



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:33 PM GMT

PDB ID : 1PKY
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
<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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

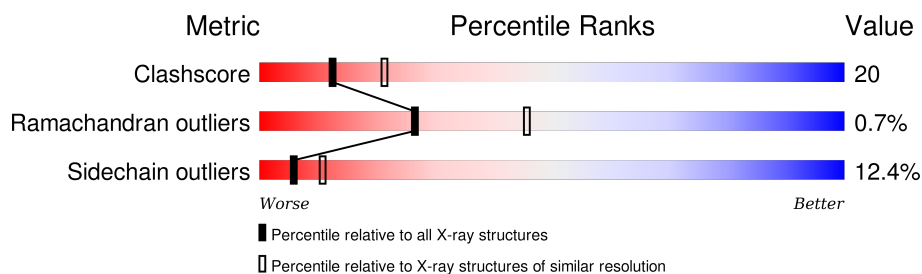
1 Overall quality at a glance ⓘ

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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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 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	470	 57% 34% 6% ..
1	B	470	 60% 31% 6% ..
1	C	470	 52% 33% 7% • 8%
1	D	470	 66% 27% 5% ..

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.

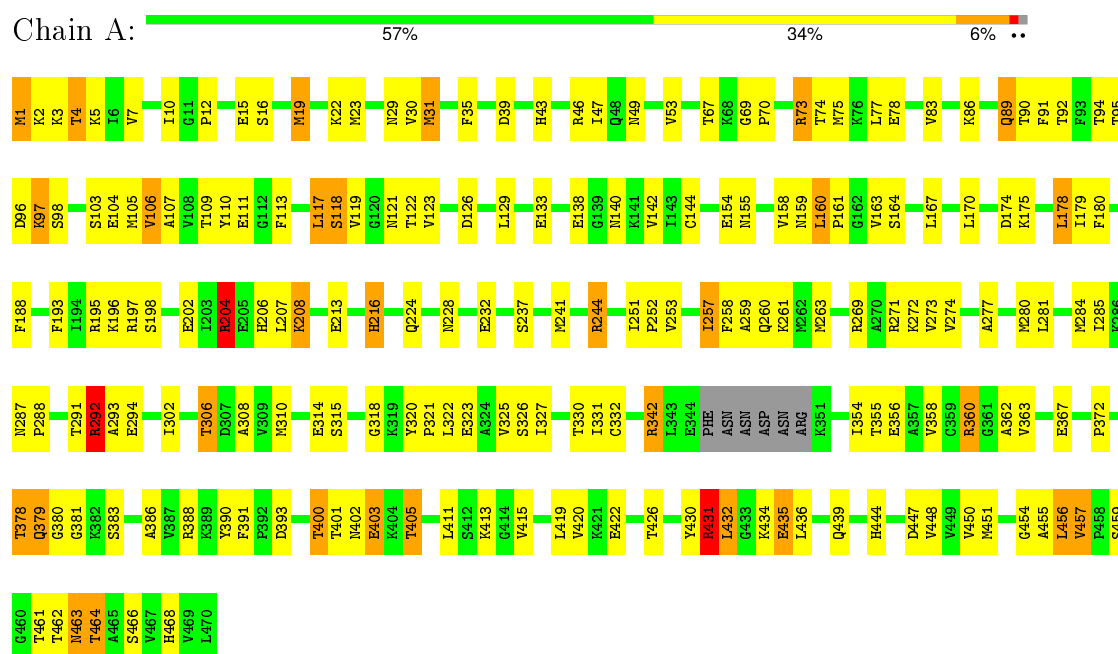
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	126	Total	O	0	0
			126	126		
2	B	137	Total	O	0	0
			137	137		
2	C	107	Total	O	0	0
			107	107		
2	D	150	Total	O	0	0
			150	150		

3 Residue-property plots

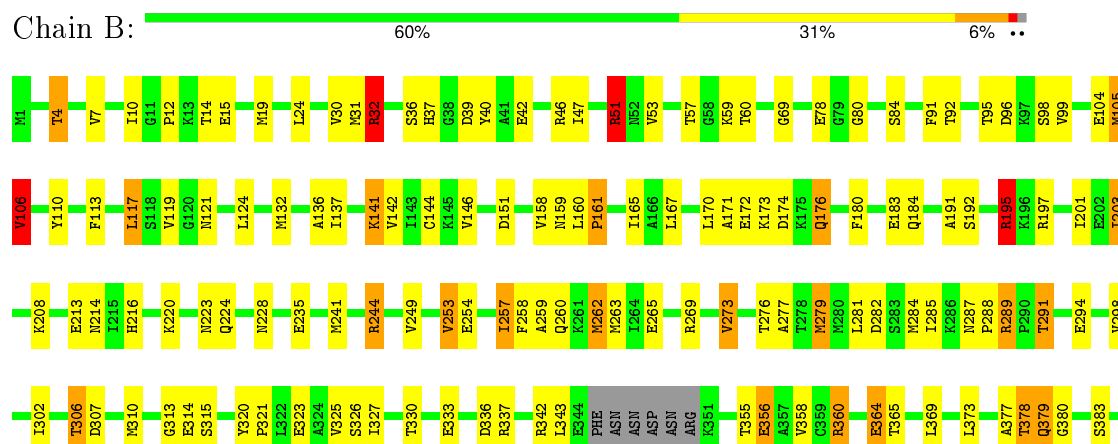
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

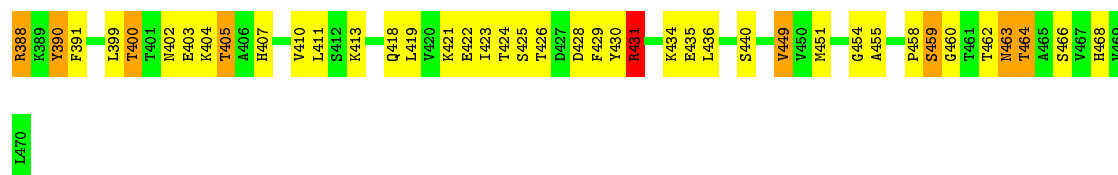
Note EDS was not executed.

• Molecule 1: PYRUVATE KINASE



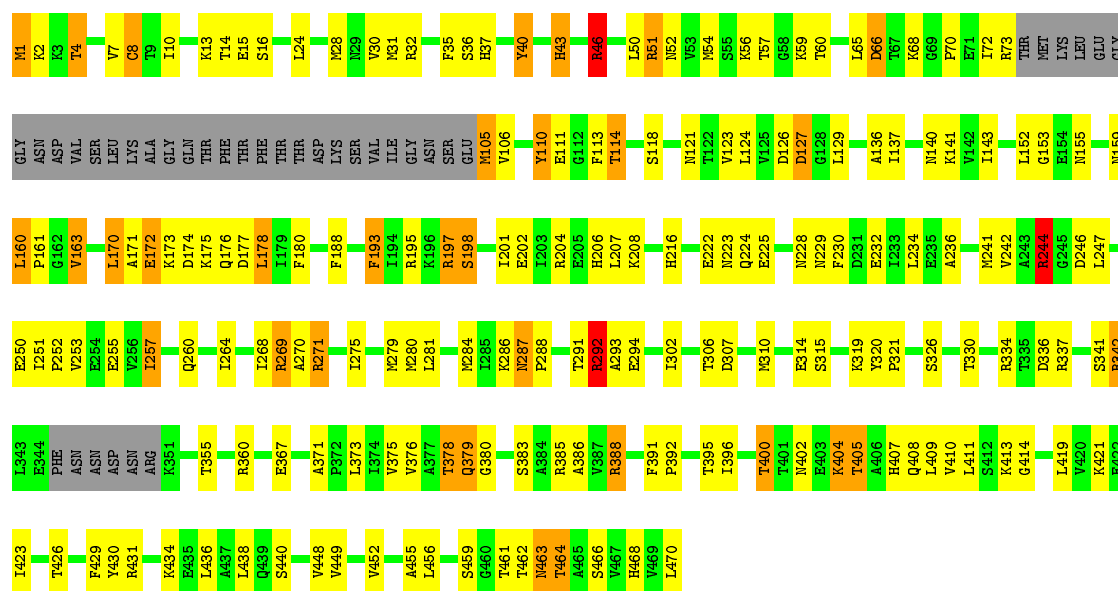
• Molecule 1: PYRUVATE KINASE





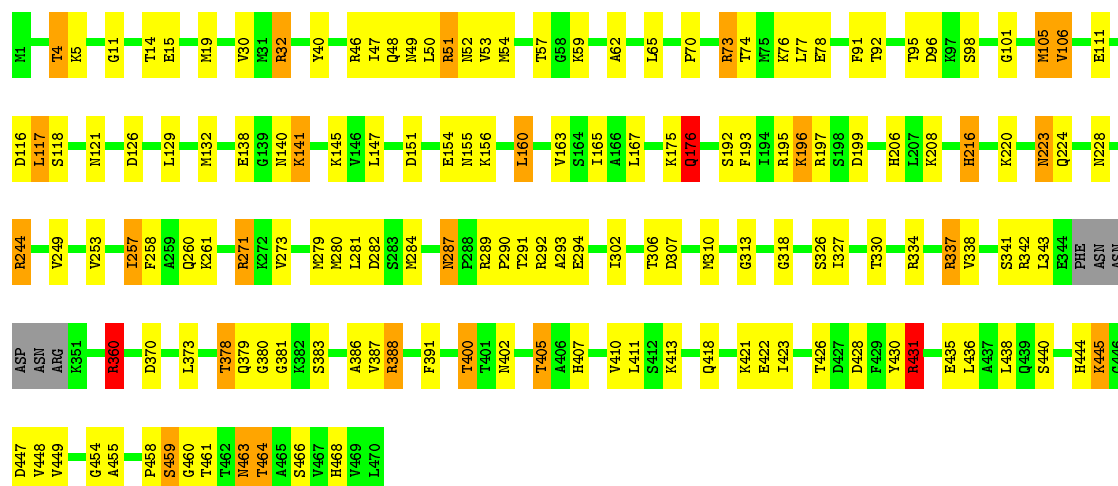
• Molecule 1: PYRUVATE KINASE

Chain C: 52% 33% 7% 8%



• Molecule 1: PYRUVATE KINASE

Chain D: 66% 27% 5%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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	0.74	1/3498 (0.0%)	0.82	6/4719 (0.1%)
1	B	0.74	1/3498 (0.0%)	0.82	4/4719 (0.1%)
1	C	0.73	1/3271 (0.0%)	0.80	1/4411 (0.0%)
1	D	0.76	0/3498	0.81	3/4719 (0.1%)
All	All	0.74	3/13765 (0.0%)	0.81	14/18568 (0.1%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	8	CYS	CB-SG	-6.36	1.71	1.82
1	A	332	CYS	CB-SG	-5.89	1.72	1.81
1	B	144	CYS	CB-SG	-5.13	1.73	1.81

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	ALA	N-CA-C	8.30	133.42	111.00
1	A	277	ALA	CB-CA-C	-8.26	97.72	110.10
1	B	51	ARG	NE-CZ-NH1	-7.92	116.34	120.30
1	A	204	ARG	NE-CZ-NH1	-7.88	116.36	120.30
1	A	292	ARG	NE-CZ-NH2	-7.22	116.69	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	431	ARG	NE-CZ-NH1	-7.00	116.80	120.30
1	B	32	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	C	292	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	B	195	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	B	195	ARG	NE-CZ-NH1	-6.13	117.24	120.30
1	D	360	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	D	32	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	431	ARG	NE-CZ-NH1	-5.76	117.42	120.30
1	A	360	ARG	NE-CZ-NH2	-5.19	117.70	120.30

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	152	0
1	B	3464	0	3541	130	0
1	C	3240	0	3327	149	0
1	D	3464	0	3541	110	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	532	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 20.

All (532) 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: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:342:ARG:HD2	2:B:585:HOH:O	1.76	0.85
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:D:244:ARG:HH11	1:D:260:GLN:HE22	1.27	0.79
1:B:355:THR:HG23	1:B:462:THR:HB	1.63	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:MET:HE1	1:A:322:LEU:HD22	1.67	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:285:ILE:HD11	1:B:313:GLY:HA3	1.65	0.76
1:B:197:ARG:HD2	2:B:550:HOH:O	1.85	0.76
1:B:137:ILE:HG12	1:B:142:VAL:HG22	1.69	0.75
1:D:326:SER:O	1:D:330:THR:HG23	1.88	0.73
1:C:463:ASN:ND2	1:C:464:THR:HG22	2.03	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:A:75:MET:HE3	1:A:97:LYS:HA	1.70	0.72
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: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:A:291:THR:HG21	2:A:570:HOH:O	1.91	0.71
1:A:206:HIS:CD2	2:A:536:HOH:O	2.43	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:19:MET:CE	1:A:322:LEU:HD22	2.23	0.68
1:C:13:LYS:HZ3	1:C:319:LYS:HA	1.57	0.67
1:A:380:GLY:HA2	1:A:405:THR:HG21	1.76	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:C:172:GLU:HG2	2:C:527:HOH:O	1.95	0.67
1:D:76:LYS:HB2	2:D:568:HOH:O	1.94	0.66
1:D:48:GLN:HG3	1:D:52:ASN:HD21	1.60	0.66
1:A:74:THR:O	1:A:155:ASN:HA	1.94	0.66
1:C:204:ARG:O	1:C:208:LYS:HG3	1.95	0.66
1:B:327:ILE:HD12	1:B:330:THR:OG1	1.93	0.66
1:D:244:ARG:HD2	1:D:260:GLN:NE2	2.11	0.66
1:C:40:TYR:HA	1:C:43:HIS:ND1	2.10	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:216:HIS:HD2	2:D:473:HOH:O	1.79	0.65
1:B:15:GLU:HB3	1:B:46:ARG:HD3	1.78	0.65
1:A:383:SER:HB3	1:A:462:THR:OG1	1.97	0.65
1:D:445:LYS:H	1:D:445:LYS:HZ2	1.44	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:D:455:ALA:H	1:D:463:ASN:ND2	1.94	0.64
1:A:92:THR:O	1:A:105:MET:HG3	1.98	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:D:257:ILE:HD12	1:D:258:PHE:CE2	2.33	0.64
1:B:92:THR:CG2	1:B:141:LYS:HG2	2.28	0.64
1:B:358:VAL:HG21	1:B:463:ASN:HA	1.79	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:D:91:PHE:HZ	1:D:106:VAL:HG22	1.63	0.63
1:C:114:THR:HG22	1:C:137:ILE:HG23	1.81	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:C:170:LEU:HD13	1:C:175:LYS:CG	2.25	0.63
1:B:10:ILE:HG12	1:B:31:MET:HG3	1.79	0.63
1:A:315:SER:HA	1:A:321:PRO:HB3	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:B:53:VAL:O	1:B:57:THR:HG23	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ILE:O	1:A:261:LYS:HG3	2.00	0.61
1:D:271:ARG:HG2	1:D:386:ALA:HA	1.81	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: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: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: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:D:337:ARG:HG3	1:D:338:VAL:HG13	1.84	0.60
1:C:284:MET:HA	1:C:287:ASN:O	2.02	0.60
1:C:30:VAL:HG21	1:C:411:LEU:HD13	1.84	0.60
1:B:434:LYS:HE2	1:B:468:HIS:HD2	1.67	0.60
1:C:379:GLN:O	1:C:405:THR:HG21	2.02	0.59
1:A:12:PRO:HG3	1:A:46:ARG:HH12	1.66	0.59
1:D:388:ARG:C	1:D:388:ARG:HD3	2.23	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:B:434:LYS:HG2	1:B:451:MET:HE1	1.83	0.58
1:B:257:ILE:HD12	1:B:258:PHE:H	1.69	0.58
1:D:249:VAL:O	1:D:249:VAL:HG12	2.02	0.58
1:D:5:LYS:HG3	1:D:410:VAL:O	2.04	0.58
1:A:466:SER:OG	1:A:468:HIS:CE1	2.57	0.58
1:A:285:ILE:HG23	1:A:318:GLY:HA2	1.86	0.58
1:D:4:THR:HG21	1:D:302:ILE:HG23	1.86	0.58
1:D:422:GLU:HB2	2:D:565:HOH:O	2.03	0.57
1:A:244:ARG:HB3	1:C:292:ARG:HE	1.69	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:ARG:HD2	2:C:511:HOH:O	2.05	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:D:341:SER:HA	1:D:391:PHE:O	2.04	0.56
1:B:333:GLU:O	1:B:337:ARG:HB2	2.05	0.56
1:C:455:ALA:H	1:C:463:ASN:ND2	2.03	0.56
1:C:402:ASN:CG	1:C:405:THR:HG23	2.26	0.56
1:C:7:VAL:HB	1:C:310:MET:HG3	1.88	0.56
1:A:170:LEU:HD22	1:A:174:ASP:HB3	1.87	0.56
1:A:77:LEU:H	1:A:154:GLU:HG2	1.71	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:C:105:MET:HG3	1:C:105:MET:O	2.06	0.56
1:C:230:PHE:CZ	1:C:234:LEU:HD22	2.41	0.56
1:C:223:ASN:OD1	1:C:225:GLU:HB3	2.06	0.56
1:C:252:PRO:HG2	1:C:255:GLU:HG3	1.88	0.56
1:B:454:GLY:HA2	1:B:463:ASN:ND2	2.21	0.55
1:A:193:PHE:CD2	1:A:195:ARG:HD2	2.41	0.55
1:B:360:ARG:NH2	1:B:364:GLU:HG3	2.21	0.55
1:D:307:ASP:HA	1:D:413:LYS:HB2	1.89	0.55
1:A:378:THR:O	1:A:400:THR:HG23	2.06	0.55
1:A:117:LEU:HD21	1:A:123:VAL:HG22	1.88	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: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: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:B:32:ARG:HD2	1:B:310:MET:HE1	1.89	0.54
1:C:188:PHE:CD1	1:C:216:HIS:HB2	2.41	0.54
1:B:4:THR:HG22	1:B:413:LYS:NZ	2.22	0.54
1:A:326:SER:O	1:A:330:THR:HG23	2.06	0.54
1:B:276:THR:OG1	1:B:306:THR:HG21	2.08	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:ASP:HB3	1:B:99:VAL:HG23	1.89	0.54
1:C:342:ARG:HD2	2:C:506:HOH:O	2.06	0.54
1:B:4:THR:HG23	1:B:336:ASP:OD1	2.08	0.54
1:D:117:LEU:HD11	1:D:160:LEU:HG	1.89	0.54
1:D:244:ARG:HD2	1:D:260:GLN:HE21	1.71	0.54
1:A:113:PHE:O	1:A:117:LEU:HB2	2.06	0.54
1:B:449:VAL:HG11	1:B:451:MET:HE2	1.90	0.54
1:A:432:LEU:HD11	1:A:436:LEU:HD11	1.90	0.54
1:A:159:ASN:O	1:A:161:PRO:HD3	2.07	0.54
1:D:50:LEU:O	1:D:54:MET:HG3	2.07	0.54
1:A:402:ASN:CG	1:A:405:THR:HG23	2.28	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:378:THR:O	1:C:400:THR:CG2	2.57	0.53
1:C:171:ALA:O	1:C:173:LYS:N	2.41	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:C:264:ILE:O	1:C:268:ILE:HG13	2.09	0.53
1:A:224:GLN:HE21	1:A:228:ASN:ND2	2.07	0.53
1:C:1:MET:SD	1:C:2:LYS:N	2.81	0.53
1:B:407:HIS:O	1:B:410:VAL:HB	2.07	0.53
1:D:438:LEU:CD2	1:D:445:LYS:HE3	2.39	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:291:THR:HG22	1:D:293:ALA:N	2.15	0.53
1:B:466:SER:OG	1:B:468:HIS:CE1	2.61	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
2:C:521:HOH:O	1:D:468:HIS:HD2	1.92	0.52
1:A:288:PRO:HB3	1:A:320:TYR:CD1	2.43	0.52
1:A:257:ILE:HG13	2:A:510:HOH:O	2.08	0.52
1:B:159:ASN:O	1:B:161:PRO:HD3	2.09	0.52
1:A:292:ARG:NH2	1:C:279:MET:HB2	2.24	0.52
1:D:327:ILE:HD12	1:D:330:THR:OG1	2.10	0.52
1:A:175:LYS:O	1:A:179:ILE:HG13	2.09	0.52
1:B:171:ALA:O	1:B:174:ASP:HB2	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:MET:HA	1:B:282:ASP:OD2	2.08	0.52
1:A:118:SER:N	1:A:121:ASN:OD1	2.42	0.52
1:C:388:ARG:HD3	1:C:388:ARG:C	2.30	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:B:24:LEU:HD13	1:B:59:LYS:HD3	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:A:271:ARG:HG2	1:A:386:ALA:HA	1.91	0.52
1:B:92:THR:O	1:B:105:MET:HA	2.09	0.52
1:C:14:THR:HG21	1:C:315:SER:O	2.09	0.52
1:B:425:SER:H	1:B:428:ASP:HB2	1.75	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: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:5:LYS:HA	1:A:29:ASN:OD1	2.10	0.51
1:C:204:ARG:HG3	1:C:204:ARG:O	2.09	0.51
1:A:7:VAL:HG22	1:A:30:VAL:HB	1.91	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:C:466:SER:OG	1:C:468:HIS:CE1	2.64	0.51
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:A:49:ASN:O	1:A:53:VAL:HG23	2.11	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:C:24:LEU:HD13	1:C:59:LYS:HD3	1.92	0.51
1:B:284:MET:HA	1:B:287:ASN:O	2.10	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: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:A:23:MET:CE	1:A:325:VAL:HG21	2.42	0.50
1:C:241:MET:CE	1:C:310:MET:HE1	2.41	0.50
1:C:193:PHE:CE2	1:C:195:ARG:HD3	2.46	0.50
1:D:463:ASN:ND2	1:D:464:THR:HG23	2.26	0.50
1:B:400:THR:HG21	1:B:405:THR:OG1	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ILE:CG2	1:B:51:ARG:HH11	2.24	0.50
1:C:222:GLU:HG2	1:C:246:ASP:HB2	1.93	0.50
1:D:196:LYS:NZ	1:D:199:ASP:OD1	2.44	0.50
1:C:126:ASP:O	1:C:129:LEU:HG	2.12	0.50
1:B:399:LEU:HD23	1:B:418:GLN:HB3	1.93	0.50
1:A:224:GLN:NE2	1:A:228:ASN:HD21	2.09	0.50
1:D:279:MET:HA	1:D:282:ASP:OD2	2.12	0.50
1:B:378:THR:O	1:B:400:THR:HG23	2.12	0.49
1:A:355:THR:HG23	1:A:462:THR:HB	1.93	0.49
1:D:11:GLY:O	1:D:15:GLU:HB3	2.12	0.49
1:C:251:ILE:HB	1:C:252:PRO:HD2	1.95	0.49
1:C:222:GLU:HG2	1:C:246:ASP:CB	2.41	0.49
1:D:458:PRO:O	1:D:460:GLY:N	2.44	0.49
1:C:241:MET:HE1	1:C:310:MET:HE1	1.94	0.49
1:D:284:MET:HA	1:D:287:ASN:O	2.12	0.49
1:C:73:ARG:HD3	1:C:155:ASN:ND2	2.24	0.49
1:D:445:LYS:NZ	1:D:445:LYS:H	2.10	0.49
1:A:292:ARG:NH2	1:C:279:MET:SD	2.81	0.49
1:C:455:ALA:N	1:C:463:ASN:HD21	2.07	0.49
1:C:373:LEU:HD23	1:C:395:THR:HB	1.95	0.49
1:B:285:ILE:HD11	1:B:313:GLY:CA	2.38	0.49
1:A:400:THR:O	1:A:419:LEU:HA	2.12	0.49
1:D:257:ILE:HD11	2:D:563:HOH:O	2.12	0.49
1:A:291:THR:HB	1:A:294:GLU:H	1.78	0.49
1:A:19:MET:O	1:A:23:MET:HG3	2.12	0.49
1:C:405:THR:HG22	2:C:534:HOH:O	2.11	0.49
1:A:121:ASN:N	1:A:121:ASN:HD22	2.11	0.49
1:D:426:THR:HG22	1:D:430:TYR:CE2	2.48	0.49
1:D:116:ASP:OD2	1:D:165:ILE:HA	2.12	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:288:PRO:HB3	1:A:320:TYR:CE1	2.48	0.48
1:A:89:GLN:NE2	1:A:103:SER:O	2.47	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:C:137:ILE:HG23	1:C:141:LYS:O	2.13	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:A:197:ARG:HB2	1:A:232:GLU:CD	2.33	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:LYS:HB2	1:C:287:ASN:ND2	2.28	0.48
1:B:262:MET:HE3	1:B:263:MET:HG3	1.96	0.48
1:A:75:MET:HE1	1:A:109:THR:HA	1.96	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:C:229:ASN:O	1:C:232:GLU:HG2	2.13	0.48
1:B:431:ARG:CZ	2:B:524:HOH:O	2.61	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: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: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:B:400:THR:O	1:B:419:LEU:HA	2.14	0.47
1:B:402:ASN:OD1	1:B:405:THR:HG23	2.14	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:165:ILE:HG22	1:B:167:LEU:H	1.80	0.47
1:B:119:VAL:HG22	1:B:136:ALA:HA	1.96	0.47
1:A:327:ILE:O	1:A:331:ILE:HG13	2.14	0.47
1:C:436:LEU:O	1:C:440:SER:HB3	2.14	0.47
1:A:175:LYS:HB3	1:A:206:HIS:NE2	2.29	0.47
1:A:10:ILE:HG13	1:A:31:MET:CG	2.45	0.47
1:B:113:PHE:O	1:B:117:LEU:HB2	2.15	0.47
1:A:259:ALA:O	1:A:263:MET:HG3	2.15	0.47
1:D:463:ASN:ND2	1:D:464:THR:CG2	2.78	0.47
1:B:378:THR:O	1:B:400:THR:CG2	2.63	0.47
1:B:191:ALA:CB	1:B:203:ILE:HD12	2.45	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:D:454:GLY:HA2	1:D:463:ASN:ND2	2.29	0.46
1:C:281:LEU:O	1:C:314:GLU:HG2	2.15	0.46
1:A:70:PRO:HB2	1:A:167:LEU:HD13	1.96	0.46
1:A:434:LYS:HG3	1:A:451:MET:CE	2.45	0.46
1:A:430:TYR:HA	1:A:451:MET:SD	2.55	0.46
1:C:271:ARG:HG2	1:C:386:ALA:HA	1.97	0.46
1:D:224:GLN:NE2	1:D:228:ASN:ND2	2.63	0.46
1:C:197:ARG:CZ	1:C:201:ILE:HD11	2.45	0.46
1:C:269:ARG:HG3	2:C:553:HOH:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:407:HIS:O	1:D:410:VAL:HB	2.16	0.46
1:C:4:THR:HG22	1:C:413:LYS:CE	2.46	0.46
1:A:224:GLN:HG3	1:A:228:ASN:OD1	2.16	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:C:288:PRO:HB3	1:C:320:TYR:CE1	2.48	0.46
1:A:463:ASN:ND2	1:A:464:THR:HG23	2.30	0.46
1:A:30:VAL:HG21	1:A:411:LEU:HD13	1.97	0.46
1:C:423:ILE:HG21	1:C:429:PHE:HB2	1.97	0.46
1:A:401:THR:HG22	1:A:420:VAL:HG23	1.98	0.46
1:A:320:TYR:N	1:A:321:PRO:HD3	2.30	0.46
1:C:7:VAL:HG21	1:C:275:ILE:HD13	1.96	0.46
1:A:280:MET:HG3	1:A:310:MET:O	2.15	0.46
1:B:265:GLU:O	1:B:269:ARG:HG3	2.16	0.46
1:A:23:MET:HE2	1:A:325:VAL:HG21	1.98	0.46
1:A:432:LEU:HA	1:A:435:GLU:HG3	1.98	0.46
1:D:77:LEU:H	1:D:154:GLU:HG2	1.81	0.46
1:C:375:VAL:HG23	1:C:449:VAL:CG1	2.46	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:C:291:THR:HG22	1:C:294:GLU:H	1.81	0.45
1:B:40:TYR:OH	1:B:176:GLN:HG2	2.15	0.45
1:C:383:SER:HB2	1:C:462:THR:OG1	2.16	0.45
1:B:192:SER:HA	1:B:220:LYS:HD3	1.99	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:224:GLN:HE21	1:B:228:ASN:ND2	2.15	0.45
1:A:291:THR:CG2	1:A:293:ALA:HB3	2.41	0.45
1:B:39:ASP:OD1	1:B:42:GLU:HB2	2.16	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:D:378:THR:HG22	1:D:381:GLY:H	1.81	0.45
1:A:378:THR:HG21	1:A:381:GLY:CA	2.46	0.45
1:D:132:MET:CA	1:D:147:LEU:HG	2.46	0.45
1:B:281:LEU:O	1:B:314:GLU:HG2	2.16	0.45
1:D:402:ASN:CG	1:D:405:THR:HG23	2.37	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:D:160:LEU:HB3	1:D:163:VAL:HB	1.98	0.44
1:D:57:THR:OG1	1:D:59:LYS:HG3	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:50:LEU:HG	1:C:54:MET:CE	2.48	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
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:14:THR:HG21	1:B:315:SER:O	2.18	0.44
1:C:423:ILE:CG2	1:C:429:PHE:HB2	2.47	0.44
1:B:180:PHE:HA	1:B:183:GLU:OE1	2.18	0.44
1:D:15:GLU:HB2	1:D:46:ARG:HD2	1.99	0.44
1:C:270:ALA:O	1:C:271:ARG:HB2	2.18	0.44
1:B:7:VAL:HG11	1:B:310:MET:HE2	1.99	0.44
1:D:445:LYS:H	1:D:445:LYS:CE	2.30	0.44
1:A:241:MET:SD	1:A:310:MET:HE1	2.58	0.44
1:B:458:PRO:O	1:B:460:GLY:N	2.51	0.44
1:D:257:ILE:O	1:D:261:LYS:HG3	2.17	0.44
1:C:281:LEU:HD23	1:C:294:GLU:HB3	1.98	0.44
1:B:78:GLU:O	1:B:80:GLY:N	2.51	0.44
1:B:402:ASN:CG	1:B:405:THR:HG23	2.38	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:A:213:GLU:CD	1:A:213:GLU:H	2.21	0.43
1:B:4:THR:HG22	1:B:413:LYS:HZ3	1.83	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:HB3	1:D:145:LYS:HE2	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:D:380:GLY:HA2	1:D:405:THR:HG21	2.00	0.43
1:A:224:GLN:HE21	1:A:228:ASN:CG	2.21	0.43
1:A:342:ARG:HD2	1:A:391:PHE:CD1	2.53	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:PHE:CE2	1:A:106:VAL:HG22	2.54	0.43
1:A:73:ARG:HD2	1:A:155:ASN:HD21	1.83	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:B:356:GLU:CD	1:B:390:TYR:HH	2.22	0.43
1:C:426:THR:HG22	1:C:430:TYR:CE2	2.53	0.43
1:B:426:THR:HG22	1:B:430:TYR:CE2	2.54	0.43
1:A:444:HIS:O	1:A:447:ASP:HB2	2.19	0.43
1:C:170:LEU:CD2	1:C:174:ASP:HB3	2.49	0.43
1:B:380:GLY:HA2	1:B:405:THR:CG2	2.41	0.43
1:A:379:GLN:HE22	1:A:402:ASN:HB2	1.84	0.43
1:D:167:LEU:C	1:D:195:ARG:HH22	2.22	0.43
1:A:354:ILE:O	1:A:358:VAL:HG13	2.19	0.43
1:D:343:LEU:O	1:D:360:ARG:HD2	2.19	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:A:19:MET:HE3	1:A:22:LYS:HD2	2.00	0.43
1:B:288:PRO:HB3	1:B:320:TYR:CE2	2.54	0.43
1:B:124:LEU:O	1:B:158:VAL:HA	2.19	0.43
1:D:257:ILE:HD12	1:D:258:PHE:CD2	2.53	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:A:436:LEU:HA	1:A:439:GLN:HB2	2.02	0.42
1:D:73:ARG:HA	1:D:156:LYS:O	2.19	0.42
1:A:142:VAL:HG12	1:A:144:CYS:SG	2.59	0.42
1:A:362:ALA:HB1	1:A:450:VAL:HG11	2.00	0.42
1:A:237:SER:O	1:A:272:LYS:HE2	2.19	0.42
1:A:96:ASP:O	1:A:98:SER:N	2.53	0.42
1:C:152:LEU:HD12	1:C:153:GLY:N	2.34	0.42
1:A:251:ILE:HB	1:A:252:PRO:HD2	2.01	0.42
1:D:313:GLY:O	1:D:318:GLY:N	2.52	0.42
1:D:223:ASN:ND2	2:D:493:HOH:O	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:C:4:THR:HG23	1:C:336:ASP:OD1	2.19	0.42
1:B:365:THR:HG22	1:B:369:LEU:HD12	2.02	0.42
1:A:444:HIS:HD2	2:A:540:HOH:O	2.02	0.42
1:C:326:SER:O	1:C:330:THR:HG23	2.20	0.42
1:A:126:ASP:HB3	1:A:129:LEU:HB3	2.01	0.42
1:A:3:LYS:NZ	1:A:393:ASP:O	2.44	0.42
1:A:257:ILE:H	1:A:257:ILE:HG13	1.47	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD3	1:C:244:ARG:H	1.85	0.42
1:C:170:LEU:O	1:C:175:LYS:HE3	2.20	0.41
1:A:455:ALA:H	1:A:457:VAL:HG22	1.83	0.41
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:B:273:VAL:HG13	2:B:531:HOH:O	2.19	0.41
1:A:292:ARG:HD3	1:C:279:MET:SD	2.60	0.41
1:B:449:VAL:CG1	1:B:451:MET:HE2	2.50	0.41
1:D:423:ILE:HA	1:D:428:ASP:OD2	2.20	0.41
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:D:463:ASN:H	1:D:463:ASN:HD22	1.67	0.41
1:D:438:LEU:HD22	1:D:445:LYS:HE3	2.02	0.41
1:D:257:ILE:CD1	1:D:258:PHE:CE2	3.02	0.41
1:A:188:PHE:CD1	1:A:216:HIS:HB2	2.55	0.41
1:C:287:ASN:N	1:C:287:ASN:ND2	2.69	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:D:448:VAL:HA	1:D:468:HIS:O	2.21	0.41
1:D:96:ASP:HB2	1:D:140:ASN:HD22	1.85	0.41
1:C:110:TYR:O	1:C:113:PHE:HB2	2.20	0.41
1:D:65:LEU:C	1:D:65:LEU:HD23	2.41	0.41
1:D:280:MET:HG3	1:D:310:MET:O	2.20	0.41
1:D:197:ARG:HD2	2:D:533:HOH:O	2.19	0.41
1:C:160:LEU:HB3	1:C:163:VAL:CB	2.45	0.41
1:D:249:VAL:CG1	1:D:249:VAL:O	2.69	0.41
1:A:1:MET:HA	1:A:1:MET:CE	2.50	0.41
1:D:466:SER:OG	1:D:468:HIS:CE1	2.74	0.41
1:C:287:ASN:HD22	1:C:287:ASN:N	2.19	0.41
1:A:426:THR:HG22	1:A:430:TYR:CE2	2.55	0.41
1:A:178:LEU:HD13	1:A:207:LEU:HD21	2.02	0.41
1:A:158:VAL:HG12	1:A:160:LEU:HD13	2.03	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:D:291:THR:HG22	1:D:292:ARG:N	2.36	0.41
1:A:378:THR:O	1:A:400:THR:CG2	2.69	0.41
1:C:178:LEU:HD13	1:C:207:LEU:HD21	2.03	0.41
1:B:289:ARG:HG2	1:B:289:ARG:NH1	2.36	0.41
1:B:463:ASN:HD22	1:B:463:ASN:N	2.12	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:ALA:HB2	1:B:464:THR:HG21	2.03	0.40
1:A:19:MET:HE3	1:A:19:MET:HA	2.02	0.40
1:C:126:ASP:O	1:C:127:ASP:C	2.59	0.40
1:A:69:GLY:HA2	1:A:174:ASP:OD2	2.22	0.40
1:D:175:LYS:O	1:D:206:HIS:HE1	2.03	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:B:117:LEU:HD12	1:B:121:ASN:OD1	2.22	0.40
1:D:118:SER:N	1:D:121:ASN:OD1	2.55	0.40
1:A:274:VAL:O	1:A:306:THR:HG22	2.21	0.40
1:D:273:VAL:HG21	1:D:411:LEU:HD23	2.02	0.40
1:C:409:LEU:HD23	1:C:409:LEU:HA	1.91	0.40
1:C:52:ASN:O	1:C:56:LYS:HB2	2.21	0.40
1:C:175:LYS:NZ	2:C:527:HOH:O	2.55	0.40
1:B:379:GLN:NE2	1:B:402:ASN:HB2	2.37	0.40
1:D:334:ARG:O	1:D:337:ARG:HG2	2.22	0.40
1:A:118:SER:O	1:A:121:ASN:CG	2.60	0.40
1:D:444:HIS:O	1:D:447:ASP:HB2	2.21	0.40
1:D:47:ILE:O	1:D:51:ARG:HG2	2.22	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%)	26	46
1	B	460/470 (98%)	434 (94%)	24 (5%)	2 (0%)	39	61
1	C	427/470 (91%)	403 (94%)	17 (4%)	7 (2%)	12	21
1	D	460/470 (98%)	441 (96%)	18 (4%)	1 (0%)	52	75

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1807/1880 (96%)	1708 (94%)	86 (5%)	13 (1%)	26	46

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
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%)	329 (87%)	48 (13%)	5	10
1	B	377/389 (97%)	328 (87%)	49 (13%)	5	9
1	C	352/389 (90%)	307 (87%)	45 (13%)	5	10
1	D	377/389 (97%)	335 (89%)	42 (11%)	8	14
All	All	1483/1556 (95%)	1299 (88%)	184 (12%)	6	11

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	16	SER
1	A	19	MET
1	A	31	MET
1	A	39	ASP
1	A	67	THR
1	A	73	ARG
1	A	78	GLU
1	A	89	GLN
1	A	104	GLU
1	A	106	VAL
1	A	111	GLU
1	A	117	LEU
1	A	118	SER
1	A	122	THR
1	A	133	GLU
1	A	138	GLU
1	A	160	LEU
1	A	178	LEU
1	A	196	LYS
1	A	204	ARG
1	A	208	LYS
1	A	216	HIS
1	A	244	ARG
1	A	253	VAL
1	A	257	ILE
1	A	273	VAL
1	A	292	ARG
1	A	306	THR
1	A	323	GLU
1	A	378	THR
1	A	379	GLN
1	A	388	ARG
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	459	SER
1	A	461	THR
1	A	463	ASN
1	A	464	THR
1	B	4	THR
1	B	19	MET
1	B	51	ARG
1	B	60	THR
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	173	LYS
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	244	ARG
1	B	253	VAL
1	B	257	ILE
1	B	262	MET
1	B	273	VAL
1	B	279	MET
1	B	289	ARG
1	B	291	THR
1	B	306	THR
1	B	356	GLU
1	B	360	ARG
1	B	364	GLU
1	B	373	LEU
1	B	378	THR
1	B	379	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	388	ARG
1	B	400	THR
1	B	403	GLU
1	B	405	THR
1	B	421	LYS
1	B	424	THR
1	B	431	ARG
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	160	LEU
1	C	170	LEU
1	C	176	GLN
1	C	178	LEU
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	269	ARG
1	C	271	ARG
1	C	287	ASN
1	C	292	ARG
1	C	306	THR
1	C	337	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	342	ARG
1	C	360	ARG
1	C	378	THR
1	C	379	GLN
1	C	388	ARG
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	151	ASP
1	D	160	LEU
1	D	176	GLN
1	D	193	PHE
1	D	196	LYS
1	D	216	HIS
1	D	223	ASN
1	D	244	ARG
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	360	ARG
1	D	370	ASP
1	D	373	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	378	THR
1	D	388	ARG
1	D	400	THR
1	D	405	THR
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	ASN
1	A	159	ASN
1	A	184	GLN
1	A	206	HIS
1	A	216	HIS
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	228	ASN
1	B	260	GLN
1	B	379	GLN
1	B	408	GLN
1	B	463	ASN
1	B	468	HIS
1	C	45	GLN
1	C	149	ASN
1	C	155	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	184	GLN
1	C	206	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	45	GLN
1	D	48	GLN
1	D	52	ASN
1	D	81	ASN
1	D	155	ASN
1	D	159	ASN
1	D	206	HIS
1	D	214	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	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 ⓘ

There are no carbohydrates 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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.