



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:25 pm BST

PDB ID : 1QGT  
Title : HUMAN HEPATITIS B VIRAL CAPSID (HBCAG)  
Authors : Leslie, A.G.W.; Wynne, S.A.; Crowther, R.A.  
Deposited on : 1999-05-05  
Resolution : 3.30 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](mailto: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.

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

MolProbity : 4.02b-467  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

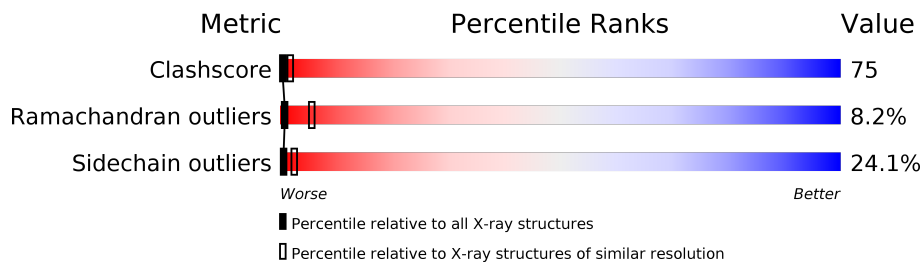
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)

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  $\geq 3$ , 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	149	21% 50% 23% • 5%
1	B	149	17% 57% 20% • •
1	C	149	15% 58% 19% • 5%
1	D	149	15% 53% 26% • •

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4560 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 PROTEIN (HBV CAPSID PROTEIN).


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	142	1136	735	188	207	6	0	0	0
1	D	143	1144	741	189	208	6	0	0	0
1	B	143	1144	741	189	208	6	0	0	0
1	A	142	1136	735	188	207	6	0	0	0

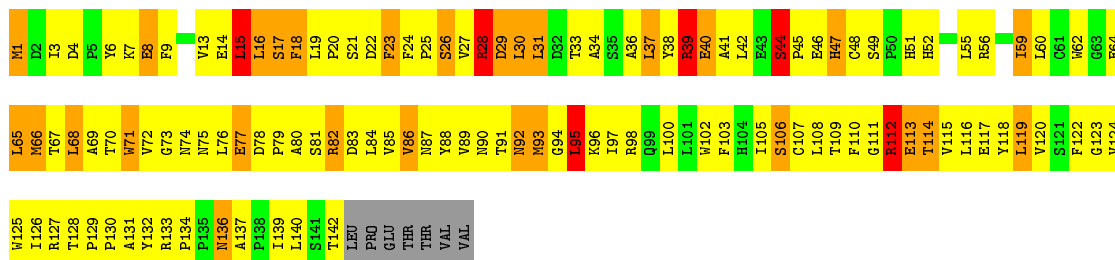
### 3 Residue-property plots [i](#)

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. 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.

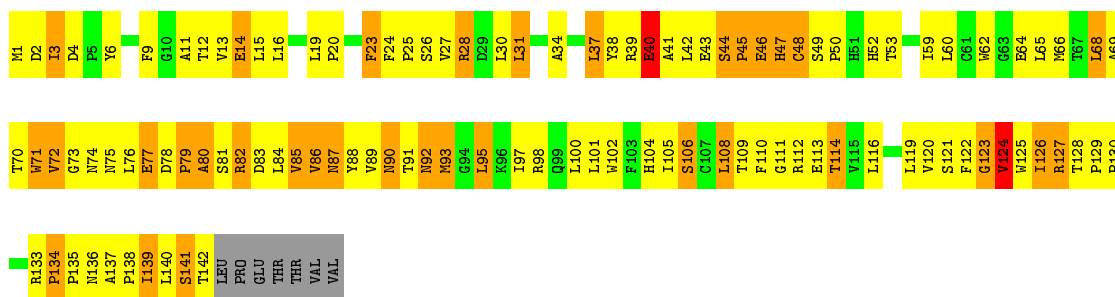
- Molecule 1: PROTEIN (HBV CAPSID PROTEIN)

Chain C: 



- Molecule 1: PROTEIN (HBV CAPSID PROTEIN)

Chain A:  21% 50% 23% 5%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	538.40Å 354.80Å 370.10Å 90.00° 132.30° 90.00°	Depositor
Resolution (Å)	8.00 – 3.30	Depositor
% Data completeness (in resolution range)	94.2 (8.00-3.30)	Depositor
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.271 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4560	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.73	0/1170	0.87	3/1602 (0.2%)
1	B	0.79	0/1178	0.96	3/1613 (0.2%)
1	C	0.73	0/1170	0.91	5/1602 (0.3%)
1	D	0.74	1/1178 (0.1%)	0.93	4/1613 (0.2%)
All	All	0.75	1/4696 (0.0%)	0.92	15/6430 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	48	CYS	CB-SG	-5.01	1.73	1.81

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	15	LEU	CA-CB-CG	-6.20	101.04	115.30
1	D	119	LEU	CA-CB-CG	-5.97	101.58	115.30
1	B	47	HIS	N-CA-C	-5.89	95.10	111.00
1	D	31	LEU	CA-CB-CG	-5.88	101.77	115.30
1	A	95	LEU	CA-CB-CG	-5.83	101.89	115.30
1	B	31	LEU	CA-CB-CG	-5.63	102.35	115.30
1	C	16	LEU	CA-CB-CG	-5.56	102.50	115.30
1	D	76	LEU	CA-CB-CG	-5.25	103.21	115.30
1	A	31	LEU	CA-CB-CG	-5.23	103.27	115.30
1	C	119	LEU	CA-CB-CG	-5.15	103.46	115.30
1	D	95	LEU	CA-CB-CG	-5.12	103.52	115.30
1	A	48	CYS	CA-CB-SG	-5.07	104.87	114.00
1	C	31	LEU	CA-CB-CG	-5.07	103.64	115.30
1	B	76	LEU	CA-CB-CG	-5.05	103.68	115.30
1	C	95	LEU	CA-CB-CG	-5.00	103.80	115.30

There are no chirality outliers.

There are no planarity outliers.

## 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	1136	0	1115	178	0
1	B	1144	0	1126	193	0
1	C	1136	0	1115	177	0
1	D	1144	0	1126	190	0
All	All	4560	0	4482	682	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 75.

All (682) 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:B:25:PRO:HG2	1:B:30:LEU:HD21	1.34	1.09
1:B:72:VAL:HG21	1:B:85:VAL:HG11	1.32	1.08
1:B:89:VAL:HA	1:B:93:MET:HE3	1.39	1.05
1:A:109:THR:HG22	1:A:110:PHE:CD1	1.91	1.04
1:A:110:PHE:HE2	1:A:140:LEU:HB3	1.19	1.03
1:B:1:MET:HG2	1:A:39:ARG:HD2	1.41	1.03
1:A:110:PHE:CE2	1:A:140:LEU:HB3	1.99	0.98
1:D:88:TYR:HA	1:D:92:ASN:ND2	1.78	0.98
1:D:82:ARG:O	1:D:86:VAL:HG23	1.66	0.96
1:B:125:TRP:CE2	1:B:133:ARG:HD2	2.01	0.94
1:C:81:SER:HA	1:C:84:LEU:HD12	1.48	0.94
1:A:72:VAL:HG21	1:A:85:VAL:HG11	1.51	0.92
1:B:89:VAL:HA	1:B:93:MET:CE	2.02	0.90
1:C:47:HIS:HA	1:C:56:ARG:NH2	1.87	0.90
1:B:25:PRO:HG2	1:B:30:LEU:CD2	2.01	0.90
1:C:120:VAL:HG22	1:B:37:LEU:HD22	1.52	0.88
1:A:25:PRO:HG2	1:A:30:LEU:HD21	1.55	0.86
1:C:122:PHE:HE1	1:C:126:ILE:HD12	1.40	0.86
1:C:72:VAL:HG13	1:C:76:LEU:HD12	1.58	0.85
1:D:140:LEU:HD23	1:D:140:LEU:N	1.91	0.85
1:A:12:THR:HG23	1:A:15:LEU:H	1.44	0.82
1:C:89:VAL:HA	1:C:93:MET:CE	2.10	0.82
1:B:79:PRO:HA	1:B:82:ARG:HG2	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:LEU:HD23	1:D:140:LEU:H	1.42	0.82
1:C:72:VAL:HG21	1:C:85:VAL:HG11	1.61	0.82
1:D:89:VAL:HA	1:D:93:MET:HG3	1.59	0.81
1:A:109:THR:HG22	1:A:110:PHE:CE1	2.14	0.81
1:C:89:VAL:HA	1:C:93:MET:HE2	1.63	0.81
1:A:72:VAL:HG11	1:A:85:VAL:HG12	1.62	0.81
1:D:25:PRO:HG2	1:D:30:LEU:HD21	1.63	0.80
1:D:11:ALA:HB2	1:D:116:LEU:HD21	1.66	0.78
1:A:110:PHE:HD2	1:A:140:LEU:HD13	1.49	0.77
1:C:25:PRO:HG2	1:C:30:LEU:HD21	1.67	0.76
1:B:6:TYR:CE2	1:B:16:LEU:HD12	2.20	0.76
1:B:34:ALA:HB2	1:B:105:ILE:HD11	1.67	0.76
1:D:112:ARG:HH12	1:D:116:LEU:HD11	1.51	0.75
1:D:72:VAL:HG21	1:D:85:VAL:HG11	1.67	0.75
1:A:69:ALA:HB2	1:A:89:VAL:HG11	1.68	0.75
1:C:123:GLY:O	1:C:127:ARG:HG3	1.86	0.75
1:C:85:VAL:HG21	1:D:85:VAL:HG21	1.66	0.75
1:A:20:PRO:O	1:A:23:PHE:HB3	1.86	0.75
1:B:133:ARG:HH11	1:B:133:ARG:HG2	1.51	0.75
1:A:24:PHE:O	1:A:98:ARG:NH1	2.20	0.75
1:A:88:TYR:HA	1:A:92:ASN:ND2	2.02	0.74
1:A:6:TYR:CD2	1:A:16:LEU:HD11	2.22	0.74
1:B:14:GLU:O	1:B:17:SER:HB3	1.87	0.73
1:B:91:THR:HG22	1:B:92:ASN:N	2.02	0.73
1:C:82:ARG:O	1:C:86:VAL:HG23	1.88	0.73
1:D:39:ARG:HG2	1:D:39:ARG:HH11	1.53	0.73
1:B:5:PRO:HG2	1:B:6:TYR:CD1	2.24	0.73
1:D:27:VAL:HG12	1:D:31:LEU:HD12	1.70	0.72
1:A:125:TRP:CZ3	1:A:126:ILE:HG12	2.24	0.72
1:C:102:TRP:O	1:C:106:SER:HB2	1.89	0.72
1:B:76:LEU:HD23	1:B:82:ARG:HA	1.71	0.72
1:A:110:PHE:CD2	1:A:140:LEU:HD13	2.25	0.72
1:D:34:ALA:HB2	1:D:105:ILE:HD11	1.72	0.72
1:B:37:LEU:HD12	1:B:38:TYR:CE2	2.25	0.72
1:B:92:ASN:H	1:B:92:ASN:ND2	1.88	0.71
1:B:71:TRP:O	1:B:75:ASN:HB2	1.91	0.71
1:C:120:VAL:O	1:C:124:VAL:HG23	1.90	0.71
1:D:39:ARG:HG2	1:D:39:ARG:NH1	2.02	0.71
1:D:82:ARG:HG2	1:D:83:ASP:N	2.06	0.71
1:D:82:ARG:CG	1:D:83:ASP:N	2.53	0.71
1:D:112:ARG:NH1	1:D:116:LEU:HD11	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:PHE:HA	1:D:138:PRO:HG2	1.72	0.71
1:A:122:PHE:O	1:A:123:GLY:C	2.29	0.71
1:B:81:SER:HB2	1:A:76:LEU:HD12	1.71	0.70
1:B:85:VAL:HG12	1:B:86:VAL:N	2.05	0.70
1:A:76:LEU:CB	1:A:82:ARG:HB2	2.22	0.70
1:A:125:TRP:CZ2	1:A:137:ALA:HB2	2.27	0.70
1:A:89:VAL:HG22	1:A:93:MET:CE	2.21	0.70
1:D:125:TRP:CZ3	1:D:126:ILE:HG12	2.27	0.70
1:B:24:PHE:CE2	1:B:99:GLN:HA	2.27	0.70
1:B:93:MET:HE1	1:A:68:LEU:HD13	1.72	0.70
1:C:41:ALA:O	1:C:44:SER:HB3	1.92	0.70
1:A:34:ALA:HB2	1:A:105:ILE:HD11	1.73	0.69
1:A:81:SER:HA	1:A:84:LEU:HB2	1.74	0.69
1:C:6:TYR:CZ	1:C:16:LEU:HD12	2.26	0.69
1:C:92:ASN:ND2	1:C:92:ASN:H	1.90	0.69
1:C:3:ILE:HG22	1:D:60:LEU:HD11	1.74	0.69
1:D:36:ALA:C	1:D:37:LEU:HD23	2.12	0.69
1:C:24:PHE:O	1:C:98:ARG:NH1	2.25	0.69
1:D:95:LEU:HD23	1:D:96:LYS:N	2.06	0.69
1:C:85:VAL:HG12	1:C:86:VAL:N	2.08	0.69
1:D:27:VAL:HG12	1:D:31:LEU:CD1	2.23	0.68
1:D:6:TYR:CD1	1:D:16:LEU:HD11	2.28	0.68
1:A:19:LEU:HD13	1:A:23:PHE:CE1	2.28	0.68
1:A:89:VAL:HG22	1:A:93:MET:HE2	1.74	0.68
1:C:125:TRP:NE1	1:C:133:ARG:HD2	2.09	0.68
1:D:40:GLU:HA	1:D:40:GLU:OE1	1.93	0.68
1:D:24:PHE:N	1:D:24:PHE:CD1	2.61	0.68
1:D:134:PRO:CB	1:D:135:PRO:HD2	2.25	0.67
1:D:20:PRO:O	1:D:23:PHE:HB3	1.95	0.67
1:B:53:THR:HA	1:B:56:ARG:HD2	1.77	0.67
1:B:125:TRP:CZ2	1:B:137:ALA:HB2	2.30	0.67
1:C:95:LEU:O	1:C:95:LEU:HG	1.89	0.67
1:C:55:LEU:O	1:C:59:ILE:HD12	1.94	0.67
1:D:134:PRO:HB2	1:D:135:PRO:HD2	1.76	0.67
1:A:70:THR:HG22	1:A:71:TRP:N	2.09	0.66
1:A:92:ASN:HD22	1:A:92:ASN:H	1.44	0.66
1:B:125:TRP:CH2	1:B:137:ALA:HB2	2.30	0.66
1:A:77:GLU:HG3	1:A:78:ASP:N	2.10	0.66
1:D:140:LEU:N	1:D:140:LEU:CD2	2.58	0.66
1:B:46:GLU:HA	1:B:46:GLU:OE1	1.94	0.66
1:C:92:ASN:H	1:C:92:ASN:HD22	1.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:PHE:O	1:A:123:GLY:O	2.14	0.66
1:D:19:LEU:HD13	1:D:23:PHE:CE1	2.31	0.66
1:D:25:PRO:HG2	1:D:30:LEU:CD2	2.25	0.65
1:B:52:HIS:HD2	1:B:108:LEU:HD21	1.61	0.65
1:B:124:VAL:HG12	1:B:125:TRP:N	2.12	0.65
1:A:125:TRP:HZ3	1:A:126:ILE:HG12	1.62	0.65
1:C:125:TRP:CE2	1:C:133:ARG:HD2	2.31	0.65
1:A:76:LEU:HB3	1:A:82:ARG:HB2	1.77	0.65
1:B:29:ASP:HA	1:B:32:ASP:HB2	1.78	0.65
1:D:71:TRP:CE3	1:D:72:VAL:HA	2.32	0.65
1:A:109:THR:CG2	1:A:110:PHE:CE1	2.80	0.65
1:D:92:ASN:HD22	1:D:92:ASN:H	1.44	0.65
1:A:82:ARG:O	1:A:86:VAL:HG23	1.96	0.65
1:C:130:PRO:HA	1:C:133:ARG:HG2	1.79	0.65
1:C:62:TRP:CE3	1:C:97:ILE:HG13	2.32	0.65
1:B:81:SER:HB2	1:A:76:LEU:CD1	2.26	0.64
1:B:52:HIS:CD2	1:B:108:LEU:HD21	2.32	0.64
1:C:123:GLY:O	1:C:126:ILE:HG22	1.96	0.64
1:B:77:GLU:O	1:B:78:ASP:C	2.36	0.64
1:C:91:THR:HG22	1:C:92:ASN:N	2.12	0.64
1:C:62:TRP:HE3	1:C:97:ILE:HG13	1.63	0.64
1:C:120:VAL:CG2	1:B:37:LEU:HD22	2.27	0.64
1:B:112:ARG:O	1:B:116:LEU:HG	1.97	0.64
1:B:16:LEU:HD21	1:B:102:TRP:HZ3	1.63	0.64
1:B:1:MET:CG	1:A:39:ARG:HD2	2.25	0.64
1:C:81:SER:HA	1:C:84:LEU:CD1	2.27	0.64
1:D:125:TRP:O	1:D:133:ARG:HD3	1.98	0.63
1:B:101:LEU:O	1:B:105:ILE:HG13	1.97	0.63
1:C:18:PHE:HZ	1:B:33:THR:HG23	1.62	0.63
1:A:92:ASN:ND2	1:A:92:ASN:H	1.96	0.63
1:B:125:TRP:CD2	1:B:133:ARG:HD2	2.32	0.63
1:B:39:ARG:NH2	1:A:1:MET:HA	2.13	0.63
1:B:42:LEU:O	1:B:56:ARG:NH1	2.32	0.62
1:B:48:CYS:HB2	1:B:52:HIS:ND1	2.14	0.62
1:A:125:TRP:HD1	1:A:134:PRO:HG2	1.64	0.62
1:B:68:LEU:HD13	1:A:93:MET:HE2	1.81	0.61
1:C:81:SER:HB3	1:D:77:GLU:OE1	1.99	0.61
1:D:95:LEU:O	1:D:98:ARG:HB2	1.99	0.61
1:B:85:VAL:HG21	1:A:85:VAL:HG21	1.83	0.61
1:C:79:PRO:HA	1:C:82:ARG:HB3	1.82	0.61
1:C:23:PHE:C	1:C:23:PHE:CD1	2.74	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:LEU:HG	1:B:59:ILE:CD1	2.30	0.61
1:D:112:ARG:O	1:D:116:LEU:HG	2.01	0.60
1:A:89:VAL:HG12	1:A:90:ASN:N	2.16	0.60
1:C:110:PHE:CD2	1:C:140:LEU:HB3	2.37	0.60
1:B:55:LEU:HG	1:B:59:ILE:HD11	1.84	0.60
1:B:77:GLU:O	1:B:79:PRO:N	2.35	0.60
1:C:80:ALA:O	1:C:84:LEU:HG	2.01	0.60
1:D:48:CYS:O	1:D:49:SER:HB3	2.01	0.60
1:C:18:PHE:CD2	1:C:123:GLY:HA3	2.37	0.60
1:B:15:LEU:HD11	1:B:119:LEU:HB3	1.82	0.60
1:B:124:VAL:CG1	1:B:125:TRP:N	2.64	0.60
1:D:125:TRP:CE3	1:D:126:ILE:HG12	2.37	0.60
1:D:5:PRO:HG2	1:D:6:TYR:CD2	2.37	0.60
1:B:37:LEU:O	1:B:38:TYR:CG	2.54	0.60
1:B:6:TYR:CZ	1:B:16:LEU:HD12	2.37	0.60
1:D:85:VAL:HG12	1:D:86:VAL:N	2.17	0.60
1:D:88:TYR:HA	1:D:92:ASN:HD21	1.64	0.60
1:A:71:TRP:O	1:A:75:ASN:HB2	2.03	0.59
1:A:77:GLU:HG3	1:A:78:ASP:H	1.66	0.59
1:A:72:VAL:HG11	1:A:85:VAL:CG1	2.30	0.59
1:C:125:TRP:CE3	1:C:126:ILE:HA	2.38	0.59
1:D:89:VAL:HG12	1:D:90:ASN:N	2.17	0.59
1:D:24:PHE:HD1	1:D:24:PHE:N	2.01	0.59
1:A:125:TRP:CE3	1:A:126:ILE:N	2.71	0.59
1:A:128:THR:O	1:A:133:ARG:NH1	2.35	0.59
1:D:24:PHE:H	1:D:24:PHE:HD1	1.51	0.59
1:B:109:THR:C	1:B:110:PHE:CD1	2.76	0.58
1:B:89:VAL:HG12	1:B:90:ASN:N	2.17	0.58
1:C:122:PHE:CE1	1:C:126:ILE:HD12	2.29	0.58
1:C:15:LEU:HD21	1:C:119:LEU:HB3	1.85	0.58
1:B:30:LEU:HD12	1:B:101:LEU:CB	2.33	0.58
1:A:95:LEU:O	1:A:98:ARG:HB2	2.02	0.58
1:C:79:PRO:HA	1:C:82:ARG:HH11	1.67	0.58
1:D:118:TYR:CD2	1:D:140:LEU:HD21	2.38	0.58
1:D:4:ASP:OD2	1:D:13:VAL:HG12	2.03	0.58
1:B:49:SER:OG	1:B:52:HIS:CD2	2.56	0.58
1:C:81:SER:HB2	1:D:76:LEU:HG	1.85	0.58
1:D:13:VAL:HG13	1:D:14:GLU:N	2.18	0.58
1:B:141:SER:OG	1:B:142:THR:N	2.34	0.58
1:B:133:ARG:NH1	1:B:133:ARG:HG2	2.19	0.58
1:C:70:THR:HG22	1:C:71:TRP:N	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:THR:HG22	1:C:110:PHE:CD1	2.38	0.58
1:C:136:ASN:H	1:C:136:ASN:ND2	2.00	0.58
1:B:95:LEU:HD23	1:B:95:LEU:C	2.24	0.57
1:C:129:PRO:HG2	1:B:23:PHE:O	2.03	0.57
1:D:11:ALA:HB2	1:D:116:LEU:CD2	2.31	0.57
1:D:47:HIS:H	1:D:47:HIS:CD2	2.21	0.57
1:A:76:LEU:HB2	1:A:82:ARG:HB2	1.86	0.57
1:B:78:ASP:OD1	1:B:78:ASP:C	2.43	0.57
1:B:68:LEU:HD23	1:B:89:VAL:CG2	2.34	0.57
1:A:121:SER:O	1:A:124:VAL:HG23	2.05	0.57
1:B:24:PHE:CD1	1:B:24:PHE:N	2.73	0.57
1:A:139:ILE:HG12	1:A:140:LEU:N	2.19	0.57
1:B:24:PHE:HB2	1:B:98:ARG:NH1	2.20	0.57
1:B:65:LEU:HD11	1:B:93:MET:SD	2.44	0.57
1:A:140:LEU:O	1:A:141:SER:HB2	2.05	0.57
1:D:112:ARG:HH11	1:D:112:ARG:HG2	1.70	0.57
1:B:1:MET:HE1	1:A:59:ILE:HD13	1.87	0.57
1:B:7:LYS:O	1:B:8:GLU:C	2.43	0.57
1:C:128:THR:CG2	1:C:133:ARG:HB3	2.35	0.56
1:C:30:LEU:H	1:C:30:LEU:HD23	1.70	0.56
1:D:72:VAL:HG11	1:D:85:VAL:CG1	2.35	0.56
1:A:72:VAL:HG12	1:A:86:VAL:HG22	1.88	0.56
1:C:4:ASP:OD2	1:C:13:VAL:HG12	2.05	0.56
1:C:39:ARG:HH11	1:C:39:ARG:HG2	1.69	0.56
1:B:3:ILE:HB	1:A:60:LEU:HD21	1.86	0.56
1:B:111:GLY:O	1:B:112:ARG:C	2.43	0.56
1:D:72:VAL:HG11	1:D:85:VAL:HG12	1.86	0.56
1:B:27:VAL:O	1:B:31:LEU:HG	2.05	0.56
1:A:82:ARG:CD	1:A:83:ASP:N	2.69	0.56
1:B:17:SER:OG	1:B:18:PHE:N	2.38	0.56
1:B:92:ASN:H	1:B:92:ASN:HD22	1.51	0.56
1:D:24:PHE:O	1:D:98:ARG:NH1	2.39	0.56
1:A:111:GLY:O	1:A:112:ARG:C	2.44	0.56
1:A:85:VAL:HG12	1:A:86:VAL:N	2.21	0.56
1:C:19:LEU:HD13	1:C:23:PHE:CE1	2.40	0.56
1:C:47:HIS:H	1:C:47:HIS:CD2	2.22	0.56
1:C:94:GLY:O	1:C:98:ARG:N	2.38	0.56
1:D:37:LEU:O	1:D:38:TYR:CG	2.59	0.56
1:D:70:THR:HG22	1:D:71:TRP:N	2.20	0.56
1:B:125:TRP:CE3	1:B:126:ILE:N	2.74	0.56
1:D:38:TYR:O	1:D:42:LEU:HG	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:TYR:CA	1:D:92:ASN:ND2	2.63	0.56
1:B:76:LEU:HB3	1:B:82:ARG:CB	2.36	0.55
1:C:25:PRO:HG2	1:C:30:LEU:CD2	2.36	0.55
1:C:27:VAL:HG12	1:C:31:LEU:HD12	1.88	0.55
1:D:137:ALA:HB1	1:D:138:PRO:CD	2.36	0.55
1:B:28:ARG:HG3	1:B:29:ASP:N	2.22	0.55
1:A:125:TRP:CD1	1:A:134:PRO:HG2	2.42	0.55
1:A:39:ARG:O	1:A:43:GLU:HG3	2.07	0.55
1:B:24:PHE:O	1:B:98:ARG:NH1	2.40	0.55
1:C:39:ARG:HH11	1:C:39:ARG:CG	2.19	0.55
1:A:120:VAL:HG12	1:A:121:SER:N	2.21	0.55
1:A:39:ARG:HH11	1:A:39:ARG:HG2	1.71	0.55
1:D:62:TRP:CE3	1:D:97:ILE:HG13	2.41	0.55
1:D:62:TRP:HE3	1:D:97:ILE:HG13	1.72	0.55
1:B:129:PRO:HG2	1:B:132:TYR:HD2	1.71	0.55
1:B:7:LYS:HD3	1:A:45:PRO:HB3	1.87	0.55
1:D:23:PHE:CD1	1:D:23:PHE:C	2.79	0.55
1:B:82:ARG:NH1	1:B:82:ARG:HG2	2.22	0.55
1:C:48:CYS:O	1:C:49:SER:HB3	2.05	0.55
1:D:48:CYS:HB2	1:D:52:HIS:CG	2.41	0.55
1:C:129:PRO:HD3	1:B:25:PRO:HB3	1.89	0.55
1:C:37:LEU:O	1:C:38:TYR:CG	2.59	0.55
1:D:42:LEU:HD21	1:D:55:LEU:HD22	1.87	0.55
1:C:132:TYR:C	1:B:139:ILE:HG22	2.28	0.54
1:B:5:PRO:HG2	1:B:6:TYR:CE1	2.41	0.54
1:A:6:TYR:CE2	1:A:16:LEU:HD11	2.42	0.54
1:D:47:HIS:HA	1:D:56:ARG:NH2	2.23	0.54
1:D:64:GLU:HA	1:D:64:GLU:OE1	2.05	0.54
1:D:89:VAL:O	1:D:91:THR:N	2.40	0.54
1:B:7:LYS:O	1:B:10:GLY:N	2.41	0.54
1:C:109:THR:HG22	1:C:110:PHE:CG	2.43	0.54
1:C:120:VAL:HG22	1:B:37:LEU:CD2	2.32	0.54
1:C:133:ARG:O	1:C:134:PRO:C	2.44	0.54
1:C:6:TYR:CE1	1:C:16:LEU:HD12	2.43	0.54
1:C:18:PHE:CZ	1:B:33:THR:HG23	2.42	0.54
1:A:123:GLY:O	1:A:124:VAL:C	2.46	0.54
1:B:62:TRP:HE3	1:B:97:ILE:HG12	1.72	0.54
1:D:92:ASN:ND2	1:D:92:ASN:H	2.05	0.54
1:B:82:ARG:HG3	1:B:83:ASP:N	2.20	0.54
1:B:27:VAL:HG11	1:B:62:TRP:CE2	2.43	0.54
1:D:48:CYS:H	1:D:56:ARG:HH22	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:HG3	1:D:35:SER:HB2	1.90	0.54
1:D:27:VAL:HG11	1:D:62:TRP:CE2	2.43	0.54
1:A:102:TRP:CH2	1:A:119:LEU:HD21	2.44	0.53
1:B:109:THR:HB	1:B:110:PHE:CE1	2.43	0.53
1:B:39:ARG:O	1:B:40:GLU:C	2.46	0.53
1:C:27:VAL:HG11	1:C:62:TRP:NE1	2.24	0.53
1:C:25:PRO:CG	1:C:30:LEU:HD21	2.37	0.53
1:A:70:THR:O	1:A:73:GLY:N	2.40	0.53
1:B:15:LEU:HD12	1:B:15:LEU:O	2.09	0.53
1:A:137:ALA:HB1	1:A:138:PRO:HD2	1.90	0.53
1:B:34:ALA:HB2	1:B:105:ILE:CD1	2.38	0.53
1:C:122:PHE:O	1:C:123:GLY:C	2.47	0.53
1:D:25:PRO:CG	1:D:30:LEU:HD21	2.36	0.53
1:B:118:TYR:HE2	1:B:139:ILE:C	2.11	0.53
1:C:76:LEU:HD22	1:D:81:SER:HB2	1.90	0.53
1:B:30:LEU:HD12	1:B:101:LEU:HB3	1.88	0.53
1:B:58:ALA:O	1:B:59:ILE:C	2.46	0.53
1:C:67:THR:O	1:C:68:LEU:C	2.46	0.53
1:D:100:LEU:O	1:D:101:LEU:C	2.47	0.53
1:C:87:ASN:O	1:C:88:TYR:C	2.48	0.53
1:A:102:TRP:O	1:A:106:SER:HB2	2.09	0.53
1:C:112:ARG:HE	1:C:116:LEU:HD11	1.72	0.53
1:C:30:LEU:CD2	1:C:30:LEU:N	2.72	0.53
1:A:86:VAL:O	1:A:86:VAL:HG12	2.09	0.53
1:C:47:HIS:CD2	1:C:47:HIS:N	2.77	0.52
1:D:53:THR:O	1:D:54:ALA:C	2.47	0.52
1:A:89:VAL:HA	1:A:93:MET:HG3	1.90	0.52
1:C:112:ARG:O	1:C:116:LEU:HG	2.09	0.52
1:C:82:ARG:C	1:C:82:ARG:HD2	2.29	0.52
1:A:26:SER:O	1:A:30:LEU:HD23	2.10	0.52
1:D:1:MET:HE3	1:D:3:ILE:HD11	1.91	0.52
1:B:55:LEU:O	1:B:59:ILE:HD12	2.09	0.52
1:C:38:TYR:O	1:C:42:LEU:HG	2.10	0.52
1:D:125:TRP:CZ2	1:D:137:ALA:HB2	2.43	0.52
1:D:37:LEU:C	1:D:38:TYR:CD1	2.83	0.52
1:A:85:VAL:O	1:A:87:ASN:N	2.42	0.52
1:B:71:TRP:C	1:B:73:GLY:N	2.63	0.52
1:A:25:PRO:O	1:A:98:ARG:HD2	2.09	0.52
1:C:1:MET:HE3	1:D:35:SER:HB2	1.91	0.52
1:A:72:VAL:HG12	1:A:73:GLY:N	2.25	0.52
1:B:76:LEU:HG	1:A:81:SER:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:THR:C	1:B:143:LEU:HG	2.29	0.52
1:D:125:TRP:O	1:D:128:THR:HB	2.10	0.52
1:A:78:ASP:OD1	1:A:78:ASP:C	2.48	0.51
1:C:82:ARG:C	1:C:82:ARG:CD	2.79	0.51
1:C:45:PRO:HA	1:D:7:LYS:HG2	1.91	0.51
1:A:41:ALA:O	1:A:44:SER:HB3	2.10	0.51
1:D:38:TYR:CE2	1:D:108:LEU:HB3	2.45	0.51
1:D:49:SER:O	1:D:50:PRO:C	2.49	0.51
1:D:73:GLY:HA2	1:D:82:ARG:HD3	1.93	0.51
1:D:82:ARG:HG2	1:D:83:ASP:H	1.74	0.51
1:A:37:LEU:HD12	1:A:38:TYR:HE2	1.76	0.51
1:B:93:MET:CE	1:A:68:LEU:HD13	2.40	0.51
1:C:86:VAL:O	1:C:86:VAL:HG12	2.11	0.51
1:D:95:LEU:C	1:D:95:LEU:HD23	2.31	0.51
1:B:5:PRO:HB3	1:A:60:LEU:HD12	1.93	0.51
1:B:1:MET:HE3	1:B:3:ILE:HD11	1.93	0.51
1:C:28:ARG:O	1:C:29:ASP:C	2.49	0.51
1:D:65:LEU:HG	1:D:93:MET:CE	2.41	0.51
1:D:9:PHE:CD2	1:D:51:HIS:CE1	2.99	0.51
1:B:17:SER:O	1:B:19:LEU:N	2.44	0.51
1:B:81:SER:C	1:B:83:ASP:N	2.62	0.51
1:C:76:LEU:HD11	1:D:85:VAL:HG23	1.93	0.51
1:A:26:SER:O	1:A:27:VAL:C	2.48	0.50
1:B:6:TYR:CE2	1:B:16:LEU:CD1	2.93	0.50
1:D:122:PHE:CE1	1:D:126:ILE:HG13	2.45	0.50
1:B:110:PHE:N	1:B:110:PHE:CD1	2.79	0.50
1:B:72:VAL:HG11	1:B:85:VAL:HG12	1.94	0.50
1:B:85:VAL:CG1	1:B:86:VAL:N	2.74	0.50
1:C:38:TYR:O	1:C:39:ARG:C	2.49	0.50
1:D:125:TRP:C	1:D:133:ARG:HD3	2.32	0.50
1:D:37:LEU:HD23	1:D:37:LEU:N	2.25	0.50
1:D:6:TYR:OH	1:D:100:LEU:HD12	2.12	0.50
1:D:135:PRO:HG2	1:D:136:ASN:H	1.77	0.50
1:D:42:LEU:O	1:D:56:ARG:HD3	2.12	0.50
1:B:46:GLU:O	1:B:47:HIS:C	2.48	0.50
1:A:13:VAL:HG13	1:A:14:GLU:N	2.25	0.50
1:D:125:TRP:HZ3	1:D:126:ILE:HG12	1.73	0.50
1:C:60:LEU:HD11	1:D:3:ILE:HG22	1.93	0.50
1:D:68:LEU:HG	1:D:68:LEU:O	2.11	0.50
1:C:8:GLU:HG2	1:C:9:PHE:CD1	2.46	0.50
1:D:71:TRP:HE3	1:D:72:VAL:N	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:GLU:O	1:A:47:HIS:C	2.51	0.50
1:A:68:LEU:HD23	1:A:89:VAL:HG21	1.94	0.50
1:A:37:LEU:O	1:A:38:TYR:CG	2.65	0.50
1:B:15:LEU:C	1:B:15:LEU:HD12	2.31	0.50
1:C:118:TYR:HH	1:C:122:PHE:HD2	1.58	0.50
1:C:128:THR:O	1:C:129:PRO:C	2.50	0.50
1:D:109:THR:CG2	1:D:110:PHE:CE1	2.95	0.50
1:A:48:CYS:HB2	1:A:52:HIS:CG	2.47	0.49
1:C:128:THR:HG21	1:C:133:ARG:HB3	1.92	0.49
1:C:65:LEU:HD21	1:D:65:LEU:HD11	1.94	0.49
1:A:135:PRO:HG2	1:A:136:ASN:H	1.78	0.49
1:A:79:PRO:O	1:A:80:ALA:C	2.50	0.49
1:B:123:GLY:O	1:B:124:VAL:C	2.50	0.49
1:B:71:TRP:HE3	1:B:72:VAL:N	2.10	0.49
1:D:68:LEU:CD2	1:D:89:VAL:HG21	2.42	0.49
1:A:12:THR:O	1:A:13:VAL:C	2.50	0.49
1:A:25:PRO:HG2	1:A:30:LEU:CD2	2.34	0.49
1:A:62:TRP:O	1:A:65:LEU:HB2	2.11	0.49
1:B:118:TYR:CE2	1:B:140:LEU:N	2.80	0.49
1:D:58:ALA:C	1:D:60:LEU:N	2.64	0.49
1:B:128:THR:HG22	1:B:129:PRO:O	2.13	0.49
1:D:112:ARG:HH12	1:D:116:LEU:CD1	2.24	0.49
1:B:104:HIS:O	1:B:105:ILE:C	2.51	0.49
1:B:76:LEU:HD11	1:A:84:LEU:HB3	1.94	0.49
1:C:113:GLU:OE1	1:C:113:GLU:HA	2.12	0.49
1:C:125:TRP:CH2	1:C:137:ALA:HB2	2.47	0.49
1:C:79:PRO:HA	1:C:82:ARG:NH1	2.28	0.49
1:D:102:TRP:HH2	1:D:119:LEU:HD21	1.77	0.49
1:A:6:TYR:CE2	1:A:16:LEU:CD1	2.95	0.49
1:C:125:TRP:CE3	1:C:126:ILE:N	2.81	0.49
1:D:130:PRO:HG2	1:D:131:ALA:H	1.78	0.49
1:A:112:ARG:O	1:A:116:LEU:HG	2.13	0.49
1:C:65:LEU:N	1:C:65:LEU:HD23	2.27	0.49
1:A:41:ALA:O	1:A:44:SER:N	2.45	0.48
1:B:142:THR:O	1:B:143:LEU:HD12	2.12	0.48
1:C:110:PHE:CE2	1:C:140:LEU:HB3	2.48	0.48
1:C:69:ALA:O	1:C:72:VAL:HB	2.13	0.48
1:D:109:THR:HG22	1:D:109:THR:O	2.12	0.48
1:A:19:LEU:HD13	1:A:23:PHE:HE1	1.75	0.48
1:B:62:TRP:CE3	1:B:97:ILE:HG12	2.47	0.48
1:C:6:TYR:CE1	1:C:16:LEU:CD1	2.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:ARG:C	1:D:86:VAL:HG23	2.33	0.48
1:C:111:GLY:O	1:C:112:ARG:C	2.52	0.48
1:C:125:TRP:HE3	1:C:126:ILE:N	2.11	0.48
1:B:109:THR:HB	1:B:110:PHE:CD1	2.48	0.48
1:C:15:LEU:HD21	1:C:119:LEU:CB	2.43	0.48
1:D:6:TYR:CZ	1:D:16:LEU:HD13	2.49	0.48
1:C:14:GLU:O	1:C:14:GLU:HG2	2.14	0.48
1:D:14:GLU:O	1:D:17:SER:OG	2.28	0.48
1:D:28:ARG:O	1:D:29:ASP:C	2.52	0.48
1:A:6:TYR:CD2	1:A:16:LEU:CD1	2.95	0.48
1:A:88:TYR:HA	1:A:92:ASN:HD21	1.73	0.48
1:D:125:TRP:CE2	1:D:137:ALA:HB2	2.48	0.48
1:B:74:ASN:N	1:B:74:ASN:ND2	2.62	0.48
1:B:76:LEU:HB3	1:B:82:ARG:HB2	1.96	0.48
1:B:50:PRO:CB	1:A:47:HIS:CD2	2.97	0.48
1:B:102:TRP:CE3	1:B:103:PHE:HA	2.49	0.48
1:A:65:LEU:HD13	1:A:93:MET:HE3	1.95	0.47
1:C:27:VAL:HG11	1:C:62:TRP:CE2	2.49	0.47
1:C:68:LEU:HB2	1:D:93:MET:SD	2.54	0.47
1:B:39:ARG:CZ	1:A:1:MET:HA	2.44	0.47
1:C:7:LYS:HG2	1:D:45:PRO:HA	1.95	0.47
1:D:122:PHE:HE1	1:D:126:ILE:HG13	1.77	0.47
1:A:126:ILE:HG22	1:A:127:ARG:N	2.28	0.47
1:B:38:TYR:CD1	1:B:108:LEU:HD13	2.50	0.47
1:B:56:ARG:O	1:B:57:GLN:C	2.51	0.47
1:D:109:THR:HG22	1:D:110:PHE:CE1	2.50	0.47
1:D:86:VAL:O	1:D:90:ASN:HB2	2.15	0.47
1:B:50:PRO:HB2	1:A:47:HIS:CD2	2.49	0.47
1:A:34:ALA:HB2	1:A:105:ILE:CD1	2.43	0.47
1:C:136:ASN:ND2	1:C:136:ASN:N	2.63	0.47
1:D:77:GLU:H	1:D:77:GLU:CD	2.16	0.47
1:A:11:ALA:HB2	1:A:116:LEU:CD2	2.45	0.47
1:B:20:PRO:HD3	1:B:126:ILE:HD12	1.95	0.47
1:B:56:ARG:HB3	1:A:3:ILE:HG21	1.97	0.47
1:C:30:LEU:CD2	1:C:30:LEU:H	2.27	0.47
1:C:82:ARG:HD3	1:C:86:VAL:HG21	1.97	0.47
1:A:27:VAL:O	1:A:31:LEU:HG	2.15	0.47
1:B:58:ALA:C	1:B:60:LEU:N	2.61	0.47
1:A:121:SER:C	1:A:124:VAL:HG23	2.35	0.47
1:A:30:LEU:N	1:A:30:LEU:CD2	2.77	0.47
1:A:79:PRO:HA	1:A:82:ARG:NH1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:ILE:HG22	1:A:60:LEU:HD11	1.95	0.47
1:B:51:HIS:O	1:B:52:HIS:C	2.51	0.47
1:A:113:GLU:O	1:A:114:THR:C	2.53	0.47
1:B:49:SER:O	1:B:50:PRO:C	2.53	0.47
1:C:84:LEU:HD13	1:D:75:ASN:O	2.15	0.47
1:C:112:ARG:O	1:C:113:GLU:C	2.53	0.46
1:C:51:HIS:O	1:C:52:HIS:C	2.51	0.46
1:D:126:ILE:HG22	1:D:127:ARG:N	2.30	0.46
1:D:65:LEU:N	1:D:65:LEU:CD1	2.77	0.46
1:B:71:TRP:CD1	1:B:75:ASN:ND2	2.84	0.46
1:C:23:PHE:O	1:C:23:PHE:CG	2.68	0.46
1:D:39:ARG:O	1:D:40:GLU:C	2.52	0.46
1:B:113:GLU:HA	1:B:113:GLU:OE1	2.14	0.46
1:D:122:PHE:O	1:D:123:GLY:C	2.54	0.46
1:A:11:ALA:HB2	1:A:116:LEU:HD21	1.97	0.46
1:A:122:PHE:HA	1:A:138:PRO:HG3	1.98	0.46
1:A:92:ASN:ND2	1:A:92:ASN:N	2.63	0.46
1:C:110:PHE:CE2	1:C:140:LEU:CB	2.98	0.46
1:D:13:VAL:HG13	1:D:14:GLU:H	1.79	0.46
1:D:89:VAL:C	1:D:91:THR:H	2.19	0.46
1:D:92:ASN:ND2	1:D:92:ASN:N	2.63	0.46
1:C:71:TRP:CD1	1:C:75:ASN:ND2	2.83	0.46
1:D:27:VAL:HG11	1:D:62:TRP:NE1	2.30	0.46
1:A:68:LEU:HD23	1:A:89:VAL:CG2	2.46	0.46
1:B:102:TRP:CH2	1:B:119:LEU:HD21	2.51	0.46
1:B:26:SER:HG	1:B:29:ASP:H	1.63	0.46
1:C:27:VAL:O	1:C:28:ARG:C	2.53	0.46
1:D:51:HIS:O	1:D:52:HIS:C	2.53	0.46
1:D:125:TRP:CE3	1:D:126:ILE:N	2.83	0.46
1:A:37:LEU:HD12	1:A:38:TYR:CE2	2.51	0.46
1:C:102:TRP:CZ3	1:C:119:LEU:HD21	2.51	0.46
1:D:38:TYR:O	1:D:39:ARG:C	2.55	0.46
1:D:71:TRP:CE3	1:D:72:VAL:CA	2.99	0.46
1:B:72:VAL:CG2	1:A:85:VAL:CG2	2.94	0.45
1:B:7:LYS:O	1:B:9:PHE:N	2.49	0.45
1:D:42:LEU:HD21	1:D:55:LEU:CD2	2.46	0.45
1:A:38:TYR:O	1:A:39:ARG:C	2.53	0.45
1:B:72:VAL:CG2	1:B:85:VAL:HG11	2.24	0.45
1:D:62:TRP:HA	1:D:62:TRP:CE3	2.51	0.45
1:A:41:ALA:O	1:A:42:LEU:C	2.54	0.45
1:A:72:VAL:CG2	1:A:85:VAL:HG11	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:ARG:O	1:C:40:GLU:C	2.54	0.45
1:D:118:TYR:HE1	1:D:138:PRO:HB2	1.82	0.45
1:B:100:LEU:HA	1:B:100:LEU:HD12	1.46	0.45
1:C:20:PRO:O	1:C:23:PHE:HB3	2.16	0.45
1:C:39:ARG:CG	1:C:39:ARG:NH1	2.76	0.45
1:C:85:VAL:O	1:C:87:ASN:N	2.50	0.45
1:C:25:PRO:O	1:C:98:ARG:HD2	2.16	0.45
1:A:65:LEU:HD23	1:A:65:LEU:HA	1.69	0.45
1:B:139:ILE:H	1:B:139:ILE:HG12	1.63	0.45
1:B:24:PHE:HD1	1:B:24:PHE:H	1.61	0.45
1:B:42:LEU:HD21	1:B:55:LEU:HD23	1.98	0.45
1:A:9:PHE:CE2	1:A:104:HIS:HE1	2.34	0.45
1:B:16:LEU:HD11	1:B:103:PHE:HB2	1.98	0.45
1:C:131:ALA:HB3	1:C:132:TYR:CE2	2.52	0.45
1:A:102:TRP:HH2	1:A:119:LEU:HD21	1.81	0.45
1:B:49:SER:C	1:B:51:HIS:N	2.68	0.45
1:D:89:VAL:HA	1:D:93:MET:CG	2.39	0.45
1:A:125:TRP:O	1:A:133:ARG:HD3	2.16	0.45
1:C:66:MET:O	1:C:69:ALA:HB3	2.16	0.45
1:C:93:MET:O	1:C:94:GLY:C	2.54	0.45
1:A:12:THR:O	1:A:15:LEU:N	2.50	0.45
1:A:3:ILE:H	1:A:3:ILE:HG12	1.63	0.45
1:B:78:ASP:O	1:B:79:PRO:C	2.52	0.45
1:D:72:VAL:HG12	1:D:73:GLY:N	2.31	0.45
1:A:71:TRP:CE3	1:A:71:TRP:C	2.90	0.44
1:B:52:HIS:O	1:B:53:THR:C	2.55	0.44
1:B:67:THR:O	1:B:68:LEU:C	2.53	0.44
1:C:28:ARG:HA	1:C:28:ARG:HD2	1.70	0.44
1:C:47:HIS:ND1	1:D:50:PRO:HB3	2.32	0.44
1:D:102:TRP:CE3	1:D:103:PHE:HA	2.52	0.44
1:D:6:TYR:CE1	1:D:16:LEU:HD11	2.52	0.44
1:D:71:TRP:C	1:D:71:TRP:CE3	2.90	0.44
1:C:34:ALA:HB2	1:C:105:ILE:HD11	1.99	0.44
1:D:123:GLY:O	1:D:124:VAL:C	2.56	0.44
1:B:58:ALA:O	1:B:60:LEU:N	2.50	0.44
1:B:72:VAL:HG11	1:B:85:VAL:CG1	2.47	0.44
1:B:95:LEU:HD23	1:B:96:LYS:N	2.33	0.44
1:D:92:ASN:O	1:D:93:MET:C	2.55	0.44
1:C:116:LEU:O	1:C:117:GLU:C	2.56	0.44
1:C:125:TRP:CE3	1:C:126:ILE:CA	3.00	0.44
1:C:87:ASN:O	1:C:90:ASN:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:SER:O	1:A:124:VAL:CG2	2.66	0.44
1:B:16:LEU:HA	1:B:16:LEU:HD23	1.90	0.44
1:B:8:GLU:OE1	1:A:47:HIS:HD2	2.00	0.44
1:B:96:LYS:O	1:B:97:ILE:C	2.56	0.44
1:C:45:PRO:O	1:D:8:GLU:HA	2.17	0.44
1:D:65:LEU:HG	1:D:93:MET:HE2	1.98	0.44
1:C:88:TYR:CE2	1:D:68:LEU:HA	2.52	0.44
1:A:125:TRP:NE1	1:A:137:ALA:HA	2.33	0.44
1:A:39:ARG:NH1	1:A:39:ARG:HG2	2.32	0.44
1:B:77:GLU:O	1:B:82:ARG:NH1	2.51	0.44
1:D:94:GLY:O	1:D:95:LEU:C	2.54	0.44
1:C:27:VAL:HG12	1:C:31:LEU:CD1	2.47	0.44
1:D:62:TRP:O	1:D:65:LEU:HB2	2.17	0.44
1:A:125:TRP:HE3	1:A:126:ILE:N	2.15	0.44
1:A:84:LEU:HA	1:A:84:LEU:HD12	1.82	0.44
1:A:97:ILE:O	1:A:101:LEU:HG	2.17	0.44
1:C:70:THR:O	1:C:72:VAL:N	2.51	0.44
1:C:72:VAL:HG12	1:C:73:GLY:N	2.31	0.44
1:D:72:VAL:C	1:D:74:ASN:H	2.21	0.44
1:B:82:ARG:CG	1:B:82:ARG:HH11	2.30	0.44
1:C:66:MET:CE	1:C:90:ASN:HD21	2.31	0.44
1:C:77:GLU:O	1:C:78:ASP:C	2.56	0.44
1:D:37:LEU:C	1:D:38:TYR:CG	2.92	0.44
1:C:68:LEU:HA	1:D:88:TYR:CE2	2.52	0.44
1:B:137:ALA:HB1	1:B:138:PRO:CD	2.48	0.43
1:B:31:LEU:HD23	1:B:31:LEU:HA	1.70	0.43
1:C:71:TRP:CE3	1:C:72:VAL:HA	2.53	0.43
1:C:77:GLU:O	1:C:79:PRO:N	2.51	0.43
1:A:38:TYR:CE1	1:A:108:LEU:HB3	2.53	0.43
1:B:74:ASN:N	1:B:74:ASN:HD22	2.16	0.43
1:B:84:LEU:HA	1:B:84:LEU:HD12	1.86	0.43
1:C:16:LEU:HA	1:C:16:LEU:HD23	1.48	0.43
1:D:85:VAL:O	1:D:87:ASN:N	2.51	0.43
1:A:19:LEU:HA	1:A:19:LEU:HD23	1.66	0.43
1:B:102:TRP:CE3	1:B:103:PHE:N	2.86	0.43
1:D:111:GLY:O	1:D:112:ARG:C	2.57	0.43
1:B:19:LEU:HA	1:B:19:LEU:HD23	1.65	0.43
1:B:76:LEU:CD1	1:A:84:LEU:HB3	2.48	0.43
1:C:76:LEU:HD23	1:C:76:LEU:HA	1.79	0.43
1:D:113:GLU:O	1:D:114:THR:C	2.56	0.43
1:B:76:LEU:HD12	1:A:84:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:HE3	1:B:3:ILE:CD1	2.48	0.43
1:B:81:SER:C	1:B:83:ASP:H	2.22	0.43
1:C:22:ASP:C	1:C:22:ASP:OD1	2.56	0.43
1:C:38:TYR:CE1	1:C:108:LEU:HD13	2.53	0.43
1:D:28:ARG:O	1:D:31:LEU:N	2.52	0.43
1:C:24:PHE:N	1:C:24:PHE:CD1	2.87	0.43
1:C:82:ARG:HH11	1:C:82:ARG:HB3	1.83	0.43
1:D:8:GLU:OE1	1:D:9:PHE:CE1	2.72	0.43
1:A:87:ASN:O	1:A:91:THR:N	2.52	0.43
1:C:112:ARG:CZ	1:C:112:ARG:HB3	2.40	0.43
1:D:41:ALA:O	1:D:42:LEU:C	2.56	0.43
1:D:49:SER:O	1:D:52:HIS:N	2.52	0.43
1:A:124:VAL:O	1:A:125:TRP:C	2.55	0.43
1:A:77:GLU:CG	1:A:78:ASP:N	2.81	0.43
1:B:99:GLN:O	1:B:102:TRP:HB3	2.18	0.43
1:C:6:TYR:OH	1:C:100:LEU:HA	2.18	0.43
1:D:61:CYS:O	1:D:65:LEU:HD13	2.19	0.43
1:D:89:VAL:C	1:D:91:THR:N	2.72	0.43
1:A:37:LEU:C	1:A:38:TYR:CD2	2.92	0.42
1:B:102:TRP:O	1:B:103:PHE:C	2.56	0.42
1:C:16:LEU:HD11	1:C:103:PHE:HB2	2.01	0.42
1:D:30:LEU:HB3	1:D:101:LEU:HD12	2.01	0.42
1:A:112:ARG:HB2	1:A:112:ARG:HE	1.62	0.42
1:A:4:ASP:C	1:A:4:ASP:OD1	2.57	0.42
1:B:15:LEU:C	1:B:17:SER:H	2.21	0.42
1:B:55:LEU:HG	1:B:59:ILE:HD12	2.01	0.42
1:C:20:PRO:HG3	1:C:126:ILE:CD1	2.50	0.42
1:C:31:LEU:HA	1:C:31:LEU:HD23	1.58	0.42
1:D:24:PHE:CE2	1:D:99:GLN:HA	2.53	0.42
1:A:140:LEU:HD23	1:A:140:LEU:HA	1.33	0.42
1:A:27:VAL:O	1:A:28:ARG:C	2.57	0.42
1:B:125:TRP:CD1	1:B:134:PRO:HD2	2.54	0.42
1:D:110:PHE:CD1	1:D:110:PHE:N	2.88	0.42
1:D:87:ASN:O	1:D:88:TYR:C	2.58	0.42
1:B:38:TYR:CE1	1:B:108:LEU:HD13	2.54	0.42
1:B:82:ARG:HH11	1:B:82:ARG:HG2	1.85	0.42
1:C:130:PRO:O	1:C:132:TYR:N	2.53	0.42
1:C:28:ARG:O	1:C:31:LEU:N	2.53	0.42
1:D:134:PRO:CB	1:D:135:PRO:CD	2.94	0.42
1:A:100:LEU:HA	1:A:100:LEU:HD12	1.53	0.42
1:A:72:VAL:HG21	1:A:85:VAL:CG1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ASN:O	1:A:88:TYR:C	2.57	0.42
1:A:9:PHE:O	1:A:112:ARG:HD3	2.20	0.42
1:C:46:GLU:O	1:C:47:HIS:C	2.58	0.42
1:D:102:TRP:CH2	1:D:119:LEU:HD21	2.55	0.42
1:C:47:HIS:CE1	1:D:50:PRO:HG2	2.54	0.42
1:D:71:TRP:CE3	1:D:72:VAL:N	2.86	0.42
1:B:26:SER:OG	1:B:29:ASP:HB2	2.19	0.42
1:B:76:LEU:HA	1:B:76:LEU:HD12	1.68	0.42
1:B:8:GLU:OE2	1:A:53:THR:HA	2.20	0.42
1:B:99:GLN:O	1:B:102:TRP:N	2.53	0.42
1:C:1:MET:HE2	1:D:35:SER:N	2.35	0.42
1:C:33:THR:O	1:C:36:ALA:HB3	2.20	0.42
1:B:94:GLY:O	1:B:95:LEU:C	2.57	0.42
1:C:71:TRP:CE3	1:C:71:TRP:C	2.93	0.42
1:D:42:LEU:HD23	1:D:42:LEU:HA	1.72	0.42
1:B:30:LEU:O	1:B:31:LEU:C	2.58	0.42
1:B:68:LEU:HD13	1:A:93:MET:CE	2.49	0.42
1:C:107:CYS:HA	1:C:115:VAL:HG21	2.01	0.42
1:D:120:VAL:O	1:D:124:VAL:HG23	2.19	0.42
1:D:60:LEU:O	1:D:61:CYS:C	2.57	0.42
1:A:85:VAL:C	1:A:87:ASN:N	2.73	0.42
1:B:15:LEU:C	1:B:17:SER:N	2.72	0.42
1:C:87:ASN:C	1:C:89:VAL:N	2.72	0.42
1:B:28:ARG:O	1:B:31:LEU:N	2.53	0.41
1:A:125:TRP:CE2	1:A:137:ALA:HB2	2.55	0.41
1:C:17:SER:O	1:C:19:LEU:N	2.53	0.41
1:C:67:THR:O	1:C:70:THR:N	2.53	0.41
1:C:83:ASP:O	1:C:84:LEU:C	2.58	0.41
1:D:39:ARG:CG	1:D:39:ARG:HH11	2.22	0.41
1:D:7:LYS:C	1:D:9:PHE:H	2.23	0.41
1:A:125:TRP:O	1:A:128:THR:HB	2.20	0.41
1:A:49:SER:O	1:A:50:PRO:C	2.57	0.41
1:A:70:THR:O	1:A:72:VAL:N	2.53	0.41
1:C:26:SER:O	1:C:27:VAL:C	2.56	0.41
1:C:55:LEU:HD11	1:C:105:ILE:HG13	2.02	0.41
1:C:84:LEU:HD12	1:D:76:LEU:HG	2.02	0.41
1:C:96:LYS:C	1:C:98:ARG:N	2.73	0.41
1:D:129:PRO:HA	1:D:130:PRO:HD2	1.72	0.41
1:C:85:VAL:HG22	1:D:72:VAL:CG2	2.50	0.41
1:A:37:LEU:C	1:A:38:TYR:CG	2.94	0.41
1:B:37:LEU:O	1:B:38:TYR:CD1	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:MET:O	1:B:69:ALA:HB3	2.21	0.41
1:B:133:ARG:NH1	1:B:133:ARG:CG	2.81	0.41
1:D:62:TRP:CZ3	1:D:94:GLY:HA2	2.56	0.41
1:A:30:LEU:N	1:A:30:LEU:HD22	2.36	0.41
1:A:70:THR:O	1:A:71:TRP:C	2.59	0.41
1:C:111:GLY:O	1:C:114:THR:N	2.53	0.41
1:A:126:ILE:HG23	1:A:126:ILE:HD12	1.72	0.41
1:B:122:PHE:HE1	1:B:126:ILE:HD12	1.86	0.41
1:B:89:VAL:HG22	1:B:93:MET:HE1	2.02	0.41
1:C:100:LEU:HD12	1:C:100:LEU:HA	1.83	0.41
1:C:26:SER:HB3	1:C:29:ASP:OD2	2.20	0.41
1:D:71:TRP:HE3	1:D:72:VAL:CA	2.34	0.41
1:A:28:ARG:O	1:A:31:LEU:N	2.53	0.41
1:D:122:PHE:CE1	1:D:126:ILE:CG1	3.04	0.41
1:A:27:VAL:O	1:A:30:LEU:HB2	2.20	0.41
1:A:68:LEU:CD2	1:A:89:VAL:HG21	2.51	0.41
1:A:81:SER:O	1:A:82:ARG:C	2.59	0.41
1:A:89:VAL:CG2	1:A:93:MET:HE2	2.47	0.41
1:A:37:LEU:HB2	1:A:38:TYR:CE2	2.56	0.41
1:B:130:PRO:O	1:B:132:TYR:N	2.54	0.41
1:B:26:SER:OG	1:B:29:ASP:N	2.49	0.41
1:A:125:TRP:O	1:A:133:ARG:CD	2.69	0.41
1:A:82:ARG:HD2	1:A:83:ASP:H	1.86	0.41
1:D:117:GLU:O	1:D:118:TYR:C	2.57	0.41
1:A:39:ARG:O	1:A:40:GLU:C	2.59	0.40
1:B:89:VAL:HG22	1:B:93:MET:CE	2.51	0.40
1:C:90:ASN:N	1:C:90:ASN:HD22	2.19	0.40
1:D:101:LEU:O	1:D:105:ILE:HB	2.21	0.40
1:D:116:LEU:HA	1:D:116:LEU:HD23	1.87	0.40
1:A:66:MET:O	1:A:69:ALA:HB3	2.20	0.40
1:C:6:TYR:CZ	1:C:16:LEU:CD1	3.00	0.40
1:D:24:PHE:HB2	1:D:98:ARG:NH1	2.36	0.40
1:D:46:GLU:O	1:D:47:HIS:C	2.56	0.40
1:A:129:PRO:HA	1:A:130:PRO:HD3	1.99	0.40
1:A:24:PHE:N	1:A:24:PHE:CD1	2.89	0.40
1:A:62:TRP:HE3	1:A:97:ILE:HG13	1.85	0.40
1:A:82:ARG:HD2	1:A:83:ASP:N	2.35	0.40
1:B:130:PRO:O	1:B:131:ALA:C	2.59	0.40
1:D:102:TRP:CE3	1:D:103:PHE:N	2.90	0.40
1:D:27:VAL:CG1	1:D:31:LEU:HD11	2.51	0.40
1:B:20:PRO:O	1:B:23:PHE:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:LEU:HB3	1:C:82:ARG:HB2	2.03	0.40
1:D:119:LEU:O	1:D:120:VAL:C	2.58	0.40
1:D:84:LEU:HD12	1:D:84:LEU:HA	1.83	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	140/149 (94%)	99 (71%)	30 (21%)	11 (8%)	1	6
1	B	141/149 (95%)	84 (60%)	46 (33%)	11 (8%)	1	6
1	C	140/149 (94%)	101 (72%)	30 (21%)	9 (6%)	1	9
1	D	141/149 (95%)	91 (64%)	35 (25%)	15 (11%)	0	3
All	All	562/596 (94%)	375 (67%)	141 (25%)	46 (8%)	1	5

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	VAL
1	C	18	PHE
1	D	8	GLU
1	D	90	ASN
1	B	8	GLU
1	B	18	PHE
1	B	44	SER
1	A	80	ALA
1	A	86	VAL
1	A	123	GLY
1	C	28	ARG
1	C	71	TRP

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Mol	Chain	Res	Type
1	C	86	VAL
1	D	135	PRO
1	B	28	ARG
1	B	38	TYR
1	A	28	ARG
1	A	40	GLU
1	C	39	ARG
1	C	40	GLU
1	C	112	ARG
1	D	28	ARG
1	D	100	LEU
1	D	124	VAL
1	D	141	SER
1	B	39	ARG
1	B	113	GLU
1	B	124	VAL
1	A	141	SER
1	C	29	ASP
1	D	44	SER
1	D	101	LEU
1	A	71	TRP
1	A	134	PRO
1	D	39	ARG
1	D	86	VAL
1	D	131	ALA
1	B	29	ASP
1	B	105	ILE
1	C	44	SER
1	D	49	SER
1	D	134	PRO
1	D	139	ILE
1	B	135	PRO
1	A	79	PRO
1	A	45	PRO

### 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	126/133 (95%)	98 (78%)	28 (22%)	1	3
1	B	127/133 (96%)	99 (78%)	28 (22%)	1	3
1	C	126/133 (95%)	95 (75%)	31 (25%)	0	2
1	D	127/133 (96%)	92 (72%)	35 (28%)	0	1
All	All	506/532 (95%)	384 (76%)	122 (24%)	0	2

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1	MET
1	C	8	GLU
1	C	15	LEU
1	C	17	SER
1	C	21	SER
1	C	23	PHE
1	C	26	SER
1	C	28	ARG
1	C	30	LEU
1	C	37	LEU
1	C	39	ARG
1	C	44	SER
1	C	47	HIS
1	C	59	ILE
1	C	64	GLU
1	C	65	LEU
1	C	66	MET
1	C	68	LEU
1	C	74	ASN
1	C	77	GLU
1	C	82	ARG
1	C	92	ASN
1	C	93	MET
1	C	95	LEU
1	C	106	SER
1	C	112	ARG
1	C	113	GLU
1	C	114	THR
1	C	136	ASN
1	C	139	ILE
1	C	142	THR
1	D	1	MET
1	D	2	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	8	GLU
1	D	12	THR
1	D	23	PHE
1	D	24	PHE
1	D	26	SER
1	D	28	ARG
1	D	37	LEU
1	D	40	GLU
1	D	44	SER
1	D	45	PRO
1	D	47	HIS
1	D	55	LEU
1	D	59	ILE
1	D	64	GLU
1	D	67	THR
1	D	68	LEU
1	D	70	THR
1	D	72	VAL
1	D	74	ASN
1	D	77	GLU
1	D	82	ARG
1	D	85	VAL
1	D	90	ASN
1	D	92	ASN
1	D	93	MET
1	D	101	LEU
1	D	112	ARG
1	D	121	SER
1	D	126	ILE
1	D	136	ASN
1	D	139	ILE
1	D	140	LEU
1	D	141	SER
1	B	1	MET
1	B	2	ASP
1	B	7	LYS
1	B	16	LEU
1	B	17	SER
1	B	21	SER
1	B	28	ARG
1	B	30	LEU
1	B	37	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	44	SER
1	B	49	SER
1	B	64	GLU
1	B	65	LEU
1	B	66	MET
1	B	70	THR
1	B	71	TRP
1	B	72	VAL
1	B	77	GLU
1	B	82	ARG
1	B	85	VAL
1	B	92	ASN
1	B	97	ILE
1	B	108	LEU
1	B	109	THR
1	B	113	GLU
1	B	124	VAL
1	B	142	THR
1	B	143	LEU
1	A	2	ASP
1	A	3	ILE
1	A	14	GLU
1	A	23	PHE
1	A	37	LEU
1	A	40	GLU
1	A	44	SER
1	A	46	GLU
1	A	47	HIS
1	A	64	GLU
1	A	68	LEU
1	A	72	VAL
1	A	74	ASN
1	A	77	GLU
1	A	82	ARG
1	A	85	VAL
1	A	87	ASN
1	A	90	ASN
1	A	92	ASN
1	A	93	MET
1	A	106	SER
1	A	108	LEU
1	A	114	THR

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Mol	Chain	Res	Type
1	A	124	VAL
1	A	126	ILE
1	A	127	ARG
1	A	139	ILE
1	A	142	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	75	ASN
1	C	90	ASN
1	C	92	ASN
1	C	136	ASN
1	D	74	ASN
1	D	92	ASN
1	B	47	HIS
1	B	52	HIS
1	B	74	ASN
1	B	75	ASN
1	B	92	ASN
1	A	47	HIS
1	A	52	HIS
1	A	92	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

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.