



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:37 pm GMT

PDB ID : 1OKV
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

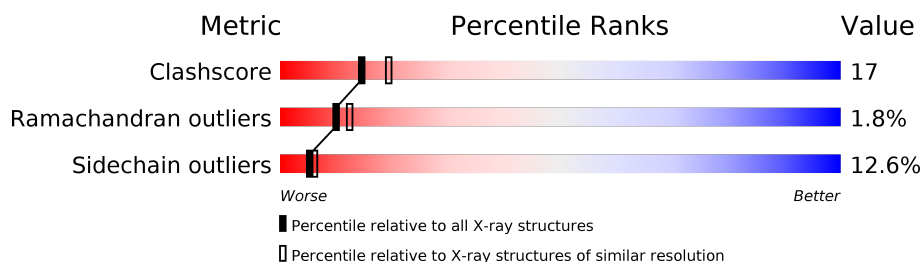
1 Overall quality at a glance

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	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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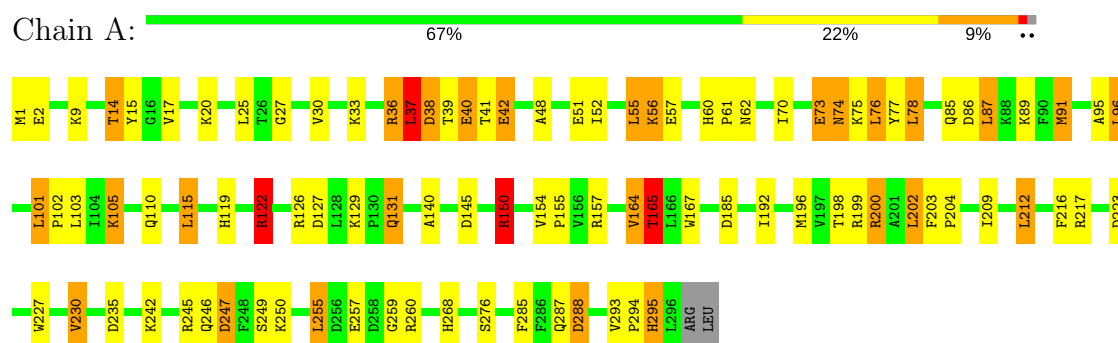
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	7	Total	O	0	0
			7	7		
4	F	8	Total	O	0	0
			8	8		

3 Residue-property plots

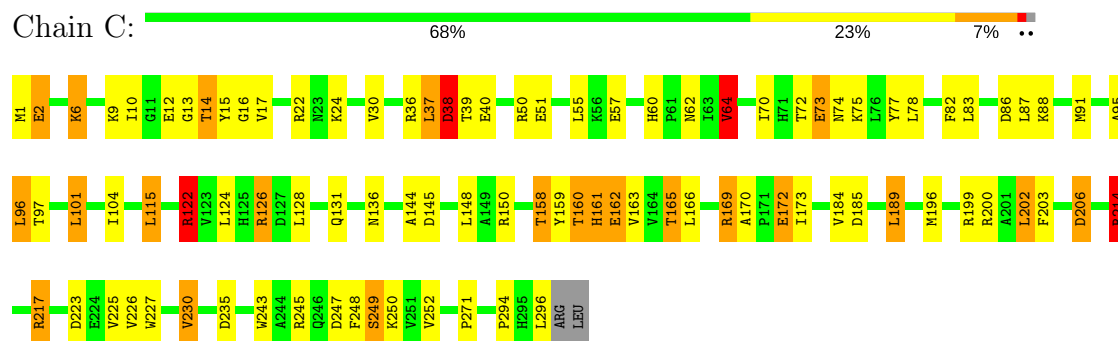
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

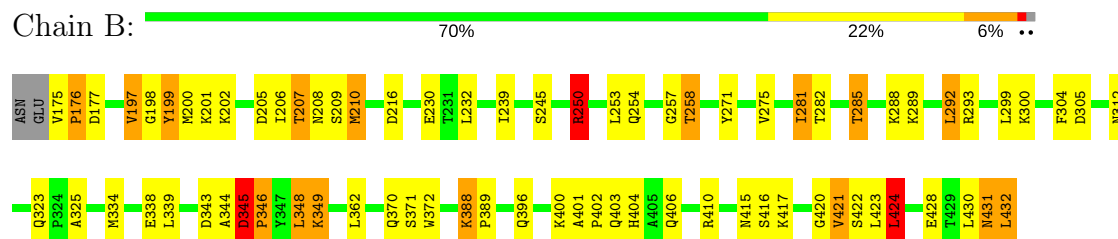
• Molecule 1: CELL DIVISION PROTEIN KINASE 2



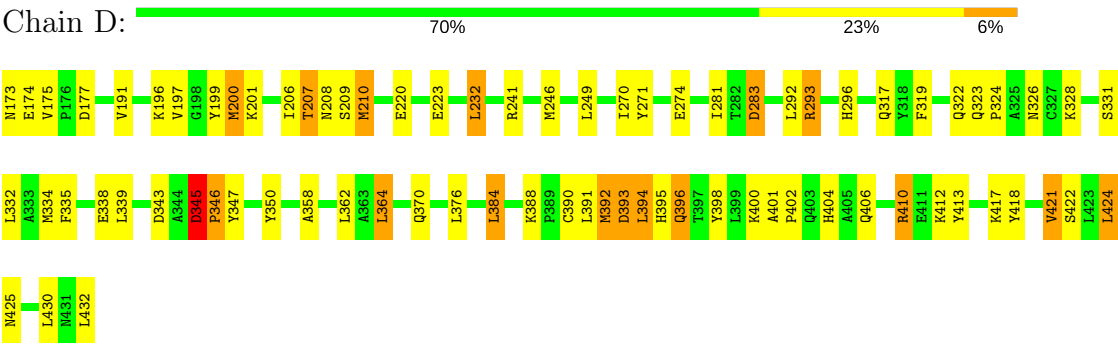
• Molecule 1: CELL DIVISION PROTEIN KINASE 2



• Molecule 2: CYCLIN A2



• Molecule 2: CYCLIN A2



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



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



4 Data and refinement statistics

Xtrriage (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.	Xtrriage
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	0.77	1/2432 (0.0%)	1.06	12/3302 (0.4%)
1	C	0.77	1/2438 (0.0%)	1.06	11/3308 (0.3%)
2	B	0.75	0/2132	1.05	8/2894 (0.3%)
2	D	0.75	1/2151 (0.0%)	0.99	5/2920 (0.2%)
3	E	0.62	0/49	1.30	0/63
3	F	0.80	0/49	1.24	1/63 (1.6%)
All	All	0.76	3/9251 (0.0%)	1.05	37/12550 (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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	210	MET	SD-CE	-7.27	1.37	1.77
1	C	73	GLU	CD-OE2	6.36	1.32	1.25
1	A	295	HIS	C-N	-5.19	1.22	1.34

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	250	ARG	NE-CZ-NH1	9.01	124.81	120.30
1	C	223	ASP	CB-CG-OD2	8.93	126.33	118.30
2	B	343	ASP	CB-CG-OD2	8.76	126.19	118.30
1	A	150	ARG	NE-CZ-NH1	8.56	124.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	ASP	CB-CG-OD2	8.27	125.74	118.30
1	C	122	ARG	NE-CZ-NH1	8.18	124.39	120.30
2	B	250	ARG	NE-CZ-NH2	-8.03	116.28	120.30
2	D	393	ASP	CB-CG-OD2	7.52	125.07	118.30
2	B	205	ASP	CB-CG-OD2	7.47	125.02	118.30
2	B	305	ASP	CB-CG-OD2	7.14	124.73	118.30
1	C	86	ASP	CB-CG-OD1	7.07	124.67	118.30
1	C	145	ASP	CB-CG-OD2	6.94	124.55	118.30
1	A	235	ASP	CB-CG-OD2	6.79	124.41	118.30
1	A	122	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	A	91	MET	CG-SD-CE	-6.62	89.60	100.20
1	C	122	ARG	NE-CZ-NH2	-6.39	117.10	120.30
1	A	288	ASP	CB-CG-OD2	6.39	124.05	118.30
1	C	247	ASP	CB-CG-OD2	6.12	123.81	118.30
2	D	241	ARG	NE-CZ-NH2	-5.98	117.31	120.30
3	F	30	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	C	64	VAL	CB-CA-C	-5.93	100.12	111.40
1	C	38	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	145	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	150	ARG	NH1-CZ-NH2	-5.89	112.92	119.40
2	B	345	ASP	CB-CG-OD2	5.85	123.56	118.30
1	C	214	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	C	235	ASP	CB-CG-OD2	5.65	123.39	118.30
1	C	245	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	247	ASP	CB-CG-OD1	5.58	123.32	118.30
2	D	246	MET	CG-SD-CE	5.50	109.01	100.20
2	B	410	ARG	NE-CZ-NH2	-5.38	117.61	120.30
2	D	232	LEU	CA-CB-CG	5.33	127.57	115.30
1	A	157	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	37	LEU	CA-CB-CG	5.27	127.42	115.30
1	A	165	THR	OG1-CB-CG2	-5.27	97.88	110.00
2	D	283	ASP	CB-CG-OD2	5.07	122.86	118.30
2	B	216	ASP	CB-CG-OD2	5.01	122.81	118.30

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	96	0
1	C	2377	0	2424	94	0
2	B	2082	0	2103	60	0
2	D	2101	0	2119	79	0
3	E	50	0	56	5	0
3	F	50	0	56	4	0
4	A	210	0	0	15	1
4	B	152	0	0	13	0
4	C	221	0	0	21	1
4	D	159	0	0	14	0
4	E	7	0	0	0	0
4	F	8	0	0	2	0
All	All	9787	0	9173	313	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 17.

All (313) 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
1:C:6:LYS:H	1:C:6:LYS:HD2	1.34	0.93
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
2:B:432:LEU:C	2:B:432:LEU:HD23	1.96	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	2:B:424:LEU:HD13	1.48	0.79
1:A:15:TYR:HD2	1:A:33:LYS:HD3	1.47	0.79
1:C:202:LEU:HD13	1:C:203:PHE:CE2	2.18	0.79
1:C:95:ALA:O	1:C:96:LEU:HB3	1.83	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:227:TRP:O	1:C:230:VAL:HG23	1.87	0.75
1:C:38:ASP:HB3	4:C:2039:HOH:O	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:O	1:C:163:VAL:HG23	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
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:N	1:C:206:ASP:OD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
2:D:388:LYS:O	2:D:392:MET:HG2	1.94	0.67
1:C:128:LEU:HD13	1:C:189:LEU:HD13	1.76	0.67
2:B:432:LEU:C	2:B:432:LEU:CD2	2.62	0.66
2:B:404:HIS:HD2	2:B:406:GLN:H	1.41	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:CG	1:C:214:ARG:HH11	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
1:A:36:ARG:C	1:A:37:LEU:HD22	2.18	0.64
1:C:126:ARG:NH1	4:C:2103:HOH:O	2.31	0.63
1:A:294:PRO:C	4:A:2206:HOH:O	2.37	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:223:GLU:CD	2:D:412:LYS:HD2	2.18	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
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
1:A:36:ARG:C	1:A:37:LEU:CD2	2.68	0.62
2:D:384:LEU:O	2:D:384:LEU:HD12	2.00	0.62
1:C:6:LYS:H	1:C:6:LYS:CD	2.05	0.62
1:C:50:ARG:HD3	1:C:150:ARG:HD2	1.82	0.61
1:C:39:THR:C	1:C:40:GLU:CA	2.69	0.61
1:C:77:TYR:OH	4:C:2070:HOH:O	2.09	0.61
1:C:75:LYS:HG3	1:C:77:TYR:CE1	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:50:ARG:NH2	4:C:2050:HOH:O	2.35	0.60
1:A:150:ARG:HH11	1:A:150:ARG:HG3	1.66	0.60
1:A:212:LEU:HD22	1:A:216:PHE:CZ	2.37	0.60
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: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:38:ASP:OD2	1:A:41:THR:C	2.41	0.57
1:A:227:TRP:CE3	1:A:230:VAL:HG13	2.40	0.57
2:B:423:LEU:O	2:B:424:LEU:C	2.42	0.57
1:A:295:HIS:N	4:A:2206:HOH:O	2.38	0.57
2:D:334:MET:HE1	4:D:2066:HOH:O	2.05	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: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:C:248:PHE:O	1:C:250:LYS:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:GLU:HG2	1:C:271:PRO:HG2	1.87	0.55
1:C:37:LEU:O	1:C:38:ASP:C	2.44	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: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
2:D:206:ILE:HG22	2:D:210:MET:HE1	1.89	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
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
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
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
1:A:38:ASP:CG	1:A:41:THR:H	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:432:LEU:C	4:D:2159:HOH:O	2.48	0.49
1:C:248:PHE:O	1:C:249:SER:C	2.51	0.49
1:A:73:GLU:CD	1:C:2:GLU:HG2	2.32	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:D:338:GLU:CD	2:D:412:LYS:NZ	2.66	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
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:105:LYS:HD2	1:A:285:PHE:CE2	2.49	0.48
1:A:51:GLU:HG3	1:A:55:LEU:HD22	1.96	0.48
1:C:126:ARG:HH12	1:C:159:TYR:HE2	1.58	0.48
2:D:393:ASP:C	2:D:394:LEU:O	2.51	0.48
1:C:159:TYR:HE1	2:D:270:ILE:CG2	2.18	0.48
1:A:1:MET:HE2	1:A:70:ILE:HD12	1.97	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:HG12	2:D:191:VAL:O	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:ARG:CZ	4:C:2103:HOH:O	2.62	0.46
1:A:41:THR:O	2:B:275:VAL:HG21	2.15	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:B:201:LYS:HE3	2:B:202:LYS:CD	2.45	0.46
2:B:420:GLY:O	2:B:421:VAL:C	2.54	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: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
2:D:413:TYR:C	2:D:422:SER:OG	2.55	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:C:72:THR:HG21	1:C:75:LYS:HZ2	1.82	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
2:B:200:MET:HG2	2:B:208:ASN:ND2	2.32	0.44
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
2:B:371:SER:O	2:B:372:TRP:C	2.56	0.44
1:A:14:THR:O	1:A:15:TYR:HB2	2.17	0.44
1:C:91:MET:HE3	1:C:196:MET:HG2	2.00	0.44
1:C:57:GLU:OE1	1:C:122:ARG:NH2	2.38	0.44
2:B:344:ALA:HB1	2:B:348:LEU:HD22	2.00	0.43
1:C:82:PHE:C	1:C:83:LEU:HG	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:PHE:C	1:C:250:LYS:N	2.71	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
1:A:33:LYS:CE	4:A:2040:HOH:O	2.61	0.43
2:B:175:VAL:HG12	2:B:175:VAL:O	2.19	0.43
2:D:421:VAL:HA	2:D:424:LEU:HD22	2.01	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
1:A:87:LEU:O	1:A:91:MET:HG3	2.18	0.43
2:B:201:LYS:HG3	2:B:202:LYS:N	2.32	0.43
2:D:394:LEU:HD12	2:D:394:LEU:HA	1.84	0.43
1:A:209:ILE:HA	1:A:209:ILE:HD12	1.85	0.42
2:B:338:GLU:O	2:B:339:LEU:C	2.55	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:C:24:LYS:HE2	4:C:2021:HOH:O	2.19	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
2:B:388:LYS:N	2:B:389:PRO:CD	2.83	0.42
2:D:376:LEU:HD23	2:D:376:LEU:HA	1.85	0.42
3:E:32:LEU:HA	3:E:32:LEU:HD23	1.97	0.42
1:C:13:GLY:O	1:C:14:THR:C	2.58	0.41
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:177:ASP:C	2:D:177:ASP:OD1	2.58	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
2:B:207:THR:HG23	2:B:209:SER:H	1.86	0.41
2:B:415:ASN:OD1	2:B:417:LYS:HB2	2.19	0.41
1:A:198:THR:O	1:A:199:ARG:HB2	2.20	0.41
1:A:76:LEU:HA	1:A:76:LEU:HD23	1.90	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
2:D:404:HIS:CD2	2:D:406:GLN:H	2.38	0.41
1:C:136:ASN:C	1:C:136:ASN:OD1	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:TYR:CD1	2:D:270:ILE:HG22	2.48	0.41
1:A:126:ARG:NH1	4:A:2099:HOH:O	2.50	0.40
1:A:38:ASP:OD2	1:A:41:THR:CB	2.69	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:C:60:HIS:HE1	4:C:2061:HOH:O	2.02	0.40
1:A:91:MET:HE1	1:A:196:MET:HA	2.03	0.40
1:A:40:GLU:O	2:B:288:LYS:CD	2.70	0.40
2:D:200:MET:HG2	2:D:208:ASN:ND2	2.36	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

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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	25	37
1	C	292/298 (98%)	274 (94%)	12 (4%)	6 (2%)	8	9
2	B	256/260 (98%)	242 (94%)	7 (3%)	7 (3%)	6	6
2	D	258/260 (99%)	248 (96%)	5 (2%)	5 (2%)	9	11
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%)	10	12

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
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 [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	260/263 (99%)	224 (86%)	36 (14%)	4	5
1	C	260/263 (99%)	227 (87%)	33 (13%)	5	6
2	B	231/234 (99%)	202 (87%)	29 (13%)	5	6
2	D	234/234 (100%)	209 (89%)	25 (11%)	8	10
3	E	5/5 (100%)	4 (80%)	1 (20%)	1	1
3	F	5/5 (100%)	4 (80%)	1 (20%)	1	1
All	All	995/1004 (99%)	870 (87%)	125 (13%)	5	6

All (125) 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	73	GLU
1	A	74	ASN
1	A	76	LEU
1	A	78	LEU
1	A	85	GLN
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	164	VAL
1	A	200	ARG
1	A	202	LEU
1	A	212	LEU
1	A	230	VAL
1	A	242	LYS
1	A	245	ARG
1	A	250	LYS
1	A	255	LEU
1	A	268	HIS
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

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Mol	Chain	Res	Type
2	B	250	ARG
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
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	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	126	ARG
1	C	158	THR

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Mol	Chain	Res	Type
1	C	160	THR
1	C	162	GLU
1	C	165	THR
1	C	169	ARG
1	C	172	GLU
1	C	189	LEU
1	C	202	LEU
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
2	D	175	VAL
2	D	196	LYS
2	D	197	VAL
2	D	199	TYR
2	D	200	MET
2	D	201	LYS
2	D	207	THR
2	D	232	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	362	LEU
2	D	364	LEU
2	D	384	LEU
2	D	392	MET
2	D	396	GLN
2	D	398	TYR
2	D	410	ARG
2	D	421	VAL
2	D	424	LEU
2	D	425	ASN
3	E	33	ILE
3	F	33	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	62	ASN
1	A	85	GLN
1	A	295	HIS
2	B	208	ASN
2	B	233	HIS
2	B	404	HIS
2	B	431	ASN
1	C	60	HIS
1	C	287	GLN
2	D	208	ASN
2	D	233	HIS
2	D	317	GLN
2	D	322	GLN
2	D	396	GLN
2	D	404	HIS
2	D	425	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 carbohydrates 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 ⓘ

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.