP:CZ3	2.51	0.46
2:B:239:ILE:HD11	2:B:257:GLY:HA2	1.98	0.46
2:B:299:LEU:HD22	2:B:304:PHE:CD1	2.51	0.46
1:A:25:LEU:HD21	2:D:293:ARG:HB3	1.97	0.45
1:C:136:ASN:OD1	1:C:136:ASN:C	2.58	0.45
1:C:166:LEU:CD2	1:C:169:ARG:NH2	2.80	0.45
1:A:257:GLU:HG3	1:A:260:ARG:NH2	2.32	0.45
2:B:253:LEU:HD23	3:E:34:PHE:CZ	2.51	0.45
1:A:129:LYS:HD3	1:A:165:THR:HG21	1.99	0.45
1:A:115:LEU:HD11	1:A:185:ASP:HB3	1.98	0.45
1:C:104:ILE:HG12	1:C:196:MET:HB3	1.99	0.45
2:D:346:PRO:CD	2:D:347:TYR:N	2.80	0.45
2:D:364:LEU:HD12	2:D:370:GLN:HB2	1.99	0.45
2:D:347:TYR:OH	2:D:394:LEU:HA	2.18	0.44
1:A:105:LYS:HE2	1:A:288:ASP:OD1	2.17	0.44
2:D:417:LYS:CD	4:D:2151:HOH:O	2.66	0.44
1:A:243:TRP:CD1	4:A:2173:HOH:O	2.69	0.44
2:B:200:MET:HG2	2:B:208:ASN:ND2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:402:PRO:HG3	2:D:410:ARG:HH21	1.83	0.44
2:B:334:MET:CE	4:B:2102:HOH:O	2.65	0.44
2:D:417:LYS:HD3	4:D:2151:HOH:O	2.17	0.44
1:A:14:THR:O	1:A:15:TYR:HB2	2.17	0.44
1:A:257:GLU:CD	1:A:257:GLU:H	2.26	0.44
1:C:57:GLU:OE1	1:C:122:ARG:NH2	2.38	0.44
2:D:420:GLY:O	2:D:421:VAL:C	2.59	0.44
2:B:344:ALA:HB1	2:B:348:LEU:HD22	2.00	0.43
1:A:101:LEU:N	1:A:102:PRO:CD	2.80	0.43
1:A:150:ARG:HH11	1:A:150:ARG:CG	2.29	0.43
1:C:170:ALA:HB1	1:C:172:GLU:OE2	2.18	0.43
1:A:110:GLN:OE1	1:A:140:ALA:HA	2.17	0.43
2:B:430:LEU:O	2:B:432:LEU:N	2.51	0.43
2:D:350:TYR:CZ	2:D:390:CYS:HA	2.53	0.43
1:A:105:LYS:CE	1:A:288:ASP:OD1	2.67	0.43
1:A:33:LYS:CE	4:A:2040:HOH:O	2.61	0.43
1:A:164:VAL:HG13	4:A:2132:HOH:O	2.18	0.43
1:A:255:LEU:HG	1:A:259:GLY:HA3	1.99	0.43
2:B:175:VAL:O	2:B:175:VAL:HG12	2.19	0.43
2:D:421:VAL:HA	2:D:424:LEU:HD22	2.01	0.43
1:A:87:LEU:O	1:A:91:MET:HG3	2.18	0.43
1:A:127:ASP:OD1	1:A:164:VAL:HG22	2.18	0.43
1:A:217:ARG:HD3	4:A:2158:HOH:O	2.17	0.43
2:B:201:LYS:HG3	2:B:202:LYS:N	2.32	0.43
1:C:138:GLU:CD	1:C:138:GLU:N	2.77	0.43
2:D:394:LEU:HA	2:D:394:LEU:HD12	1.84	0.43
1:A:209:ILE:HD12	1:A:209:ILE:HA	1.85	0.42
2:B:406:GLN:C	2:B:407:GLN:HG2	2.44	0.42
2:D:219:VAL:O	2:D:220:GLU:C	2.60	0.42
2:D:234:LEU:O	2:D:235:ALA:C	2.61	0.42
2:D:323:GLN:HA	2:D:324:PRO:HA	1.84	0.42
2:D:335:PHE:CZ	2:D:339:LEU:HD11	2.54	0.42
1:A:229:GLY:O	1:A:230:VAL:C	2.61	0.42
1:C:24:LYS:HE2	4:C:2021:HOH:O	2.19	0.42
2:D:263:LEU:O	2:D:264:ALA:C	2.61	0.42
2:B:199:TYR:CD1	2:B:199:TYR:C	2.97	0.42
2:D:390:CYS:SG	4:D:2135:HOH:O	2.02	0.42
2:D:404:HIS:CD2	2:D:406:GLN:HB2	2.53	0.42
1:A:2:GLU:HG2	1:C:73:GLU:CD	2.45	0.42
1:C:1:MET:HE2	1:C:1:MET:HA	2.02	0.42
2:B:388:LYS:N	2:B:389:PRO:CD	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:376:LEU:HD23	2:D:376:LEU:HA	1.85	0.42
3:E:32:LEU:HD23	3:E:32:LEU:HA	1.97	0.42
1:A:86:ASP:OD2	1:A:89:LYS:HD2	2.19	0.41
2:B:345:ASP:CB	2:B:346:PRO:HD3	2.22	0.41
2:D:331:SER:HB3	2:D:421:VAL:HG21	2.02	0.41
2:D:207:THR:HG22	2:D:210:MET:H	1.85	0.41
1:A:62:ASN:ND2	1:A:110:GLN:HB3	2.35	0.41
1:C:9:LYS:HD2	1:C:17:VAL:CG1	2.51	0.41
1:A:38:ASP:CG	1:A:41:THR:HB	2.45	0.41
2:B:207:THR:HG23	2:B:209:SER:H	1.86	0.41
2:B:294:MET:O	2:B:295:GLU:C	2.61	0.41
2:B:415:ASN:OD1	2:B:417:LYS:HB2	2.19	0.41
1:A:76:LEU:HD23	1:A:76:LEU:HA	1.90	0.41
1:A:198:THR:O	1:A:199:ARG:HB2	2.20	0.41
1:C:159:TYR:CE1	2:D:270:ILE:HG22	2.51	0.41
1:A:103:LEU:HD21	1:A:294:PRO:HB3	2.03	0.41
2:B:401:ALA:N	2:B:402:PRO:CD	2.83	0.41
2:B:424:LEU:N	4:B:2144:HOH:O	2.54	0.41
1:C:294:PRO:HG2	1:C:296:LEU:HD21	2.03	0.41
1:A:154:VAL:CG1	4:B:2070:HOH:O	2.68	0.41
1:C:159:TYR:CD1	2:D:270:ILE:HG22	2.48	0.41
2:D:404:HIS:CD2	2:D:406:GLN:H	2.38	0.41
2:B:175:VAL:C	2:B:177:ASP:H	2.26	0.41
1:A:38:ASP:OD2	1:A:41:THR:CB	2.69	0.40
1:A:126:ARG:NH1	4:A:2099:HOH:O	2.50	0.40
1:C:60:HIS:HE1	4:C:2061:HOH:O	2.02	0.40
1:C:64:VAL:HG22	1:C:144:ALA:HA	2.03	0.40
1:C:96:LEU:O	1:C:199:ARG:NH1	2.54	0.40
1:A:40:GLU:O	2:B:288:LYS:CD	2.70	0.40
2:B:198:GLY:C	2:B:201:LYS:HG2	2.45	0.40
1:C:272:ASN:CG	4:C:2199:HOH:O	2.64	0.40
2:D:200:MET:HG2	2:D:208:ASN:ND2	2.36	0.40
2:B:350:TYR:OH	2:B:393:ASP:OD2	2.39	0.40
2:B:430:LEU:C	2:B:432:LEU:N	2.79	0.40
2:B:275:VAL:HG11	2:B:292:LEU:HD11	2.03	0.40
2:D:296:HIS:CG	4:D:2092:HOH:O	2.73	0.40
2:D:312:ASN:OD1	2:D:334:MET:HE1	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)
4:A:2129:HOH:O	4:C:2005:HOH:O[4_455]	2.17	0.03

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	294/298 (99%)	276 (94%)	16 (5%)	2 (1%)	18	28
1	C	292/298 (98%)	274 (94%)	12 (4%)	6 (2%)	5	7
2	B	256/260 (98%)	242 (94%)	7 (3%)	7 (3%)	4	4
2	D	258/260 (99%)	248 (96%)	5 (2%)	5 (2%)	6	8
3	E	4/6 (67%)	4 (100%)	0	0	100	100
3	F	4/6 (67%)	4 (100%)	0	0	100	100
All	All	1108/1128 (98%)	1048 (95%)	40 (4%)	20 (2%)	6	9

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	THR
2	B	199	TYR
2	B	424	LEU
1	C	96	LEU
2	D	345	ASP
2	D	346	PRO
2	D	394	LEU
2	D	395	HIS
1	A	96	LEU
2	B	346	PRO
2	B	421	VAL
2	B	431	ASN
1	C	38	ASP
1	C	249	SER
2	D	174	GLU

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Mol	Chain	Res	Type
2	B	176	PRO
2	B	345	ASP
1	C	14	THR
1	C	15	TYR
1	C	161	HIS

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	260/263 (99%)	223 (86%)	37 (14%)	3	4
1	C	260/263 (99%)	221 (85%)	39 (15%)	3	3
2	B	231/234 (99%)	199 (86%)	32 (14%)	3	4
2	D	234/234 (100%)	207 (88%)	27 (12%)	5	8
3	E	5/5 (100%)	4 (80%)	1 (20%)	1	2
3	F	5/5 (100%)	3 (60%)	2 (40%)	0	0
All	All	995/1004 (99%)	857 (86%)	138 (14%)	3	4

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	9	LYS
1	A	14	THR
1	A	17	VAL
1	A	30	VAL
1	A	36	ARG
1	A	37	LEU
1	A	38	ASP
1	A	40	GLU
1	A	42	GLU
1	A	55	LEU
1	A	56	LYS
1	A	70	ILE

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Mol	Chain	Res	Type
1	A	73	GLU
1	A	74	ASN
1	A	76	LEU
1	A	78	LEU
1	A	87	LEU
1	A	101	LEU
1	A	105	LYS
1	A	115	LEU
1	A	122	ARG
1	A	131	GLN
1	A	150	ARG
1	A	163	VAL
1	A	164	VAL
1	A	200	ARG
1	A	202	LEU
1	A	212	LEU
1	A	230	VAL
1	A	245	ARG
1	A	250	LYS
1	A	255	LEU
1	A	268	HIS
1	A	278	LYS
1	A	287	GLN
1	A	293	VAL
2	B	197	VAL
2	B	199	TYR
2	B	207	THR
2	B	210	MET
2	B	232	LEU
2	B	245	SER
2	B	249	LEU
2	B	250	ARG
2	B	256	VAL
2	B	258	THR
2	B	271	TYR
2	B	281	ILE
2	B	285	THR
2	B	289	LYS
2	B	292	LEU
2	B	293	ARG
2	B	300	LYS
2	B	323	GLN

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Mol	Chain	Res	Type
2	B	345	ASP
2	B	348	LEU
2	B	349	LYS
2	B	362	LEU
2	B	370	GLN
2	B	388	LYS
2	B	396	GLN
2	B	400	LYS
2	B	403	GLN
2	B	416	SER
2	B	424	LEU
2	B	428	GLU
2	B	431	ASN
2	B	432	LEU
1	C	2	GLU
1	C	6	LYS
1	C	10	ILE
1	C	12	GLU
1	C	22	ARG
1	C	30	VAL
1	C	36	ARG
1	C	37	LEU
1	C	64	VAL
1	C	74	ASN
1	C	78	LEU
1	C	87	LEU
1	C	88	LYS
1	C	97	THR
1	C	101	LEU
1	C	115	LEU
1	C	122	ARG
1	C	124	LEU
1	C	126	ARG
1	C	154	VAL
1	C	158	THR
1	C	160	THR
1	C	162	GLU
1	C	163	VAL
1	C	165	THR
1	C	169	ARG
1	C	189	LEU
1	C	202	LEU

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Mol	Chain	Res	Type
1	C	206	ASP
1	C	214	ARG
1	C	217	ARG
1	C	225	VAL
1	C	226	VAL
1	C	230	VAL
1	C	252	VAL
1	C	257	GLU
1	C	291	LYS
1	C	293	VAL
1	C	296	LEU
2	D	174	GLU
2	D	175	VAL
2	D	197	VAL
2	D	200	MET
2	D	201	LYS
2	D	207	THR
2	D	232	LEU
2	D	249	LEU
2	D	274	GLU
2	D	281	ILE
2	D	292	LEU
2	D	293	ARG
2	D	317	GLN
2	D	328	LYS
2	D	345	ASP
2	D	348	LEU
2	D	362	LEU
2	D	364	LEU
2	D	384	LEU
2	D	392	MET
2	D	396	GLN
2	D	403	GLN
2	D	410	ARG
2	D	421	VAL
2	D	424	LEU
2	D	425	ASN
2	D	431	ASN
3	E	33	ILE
3	F	30	ARG
3	F	33	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	60	HIS
1	A	62	ASN
1	A	85	GLN
1	A	113	GLN
1	A	131	GLN
1	A	161	HIS
1	A	295	HIS
2	B	208	ASN
2	B	296	HIS
2	B	323	GLN
2	B	404	HIS
2	B	406	GLN
2	B	431	ASN
1	C	5	GLN
1	C	60	HIS
1	C	62	ASN
1	C	287	GLN
2	D	208	ASN
2	D	233	HIS
2	D	313	GLN
2	D	317	GLN
2	D	322	GLN
2	D	361	HIS
2	D	395	HIS
2	D	396	GLN
2	D	404	HIS
2	D	406	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.