



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:05 AM UTC

PDB ID : 1PKY / pdb_00001pky
Title : PYRUVATE KINASE FROM E. COLI IN THE T-STATE
Authors : Mattevi, A.
Deposited on : 1995-04-27
Resolution : 2.50 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

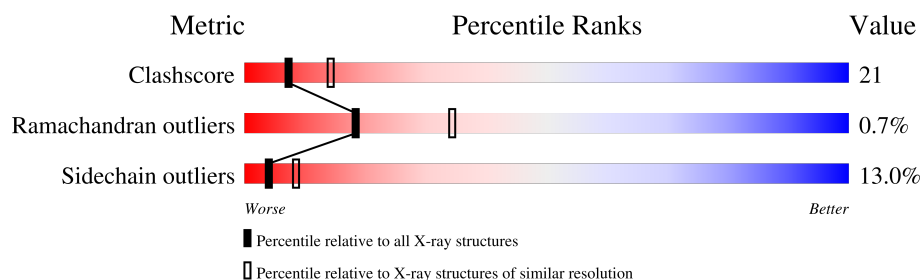
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	470	
1	B	470	
1	C	470	
1	D	470	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14152 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 PYRUVATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	26	0	0
			3464	2159	600	680	25			
1	B	464	Total	C	N	O	S	16	0	0
			3464	2159	600	680	25			
1	C	433	Total	C	N	O	S	65	0	0
			3240	2022	564	630	24			
1	D	464	Total	C	N	O	S	11	0	0
			3464	2159	600	680	25			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	MET	GLN	conflict	UNP P14178
B	279	MET	GLN	conflict	UNP P14178
C	279	MET	GLN	conflict	UNP P14178
D	279	MET	GLN	conflict	UNP P14178

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	126	Total	O	0	0
			126	126		
2	B	137	Total	O	0	0
			137	137		
2	C	107	Total	O	0	0
			107	107		
2	D	150	Total	O	0	0
			150	150		

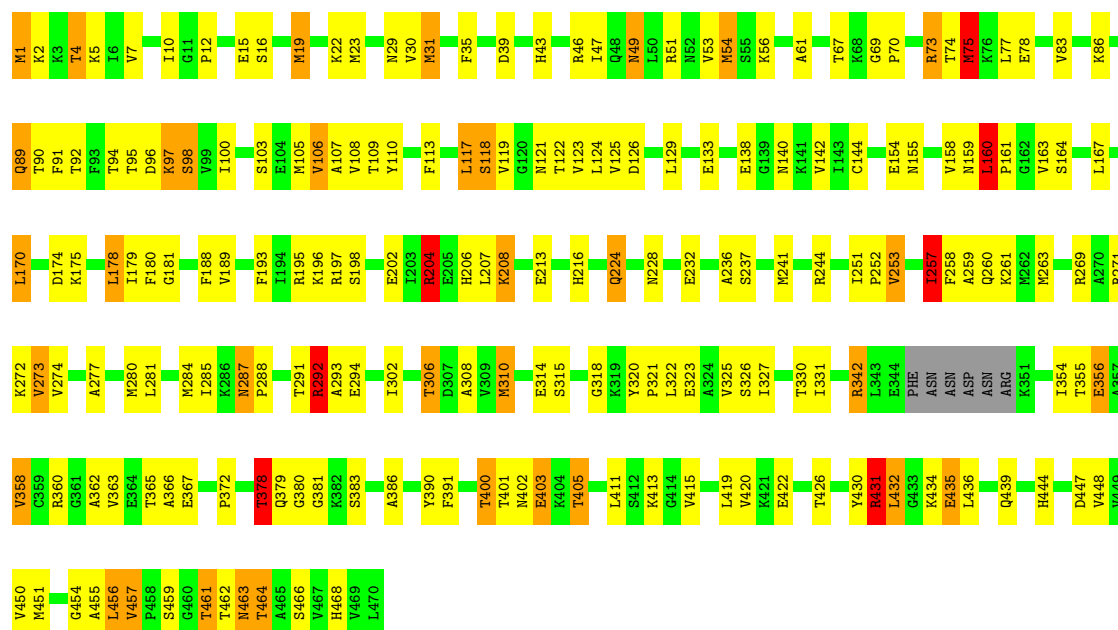
3 Residue-property plots

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.

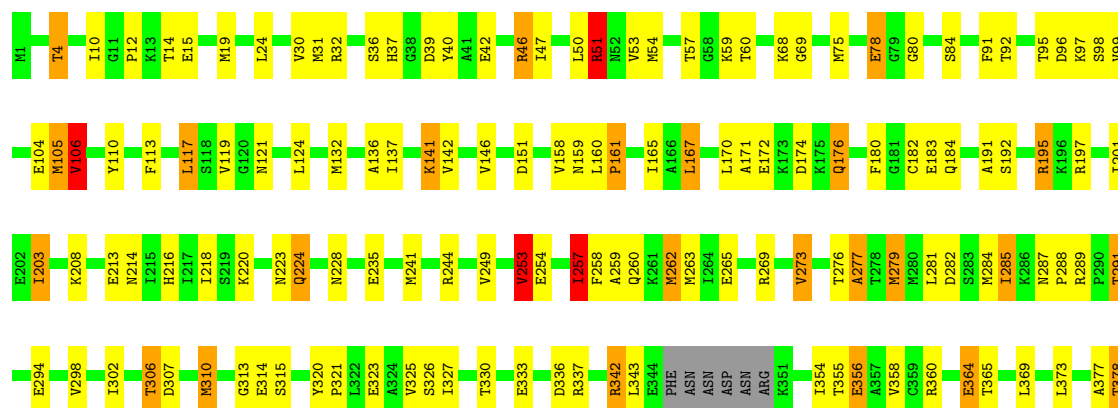
• Molecule 1: PYRUVATE KINASE

Chain A: 



• Molecule 1: PYRUVATE KINASE

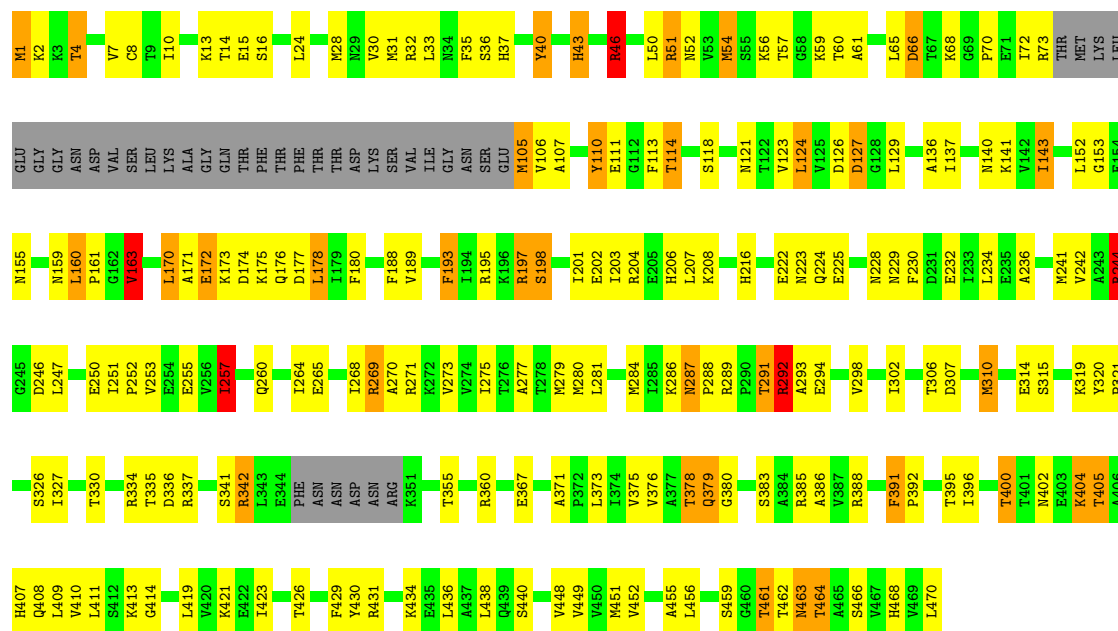
Chain B: 





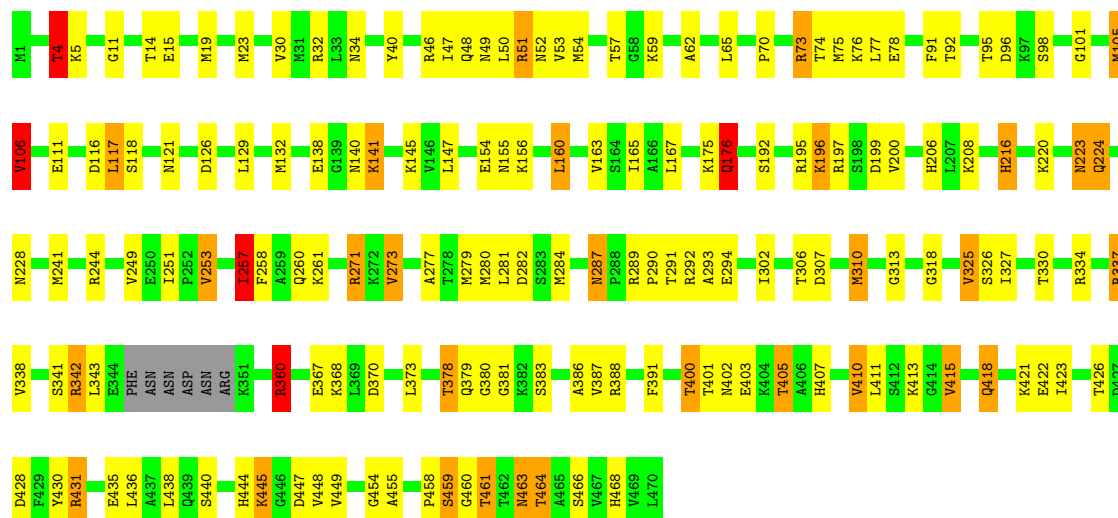
• Molecule 1: PYRUVATE KINASE

Chain C: 49% 35% 7% 8%



• Molecule 1: PYRUVATE KINASE

Chain D: 64% 28% 6%



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	73.91Å 129.58Å 241.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.50	Depositor
% Data completeness (in resolution range)	99.9 (6.00-2.50)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.203 , 0.305	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14152	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.96	3/3498 (0.1%)	1.12	16/4719 (0.3%)
1	B	0.96	2/3498 (0.1%)	1.08	11/4719 (0.2%)
1	C	0.97	3/3271 (0.1%)	1.10	7/4411 (0.2%)
1	D	1.00	5/3498 (0.1%)	1.10	12/4719 (0.3%)
All	All	0.97	13/13765 (0.1%)	1.10	46/18568 (0.2%)

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	A	0	7
1	B	0	8
1	C	0	8
1	D	0	5
All	All	0	28

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	310	MET	SD-CE	-7.41	1.61	1.79
1	A	54	MET	SD-CE	-7.26	1.61	1.79
1	D	4	THR	CA-CB	6.19	1.62	1.53
1	A	125	VAL	CA-CB	6.08	1.62	1.54
1	D	415	VAL	CA-CB	5.96	1.62	1.54
1	B	218	ILE	CA-CB	5.94	1.60	1.53
1	B	310	MET	SD-CE	-5.93	1.64	1.79
1	D	251	ILE	CA-CB	5.72	1.60	1.55
1	C	273	VAL	CA-CB	5.61	1.59	1.54
1	D	75	MET	SD-CE	-5.58	1.65	1.79
1	C	451	MET	SD-CE	-5.39	1.66	1.79
1	D	273	VAL	CA-CB	5.37	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	391	PHE	C-O	5.19	1.26	1.23

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	ALA	N-CA-C	15.22	133.42	111.96
1	C	277	ALA	N-CA-C	8.34	123.94	113.43
1	B	277	ALA	N-CA-C	7.58	123.10	113.55
1	A	277	ALA	CB-CA-C	-7.44	97.72	110.88
1	D	277	ALA	N-CA-C	7.21	122.09	111.34
1	D	253	VAL	CB-CA-C	-7.20	102.67	111.88
1	D	257	ILE	CB-CA-C	-6.74	103.04	112.14
1	A	75	MET	N-CA-C	6.54	115.03	108.75
1	D	403	GLU	N-CA-C	6.40	117.92	111.07
1	B	257	ILE	N-CA-CB	6.29	117.91	110.55
1	C	257	ILE	CB-CA-C	-6.08	103.94	112.14
1	A	257	ILE	CB-CA-C	-6.04	104.13	112.04
1	B	224	GLN	N-CA-C	6.03	117.85	111.28
1	D	310	MET	N-CA-C	5.95	118.65	109.07
1	B	257	ILE	CB-CA-C	-5.90	104.42	111.97
1	C	203	ILE	N-CA-C	-5.67	105.20	110.53
1	A	236	ALA	N-CA-C	5.64	118.36	111.82
1	C	461	THR	N-CA-C	5.62	118.65	109.59
1	B	354	ILE	N-CA-C	5.55	115.64	110.42
1	A	253	VAL	CB-CA-C	-5.49	103.65	112.16
1	D	325	VAL	CB-CA-C	-5.48	104.87	111.88
1	D	418	GLN	N-CA-C	5.43	117.36	108.55
1	D	461	THR	N-CA-C	5.43	117.75	108.90
1	A	160	LEU	CA-C-N	-5.39	114.20	119.76
1	A	160	LEU	C-N-CA	-5.39	114.20	119.76
1	C	107	ALA	N-CA-C	5.39	117.31	108.52
1	B	310	MET	N-CA-C	5.30	117.60	109.07
1	B	106	VAL	CB-CA-C	-5.29	102.23	110.69
1	D	224	GLN	N-CA-C	5.29	117.73	111.33
1	A	378	THR	N-CA-C	5.24	118.10	109.72
1	A	181	GLY	N-CA-C	5.23	119.00	112.73
1	C	310	MET	N-CA-C	5.18	117.93	109.59
1	A	49	ASN	N-CA-C	5.16	117.30	111.11
1	B	51	ARG	NE-CZ-NH1	-5.16	116.34	121.50
1	D	401	THR	N-CA-C	-5.16	107.04	113.38
1	A	204	ARG	NE-CZ-NH1	-5.14	116.36	121.50
1	B	253	VAL	CB-CA-C	-5.12	102.90	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	106	VAL	CB-CA-C	-5.12	104.18	111.19
1	A	224	GLN	N-CA-C	5.09	116.91	111.36
1	A	273	VAL	CB-CA-C	-5.09	104.25	111.28
1	C	54	MET	N-CA-C	5.09	116.52	110.97
1	B	167	LEU	CA-C-N	-5.03	115.54	120.52
1	B	167	LEU	C-N-CA	-5.03	115.54	120.52
1	D	200	VAL	CB-CA-C	-5.02	105.37	112.14
1	A	461	THR	N-CA-C	5.01	117.98	109.76
1	A	356	GLU	N-CA-C	-5.00	105.83	111.28

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	TYR	Sidechain
1	A	204	ARG	Sidechain
1	A	269	ARG	Sidechain
1	A	292	ARG	Sidechain
1	A	342	ARG	Sidechain
1	A	360	ARG	Sidechain
1	A	431	ARG	Sidechain
1	B	106	VAL	Mainchain
1	B	110	TYR	Sidechain
1	B	195	ARG	Sidechain
1	B	32	ARG	Sidechain
1	B	388	ARG	Sidechain
1	B	390	TYR	Sidechain
1	B	431	ARG	Sidechain
1	B	51	ARG	Sidechain
1	C	110	TYR	Sidechain
1	C	193	PHE	Sidechain
1	C	244	ARG	Sidechain
1	C	292	ARG	Sidechain
1	C	334	ARG	Sidechain
1	C	40	TYR	Sidechain
1	C	46	ARG	Sidechain
1	C	51	ARG	Sidechain
1	D	176	GLN	Mainchain
1	D	208	LYS	Mainchain
1	D	32	ARG	Sidechain
1	D	360	ARG	Sidechain
1	D	431	ARG	Sidechain

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	3464	0	3541	159	0
1	B	3464	0	3541	137	0
1	C	3240	0	3327	158	0
1	D	3464	0	3541	118	0
2	A	126	0	0	8	0
2	B	137	0	0	10	0
2	C	107	0	0	12	0
2	D	150	0	0	9	0
All	All	14152	0	13950	563	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (563) 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:A:291:THR:HG22	1:A:293:ALA:H	1.18	1.07
1:A:4:THR:HG22	1:A:413:LYS:HE3	1.39	1.04
1:C:172:GLU:HA	1:C:175:LYS:HD2	1.43	0.96
1:A:23:MET:HE2	1:A:325:VAL:HG21	1.53	0.91
1:A:291:THR:HG22	1:A:293:ALA:N	1.85	0.91
1:D:291:THR:HG22	1:D:293:ALA:H	1.35	0.90
1:C:15:GLU:HB3	1:C:46:ARG:HD3	1.56	0.88
1:B:291:THR:HG22	1:B:294:GLU:H	1.39	0.87
1:C:170:LEU:HD13	1:C:175:LYS:HG2	1.55	0.86
1:B:75:MET:HE1	1:B:97:LYS:HB3	1.58	0.85
1:B:342:ARG:HD2	2:B:585:HOH:O	1.76	0.85
1:A:19:MET:HE1	1:A:322:LEU:HD22	1.59	0.84
1:A:95:THR:HB	1:A:140:ASN:HB2	1.60	0.83
1:D:455:ALA:H	1:D:463:ASN:HD21	1.28	0.81
1:A:1:MET:SD	1:A:2:LYS:N	2.53	0.81
1:B:380:GLY:HA2	1:B:405:THR:HG21	1.64	0.80
1:C:73:ARG:HD3	1:C:155:ASN:HD21	1.47	0.80
1:A:75:MET:HE1	1:A:97:LYS:HG2	1.64	0.80
1:B:355:THR:HG23	1:B:462:THR:HB	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:ARG:HH11	1:D:260:GLN:HE22	1.27	0.79
1:C:288:PRO:HB3	1:C:320:TYR:CD1	2.18	0.79
1:B:463:ASN:ND2	1:B:464:THR:HG22	1.99	0.78
1:C:13:LYS:NZ	1:C:319:LYS:HA	1.99	0.77
1:A:75:MET:HE2	1:A:108:VAL:C	2.10	0.77
1:D:40:TYR:OH	1:D:176:GLN:HG2	1.85	0.77
1:A:454:GLY:HA2	1:A:463:ASN:ND2	2.00	0.77
1:B:197:ARG:HD2	2:B:550:HOH:O	1.85	0.76
1:B:285:ILE:HD11	1:B:313:GLY:HA3	1.65	0.76
1:B:137:ILE:HG12	1:B:142:VAL:HG22	1.69	0.75
1:C:463:ASN:ND2	1:C:464:THR:HG22	2.03	0.73
1:D:326:SER:O	1:D:330:THR:HG23	1.88	0.73
1:D:379:GLN:O	1:D:405:THR:HG21	1.89	0.73
1:A:405:THR:HG22	2:A:494:HOH:O	1.89	0.73
1:C:10:ILE:HG13	1:C:31:MET:HG3	1.70	0.73
1:B:342:ARG:HD3	1:B:391:PHE:CD1	2.25	0.72
1:A:291:THR:HG21	1:A:293:ALA:HB3	1.71	0.71
1:C:400:THR:HG21	1:C:405:THR:OG1	1.91	0.71
1:D:50:LEU:HG	1:D:54:MET:HE2	1.72	0.71
1:C:160:LEU:HB3	1:C:163:VAL:HB	1.71	0.71
1:D:342:ARG:HD2	2:D:520:HOH:O	1.90	0.71
1:A:198:SER:O	1:A:202:GLU:HG3	1.91	0.71
1:C:50:LEU:HG	1:C:54:MET:HE3	1.73	0.71
1:A:206:HIS:CD2	2:A:536:HOH:O	2.43	0.71
1:A:291:THR:HG21	2:A:570:HOH:O	1.91	0.71
1:D:291:THR:HB	1:D:294:GLU:HG3	1.72	0.70
1:D:91:PHE:CZ	1:D:106:VAL:HG22	2.27	0.70
1:C:455:ALA:H	1:C:463:ASN:HD21	1.37	0.70
1:C:15:GLU:CB	1:C:46:ARG:HD3	2.21	0.70
1:B:244:ARG:HH11	1:B:260:GLN:HE22	1.39	0.69
1:B:360:ARG:O	1:B:364:GLU:HB2	1.92	0.69
1:D:455:ALA:N	1:D:463:ASN:HD21	1.90	0.68
1:C:438:LEU:HG	1:C:470:LEU:HD13	1.76	0.68
1:A:380:GLY:HA2	1:A:405:THR:HG21	1.76	0.67
1:C:241:MET:CE	1:C:310:MET:HE1	2.24	0.67
1:D:342:ARG:HD3	1:D:391:PHE:CD1	2.28	0.67
1:A:91:PHE:CZ	1:A:106:VAL:HG22	2.29	0.67
1:A:19:MET:CE	1:A:322:LEU:HD22	2.23	0.67
1:C:172:GLU:HG2	2:C:527:HOH:O	1.95	0.67
1:D:48:GLN:HG3	1:D:52:ASN:HD21	1.60	0.66
1:D:76:LYS:HB2	2:D:568:HOH:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:THR:O	1:A:155:ASN:HA	1.94	0.66
1:B:327:ILE:HD12	1:B:330:THR:OG1	1.93	0.66
1:C:204:ARG:O	1:C:208:LYS:HG3	1.95	0.66
1:C:40:TYR:HA	1:C:43:HIS:ND1	2.10	0.66
1:D:244:ARG:HD2	1:D:260:GLN:NE2	2.11	0.66
1:B:430:TYR:O	1:B:434:LYS:HG3	1.96	0.66
1:A:206:HIS:HD2	2:A:536:HOH:O	1.76	0.66
1:A:241:MET:SD	1:A:310:MET:HE1	2.36	0.66
1:B:343:LEU:HD13	1:B:364:GLU:HG2	1.78	0.66
1:D:378:THR:O	1:D:400:THR:HG23	1.95	0.66
1:C:106:VAL:HG11	1:C:152:LEU:HD21	1.78	0.66
1:B:310:MET:SD	2:B:602:HOH:O	2.53	0.66
1:B:455:ALA:H	1:B:463:ASN:HD21	1.44	0.65
1:C:10:ILE:CG1	1:C:31:MET:HG3	2.26	0.65
1:C:380:GLY:HA2	1:C:405:THR:HG21	1.78	0.65
1:A:383:SER:HB3	1:A:462:THR:OG1	1.97	0.65
1:B:15:GLU:HB3	1:B:46:ARG:HD3	1.78	0.65
1:D:216:HIS:HD2	2:D:473:HOH:O	1.79	0.65
1:D:445:LYS:H	1:D:445:LYS:HZ2	1.43	0.65
1:A:2:LYS:HD2	1:A:4:THR:O	1.96	0.65
1:D:224:GLN:HE21	1:D:228:ASN:ND2	1.95	0.65
1:A:378:THR:HG23	1:A:383:SER:OG	1.97	0.64
1:A:92:THR:O	1:A:105:MET:HG3	1.98	0.64
1:D:455:ALA:H	1:D:463:ASN:ND2	1.94	0.64
1:C:170:LEU:CD1	1:C:175:LYS:HG2	2.28	0.64
1:B:30:VAL:HG21	1:B:411:LEU:HD13	1.80	0.64
1:B:92:THR:CG2	1:B:141:LYS:HG2	2.28	0.64
1:D:257:ILE:HD12	1:D:258:PHE:CE2	2.33	0.64
1:B:358:VAL:HG21	1:B:463:ASN:HA	1.79	0.64
1:D:388:ARG:HD3	1:D:388:ARG:C	2.23	0.64
1:C:342:ARG:HD3	1:C:391:PHE:CD1	2.32	0.64
1:B:399:LEU:HD22	1:B:418:GLN:HG2	1.80	0.64
1:C:114:THR:HG22	1:C:137:ILE:HG23	1.81	0.63
1:D:91:PHE:HZ	1:D:106:VAL:HG22	1.63	0.63
1:B:259:ALA:O	1:B:263:MET:HG3	1.98	0.63
1:C:376:VAL:HG22	1:C:452:VAL:HB	1.79	0.63
1:C:50:LEU:O	1:C:54:MET:HG3	1.98	0.63
1:D:405:THR:HG22	2:D:506:HOH:O	1.98	0.63
1:B:10:ILE:HG12	1:B:31:MET:HG3	1.79	0.63
1:C:170:LEU:HD13	1:C:175:LYS:CG	2.25	0.63
1:A:315:SER:HA	1:A:321:PRO:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:LYS:HG3	1:A:451:MET:HE1	1.81	0.63
1:C:280:MET:HG3	1:C:310:MET:O	1.99	0.62
1:C:230:PHE:CE2	1:C:234:LEU:HD22	2.34	0.62
1:A:284:MET:HA	1:A:287:ASN:O	1.98	0.62
1:D:132:MET:HA	1:D:147:LEU:HG	1.82	0.62
1:A:117:LEU:HD13	1:A:163:VAL:HG21	1.82	0.62
1:B:92:THR:HG21	1:B:141:LYS:HG2	1.79	0.62
1:C:54:MET:HE2	1:C:61:ALA:HB3	1.80	0.62
1:B:53:VAL:O	1:B:57:THR:HG23	2.00	0.61
1:A:257:ILE:O	1:A:261:LYS:HG3	2.00	0.61
1:A:86:LYS:O	1:A:89:GLN:HB3	2.00	0.61
1:C:32:ARG:HD2	1:C:66:ASP:OD2	2.00	0.61
1:D:271:ARG:HG2	1:D:386:ALA:HA	1.81	0.61
1:A:292:ARG:HH21	1:C:279:MET:HB2	1.65	0.61
1:C:208:LYS:HD2	2:C:571:HOH:O	2.00	0.61
1:A:23:MET:HE2	1:A:325:VAL:CG2	2.30	0.61
1:A:91:PHE:HZ	1:A:106:VAL:HG22	1.66	0.61
1:D:192:SER:HA	1:D:220:LYS:HD3	1.82	0.61
1:C:400:THR:O	1:C:419:LEU:HA	2.00	0.61
1:B:216:HIS:HD2	2:B:472:HOH:O	1.83	0.61
1:A:1:MET:HA	1:A:1:MET:HE2	1.83	0.60
1:B:377:ALA:HB2	1:B:429:PHE:CE1	2.36	0.60
1:C:242:VAL:HG11	1:C:260:GLN:HG3	1.82	0.60
1:C:291:THR:HG22	1:C:293:ALA:H	1.66	0.60
1:B:132:MET:HG2	1:B:146:VAL:HA	1.84	0.60
1:C:174:ASP:HB2	2:C:520:HOH:O	1.99	0.60
1:B:463:ASN:HD22	1:B:463:ASN:H	1.48	0.60
1:A:216:HIS:HD2	2:A:472:HOH:O	1.84	0.60
1:C:402:ASN:CG	1:C:405:THR:HG23	2.26	0.60
1:D:51:ARG:HA	1:D:54:MET:HE3	1.82	0.60
1:D:337:ARG:HG3	1:D:338:VAL:HG13	1.84	0.60
1:C:30:VAL:HG21	1:C:411:LEU:HD13	1.84	0.60
1:C:284:MET:HA	1:C:287:ASN:O	2.02	0.60
1:B:434:LYS:HE2	1:B:468:HIS:HD2	1.67	0.60
1:A:12:PRO:HG3	1:A:46:ARG:HH12	1.66	0.59
1:C:379:GLN:O	1:C:405:THR:HG21	2.02	0.59
1:C:466:SER:OG	1:C:468:HIS:HE1	1.86	0.59
1:D:378:THR:HG21	1:D:381:GLY:CA	2.33	0.59
1:A:402:ASN:CG	1:A:405:THR:HG23	2.28	0.58
1:B:257:ILE:HD12	1:B:258:PHE:H	1.69	0.58
1:D:5:LYS:HG3	1:D:410:VAL:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:VAL:O	1:D:249:VAL:HG12	2.02	0.58
1:A:285:ILE:HG23	1:A:318:GLY:HA2	1.86	0.58
1:A:466:SER:OG	1:A:468:HIS:CE1	2.57	0.58
1:D:241:MET:CE	1:D:310:MET:HE1	2.33	0.58
1:D:4:THR:HG21	1:D:302:ILE:HG23	1.86	0.58
1:A:244:ARG:HB3	1:C:292:ARG:HE	1.69	0.57
1:D:422:GLU:HB2	2:D:565:HOH:O	2.03	0.57
1:D:78:GLU:HG3	1:D:101:GLY:O	2.04	0.57
1:A:464:THR:HG22	1:B:466:SER:OG	2.03	0.57
1:A:292:ARG:HH21	1:C:279:MET:CB	2.17	0.57
1:C:136:ALA:O	1:C:143:ILE:HD12	2.05	0.57
1:C:198:SER:O	1:C:202:GLU:HG3	2.04	0.57
1:B:257:ILE:HG13	2:B:517:HOH:O	2.05	0.57
1:C:195:ARG:HD2	2:C:511:HOH:O	2.05	0.57
1:C:388:ARG:C	1:C:388:ARG:HD3	2.30	0.57
1:C:159:ASN:O	1:C:161:PRO:HD3	2.05	0.56
1:B:326:SER:O	1:B:330:THR:HG23	2.04	0.56
1:C:385:ARG:NH1	2:C:491:HOH:O	2.38	0.56
1:B:244:ARG:HB3	1:D:292:ARG:HD3	1.88	0.56
1:B:379:GLN:O	1:B:405:THR:HG21	2.04	0.56
1:B:449:VAL:HG11	1:B:451:MET:HE2	1.87	0.56
1:B:333:GLU:O	1:B:337:ARG:HB2	2.05	0.56
1:D:341:SER:HA	1:D:391:PHE:O	2.04	0.56
1:A:77:LEU:H	1:A:154:GLU:HG2	1.71	0.56
1:A:170:LEU:HD22	1:A:174:ASP:HB3	1.87	0.56
1:B:241:MET:HE2	1:B:310:MET:HE1	1.86	0.56
1:C:7:VAL:HB	1:C:310:MET:HG3	1.88	0.56
1:C:455:ALA:H	1:C:463:ASN:ND2	2.03	0.56
1:C:13:LYS:HZ3	1:C:319:LYS:HA	1.69	0.56
1:C:284:MET:HE3	1:C:288:PRO:C	2.31	0.56
1:D:244:ARG:HH11	1:D:260:GLN:NE2	2.01	0.56
1:D:378:THR:HG21	1:D:381:GLY:HA2	1.87	0.56
1:A:454:GLY:HA2	1:A:463:ASN:HD22	1.70	0.56
1:B:434:LYS:HG2	1:B:451:MET:HE1	1.86	0.56
1:C:105:MET:O	1:C:105:MET:HG3	2.06	0.56
1:C:223:ASN:OD1	1:C:225:GLU:HB3	2.06	0.56
1:C:230:PHE:CZ	1:C:234:LEU:HD22	2.41	0.56
1:C:252:PRO:HG2	1:C:255:GLU:HG3	1.88	0.56
1:A:193:PHE:CD2	1:A:195:ARG:HD2	2.41	0.55
1:B:454:GLY:HA2	1:B:463:ASN:ND2	2.21	0.55
1:B:360:ARG:NH2	1:B:364:GLU:HG3	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:ASP:HA	1:D:413:LYS:HB2	1.89	0.55
1:A:117:LEU:HD21	1:A:123:VAL:HG22	1.88	0.55
1:A:378:THR:O	1:A:400:THR:HG23	2.06	0.55
1:B:320:TYR:HB3	1:B:323:GLU:HB2	1.88	0.55
1:C:244:ARG:HH11	1:C:260:GLN:HE22	1.55	0.55
1:A:204:ARG:HG3	1:A:208:LYS:HE3	1.89	0.55
1:A:431:ARG:HG3	1:A:432:LEU:N	2.21	0.55
1:D:23:MET:HE2	1:D:325:VAL:HG21	1.88	0.55
1:A:356:GLU:HG2	1:A:390:TYR:OH	2.06	0.55
1:C:40:TYR:HA	1:C:43:HIS:HD1	1.70	0.55
1:A:326:SER:O	1:A:330:THR:HG23	2.06	0.54
1:B:4:THR:HG22	1:B:413:LYS:NZ	2.22	0.54
1:B:244:ARG:HD2	1:B:260:GLN:NE2	2.22	0.54
1:B:291:THR:HG22	1:B:294:GLU:N	2.16	0.54
1:C:188:PHE:CD1	1:C:216:HIS:HB2	2.41	0.54
1:B:276:THR:OG1	1:B:306:THR:HG21	2.08	0.54
1:B:96:ASP:HB3	1:B:99:VAL:HG23	1.89	0.54
1:D:74:THR:O	1:D:155:ASN:HA	2.07	0.54
1:D:167:LEU:O	1:D:195:ARG:NH2	2.39	0.54
1:B:4:THR:HG23	1:B:336:ASP:OD1	2.08	0.54
1:C:342:ARG:HD2	2:C:506:HOH:O	2.06	0.54
1:D:117:LEU:HD11	1:D:160:LEU:HG	1.89	0.54
1:A:113:PHE:O	1:A:117:LEU:HB2	2.06	0.54
1:C:400:THR:HG21	1:C:405:THR:HG1	1.72	0.54
1:D:244:ARG:HD2	1:D:260:GLN:HE21	1.71	0.54
1:A:159:ASN:O	1:A:161:PRO:HD3	2.07	0.54
1:A:432:LEU:HD11	1:A:436:LEU:HD11	1.90	0.54
1:D:50:LEU:O	1:D:54:MET:HG3	2.07	0.54
1:A:281:LEU:O	1:A:314:GLU:HG2	2.07	0.54
1:B:47:ILE:HG21	1:B:184:GLN:HE21	1.73	0.54
1:C:57:THR:OG1	1:C:59:LYS:HD2	2.08	0.54
1:B:92:THR:HB	1:B:105:MET:HG2	1.90	0.53
1:C:171:ALA:O	1:C:173:LYS:N	2.41	0.53
1:C:378:THR:O	1:C:400:THR:CG2	2.57	0.53
1:B:241:MET:CE	1:B:310:MET:HE1	2.38	0.53
1:C:70:PRO:HG3	1:C:195:ARG:HH12	1.73	0.53
1:A:94:THR:O	1:A:107:ALA:HA	2.08	0.53
1:A:175:LYS:HB3	1:A:206:HIS:CE1	2.43	0.53
1:C:307:ASP:HA	1:C:413:LYS:HB2	1.90	0.53
1:B:466:SER:OG	1:B:468:HIS:HE1	1.90	0.53
1:A:224:GLN:HE21	1:A:228:ASN:ND2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:HIS:O	1:B:410:VAL:HB	2.07	0.53
1:C:1:MET:SD	1:C:2:LYS:N	2.81	0.53
1:C:264:ILE:O	1:C:268:ILE:HG13	2.09	0.53
1:A:197:ARG:HB2	1:A:232:GLU:CD	2.33	0.53
1:C:4:THR:HG21	1:C:302:ILE:HG23	1.91	0.53
1:D:383:SER:O	1:D:387:VAL:HG23	2.08	0.53
1:D:438:LEU:CD2	1:D:445:LYS:HE3	2.39	0.53
1:B:466:SER:OG	1:B:468:HIS:CE1	2.61	0.53
1:D:291:THR:HG22	1:D:293:ALA:N	2.15	0.53
1:C:407:HIS:O	1:C:410:VAL:HB	2.09	0.53
1:B:12:PRO:HA	1:B:15:GLU:OE2	2.09	0.52
1:A:257:ILE:HG13	2:A:510:HOH:O	2.08	0.52
1:A:288:PRO:HB3	1:A:320:TYR:CD1	2.43	0.52
1:B:159:ASN:O	1:B:161:PRO:HD3	2.09	0.52
2:C:521:HOH:O	1:D:468:HIS:HD2	1.92	0.52
1:D:241:MET:HE2	1:D:310:MET:HE1	1.90	0.52
1:A:175:LYS:O	1:A:179:ILE:HG13	2.09	0.52
1:A:292:ARG:NH2	1:C:279:MET:HB2	2.24	0.52
1:B:171:ALA:O	1:B:174:ASP:HB2	2.09	0.52
1:B:279:MET:HA	1:B:282:ASP:OD2	2.08	0.52
1:D:327:ILE:HD12	1:D:330:THR:OG1	2.10	0.52
1:A:118:SER:N	1:A:121:ASN:OD1	2.42	0.52
1:B:24:LEU:HD13	1:B:59:LYS:HD3	1.91	0.52
1:B:244:ARG:HD2	1:B:260:GLN:HE21	1.74	0.52
1:D:138:GLU:O	1:D:141:LYS:HB2	2.09	0.52
1:A:271:ARG:HG2	1:A:386:ALA:HA	1.91	0.52
1:B:455:ALA:N	1:B:463:ASN:HD21	2.07	0.52
1:C:291:THR:HG22	1:C:293:ALA:N	2.25	0.52
1:B:92:THR:O	1:B:105:MET:HA	2.09	0.52
1:B:425:SER:H	1:B:428:ASP:HB2	1.75	0.52
1:C:14:THR:HG21	1:C:315:SER:O	2.09	0.52
1:A:463:ASN:HD22	1:A:463:ASN:H	1.56	0.52
1:B:91:PHE:CZ	1:B:106:VAL:HG22	2.45	0.52
1:A:5:LYS:HA	1:A:29:ASN:OD1	2.10	0.51
1:B:244:ARG:HH11	1:B:260:GLN:NE2	2.06	0.51
1:C:378:THR:O	1:C:400:THR:HG22	2.10	0.51
1:A:7:VAL:HG22	1:A:30:VAL:HB	1.91	0.51
1:C:204:ARG:O	1:C:204:ARG:HG3	2.09	0.51
1:C:174:ASP:O	1:C:177:ASP:HB2	2.09	0.51
1:C:204:ARG:NH2	1:C:236:ALA:O	2.44	0.51
1:A:49:ASN:O	1:A:53:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:LYS:O	1:B:407:HIS:HB2	2.10	0.51
1:C:404:LYS:O	1:C:408:GLN:HG3	2.10	0.51
1:C:466:SER:OG	1:C:468:HIS:CE1	2.64	0.51
1:A:204:ARG:NH1	2:A:516:HOH:O	2.43	0.51
1:B:253:VAL:HG23	1:B:254:GLU:H	1.75	0.51
1:B:284:MET:HA	1:B:287:ASN:O	2.10	0.51
1:C:24:LEU:HD13	1:C:59:LYS:HD3	1.92	0.51
1:A:19:MET:CE	1:A:22:LYS:HD2	2.41	0.51
1:A:4:THR:HG21	1:A:302:ILE:HG23	1.92	0.51
1:D:48:GLN:O	1:D:52:ASN:ND2	2.44	0.51
1:A:288:PRO:HD3	1:A:320:TYR:CE2	2.45	0.50
1:A:10:ILE:HG13	1:A:31:MET:HG3	1.94	0.50
1:B:50:LEU:HG	1:B:54:MET:HE2	1.92	0.50
1:B:426:THR:O	1:B:429:PHE:HB3	2.11	0.50
1:C:202:GLU:O	1:C:206:HIS:HD2	1.95	0.50
1:C:193:PHE:CE2	1:C:195:ARG:HD3	2.46	0.50
1:B:47:ILE:CG2	1:B:51:ARG:HH11	2.24	0.50
1:B:400:THR:HG21	1:B:405:THR:OG1	2.11	0.50
1:C:126:ASP:O	1:C:129:LEU:HG	2.12	0.50
1:C:222:GLU:HG2	1:C:246:ASP:HB2	1.93	0.50
1:C:241:MET:HE2	1:C:310:MET:HE1	1.93	0.50
1:D:196:LYS:NZ	1:D:199:ASP:OD1	2.44	0.50
1:D:463:ASN:ND2	1:D:464:THR:HG23	2.26	0.50
1:A:224:GLN:NE2	1:A:228:ASN:HD21	2.09	0.50
1:B:399:LEU:HD23	1:B:418:GLN:HB3	1.93	0.50
1:D:279:MET:HA	1:D:282:ASP:OD2	2.12	0.50
1:A:355:THR:HG23	1:A:462:THR:HB	1.93	0.49
1:B:378:THR:O	1:B:400:THR:HG23	2.12	0.49
1:D:11:GLY:O	1:D:15:GLU:HB3	2.12	0.49
1:A:54:MET:HE3	1:A:61:ALA:H	1.77	0.49
1:A:54:MET:HE3	1:A:61:ALA:N	2.27	0.49
1:C:222:GLU:HG2	1:C:246:ASP:CB	2.41	0.49
1:C:251:ILE:HB	1:C:252:PRO:HD2	1.95	0.49
1:D:458:PRO:O	1:D:460:GLY:N	2.44	0.49
1:B:262:MET:HE3	1:B:263:MET:HG3	1.95	0.49
1:D:284:MET:HA	1:D:287:ASN:O	2.12	0.49
1:D:402:ASN:CG	1:D:405:THR:HG23	2.37	0.49
1:C:73:ARG:HD3	1:C:155:ASN:ND2	2.24	0.49
1:D:445:LYS:H	1:D:445:LYS:NZ	2.10	0.49
1:A:292:ARG:NH2	1:C:279:MET:SD	2.81	0.49
1:C:373:LEU:HD23	1:C:395:THR:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:ALA:N	1:C:463:ASN:HD21	2.07	0.49
1:A:400:THR:O	1:A:419:LEU:HA	2.12	0.49
1:B:285:ILE:HD11	1:B:313:GLY:CA	2.38	0.49
1:D:257:ILE:HD11	2:D:563:HOH:O	2.12	0.49
1:A:19:MET:O	1:A:23:MET:HG3	2.12	0.49
1:A:121:ASN:N	1:A:121:ASN:HD22	2.11	0.49
1:A:291:THR:HB	1:A:294:GLU:H	1.78	0.49
1:C:405:THR:HG22	2:C:534:HOH:O	2.11	0.49
1:D:116:ASP:OD2	1:D:165:ILE:HA	2.12	0.49
1:D:426:THR:HG22	1:D:430:TYR:CE2	2.48	0.49
1:A:15:GLU:HB3	1:A:46:ARG:HD3	1.94	0.49
1:C:123:VAL:O	1:C:124:LEU:HD23	2.13	0.48
1:B:360:ARG:CZ	1:B:364:GLU:HG3	2.43	0.48
1:A:89:GLN:NE2	1:A:103:SER:O	2.47	0.48
1:A:224:GLN:HE21	1:A:228:ASN:CG	2.21	0.48
1:A:288:PRO:HB3	1:A:320:TYR:CE1	2.48	0.48
1:B:402:ASN:CG	1:B:405:THR:HG23	2.38	0.48
1:C:291:THR:CG2	1:C:293:ALA:H	2.26	0.48
1:C:314:GLU:O	1:C:321:PRO:HA	2.14	0.48
1:C:392:PRO:HG3	1:C:396:ILE:HD11	1.95	0.48
1:B:249:VAL:HG12	1:B:249:VAL:O	2.13	0.48
1:B:321:PRO:HD2	2:B:590:HOH:O	2.13	0.48
1:C:137:ILE:HG23	1:C:141:LYS:O	2.13	0.48
1:C:284:MET:HE3	1:C:289:ARG:N	2.29	0.48
1:C:286:LYS:HB2	1:C:287:ASN:ND2	2.28	0.48
1:A:257:ILE:HD12	1:A:258:PHE:CD2	2.49	0.48
1:B:69:GLY:HA2	1:B:174:ASP:OD2	2.14	0.48
1:B:431:ARG:CZ	2:B:524:HOH:O	2.61	0.48
1:C:229:ASN:O	1:C:232:GLU:HG2	2.13	0.48
1:C:140:ASN:OD1	1:C:141:LYS:HD2	2.13	0.47
1:C:341:SER:HB3	1:C:367:GLU:OE2	2.14	0.47
1:A:213:GLU:CD	1:A:213:GLU:H	2.21	0.47
1:A:455:ALA:N	1:A:463:ASN:HD21	2.12	0.47
1:D:49:ASN:O	1:D:53:VAL:HG23	2.13	0.47
1:D:167:LEU:C	1:D:195:ARG:HH22	2.22	0.47
1:A:291:THR:HG22	1:A:292:ARG:N	2.29	0.47
1:B:4:THR:HG21	1:B:302:ILE:HG23	1.95	0.47
1:C:224:GLN:HG3	1:C:228:ASN:OD1	2.13	0.47
1:A:224:GLN:HE21	1:A:228:ASN:HD21	1.61	0.47
1:A:363:VAL:O	1:A:367:GLU:HG3	2.14	0.47
1:B:400:THR:O	1:B:419:LEU:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:ASN:OD1	1:B:405:THR:HG23	2.14	0.47
1:A:327:ILE:O	1:A:331:ILE:HG13	2.14	0.47
1:B:119:VAL:HG22	1:B:136:ALA:HA	1.96	0.47
1:B:165:ILE:HG22	1:B:167:LEU:H	1.80	0.47
1:C:436:LEU:O	1:C:440:SER:HB3	2.14	0.47
1:A:10:ILE:HG13	1:A:31:MET:CG	2.45	0.47
1:A:175:LYS:HB3	1:A:206:HIS:NE2	2.29	0.47
1:A:259:ALA:O	1:A:263:MET:HG3	2.15	0.47
1:B:113:PHE:O	1:B:117:LEU:HB2	2.15	0.47
1:C:241:MET:HE1	1:C:310:MET:HE1	1.94	0.47
1:B:191:ALA:CB	1:B:203:ILE:HD12	2.45	0.47
1:B:378:THR:O	1:B:400:THR:CG2	2.63	0.47
1:C:241:MET:HE2	1:C:310:MET:CE	2.45	0.47
1:D:463:ASN:ND2	1:D:464:THR:CG2	2.78	0.47
1:A:403:GLU:HG3	1:A:419:LEU:HD22	1.97	0.47
1:B:422:GLU:O	1:B:423:ILE:HG13	2.15	0.47
1:C:414:GLY:HA2	2:C:483:HOH:O	2.14	0.47
1:A:70:PRO:HB2	1:A:167:LEU:HD13	1.96	0.46
1:A:430:TYR:HA	1:A:451:MET:SD	2.55	0.46
1:A:434:LYS:HG3	1:A:451:MET:CE	2.45	0.46
1:C:281:LEU:O	1:C:314:GLU:HG2	2.15	0.46
1:D:454:GLY:HA2	1:D:463:ASN:ND2	2.29	0.46
1:C:271:ARG:HG2	1:C:386:ALA:HA	1.97	0.46
1:C:197:ARG:CZ	1:C:201:ILE:HD11	2.45	0.46
1:D:224:GLN:NE2	1:D:228:ASN:ND2	2.63	0.46
1:C:31:MET:HE3	1:C:33:LEU:HD11	1.97	0.46
1:C:269:ARG:HG3	2:C:553:HOH:O	2.15	0.46
1:A:19:MET:HE3	1:A:22:LYS:HD2	1.97	0.46
1:D:407:HIS:O	1:D:410:VAL:HB	2.16	0.46
1:A:31:MET:HE1	1:A:46:ARG:O	2.14	0.46
1:A:224:GLN:HG3	1:A:228:ASN:OD1	2.16	0.46
1:C:4:THR:HG22	1:C:413:LYS:CE	2.46	0.46
1:A:463:ASN:HD22	1:A:463:ASN:N	2.11	0.46
1:D:126:ASP:OD2	1:D:129:LEU:HD22	2.15	0.46
1:A:30:VAL:HG21	1:A:411:LEU:HD13	1.97	0.46
1:A:401:THR:HG22	1:A:420:VAL:HG23	1.98	0.46
1:A:463:ASN:ND2	1:A:464:THR:HG23	2.30	0.46
1:C:288:PRO:HB3	1:C:320:TYR:CE1	2.48	0.46
1:C:423:ILE:HG21	1:C:429:PHE:HB2	1.97	0.46
1:D:65:LEU:HD23	1:D:65:LEU:C	2.41	0.46
1:A:280:MET:HG3	1:A:310:MET:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:TYR:N	1:A:321:PRO:HD3	2.30	0.46
1:B:265:GLU:O	1:B:269:ARG:HG3	2.16	0.46
1:C:7:VAL:HG21	1:C:275:ILE:HD13	1.96	0.46
1:D:284:MET:HE2	1:D:284:MET:HB3	1.78	0.46
1:A:432:LEU:HA	1:A:435:GLU:HG3	1.98	0.46
1:C:375:VAL:HG23	1:C:449:VAL:CG1	2.46	0.46
1:D:77:LEU:H	1:D:154:GLU:HG2	1.81	0.46
1:D:436:LEU:O	1:D:440:SER:HB3	2.16	0.46
1:C:46:ARG:HE	1:C:46:ARG:HB2	1.41	0.45
1:B:40:TYR:OH	1:B:176:GLN:HG2	2.15	0.45
1:B:192:SER:HA	1:B:220:LYS:HD3	1.99	0.45
1:C:291:THR:HG22	1:C:294:GLU:H	1.81	0.45
1:C:383:SER:HB2	1:C:462:THR:OG1	2.16	0.45
1:A:89:GLN:HG3	1:A:90:THR:O	2.15	0.45
1:A:372:PRO:HD2	1:A:448:VAL:O	2.17	0.45
1:B:50:LEU:CD2	1:B:54:MET:HE2	2.46	0.45
1:B:224:GLN:HE21	1:B:228:ASN:ND2	2.15	0.45
1:C:126:ASP:O	1:C:127:ASP:C	2.59	0.45
1:A:291:THR:CG2	1:A:293:ALA:HB3	2.41	0.45
1:B:449:VAL:CG1	1:B:451:MET:HE2	2.46	0.45
1:A:75:MET:HE2	1:A:109:THR:N	2.31	0.45
1:B:39:ASP:OD1	1:B:42:GLU:HB2	2.16	0.45
1:A:118:SER:O	1:A:121:ASN:CG	2.60	0.45
1:B:436:LEU:O	1:B:440:SER:HB3	2.16	0.45
1:D:30:VAL:HG22	1:D:62:ALA:HB3	1.98	0.45
1:A:378:THR:HG21	1:A:381:GLY:CA	2.46	0.45
1:B:281:LEU:O	1:B:314:GLU:HG2	2.16	0.45
1:D:132:MET:CA	1:D:147:LEU:HG	2.46	0.45
1:D:378:THR:HG22	1:D:381:GLY:H	1.81	0.45
1:C:257:ILE:H	1:C:257:ILE:HG13	1.71	0.45
1:B:383:SER:HB3	1:B:462:THR:OG1	2.17	0.45
1:D:14:THR:HA	1:D:19:MET:HG2	1.98	0.45
1:B:51:ARG:HA	1:B:54:MET:HE3	1.98	0.44
1:D:57:THR:OG1	1:D:59:LYS:HG3	2.16	0.44
1:D:160:LEU:HB3	1:D:163:VAL:HB	1.98	0.44
1:A:121:ASN:N	1:A:121:ASN:ND2	2.64	0.44
1:C:8:CYS:SG	1:C:28:MET:HG3	2.57	0.44
1:A:197:ARG:HB2	1:A:232:GLU:HG3	1.98	0.44
1:C:178:LEU:HD13	1:C:207:LEU:CD2	2.47	0.44
1:A:83:VAL:HB	1:A:103:SER:HB3	2.00	0.44
1:A:244:ARG:HH11	1:A:260:GLN:HE22	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:THR:HG21	1:B:315:SER:O	2.18	0.44
1:B:321:PRO:O	1:B:325:VAL:HG23	2.18	0.44
1:B:422:GLU:HA	2:B:543:HOH:O	2.17	0.44
1:B:180:PHE:HA	1:B:183:GLU:OE1	2.18	0.44
1:C:423:ILE:CG2	1:C:429:PHE:HB2	2.47	0.44
1:C:270:ALA:O	1:C:271:ARG:HB2	2.18	0.44
1:D:15:GLU:HB2	1:D:46:ARG:HD2	1.99	0.44
1:B:458:PRO:O	1:B:460:GLY:N	2.51	0.44
1:D:445:LYS:H	1:D:445:LYS:CE	2.30	0.44
1:B:78:GLU:O	1:B:80:GLY:N	2.51	0.44
1:C:281:LEU:HD23	1:C:294:GLU:HB3	1.98	0.44
1:D:257:ILE:O	1:D:261:LYS:HG3	2.17	0.44
1:D:96:ASP:HB2	1:D:140:ASN:ND2	2.33	0.44
1:B:425:SER:O	1:B:428:ASP:HB2	2.18	0.43
1:D:92:THR:O	1:D:105:MET:HA	2.18	0.43
1:B:36:SER:O	1:B:37:HIS:CD2	2.70	0.43
1:A:77:LEU:N	1:A:154:GLU:HG2	2.33	0.43
1:B:307:ASP:HA	1:B:413:LYS:HB2	2.01	0.43
1:B:431:ARG:NH1	1:B:435:GLU:OE2	2.52	0.43
1:D:145:LYS:HE2	1:D:145:LYS:HB3	1.45	0.43
1:D:15:GLU:CB	1:D:46:ARG:HD2	2.48	0.43
1:D:70:PRO:HA	2:D:579:HOH:O	2.17	0.43
1:D:281:LEU:HD22	1:D:290:PRO:HB3	1.99	0.43
1:A:291:THR:CG2	1:A:293:ALA:H	2.09	0.43
1:A:342:ARG:HD2	1:A:391:PHE:CD1	2.53	0.43
1:D:380:GLY:HA2	1:D:405:THR:HG21	2.00	0.43
1:A:466:SER:OG	1:A:468:HIS:HE1	2.01	0.43
1:C:216:HIS:HD2	2:C:473:HOH:O	2.01	0.43
1:A:73:ARG:HD2	1:A:155:ASN:HD21	1.83	0.43
1:A:91:PHE:CE2	1:A:106:VAL:HG22	2.54	0.43
1:B:277:ALA:HA	1:B:310:MET:HB3	2.01	0.43
1:C:193:PHE:HE2	1:C:195:ARG:HD3	1.84	0.43
1:C:426:THR:HG22	1:C:430:TYR:CE2	2.53	0.43
1:A:444:HIS:O	1:A:447:ASP:HB2	2.19	0.43
1:B:426:THR:HG22	1:B:430:TYR:CE2	2.54	0.43
1:A:354:ILE:O	1:A:358:VAL:HG13	2.19	0.43
1:A:379:GLN:HE22	1:A:402:ASN:HB2	1.84	0.43
1:B:380:GLY:HA2	1:B:405:THR:CG2	2.41	0.43
1:C:36:SER:OG	1:C:37:HIS:CE1	2.72	0.43
1:C:72:ILE:HD11	1:C:110:TYR:CD2	2.54	0.43
1:C:170:LEU:CD2	1:C:174:ASP:HB3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:LEU:O	1:D:360:ARG:HD2	2.19	0.43
1:B:124:LEU:O	1:B:158:VAL:HA	2.19	0.43
1:B:288:PRO:HB3	1:B:320:TYR:CE2	2.54	0.43
1:D:257:ILE:HD12	1:D:258:PHE:CD2	2.53	0.42
1:A:142:VAL:HG12	1:A:144:CYS:SG	2.59	0.42
1:A:390:TYR:O	1:A:391:PHE:C	2.61	0.42
1:A:436:LEU:HA	1:A:439:GLN:HB2	2.02	0.42
1:C:170:LEU:HD22	1:C:174:ASP:HB3	2.01	0.42
1:C:244:ARG:HH11	1:C:260:GLN:NE2	2.17	0.42
1:C:280:MET:HE3	1:C:298:VAL:HG22	2.01	0.42
1:D:73:ARG:HA	1:D:156:LYS:O	2.19	0.42
1:A:96:ASP:O	1:A:98:SER:N	2.53	0.42
1:A:237:SER:O	1:A:272:LYS:HE2	2.19	0.42
1:A:362:ALA:HB1	1:A:450:VAL:HG11	2.00	0.42
1:A:251:ILE:HB	1:A:252:PRO:HD2	2.01	0.42
1:C:152:LEU:HD12	1:C:153:GLY:N	2.34	0.42
1:D:313:GLY:O	1:D:318:GLY:N	2.52	0.42
1:C:35:PHE:HZ	1:C:180:PHE:CE2	2.38	0.42
1:C:371:ALA:HB2	1:C:448:VAL:HG12	2.02	0.42
1:D:23:MET:HE2	1:D:325:VAL:CG2	2.48	0.42
1:D:223:ASN:ND2	2:D:493:HOH:O	2.52	0.42
1:B:365:THR:HG22	1:B:369:LEU:HD12	2.02	0.42
1:C:4:THR:HG23	1:C:336:ASP:OD1	2.19	0.42
1:A:126:ASP:HB3	1:A:129:LEU:HB3	2.01	0.42
1:A:444:HIS:HD2	2:A:540:HOH:O	2.02	0.42
1:B:4:THR:HG22	1:B:413:LYS:HZ2	1.83	0.42
1:B:356:GLU:CD	1:B:390:TYR:OH	2.63	0.42
1:B:431:ARG:C	1:B:431:ARG:HE	2.28	0.42
1:C:326:SER:O	1:C:330:THR:HG23	2.20	0.42
1:A:257:ILE:HG13	1:A:257:ILE:H	1.47	0.42
1:C:426:THR:HG22	1:C:430:TYR:CZ	2.55	0.42
1:C:464:THR:HB	1:D:466:SER:CB	2.50	0.42
1:C:244:ARG:H	1:C:244:ARG:HD3	1.85	0.42
1:A:5:LYS:O	1:A:308:ALA:HA	2.20	0.41
1:A:35:PHE:HZ	1:A:180:PHE:CE2	2.37	0.41
1:A:455:ALA:H	1:A:457:VAL:HG22	1.83	0.41
1:B:273:VAL:HG13	2:B:531:HOH:O	2.19	0.41
1:C:170:LEU:O	1:C:175:LYS:HE3	2.20	0.41
1:A:284:MET:HE2	1:A:284:MET:HB3	1.82	0.41
1:A:292:ARG:HD3	1:C:279:MET:SD	2.60	0.41
1:D:423:ILE:HA	1:D:428:ASP:OD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:MET:CG	1:B:277:ALA:HB2	2.49	0.41
1:C:4:THR:HG22	1:C:413:LYS:HE3	2.02	0.41
1:A:188:PHE:CD1	1:A:216:HIS:HB2	2.55	0.41
1:C:287:ASN:ND2	1:C:287:ASN:N	2.69	0.41
1:D:257:ILE:CD1	1:D:258:PHE:CE2	3.02	0.41
1:D:438:LEU:HD22	1:D:445:LYS:HE3	2.02	0.41
1:D:463:ASN:HD22	1:D:463:ASN:H	1.67	0.41
1:A:7:VAL:HB	1:A:310:MET:HG3	2.02	0.41
1:A:43:HIS:O	1:A:47:ILE:HG13	2.20	0.41
1:B:78:GLU:C	1:B:80:GLY:N	2.79	0.41
1:C:110:TYR:O	1:C:113:PHE:HB2	2.20	0.41
1:D:96:ASP:HB2	1:D:140:ASN:HD22	1.85	0.41
1:D:448:VAL:HA	1:D:468:HIS:O	2.21	0.41
1:D:197:ARG:HD2	2:D:533:HOH:O	2.19	0.41
1:D:280:MET:HG3	1:D:310:MET:O	2.20	0.41
1:C:160:LEU:HB3	1:C:163:VAL:CB	2.45	0.41
1:D:249:VAL:O	1:D:249:VAL:CG1	2.69	0.41
1:A:158:VAL:HG12	1:A:160:LEU:HD13	2.03	0.41
1:A:178:LEU:HD13	1:A:207:LEU:HD21	2.02	0.41
1:A:365:THR:O	1:A:366:ALA:C	2.64	0.41
1:A:426:THR:HG22	1:A:430:TYR:CE2	2.55	0.41
1:A:456:LEU:HD23	1:A:456:LEU:N	2.35	0.41
1:B:214:ASN:HB2	2:B:528:HOH:O	2.21	0.41
1:C:287:ASN:N	1:C:287:ASN:HD22	2.19	0.41
1:D:466:SER:OG	1:D:468:HIS:CE1	2.74	0.41
1:A:378:THR:O	1:A:400:THR:CG2	2.69	0.41
1:B:289:ARG:NH1	1:B:289:ARG:HG2	2.36	0.41
1:C:178:LEU:HD13	1:C:207:LEU:HD21	2.03	0.41
1:D:291:THR:HG22	1:D:292:ARG:N	2.36	0.41
1:B:455:ALA:HB2	1:B:464:THR:HG21	2.03	0.40
1:B:463:ASN:HD22	1:B:463:ASN:N	2.12	0.40
1:C:335:THR:O	1:C:336:ASP:C	2.63	0.40
1:A:69:GLY:HA2	1:A:174:ASP:OD2	2.22	0.40
1:A:372:PRO:HG3	1:A:447:ASP:CG	2.47	0.40
1:D:175:LYS:O	1:D:206:HIS:HE1	2.03	0.40
1:A:274:VAL:O	1:A:306:THR:HG22	2.21	0.40
1:B:117:LEU:HD12	1:B:121:ASN:OD1	2.22	0.40
1:B:182:CYS:O	1:B:183:GLU:C	2.63	0.40
1:B:294:GLU:O	1:B:298:VAL:HG23	2.20	0.40
1:B:399:LEU:HA	1:B:418:GLN:O	2.21	0.40
1:C:52:ASN:O	1:C:56:LYS:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:409:LEU:HD23	1:C:409:LEU:HA	1.91	0.40
1:D:118:SER:N	1:D:121:ASN:OD1	2.55	0.40
1:D:273:VAL:HG21	1:D:411:LEU:HD23	2.02	0.40
1:B:379:GLN:NE2	1:B:402:ASN:HB2	2.37	0.40
1:C:175:LYS:NZ	2:C:527:HOH:O	2.55	0.40
1:D:34:ASN:OD1	1:D:34:ASN:C	2.62	0.40
1:D:47:ILE:O	1:D:51:ARG:HG2	2.22	0.40
1:D:334:ARG:O	1:D:337:ARG:HG2	2.22	0.40
1:D:444:HIS:O	1:D:447:ASP:HB2	2.21	0.40
1:B:15:GLU:CB	1:B:46:ARG:HD3	2.50	0.40
1:B:84:SER:HA	1:B:151:ASP:HA	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	460/470 (98%)	430 (94%)	27 (6%)	3 (1%)	18	34
1	B	460/470 (98%)	434 (94%)	24 (5%)	2 (0%)	30	49
1	C	427/470 (91%)	403 (94%)	17 (4%)	7 (2%)	7	14
1	D	460/470 (98%)	441 (96%)	18 (4%)	1 (0%)	43	63
All	All	1807/1880 (96%)	1708 (94%)	86 (5%)	13 (1%)	18	34

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	459	SER
1	C	459	SER
1	D	459	SER
1	A	97	LYS

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Mol	Chain	Res	Type
1	A	164	SER
1	C	163	VAL
1	C	172	GLU
1	C	121	ASN
1	C	127	ASP
1	C	456	LEU
1	C	355	THR
1	B	161	PRO
1	A	119	VAL

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	377/389 (97%)	325 (86%)	52 (14%)	3	7
1	B	377/389 (97%)	329 (87%)	48 (13%)	4	9
1	C	352/389 (90%)	302 (86%)	50 (14%)	3	7
1	D	377/389 (97%)	334 (89%)	43 (11%)	5	12
All	All	1483/1556 (95%)	1290 (87%)	193 (13%)	4	8

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	THR
1	A	16	SER
1	A	19	MET
1	A	31	MET
1	A	39	ASP
1	A	51	ARG
1	A	56	LYS
1	A	67	THR
1	A	73	ARG
1	A	75	MET
1	A	78	GLU

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Mol	Chain	Res	Type
1	A	89	GLN
1	A	98	SER
1	A	100	ILE
1	A	106	VAL
1	A	117	LEU
1	A	118	SER
1	A	122	THR
1	A	124	LEU
1	A	133	GLU
1	A	138	GLU
1	A	160	LEU
1	A	170	LEU
1	A	178	LEU
1	A	189	VAL
1	A	196	LYS
1	A	204	ARG
1	A	208	LYS
1	A	253	VAL
1	A	257	ILE
1	A	273	VAL
1	A	287	ASN
1	A	292	ARG
1	A	306	THR
1	A	323	GLU
1	A	358	VAL
1	A	378	THR
1	A	400	THR
1	A	403	GLU
1	A	405	THR
1	A	415	VAL
1	A	422	GLU
1	A	431	ARG
1	A	432	LEU
1	A	435	GLU
1	A	456	LEU
1	A	457	VAL
1	A	459	SER
1	A	461	THR
1	A	463	ASN
1	A	464	THR
1	B	4	THR
1	B	19	MET

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Mol	Chain	Res	Type
1	B	46	ARG
1	B	60	THR
1	B	68	LYS
1	B	78	GLU
1	B	95	THR
1	B	98	SER
1	B	104	GLU
1	B	105	MET
1	B	106	VAL
1	B	117	LEU
1	B	141	LYS
1	B	160	LEU
1	B	170	LEU
1	B	172	GLU
1	B	176	GLN
1	B	195	ARG
1	B	201	ILE
1	B	203	ILE
1	B	208	LYS
1	B	213	GLU
1	B	223	ASN
1	B	235	GLU
1	B	253	VAL
1	B	257	ILE
1	B	262	MET
1	B	273	VAL
1	B	279	MET
1	B	285	ILE
1	B	291	THR
1	B	306	THR
1	B	342	ARG
1	B	356	GLU
1	B	364	GLU
1	B	373	LEU
1	B	378	THR
1	B	400	THR
1	B	403	GLU
1	B	405	THR
1	B	415	VAL
1	B	421	LYS
1	B	424	THR
1	B	431	ARG

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Mol	Chain	Res	Type
1	B	449	VAL
1	B	459	SER
1	B	463	ASN
1	B	464	THR
1	C	1	MET
1	C	4	THR
1	C	16	SER
1	C	43	HIS
1	C	46	ARG
1	C	51	ARG
1	C	60	THR
1	C	65	LEU
1	C	66	ASP
1	C	68	LYS
1	C	105	MET
1	C	111	GLU
1	C	114	THR
1	C	118	SER
1	C	124	LEU
1	C	143	ILE
1	C	160	LEU
1	C	163	VAL
1	C	170	LEU
1	C	176	GLN
1	C	178	LEU
1	C	189	VAL
1	C	197	ARG
1	C	198	SER
1	C	244	ARG
1	C	247	LEU
1	C	250	GLU
1	C	253	VAL
1	C	257	ILE
1	C	265	GLU
1	C	269	ARG
1	C	287	ASN
1	C	291	THR
1	C	292	ARG
1	C	306	THR
1	C	327	ILE
1	C	337	ARG
1	C	342	ARG

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Mol	Chain	Res	Type
1	C	360	ARG
1	C	378	THR
1	C	379	GLN
1	C	400	THR
1	C	404	LYS
1	C	405	THR
1	C	421	LYS
1	C	431	ARG
1	C	434	LYS
1	C	461	THR
1	C	463	ASN
1	C	464	THR
1	D	4	THR
1	D	51	ARG
1	D	73	ARG
1	D	95	THR
1	D	98	SER
1	D	105	MET
1	D	106	VAL
1	D	111	GLU
1	D	117	LEU
1	D	141	LYS
1	D	160	LEU
1	D	176	GLN
1	D	196	LYS
1	D	216	HIS
1	D	223	ASN
1	D	253	VAL
1	D	257	ILE
1	D	271	ARG
1	D	287	ASN
1	D	289	ARG
1	D	306	THR
1	D	337	ARG
1	D	342	ARG
1	D	360	ARG
1	D	367	GLU
1	D	368	LYS
1	D	370	ASP
1	D	373	LEU
1	D	378	THR
1	D	400	THR

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Mol	Chain	Res	Type
1	D	405	THR
1	D	410	VAL
1	D	415	VAL
1	D	418	GLN
1	D	421	LYS
1	D	431	ARG
1	D	435	GLU
1	D	445	LYS
1	D	449	VAL
1	D	459	SER
1	D	461	THR
1	D	463	ASN
1	D	464	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	155	ASN
1	A	159	ASN
1	A	184	GLN
1	A	206	HIS
1	A	216	HIS
1	A	223	ASN
1	A	224	GLN
1	A	260	GLN
1	A	287	ASN
1	A	408	GLN
1	A	463	ASN
1	A	468	HIS
1	B	37	HIS
1	B	184	GLN
1	B	216	HIS
1	B	223	ASN
1	B	224	GLN
1	B	228	ASN
1	B	260	GLN
1	B	300	ASN
1	B	379	GLN
1	B	408	GLN
1	B	444	HIS
1	B	463	ASN

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Mol	Chain	Res	Type
1	B	468	HIS
1	C	34	ASN
1	C	45	GLN
1	C	48	GLN
1	C	149	ASN
1	C	155	ASN
1	C	184	GLN
1	C	206	HIS
1	C	210	HIS
1	C	216	HIS
1	C	224	GLN
1	C	260	GLN
1	C	287	ASN
1	C	408	GLN
1	C	463	ASN
1	C	468	HIS
1	D	37	HIS
1	D	48	GLN
1	D	52	ASN
1	D	155	ASN
1	D	216	HIS
1	D	223	ASN
1	D	228	ASN
1	D	260	GLN
1	D	287	ASN
1	D	407	HIS
1	D	408	GLN
1	D	444	HIS
1	D	463	ASN
1	D	468	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.