



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:03 pm BST

PDB ID : 1NJ9
Title : Cocaine hydrolytic antibody 15A10
Authors : Larsen, N.A.; de Prada, P.; Deng, S.X.; Zhu, X.; Landry, D.W.; Wilson, I.A.
Deposited on : 2002-12-30
Resolution : 2.35 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 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

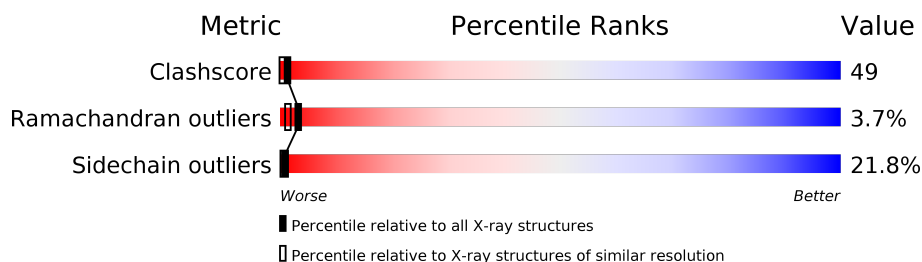
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)

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 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	212	31% 49% 20%
1	L	212	24% 58% 16% .
2	B	215	36% 50% 13% .
2	H	215	32% 51% 16%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6579 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 immunoglobulin variable chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	212	Total 1616	C 1010	N 271	O 329	S 6	0	0	0
1	A	212	Total 1616	C 1010	N 271	O 329	S 6	0	0	0

- Molecule 2 is a protein called immunoglobulin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	215	Total 1620	C 1027	N 265	O 321	S 7	0	0	0
2	B	215	Total 1612	C 1020	N 265	O 320	S 7	0	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	3	Total 3	Na 3	0	0
3	B	2	Total 2	Na 2	0	0
3	A	1	Total 1	Na 1	0	0
3	L	2	Total 2	Na 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	25	Total 25	O 25	0	0
4	H	29	Total 29	O 29	0	0

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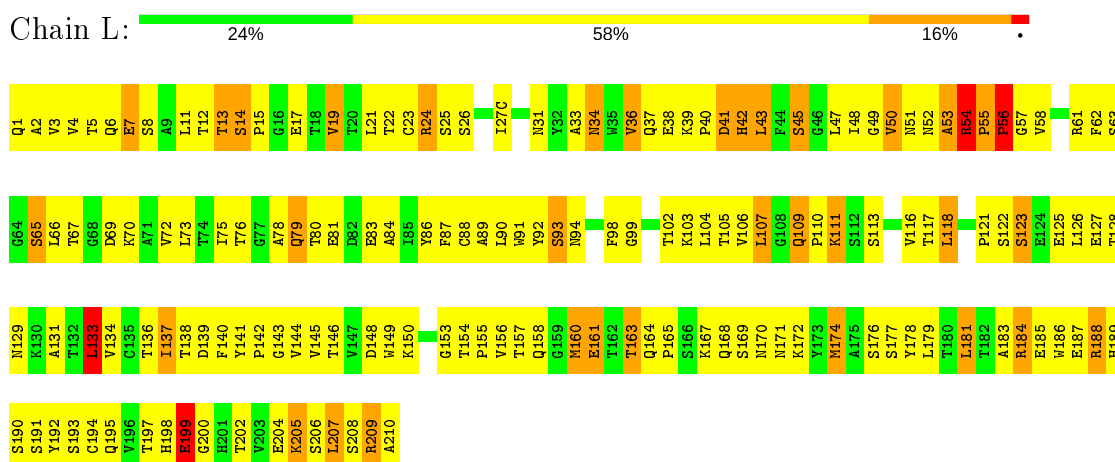
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total 23	O 23	0	0
4	B	30	Total 30	O 30	0	0

3 Residue-property plots

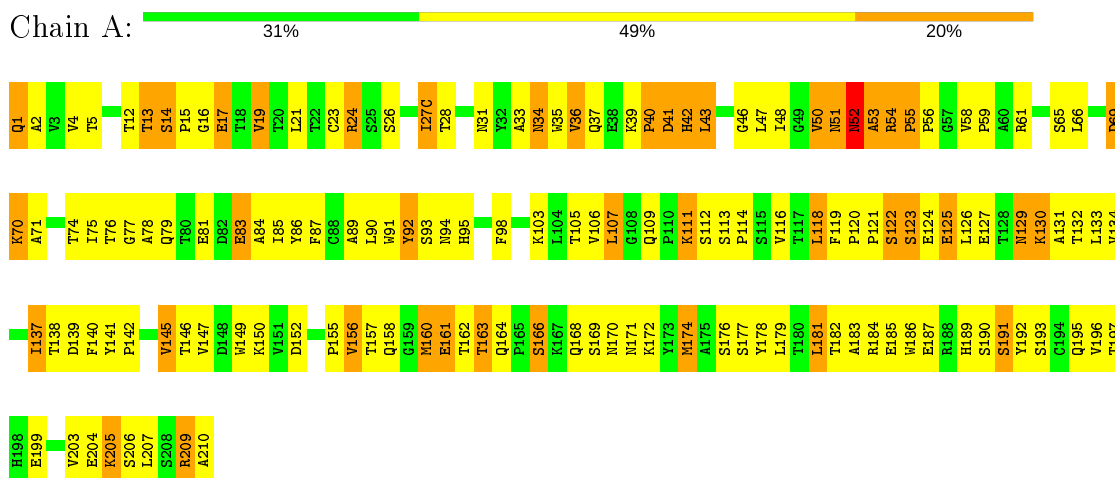
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

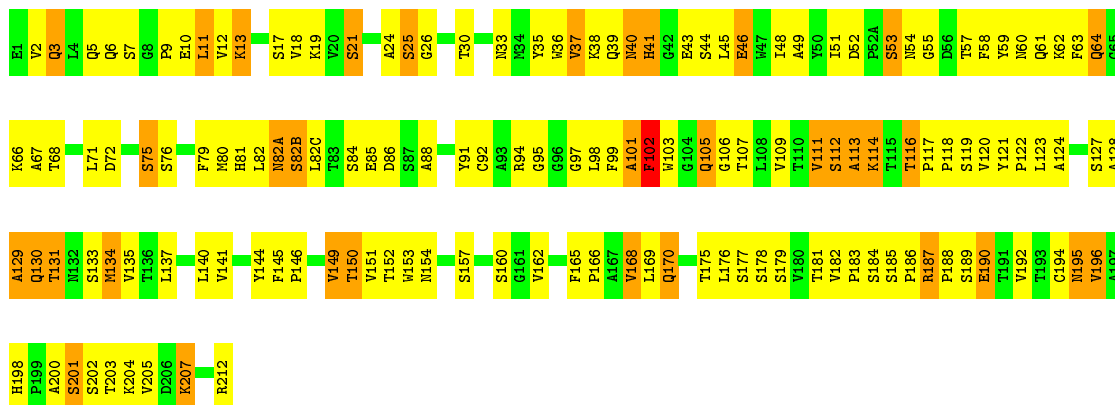


- Molecule 1: immunoglobulin variable chain



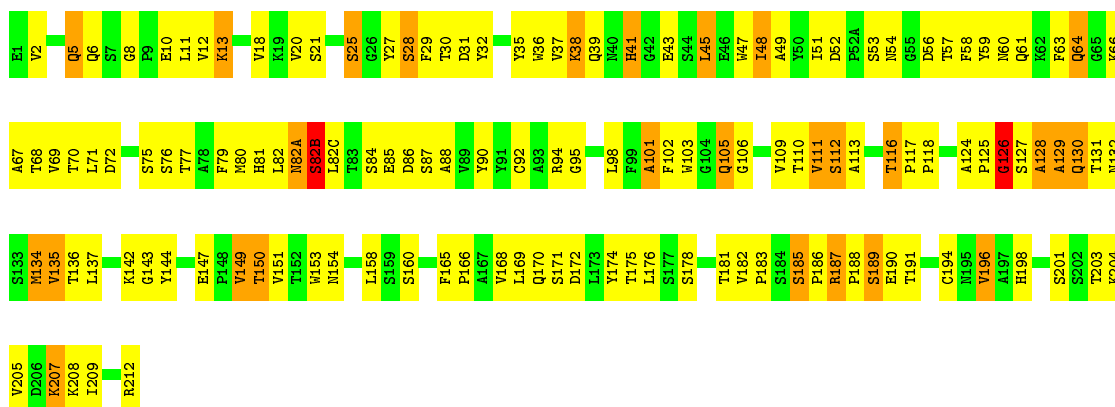
- Molecule 2: immunoglobulin heavy chain





- Molecule 2: immunoglobulin heavy chain

Chain B: 36% 50% 13%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	37.50Å 108.40Å 111.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.35	Depositor
% Data completeness (in resolution range)	80.0 (30.00-2.35)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS 1.1, SHELXL-97 & CNS1.1	Depositor
R, R_{free}	0.199 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6579	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.44	0/1655	0.84	3/2262 (0.1%)
1	L	0.51	1/1655 (0.1%)	1.03	14/2262 (0.6%)
2	B	0.45	0/1656	0.86	2/2261 (0.1%)
2	H	0.50	0/1664	0.91	2/2273 (0.1%)
All	All	0.47	1/6630 (0.0%)	0.91	21/9058 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	55	PRO	CB-CG	-5.13	1.24	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	55	PRO	N-CA-C	13.41	146.97	112.10
1	L	56	PRO	N-CA-C	-9.91	86.34	112.10
1	L	93	SER	CA-C-N	-9.21	96.93	117.20
2	B	126	GLY	N-CA-C	-8.72	91.30	113.10
1	L	93	SER	N-CA-C	8.61	134.23	111.00
2	B	126	GLY	C-N-CA	-6.91	104.43	121.70
1	A	92	TYR	C-N-CA	-6.24	106.10	121.70
1	L	55	PRO	C-N-CD	-6.22	106.92	120.60
1	L	41	ASP	N-CA-C	-6.05	94.67	111.00
1	L	92	TYR	C-N-CA	-5.98	106.75	121.70
1	A	69	ASP	N-CA-C	-5.97	94.89	111.00
2	H	101	ALA	C-N-CA	-5.95	106.83	121.70
2	H	102	PHE	CB-CG-CD2	-5.77	116.76	120.80
1	L	43	LEU	CA-CB-CG	5.63	128.26	115.30
1	L	133	LEU	CA-CB-CG	5.49	127.93	115.30
1	L	93	SER	O-C-N	5.43	131.40	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	93	SER	CA-C-O	5.32	131.27	120.10
1	L	55	PRO	CA-N-CD	-5.30	104.09	111.50
1	A	93	SER	CA-C-N	-5.11	105.97	117.20
1	L	55	PRO	CB-CA-C	-5.07	99.32	112.00
1	L	93	SER	C-N-CA	5.00	134.21	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1616	0	1556	181	0
1	L	1616	0	1556	161	0
2	B	1612	0	1552	160	0
2	H	1620	0	1574	159	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	H	3	0	0	0	0
3	L	2	0	0	0	0
4	A	23	0	0	4	0
4	B	30	0	0	6	0
4	H	29	0	0	5	0
4	L	25	0	0	4	0
All	All	6579	0	6238	624	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 49.

All (624) 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:L:2:ALA:HB1	1:L:26:SER:OG	1.34	1.24
1:L:54:ARG:HB3	1:L:55:PRO:HD3	1.21	1.12
1:L:45:SER:HB3	2:H:102:PHE:HE2	1.05	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:PRO:HG3	2:B:126:GLY:HA2	1.30	1.06
2:B:125:PRO:O	2:B:126:GLY:O	1.71	1.06
1:L:45:SER:HB3	2:H:102:PHE:CE2	1.90	1.05
1:L:54:ARG:HB3	1:L:55:PRO:CD	1.89	1.03
2:H:52:ASP:HB3	2:H:54:ASN:OD1	1.59	1.02
2:B:183:PRO:HD2	2:B:186:PRO:HG2	1.44	0.99
1:L:118:LEU:HB2	1:L:205:LYS:HG2	1.43	0.97
1:A:19:VAL:HG13	1:A:75:ILE:HB	1.46	0.97
1:A:116:VAL:HG12	1:A:205:LYS:HD2	1.41	0.97
1:L:19:VAL:HG13	1:L:75:ILE:HB	1.44	0.96
1:L:168:GLN:HE21	1:L:174:MET:HB3	1.32	0.94
2:H:183:PRO:HD2	2:H:186:PRO:HG2	1.50	0.94
1:A:107:LEU:HD22	1:A:111:LYS:HE2	1.51	0.93
1:A:5:THR:HB	1:A:24:ARG:HE	1.30	0.93
1:L:45:SER:CB	2:H:102:PHE:HE2	1.80	0.93
1:A:111:LYS:HG3	1:A:142:PRO:HD3	1.51	0.92
1:L:39:LYS:HD3	1:L:84:ALA:HB2	1.51	0.92
1:A:51:ASN:HD22	1:A:65:SER:N	1.67	0.91
2:H:137:LEU:HD11	2:H:187:ARG:HG3	1.52	0.91
2:B:52:ASP:OD1	2:B:54:ASN:ND2	2.06	0.89
1:A:190:SER:HB3	1:A:210:ALA:HB3	1.54	0.89
1:L:54:ARG:CB	1:L:55:PRO:CD	2.51	0.89
2:B:187:ARG:HB3	2:B:187:ARG:HH11	1.38	0.88
1:L:50:VAL:O	1:L:52:ASN:ND2	2.07	0.87
1:A:168:GLN:HG2	1:A:174:MET:HE3	1.55	0.87
1:A:39:LYS:HB2	1:A:43:LEU:HB3	1.56	0.87
2:H:122:PRO:HD3	2:H:207:LYS:HE2	1.54	0.86
1:A:168:GLN:HE21	1:A:174:MET:HB3	1.40	0.86
1:L:56:PRO:HD2	1:L:58:VAL:HG23	1.55	0.85
2:B:72:ASP:OD2	2:B:75:SER:HB3	1.77	0.84
1:L:139:ASP:H	1:L:168:GLN:HE22	1.24	0.84
2:B:125:PRO:C	2:B:126:GLY:O	2.11	0.84
2:B:187:ARG:HD2	2:B:188:PRO:HA	1.57	0.84
2:B:135:VAL:HG13	2:B:182:VAL:HG23	1.59	0.84
2:H:187:ARG:HD2	2:H:188:PRO:HA	1.60	0.84
1:L:168:GLN:HG2	1:L:174:MET:HE3	1.60	0.84
1:A:193:SER:HB2	1:A:206:SER:HB3	1.60	0.83
2:H:205:VAL:HG21	2:B:191:THR:HG23	1.60	0.83
1:L:2:ALA:CB	1:L:26:SER:OG	2.24	0.83
2:B:127:SER:O	2:B:128:ALA:HB2	1.78	0.83
1:A:51:ASN:ND2	1:A:65:SER:H	1.77	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ASP:H	1:A:168:GLN:HE22	1.27	0.82
1:A:195:GLN:HG3	1:A:204:GLU:HG3	1.60	0.82
2:B:154:ASN:ND2	2:B:158:LEU:HD11	1.95	0.82
1:A:120:PRO:CG	2:B:126:GLY:HA2	2.09	0.82
1:A:131:ALA:HB3	1:A:181:LEU:CD1	2.10	0.81
2:B:198:HIS:HB3	2:B:203:THR:HB	1.63	0.81
1:A:4:VAL:HG22	1:A:90:LEU:HD12	1.63	0.79
2:H:187:ARG:HH11	2:H:187:ARG:HB3	1.46	0.79
2:H:137:LEU:HD12	2:H:192:VAL:HG11	1.65	0.79
1:A:116:VAL:O	1:A:205:LYS:HE3	1.83	0.78
1:A:51:ASN:HD22	1:A:65:SER:H	1.26	0.78
1:L:209:ARG:NH1	1:L:210:ALA:HB3	2.00	0.77
1:L:15:PRO:HA	1:L:78:ALA:O	1.84	0.77
2:H:19:LYS:HE2	2:H:79:PHE:HB3	1.67	0.76
2:H:130:GLN:HB3	2:H:184:SER:HB3	1.68	0.76
1:L:12:THR:HG21	1:L:107:LEU:HD21	1.67	0.76
2:B:198:HIS:ND1	2:B:201:SER:OG	2.15	0.76
2:H:2:VAL:HA	2:H:26:GLY:HA3	1.67	0.76
1:A:129:ASN:ND2	1:A:182:THR:HB	2.00	0.76
1:L:168:GLN:HB2	1:L:170:ASN:OD1	1.85	0.76
1:A:34:ASN:ND2	1:A:89:ALA:HB3	2.02	0.75
1:L:51:ASN:HD22	1:L:66:LEU:HD11	1.50	0.74
2:B:170:GLN:OE1	4:B:1024:HOH:O	2.03	0.74
1:A:51:ASN:ND2	1:A:65:SER:O	2.21	0.73
1:L:2:ALA:HB1	1:L:26:SER:HG	1.50	0.73
2:B:183:PRO:HD2	2:B:186:PRO:CG	2.17	0.73
1:A:163:THR:HG23	1:A:176:SER:O	1.89	0.73
2:B:187:ARG:NH1	2:B:187:ARG:HB3	2.03	0.73
1:A:2:ALA:HB1	1:A:26:SER:OG	1.89	0.73
1:A:168:GLN:HB2	1:A:170:ASN:OD1	1.89	0.73
2:B:59:TYR:HB2	2:B:64:GLN:HG3	1.70	0.72
2:B:48:ILE:HG13	2:B:49:ALA:N	2.05	0.72
2:H:119:SER:HB2	4:H:1009:HOH:O	1.87	0.72
2:H:37:VAL:HG12	2:H:91:TYR:HB2	1.70	0.72
1:A:116:VAL:CG1	1:A:205:LYS:HD2	2.19	0.72
1:L:133:LEU:HB2	1:L:179:LEU:HB3	1.71	0.72
1:L:118:LEU:N	1:L:205:LYS:HD3	2.03	0.72
1:L:195:GLN:HB2	1:L:202:THR:HG22	1.70	0.72
2:H:40:ASN:OD1	2:H:43:GLU:HB2	1.90	0.71
1:A:170:ASN:HD21	1:A:172:LYS:HB2	1.55	0.71
2:H:39:GLN:O	2:H:88:ALA:HB1	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:144:VAL:O	1:L:198:HIS:HD2	1.72	0.71
1:L:5:THR:HB	1:L:24:ARG:HB3	1.73	0.71
1:L:11:LEU:O	1:L:104:LEU:HA	1.91	0.71
1:A:46:GLY:CA	2:B:98:LEU:HD11	2.21	0.70
2:H:205:VAL:HG22	2:B:190:GLU:HA	1.72	0.70
1:A:116:VAL:HG12	1:A:205:LYS:CD	2.17	0.70
2:B:183:PRO:O	2:B:186:PRO:HD2	1.90	0.70
1:A:52:ASN:HD22	1:A:53:ALA:H	1.40	0.70
2:B:118:PRO:HB3	2:B:144:TYR:HB3	1.71	0.70
2:B:75:SER:O	2:B:76:SER:OG	2.06	0.70
2:H:9:PRO:HG3	4:H:1006:HOH:O	1.90	0.70
2:H:52:ASP:OD1	2:H:54:ASN:ND2	2.24	0.70
1:L:36:VAL:HG11	2:H:103:TRP:HZ2	1.56	0.70
2:B:125:PRO:O	2:B:212:ARG:HG3	1.91	0.70
2:H:66:LYS:HE3	2:H:86:ASP:OD2	1.92	0.69
2:B:82:LEU:HB3	2:B:82(C):LEU:HD21	1.74	0.69
2:B:203:THR:O	2:B:204:LYS:HG3	1.91	0.69
2:B:2:VAL:HG22	2:B:27:TYR:HB3	1.73	0.69
2:B:59:TYR:HB3	2:B:64:GLN:HA	1.72	0.69
1:A:52:ASN:ND2	1:A:53:ALA:H	1.90	0.69
1:L:116:VAL:HG12	1:L:205:LYS:HD2	1.73	0.68
1:A:23:CYS:O	1:A:70:LYS:HB2	1.92	0.68
2:B:81:HIS:HE1	2:B:82(A):ASN:HB3	1.59	0.68
2:B:98:LEU:O	2:B:101:ALA:N	2.27	0.68
1:A:51:ASN:ND2	1:A:65:SER:N	2.35	0.68
1:L:163:THR:HG23	1:L:176:SER:O	1.93	0.68
2:H:2:VAL:HA	2:H:25:SER:O	1.93	0.68
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.76	0.67
2:B:150:THR:O	2:B:196:VAL:HA	1.95	0.67
2:H:130:GLN:HG3	2:H:184:SER:OG	1.94	0.67
2:H:134:MET:HG2	2:H:181:THR:HG22	1.77	0.67
1:L:118:LEU:H	1:L:205:LYS:HD3	1.60	0.67
2:H:38:LYS:HB2	2:H:48:ILE:HD11	1.76	0.67
1:A:14:SER:O	1:A:17:GLU:HB2	1.94	0.66
1:L:107:LEU:HA	1:L:141:TYR:OH	1.94	0.66
1:L:93:SER:OG	1:L:94:ASN:N	2.26	0.66
1:A:133:LEU:HD11	1:A:186:TRP:HZ3	1.59	0.66
1:L:49:GLY:HA3	2:H:97:GLY:O	1.94	0.66
2:H:149:VAL:HG11	2:H:176:LEU:HD22	1.78	0.66
1:L:109:GLN:HA	4:L:1026:HOH:O	1.95	0.66
1:L:118:LEU:HD12	1:L:205:LYS:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:128:ALA:O	2:H:129:ALA:HB2	1.95	0.66
2:H:187:ARG:HB3	2:H:187:ARG:NH1	2.11	0.65
1:L:146:THR:HB	1:L:197:THR:HB	1.77	0.65
2:B:137:LEU:HD23	4:B:1035:HOH:O	1.95	0.65
1:A:152:ASP:HA	1:A:191:SER:HB3	1.78	0.65
1:L:121:PRO:HG3	1:L:131:ALA:HB1	1.79	0.65
1:A:189:HIS:O	1:A:209:ARG:HD3	1.96	0.65
1:A:46:GLY:HA3	2:B:98:LEU:HD11	1.79	0.65
2:H:11:LEU:HB2	4:H:1013:HOH:O	1.96	0.65
1:A:168:GLN:NE2	1:A:174:MET:HB3	2.12	0.65
1:A:189:HIS:HB2	1:A:192:TYR:OH	1.97	0.65
1:A:27(C):ILE:HD11	1:A:33:ALA:HB2	1.79	0.65
2:H:118:PRO:HB3	2:H:144:TYR:HB3	1.79	0.65
2:H:94:ARG:HG2	2:H:95:GLY:N	2.11	0.65
1:A:182:THR:HG23	1:A:185:GLU:OE1	1.97	0.65
2:H:66:LYS:HD2	2:H:82(A):ASN:O	1.97	0.65
2:B:61:GLN:HA	2:B:64:GLN:OE1	1.96	0.64
1:A:5:THR:HB	1:A:24:ARG:NE	2.09	0.64
2:B:39:GLN:O	2:B:88:ALA:HB1	1.97	0.64
2:B:81:HIS:O	2:B:82:LEU:HD23	1.97	0.64
2:B:137:LEU:HD11	2:B:187:ARG:HG3	1.78	0.64
1:L:36:VAL:HG11	2:H:103:TRP:CZ2	2.32	0.64
1:L:195:GLN:HA	1:L:204:GLU:HA	1.79	0.64
1:L:51:ASN:ND2	1:L:66:LEU:HD11	2.13	0.64
1:A:142:PRO:HD2	1:A:199:GLU:OE2	1.98	0.64
1:A:34:ASN:HD22	1:A:89:ALA:HB3	1.61	0.63
2:B:36:TRP:O	2:B:48:ILE:HG23	1.98	0.63
2:H:67:ALA:HA	2:H:81:HIS:O	1.99	0.63
1:L:34:ASN:HD22	1:L:89:ALA:HB3	1.62	0.63
2:B:72:ASP:HB3	2:B:77:THR:O	1.99	0.63
1:A:122:SER:OG	1:A:125:GLU:HB3	1.99	0.63
1:A:47:LEU:O	1:A:58:VAL:HG21	1.99	0.63
1:L:56:PRO:HD2	1:L:58:VAL:CG2	2.27	0.63
2:H:146:PRO:HD2	2:H:200:ALA:CB	2.28	0.63
1:L:42:HIS:CE1	4:L:1017:HOH:O	2.51	0.63
2:B:171:SER:O	2:B:172:ASP:HB2	1.99	0.62
2:B:127:SER:O	2:B:128:ALA:CB	2.46	0.62
1:A:123:SER:O	1:A:126:LEU:N	2.32	0.62
1:L:123:SER:H	2:H:212:ARG:NH2	1.97	0.62
1:A:85:ILE:HA	1:A:103:LYS:HA	1.80	0.62
1:L:7:GLU:HB2	1:L:102:THR:HG23	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:PRO:HB3	2:B:144:TYR:CD1	2.34	0.62
1:A:133:LEU:HD21	1:A:186:TRP:CH2	2.35	0.62
1:L:47:LEU:O	1:L:48:ILE:HD13	2.00	0.62
1:A:40:PRO:O	1:A:41:ASP:HB2	1.99	0.61
2:H:120:VAL:HA	2:H:140:LEU:O	2.00	0.61
2:H:37:VAL:HG11	2:H:103:TRP:HZ3	1.64	0.61
1:L:111:LYS:HG2	1:L:142:PRO:HD3	1.82	0.61
1:A:122:SER:O	1:A:126:LEU:HD12	2.00	0.61
1:L:183:ALA:O	1:L:187:GLU:HG3	2.00	0.61
1:L:161:GLU:HG3	2:H:168:VAL:HG21	1.81	0.61
1:A:1:GLN:HG3	1:A:95:HIS:CE1	2.36	0.61
2:H:40:ASN:HD21	2:H:43:GLU:HG3	1.66	0.61
1:L:139:ASP:H	1:L:168:GLN:NE2	1.97	0.61
2:B:118:PRO:CB	2:B:144:TYR:HB3	2.30	0.61
2:B:13:LYS:HD2	4:B:1008:HOH:O	2.01	0.60
2:B:54:ASN:OD1	2:B:56:ASP:HB2	2.00	0.60
2:H:72:ASP:OD1	2:H:75:SER:HB3	2.01	0.60
1:L:12:THR:CG2	1:L:107:LEU:HD21	2.30	0.60
2:H:183:PRO:O	2:H:186:PRO:HD2	2.02	0.60
1:L:80:THR:HA	1:L:106:VAL:HG11	1.84	0.60
2:B:11:LEU:HD12	2:B:110:THR:HB	1.82	0.60
2:B:29:PHE:CE2	2:B:76:SER:HA	2.36	0.60
2:B:82(A):ASN:ND2	2:B:82(B):SER:HB3	2.16	0.60
2:B:41:HIS:C	2:B:43:GLU:H	2.06	0.59
2:H:112:SER:OG	2:H:113:ALA:N	2.32	0.59
2:H:198:HIS:ND1	2:H:201:SER:OG	2.35	0.59
1:L:143:GLY:O	1:L:165:PRO:HG2	2.01	0.59
1:L:142:PRO:O	1:L:198:HIS:NE2	2.34	0.59
2:B:6:GLN:NE2	2:B:106:GLY:H	2.00	0.59
1:L:111:LYS:NZ	1:L:199:GLU:OE1	2.32	0.59
1:A:145:VAL:HG23	1:A:196:VAL:HG13	1.85	0.59
1:A:209:ARG:CZ	1:A:210:ALA:HB2	2.33	0.59
2:B:48:ILE:CD1	2:B:67:ALA:HB3	2.32	0.59
2:H:153:TRP:CZ3	2:H:194:CYS:HB3	2.37	0.59
2:B:72:ASP:HB2	2:B:79:PHE:HE1	1.68	0.59
1:L:153:GLY:O	1:L:155:PRO:HD3	2.03	0.59
2:B:170:GLN:HB3	4:B:1024:HOH:O	2.02	0.58
2:H:18:VAL:HG13	2:H:82(C):LEU:CD1	2.33	0.58
1:L:187:GLU:HA	1:L:209:ARG:HH21	1.67	0.58
2:B:41:HIS:CE1	2:B:87:SER:O	2.57	0.58
2:B:54:ASN:OD1	2:B:56:ASP:CB	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:54:ARG:CB	1:L:55:PRO:HD2	2.30	0.58
1:A:162:THR:HA	1:A:177:SER:HA	1.85	0.58
1:L:111:LYS:CG	1:L:142:PRO:HD3	2.33	0.58
2:H:130:GLN:HG2	2:H:130:GLN:O	2.04	0.58
1:A:170:ASN:HD22	1:A:172:LYS:HE3	1.67	0.58
1:A:19:VAL:CG1	1:A:75:ILE:HB	2.29	0.58
2:B:153:TRP:CZ3	2:B:194:CYS:HB3	2.39	0.58
1:L:161:GLU:HG3	2:H:168:VAL:CG2	2.33	0.58
1:A:27(C):ILE:HD13	1:A:66:LEU:HD22	1.86	0.58
1:A:161:GLU:O	1:A:178:TYR:HD2	1.87	0.58
2:H:52:ASP:OD1	2:H:53:SER:HB2	2.04	0.58
2:B:45:LEU:N	2:B:45:LEU:HD23	2.18	0.57
2:H:120:VAL:HG21	2:H:196:VAL:HG11	1.86	0.57
2:H:187:ARG:HD2	2:H:188:PRO:CA	2.33	0.57
1:L:34:ASN:ND2	2:H:99:PHE:HD1	2.02	0.57
1:A:61:ARG:HB2	1:A:76:THR:O	2.04	0.57
1:L:168:GLN:HE21	1:L:174:MET:CB	2.13	0.57
1:L:187:GLU:HA	1:L:209:ARG:NH2	2.20	0.57
1:A:59:PRO:HB2	1:A:61:ARG:HG2	1.85	0.57
1:A:114:PRO:HB3	1:A:140:PHE:HB3	1.86	0.57
1:A:209:ARG:NH1	1:A:210:ALA:HB2	2.18	0.57
2:B:203:THR:C	2:B:204:LYS:HG3	2.24	0.57
2:B:2:VAL:HG13	2:B:27:TYR:CD1	2.40	0.57
2:B:59:TYR:OH	2:B:68:THR:HA	2.05	0.57
1:A:129:ASN:HD22	1:A:182:THR:HB	1.69	0.56
2:H:3:GLN:O	2:H:24:ALA:HA	2.05	0.56
2:H:52:ASP:HB3	2:H:54:ASN:CG	2.24	0.56
2:B:124:ALA:HB1	2:B:125:PRO:HD2	1.85	0.56
2:B:130:GLN:N	2:B:130:GLN:OE1	2.38	0.56
2:B:134:MET:HG2	2:B:182:VAL:O	2.05	0.56
2:B:48:ILE:CD1	2:B:67:ALA:CB	2.82	0.56
1:A:54:ARG:HD2	1:A:58:VAL:HB	1.87	0.56
1:L:3:VAL:HB	1:L:24:ARG:NH2	2.19	0.56
2:B:137:LEU:CD1	2:B:187:ARG:HG3	2.35	0.56
2:H:41:HIS:H	2:H:41:HIS:CD2	2.23	0.56
1:L:123:SER:H	2:H:212:ARG:HH22	1.54	0.56
1:A:170:ASN:O	1:A:171:ASN:HB2	2.05	0.56
1:A:94:ASN:ND2	4:A:1013:HOH:O	2.38	0.56
1:L:39:LYS:CD	1:L:84:ALA:HB2	2.31	0.56
1:A:133:LEU:HD12	1:A:179:LEU:HD23	1.88	0.56
1:A:36:VAL:HG23	1:A:87:PHE:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:TRP:CE2	2:B:80:MET:HB2	2.42	0.55
2:H:36:TRP:O	2:H:48:ILE:HB	2.06	0.55
1:A:95:HIS:HA	2:B:47:TRP:CZ3	2.41	0.55
2:H:19:LYS:HE2	2:H:79:PHE:CB	2.36	0.55
2:H:2:VAL:CA	2:H:26:GLY:HA3	2.36	0.55
2:B:18:VAL:HG22	2:B:82(C):LEU:HD11	1.87	0.55
2:H:203:THR:HG23	2:H:205:VAL:HG23	1.87	0.55
2:H:18:VAL:HG13	2:H:82(C):LEU:HD11	1.88	0.55
1:A:36:VAL:HG11	2:B:103:TRP:CZ2	2.42	0.55
1:L:45:SER:CB	2:H:102:PHE:CE2	2.71	0.55
2:H:51:ILE:HB	2:H:57:THR:HG22	1.89	0.54
2:B:203:THR:HG23	2:B:205:VAL:HG23	1.90	0.54
1:A:1:GLN:HG3	1:A:95:HIS:ND1	2.22	0.54
1:A:85:ILE:N	1:A:85:ILE:HD12	2.22	0.54
2:H:39:GLN:HB2	2:H:45:LEU:CD2	2.37	0.54
1:A:118:LEU:HB2	1:A:205:LYS:HG2	1.90	0.54
1:A:121:PRO:HD3	1:A:133:LEU:CD2	2.37	0.54
1:A:39:LYS:HD2	1:A:84:ALA:HB2	1.90	0.54
2:B:5:GLN:HA	2:B:105:GLN:OE1	2.07	0.54
2:B:59:TYR:CE2	2:B:68:THR:HA	2.42	0.54
1:L:178:TYR:OH	2:H:177:SER:HB2	2.08	0.54
1:A:138:THR:CG2	1:A:139:ASP:N	2.70	0.54
2:H:146:PRO:HD2	2:H:200:ALA:HB3	1.90	0.54
1:A:183:ALA:O	1:A:187:GLU:HG3	2.08	0.54
1:A:42:HIS:N	1:A:42:HIS:ND1	2.56	0.54
2:H:18:VAL:HG22	2:H:82:LEU:HB2	1.89	0.54
1:L:24:ARG:HA	1:L:70:LYS:HB3	1.91	0.53
1:A:116:VAL:O	1:A:205:LYS:CE	2.56	0.53
1:A:90:LEU:HD12	1:A:92:TYR:OH	2.07	0.53
2:B:12:VAL:O	2:B:111:VAL:HA	2.08	0.53
2:H:131:THR:N	4:H:1028:HOH:O	2.39	0.53
1:A:121:PRO:HD3	1:A:133:LEU:HD23	1.91	0.53
2:H:60:ASN:HB3	2:H:63:PHE:HD2	1.73	0.53
1:A:55:PRO:HG2	1:A:58:VAL:HG23	1.90	0.53
1:L:168:GLN:HG3	1:L:172:LYS:O	2.07	0.53
1:L:133:LEU:HG	1:L:179:LEU:HD23	1.90	0.53
1:A:156:VAL:HG13	1:A:158:GLN:O	2.08	0.53
1:A:170:ASN:ND2	1:A:172:LYS:HB2	2.24	0.53
1:L:49:GLY:HA3	2:H:98:LEU:HB3	1.90	0.53
1:A:131:ALA:HB3	1:A:181:LEU:HD11	1.91	0.53
2:B:187:ARG:HD2	2:B:188:PRO:CA	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:36:VAL:HG23	1:L:87:PHE:HB2	1.90	0.53
1:A:118:LEU:HD13	1:A:207:LEU:CD2	2.39	0.53
2:H:52:ASP:O	2:H:55:GLY:N	2.38	0.53
2:H:6:GLN:HB2	2:H:105:GLN:OE1	2.09	0.53
1:L:184:ARG:O	1:L:188:ARG:HD2	2.09	0.53
1:L:3:VAL:HB	1:L:24:ARG:HH22	1.74	0.53
1:A:28:THR:O	1:A:31:ASN:HB2	2.09	0.53
1:L:19:VAL:CG1	1:L:75:ILE:HB	2.31	0.53
2:B:68:THR:HB	2:B:81:HIS:HB3	1.90	0.52
2:B:49:ALA:HB1	2:B:58:PHE:O	2.10	0.52
1:A:125:GLU:HG3	1:A:130:LYS:O	2.09	0.52
1:A:133:LEU:HD21	1:A:186:TRP:CZ3	2.45	0.52
1:A:204:GLU:HG2	1:A:205:LYS:N	2.25	0.52
2:H:201:SER:O	2:H:202:SER:HB2	2.10	0.52
2:B:20:VAL:O	2:B:79:PHE:HA	2.10	0.52
2:H:124:ALA:HB3	2:H:212:ARG:HD3	1.92	0.52
2:H:134:MET:HG3	2:H:182:VAL:O	2.09	0.52
1:A:91:TRP:CZ2	1:A:94:ASN:HA	2.44	0.52
2:H:7:SER:O	2:H:107:THR:HG23	2.10	0.52
2:H:82(B):SER:O	2:H:82(B):SER:OG	2.25	0.52
1:L:4:VAL:HG13	1:L:23:CYS:SG	2.50	0.52
1:A:119:PHE:HB2	1:A:134:VAL:HB	1.92	0.52
2:B:94:ARG:HG2	2:B:95:GLY:N	2.25	0.52
1:L:34:ASN:ND2	2:H:99:PHE:CD1	2.78	0.51
1:L:21:LEU:O	1:L:72:VAL:HG13	2.10	0.51
1:L:33:ALA:HB3	1:L:51:ASN:OD1	2.11	0.51
1:A:35:TRP:HB3	4:A:1009:HOH:O	2.11	0.51
1:A:122:SER:O	1:A:126:LEU:CD1	2.58	0.51
1:A:190:SER:CB	1:A:210:ALA:HB3	2.35	0.51
2:H:203:THR:O	2:H:204:LYS:HG3	2.09	0.51
2:H:61:GLN:HA	2:H:64:GLN:NE2	2.26	0.51
1:L:118:LEU:HD13	1:L:207:LEU:CD2	2.40	0.51
1:L:31:ASN:O	1:L:91:TRP:HB3	2.11	0.51
1:A:161:GLU:OE1	1:A:161:GLU:HA	2.09	0.51
2:H:168:VAL:HG12	2:H:175:THR:HB	1.91	0.51
1:L:170:ASN:HD21	1:L:172:LYS:HB2	1.76	0.51
2:B:154:ASN:ND2	2:B:158:LEU:CD1	2.70	0.51
2:H:49:ALA:HB1	2:H:58:PHE:O	2.09	0.51
1:A:131:ALA:O	1:A:181:LEU:HD12	2.11	0.51
1:A:118:LEU:HD13	1:A:207:LEU:HD23	1.92	0.51
2:B:118:PRO:CA	2:B:144:TYR:HB3	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:HIS:CE1	2:B:82(A):ASN:HB3	2.42	0.51
1:A:13:THR:HG23	1:A:14:SER:N	2.24	0.51
1:A:47:LEU:O	1:A:48:ILE:HD13	2.11	0.51
2:H:62:LYS:O	2:H:62:LYS:HG2	2.11	0.51
2:H:130:GLN:CG	2:H:133:SER:HA	2.41	0.50
2:H:75:SER:O	2:H:76:SER:OG	2.26	0.50
1:L:116:VAL:HG12	1:L:205:LYS:CD	2.39	0.50
1:A:133:LEU:HD11	1:A:186:TRP:CZ3	2.44	0.50
2:B:10:GLU:HG3	2:B:109:VAL:HG22	1.94	0.50
2:H:111:VAL:O	2:H:112:SER:HB2	2.11	0.50
1:L:25:SER:HB2	1:L:90:LEU:CD1	2.41	0.50
1:A:137:ILE:HD12	1:A:145:VAL:HG21	1.93	0.50
2:B:38:LYS:HD3	2:B:63:PHE:HZ	1.77	0.50
2:H:17:SER:HB2	2:H:82(A):ASN:HA	1.94	0.50
1:A:125:GLU:OE2	1:A:132:THR:N	2.44	0.50
1:L:5:THR:O	1:L:23:CYS:HA	2.11	0.50
2:B:116:THR:O	2:B:144:TYR:HA	2.12	0.49
1:L:170:ASN:ND2	1:L:172:LYS:HB2	2.27	0.49
2:H:117:PRO:HG2	2:B:208:LYS:HD2	1.94	0.49
1:L:110:PRO:HD3	4:L:1026:HOH:O	2.11	0.49
2:H:204:LYS:O	2:B:189:SER:O	2.30	0.49
2:B:51:ILE:HG12	2:B:71:LEU:HD13	1.94	0.49
2:H:146:PRO:O	2:H:198:HIS:NE2	2.39	0.49
1:L:140:PHE:CE1	1:L:143:GLY:HA2	2.48	0.49
1:A:137:ILE:CD1	1:A:145:VAL:HG21	2.43	0.49
2:B:143:GLY:HA2	4:B:1024:HOH:O	2.12	0.49
2:B:28:SER:HB2	2:B:31:ASP:HB2	1.95	0.49
2:B:59:TYR:CZ	2:B:68:THR:HA	2.47	0.49
1:L:117:THR:HA	1:L:205:LYS:HE2	1.93	0.49
1:L:158:GLN:HE22	1:L:181:LEU:HD23	1.78	0.49
1:L:67:THR:O	1:L:67:THR:HG22	2.13	0.49
1:L:80:THR:HA	1:L:106:VAL:CG1	2.42	0.49
1:L:170:ASN:O	1:L:171:ASN:HB2	2.13	0.49
2:B:80:MET:HE3	2:B:82:LEU:HG	1.94	0.49
1:A:168:GLN:CG	1:A:174:MET:HE3	2.35	0.48
1:A:37:GLN:HG3	1:A:86:TYR:CE2	2.47	0.48
1:L:193:SER:HB2	1:L:206:SER:OG	2.13	0.48
1:A:85:ILE:HG13	1:A:103:LYS:HG3	1.95	0.48
2:H:3:GLN:HB3	2:H:5:GLN:NE2	2.28	0.48
2:B:37:VAL:HG11	2:B:103:TRP:HZ3	1.78	0.48
2:H:128:ALA:O	2:H:129:ALA:CB	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:65:SER:OG	1:L:66:LEU:N	2.43	0.48
2:B:2:VAL:HG13	2:B:27:TYR:HD1	1.78	0.48
2:B:51:ILE:HB	2:B:57:THR:HG22	1.95	0.48
2:B:80:MET:CE	2:B:82:LEU:HG	2.44	0.48
2:H:51:ILE:HD13	2:H:71:LEU:HB2	1.95	0.48
1:L:34:ASN:HD21	2:H:99:PHE:HD1	1.59	0.48
2:B:149:VAL:HG11	2:B:176:LEU:HD22	1.95	0.48
1:L:195:GLN:HB2	1:L:202:THR:CG2	2.41	0.48
2:B:147:GLU:HG3	2:B:174:TYR:CE1	2.48	0.48
2:B:151:VAL:HG11	2:B:178:SER:CB	2.44	0.48
2:H:38:LYS:O	2:H:46:GLU:HB2	2.13	0.48
2:H:97:GLY:O	2:H:98:LEU:HB3	2.14	0.48
1:L:79:GLN:HA	1:L:79:GLN:OE1	2.14	0.48
2:B:2:VAL:HA	2:B:25:SER:O	2.13	0.48
1:A:138:THR:HG22	1:A:139:ASP:OD2	2.14	0.47
1:A:13:THR:HG22	1:A:106:VAL:HG22	1.95	0.47
2:H:12:VAL:HG23	2:H:13:LYS:N	2.29	0.47
2:H:116:THR:N	2:H:145:PHE:O	2.39	0.47
1:A:121:PRO:HG3	1:A:131:ALA:HB1	1.96	0.47
1:A:147:VAL:HG22	1:A:196:VAL:HG22	1.96	0.47
1:A:166:SER:OG	2:B:166:PRO:HD3	2.14	0.47
2:H:154:ASN:O	2:H:157:SER:HB2	2.14	0.47
2:H:130:GLN:CB	2:H:184:SER:HB3	2.43	0.47
1:A:149:TRP:CE3	1:A:179:LEU:HD22	2.49	0.47
1:L:139:ASP:OD1	1:L:168:GLN:OE1	2.33	0.47
1:L:61:ARG:HB2	1:L:76:THR:O	2.15	0.47
2:B:183:PRO:HD2	2:B:186:PRO:CD	2.44	0.47
1:A:2:ALA:HB1	1:A:26:SER:HG	1.80	0.47
1:A:39:LYS:HB2	1:A:43:LEU:CB	2.38	0.47
2:B:132:ASN:O	2:B:132:ASN:OD1	2.33	0.47
2:H:153:TRP:CH2	2:H:194:CYS:HB3	2.50	0.47
1:A:204:GLU:HG2	1:A:205:LYS:H	1.79	0.47
2:B:128:ALA:O	2:B:129:ALA:HB2	2.13	0.47
1:A:164:GLN:CD	1:A:164:GLN:H	2.18	0.47
1:A:51:ASN:HD22	1:A:65:SER:CA	2.27	0.47
2:H:21:SER:HB2	2:H:79:PHE:CE2	2.50	0.47
1:L:168:GLN:NE2	1:L:174:MET:HB3	2.14	0.47
1:L:191:SER:HB3	4:L:1015:HOH:O	2.14	0.47
1:L:62:PHE:CD2	1:L:75:ILE:HG12	2.50	0.47
1:L:121:PRO:HD2	1:L:186:TRP:CH2	2.50	0.47
1:L:148:ASP:HB2	1:L:195:GLN:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:VAL:HG12	1:A:50:VAL:O	2.15	0.47
2:H:118:PRO:CB	2:H:144:TYR:HB3	2.43	0.47
2:H:183:PRO:C	2:H:186:PRO:HD2	2.35	0.47
1:A:95:HIS:HA	2:B:47:TRP:HZ3	1.80	0.46
2:B:67:ALA:HA	2:B:81:HIS:O	2.16	0.46
2:H:121:TYR:HB2	2:H:140:LEU:HB3	1.97	0.46
2:H:2:VAL:N	2:H:26:GLY:HA3	2.30	0.46
1:L:12:THR:HG23	1:L:105:THR:HB	1.96	0.46
1:L:2:ALA:HB1	1:L:3:VAL:H	1.54	0.46
1:A:39:LYS:HD2	1:A:39:LYS:HA	1.82	0.46
1:A:69:ASP:HB2	4:A:1004:HOH:O	2.16	0.46
2:B:59:TYR:CB	2:B:64:GLN:HA	2.42	0.46
1:L:170:ASN:ND2	1:L:172:LYS:HD2	2.30	0.46
1:A:131:ALA:O	1:A:181:LEU:CD1	2.64	0.46
1:L:81:GLU:CD	1:L:81:GLU:H	2.19	0.46
1:A:170:ASN:ND2	1:A:172:LYS:HE3	2.31	0.46
1:A:85:ILE:HG13	1:A:103:LYS:HB2	1.97	0.46
1:L:5:THR:OG1	1:L:24:ARG:NH2	2.48	0.46
1:A:12:THR:HG23	1:A:105:THR:HB	1.98	0.46
1:A:59:PRO:HG2	1:A:61:ARG:CZ	2.46	0.46
2:B:38:LYS:HD3	2:B:63:PHE:CZ	2.50	0.46
1:L:27(C):ILE:HD12	1:L:90:LEU:HD11	1.98	0.46
2:B:90:TYR:HE1	2:B:109:VAL:HB	1.80	0.46
2:B:135:VAL:CG1	2:B:182:VAL:HG23	2.40	0.46
1:L:50:VAL:HG12	1:L:50:VAL:O	2.16	0.46
1:A:33:ALA:O	1:A:50:VAL:N	2.49	0.46
1:L:22:THR:HG22	1:L:72:VAL:HG22	1.98	0.46
1:L:48:ILE:HG23	1:L:53:ALA:O	2.16	0.46
1:L:37:GLN:HG3	1:L:86:TYR:CE2	2.51	0.46
2:B:35:TYR:O	2:B:92:CYS:HA	2.16	0.45
1:A:46:GLY:C	2:B:98:LEU:HD11	2.36	0.45
2:H:67:ALA:HB2	2:H:82:LEU:HD23	1.97	0.45
1:L:150:LYS:HA	1:L:154:THR:O	2.16	0.45
2:B:27:TYR:HD2	2:B:28:SER:O	1.99	0.45
2:H:186:PRO:O	2:H:190:GLU:N	2.46	0.45
1:L:140:PHE:CZ	1:L:165:PRO:HB3	2.52	0.45
1:L:123:SER:N	2:H:212:ARG:NH2	2.63	0.45
1:L:199:GLU:HB3	1:L:200:GLY:H	1.51	0.45
1:L:3:VAL:O	1:L:24:ARG:NH2	2.49	0.45
1:L:7:GLU:OE2	1:L:22:THR:N	2.46	0.45
1:A:36:VAL:HG11	2:B:103:TRP:HZ2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:HIS:O	2:B:43:GLU:HG3	2.17	0.45
2:B:48:ILE:HA	2:B:63:PHE:CD2	2.51	0.45
2:H:12:VAL:HG23	2:H:13:LYS:O	2.17	0.45
1:L:83:GLU:OE2	1:L:105:THR:HG23	2.17	0.45
1:L:88:CYS:O	1:L:98:PHE:HA	2.15	0.45
1:A:149:TRP:O	1:A:155:PRO:HA	2.17	0.45
1:A:40:PRO:O	1:A:41:ASP:CB	2.65	0.45
1:A:39:LYS:NZ	1:A:83:GLU:O	2.50	0.45
2:H:59:TYR:OH	2:H:68:THR:HA	2.16	0.45
2:H:152:THR:OG1	2:H:195:ASN:OD1	2.34	0.45
2:B:87:SER:OG	2:B:111:VAL:HG23	2.17	0.45
1:A:24:ARG:HB2	1:A:70:LYS:HB3	1.99	0.45
1:A:83:GLU:OE1	1:A:106:VAL:N	2.33	0.45
1:A:131:ALA:HB3	1:A:181:LEU:HD12	1.97	0.45
2:B:60:ASN:HB3	2:B:63:PHE:HB2	1.98	0.45
2:H:165:PHE:HB3	2:H:166:PRO:HD2	1.99	0.45
2:H:40:ASN:CG	2:H:43:GLU:HB2	2.37	0.45
1:L:50:VAL:C	1:L:52:ASN:H	2.19	0.45
2:B:29:PHE:CD2	2:B:76:SER:HA	2.52	0.45
2:H:176:LEU:HD23	2:H:177:SER:N	2.32	0.45
2:H:187:ARG:HA	2:H:188:PRO:HA	1.76	0.45
2:H:38:LYS:CB	2:H:48:ILE:HD11	2.45	0.45
1:A:16:GLY:O	1:A:77:GLY:HA2	2.17	0.44
1:A:51:ASN:HD22	1:A:65:SER:C	2.20	0.44
2:B:151:VAL:HG11	2:B:178:SER:HB3	1.99	0.44
1:A:85:ILE:HG13	1:A:103:LYS:CB	2.47	0.44
1:L:6:GLN:HG3	1:L:99:GLY:HA3	1.98	0.44
1:A:79:GLN:HB3	1:A:81:GLU:OE1	2.17	0.44
2:B:82(B):SER:O	2:B:82(B):SER:OG	2.29	0.44
2:H:124:ALA:HB3	2:H:212:ARG:CD	2.47	0.44
1:L:128:THR:O	1:L:129:ASN:HB2	2.18	0.44
1:L:79:GLN:HB3	1:L:81:GLU:CD	2.38	0.44
1:A:120:PRO:CD	2:B:126:GLY:HA2	2.47	0.44
1:A:98:PHE:CE2	2:B:45:LEU:HD12	2.52	0.44
2:H:122:PRO:O	2:H:123:LEU:HD23	2.18	0.44
2:H:150:THR:O	2:H:150:THR:HG22	2.18	0.44
1:A:182:THR:O	1:A:185:GLU:HB2	2.17	0.44
2:B:2:VAL:HG11	2:B:102:PHE:CD1	2.53	0.44
2:B:207:LYS:HA	2:B:207:LYS:HD3	1.30	0.44
2:H:33:ASN:O	2:H:95:GLY:N	2.51	0.44
1:L:14:SER:O	1:L:17:GLU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:LYS:HA	2:B:175:THR:HG23	1.98	0.44
2:B:185:SER:OG	2:B:186:PRO:HD3	2.18	0.44
2:H:145:PHE:HA	2:H:146:PRO:HA	1.70	0.44
1:L:79:GLN:HB3	1:L:81:GLU:OE2	2.17	0.44
1:A:21:LEU:HD12	1:A:21:LEU:N	2.33	0.44
2:B:6:GLN:NE2	2:B:106:GLY:N	2.66	0.44
2:H:162:VAL:HA	2:H:179:SER:O	2.18	0.44
1:L:137:ILE:O	1:L:174:MET:HA	2.18	0.44
2:H:35:TYR:O	2:H:92:CYS:HA	2.17	0.43
1:L:145:VAL:HA	1:L:197:THR:O	2.17	0.43
1:A:182:THR:H	1:A:185:GLU:CD	2.22	0.43
1:A:112:SER:N	1:A:141:TYR:O	2.49	0.43
2:H:116:THR:O	2:H:144:TYR:HA	2.18	0.43
2:H:94:ARG:HG2	2:H:95:GLY:H	1.83	0.43
1:L:116:VAL:HA	1:L:136:THR:O	2.18	0.43
1:L:150:LYS:HG3	1:L:195:GLN:HE22	1.82	0.43
1:L:38:GLU:OE2	1:L:42:HIS:HA	2.17	0.43
1:A:1:GLN:HB3	1:A:2:ALA:H	1.57	0.43
1:L:121:PRO:HB2	1:L:126:LEU:HG	2.00	0.43
1:L:189:HIS:HB2	1:L:192:TYR:OH	2.18	0.43
1:A:195:GLN:HA	1:A:204:GLU:HA	2.00	0.43
2:B:41:HIS:C	2:B:43:GLU:N	2.71	0.43
2:B:66:LYS:NZ	2:B:82(B):SER:O	2.51	0.43
2:H:187:ARG:HH11	2:H:187:ARG:CB	2.25	0.43
2:H:207:LYS:HA	2:H:207:LYS:HD2	1.81	0.43
2:H:51:ILE:CB	2:H:57:THR:HG22	2.47	0.43
1:L:149:TRP:HB2	1:L:156:VAL:HB	2.00	0.43
1:A:34:ASN:OD1	2:B:98:LEU:HB2	2.19	0.43
1:L:156:VAL:HG12	1:L:160:MET:SD	2.59	0.43
1:A:35:TRP:HE3	4:A:1009:HOH:O	2.01	0.43
2:H:44:SER:HB3	2:H:45:LEU:H	1.56	0.43
1:L:21:LEU:HD22	1:L:73:LEU:HD23	2.00	0.43
1:A:4:VAL:HG13	1:A:23:CYS:SG	2.59	0.43
2:H:102:PHE:HD2	2:H:102:PHE:HA	1.38	0.43
1:L:126:LEU:HD21	1:L:131:ALA:HB2	2.01	0.43
1:L:50:VAL:HG12	1:L:52:ASN:HD21	1.83	0.43
1:A:120:PRO:HA	1:A:133:LEU:HD23	2.00	0.43
1:A:145:VAL:CG2	1:A:196:VAL:HG13	2.48	0.43
2:B:153:TRP:HB2	2:B:158:LEU:HB2	2.01	0.43
2:H:38:LYS:O	2:H:46:GLU:N	2.51	0.43
1:L:79:GLN:O	1:L:106:VAL:HG21	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:80:MET:HB3	2:H:80:MET:HE2	1.69	0.43
1:L:7:GLU:H	1:L:7:GLU:HG2	1.30	0.43
2:H:59:TYR:CE2	2:H:68:THR:HA	2.54	0.42
1:L:145:VAL:HG23	1:L:146:THR:N	2.33	0.42
1:A:79:GLN:O	1:A:106:VAL:HG21	2.20	0.42
1:L:12:THR:HA	1:L:105:THR:O	2.19	0.42
2:H:119:SER:OG	2:B:208:LYS:HE2	2.19	0.42
2:H:36:TRP:CD2	2:H:80:MET:HB2	2.54	0.42
2:H:46:GLU:OE2	2:H:63:PHE:HZ	2.02	0.42
1:L:27(C):ILE:HD11	1:L:90:LEU:HD21	2.02	0.42
2:B:137:LEU:HD22	2:B:209:ILE:HG21	2.00	0.42
2:H:105:GLN:NE2	2:H:106:GLY:O	2.52	0.42
2:B:60:ASN:O	2:B:64:GLN:N	2.43	0.42
2:H:151:VAL:HG11	2:H:178:SER:HB3	2.02	0.42
1:A:24:ARG:CB	1:A:70:LYS:HD3	2.49	0.42
2:H:122:PRO:CD	2:H:207:LYS:HE2	2.37	0.42
1:L:185:GLU:O	1:L:188:ARG:HB2	2.20	0.42
1:A:85:ILE:CD1	1:A:103:LYS:HG3	2.49	0.42
1:A:193:SER:CB	1:A:206:SER:HB3	2.42	0.42
2:B:134:MET:HG3	2:B:183:PRO:HA	2.01	0.42
2:H:35:TYR:CG	2:H:99:PHE:HE2	2.37	0.42
2:H:114:LYS:HE3	1:A:124:GLU:HG3	2.01	0.42
1:A:15:PRO:HA	1:A:78:ALA:O	2.20	0.42
1:A:186:TRP:CE2	1:A:209:ARG:HG3	2.55	0.42
2:B:98:LEU:C	2:B:101:ALA:N	2.72	0.42
2:B:124:ALA:O	2:B:125:PRO:C	2.57	0.42
1:L:150:LYS:HG3	1:L:195:GLN:NE2	2.35	0.42
1:L:190:SER:O	1:L:208:SER:HA	2.20	0.42
1:A:146:THR:HB	1:A:197:THR:HB	2.02	0.42
2:B:28:SER:O	2:B:32:TYR:HD1	2.02	0.42
2:H:17:SER:HB2	2:H:82:LEU:O	2.20	0.42
1:L:4:VAL:CG1	1:L:23:CYS:SG	3.07	0.42
2:B:149:VAL:CG1	2:B:176:LEU:HD22	2.49	0.41
2:H:37:VAL:HG11	2:H:103:TRP:CZ3	2.49	0.41
2:B:165:PHE:HB3	2:B:166:PRO:HD2	2.02	0.41
2:H:130:GLN:CG	2:H:130:GLN:O	2.69	0.41
1:L:13:THR:HG23	1:L:14:SER:N	2.33	0.41
1:A:59:PRO:HG2	1:A:61:ARG:NH2	2.36	0.41
2:B:6:GLN:OE1	2:B:90:TYR:O	2.37	0.41
2:H:72:ASP:O	2:H:76:SER:N	2.53	0.41
1:L:23:CYS:O	1:L:70:LYS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:THR:O	1:A:106:VAL:HA	2.19	0.41
2:B:150:THR:HG22	2:B:150:THR:O	2.19	0.41
2:H:170:GLN:HE21	2:H:170:GLN:HA	1.85	0.41
2:B:82(C):LEU:HD23	2:B:86:ASP:OD2	2.21	0.41
1:A:114:PRO:HB2	1:A:137:ILE:CG2	2.51	0.41
1:A:186:TRP:CZ2	1:A:209:ARG:HB2	2.55	0.41
1:A:39:LYS:NZ	1:A:81:GLU:O	2.50	0.41
2:B:90:TYR:CE1	2:B:109:VAL:HB	2.56	0.41
2:B:27:TYR:CD2	2:B:28:SER:O	2.73	0.41
1:A:122:SER:OG	1:A:123:SER:N	2.52	0.41
1:A:23:CYS:HB3	1:A:71:ALA:HB3	2.03	0.41
2:B:187:ARG:HE	2:B:209:ILE:HG22	1.85	0.41
2:B:203:THR:O	2:B:204:LYS:CG	2.64	0.41
2:B:112:SER:OG	2:B:113:ALA:N	2.50	0.41
2:H:118:PRO:CA	2:H:144:TYR:HB3	2.51	0.41
2:H:141:VAL:HB	2:H:176:LEU:HB3	2.02	0.41
2:H:44:SER:HA	4:H:1011:HOH:O	2.20	0.41
1:A:137:ILE:O	1:A:174:MET:HA	2.20	0.41
1:A:114:PRO:HG2	1:A:203:VAL:HG21	2.03	0.41
2:B:125:PRO:HD3	4:B:1035:HOH:O	2.21	0.41
1:A:189:HIS:HB2	1:A:192:TYR:CZ	2.55	0.41
2:B:105:GLN:HE21	2:B:105:GLN:HB3	1.61	0.41
2:H:10:GLU:HB2	2:H:109:VAL:HG22	2.03	0.41
2:B:116:THR:HA	2:B:117:PRO:HD2	1.99	0.41
2:B:154:ASN:HB2	2:B:158:LEU:HG	2.03	0.41
2:B:203:THR:CG2	2:B:205:VAL:HG23	2.50	0.41
2:H:6:GLN:HB2	2:H:105:GLN:CD	2.42	0.41
1:L:118:LEU:HD13	1:L:207:LEU:HD21	2.02	0.41
1:L:81:GLU:OE1	1:L:81:GLU:N	2.45	0.41
1:A:17:GLU:O	1:A:78:ALA:N	2.47	0.40
1:A:129:ASN:HD21	1:A:182:THR:HB	1.83	0.40
2:B:136:THR:OG1	2:B:181:THR:HG23	2.20	0.40
1:A:121:PRO:O	2:B:212:ARG:NH2	2.54	0.40
2:H:122:PRO:HD3	2:H:207:LYS:CE	2.40	0.40
2:H:150:THR:O	2:H:196:VAL:HA	2.21	0.40
1:L:122:SER:OG	1:L:125:GLU:HB3	2.21	0.40
1:L:133:LEU:HG	1:L:179:LEU:CD2	2.51	0.40
2:B:187:ARG:HH21	2:B:209:ILE:HG22	1.86	0.40
1:L:134:VAL:HG22	1:L:178:TYR:CD1	2.56	0.40
1:A:114:PRO:CB	1:A:140:PHE:HB3	2.50	0.40
1:A:170:ASN:HD21	1:A:172:LYS:CB	2.31	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:SER:OG	1:A:66:LEU:N	2.55	0.40
1:L:194:CYS:O	1:L:205:LYS:N	2.54	0.40
1:A:138:THR:HG23	1:A:139:ASP:N	2.36	0.40
2:B:147:GLU:HG3	2:B:174:TYR:CD1	2.57	0.40
2:B:59:TYR:OH	2:B:69:VAL:N	2.50	0.40
2:H:33:ASN:OD1	2:H:52:ASP:OD2	2.40	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	210/212 (99%)	185 (88%)	15 (7%)	10 (5%)	2	0
1	L	210/212 (99%)	188 (90%)	14 (7%)	8 (4%)	3	1
2	B	213/215 (99%)	182 (85%)	23 (11%)	8 (4%)	3	1
2	H	213/215 (99%)	191 (90%)	17 (8%)	5 (2%)	6	4
All	All	846/854 (99%)	746 (88%)	69 (8%)	31 (4%)	3	1

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	160	MET
2	H	129	ALA
1	A	41	ASP
1	A	160	MET
2	B	126	GLY
2	B	128	ALA
2	H	101	ALA
1	A	50	VAL
1	A	52	ASN

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Mol	Chain	Res	Type
2	B	8	GLY
2	B	129	ALA
1	L	53	ALA
1	L	56	PRO
2	H	112	SER
2	H	113	ALA
1	A	40	PRO
1	L	40	PRO
1	L	57	GLY
1	L	199	GLU
2	H	41	HIS
1	A	53	ALA
1	A	107	LEU
2	B	101	ALA
1	L	54	ARG
1	A	55	PRO
1	A	122	SER
2	B	41	HIS
2	B	82(B)	SER
2	B	112	SER
1	L	50	VAL
1	A	56	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	183/183 (100%)	141 (77%)	42 (23%)	1	0
1	L	183/183 (100%)	139 (76%)	44 (24%)	0	0
2	B	181/184 (98%)	148 (82%)	33 (18%)	1	1
2	H	184/184 (100%)	144 (78%)	40 (22%)	1	0
All	All	731/734 (100%)	572 (78%)	159 (22%)	1	0

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	GLN
1	L	7	GLU
1	L	8	SER
1	L	13	THR
1	L	14	SER
1	L	19	VAL
1	L	24	ARG
1	L	34	ASN
1	L	36	VAL
1	L	41	ASP
1	L	42	HIS
1	L	43	LEU
1	L	45	SER
1	L	54	ARG
1	L	63	SER
1	L	65	SER
1	L	69	ASP
1	L	79	GLN
1	L	103	LYS
1	L	107	LEU
1	L	109	GLN
1	L	111	LYS
1	L	113	SER
1	L	118	LEU
1	L	123	SER
1	L	127	GLU
1	L	133	LEU
1	L	137	ILE
1	L	138	THR
1	L	157	THR
1	L	161	GLU
1	L	163	THR
1	L	164	GLN
1	L	167	LYS
1	L	169	SER
1	L	174	MET
1	L	177	SER
1	L	181	LEU
1	L	184	ARG
1	L	188	ARG
1	L	199	GLU
1	L	205	LYS
1	L	207	LEU

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Mol	Chain	Res	Type
1	L	209	ARG
2	H	3	GLN
2	H	11	LEU
2	H	13	LYS
2	H	21	SER
2	H	25	SER
2	H	30	THR
2	H	37	VAL
2	H	40	ASN
2	H	46	GLU
2	H	53	SER
2	H	64	GLN
2	H	75	SER
2	H	82(A)	ASN
2	H	82(B)	SER
2	H	84	SER
2	H	85	GLU
2	H	102	PHE
2	H	105	GLN
2	H	111	VAL
2	H	114	LYS
2	H	116	THR
2	H	127	SER
2	H	130	GLN
2	H	131	THR
2	H	134	MET
2	H	135	VAL
2	H	149	VAL
2	H	150	THR
2	H	160	SER
2	H	168	VAL
2	H	169	LEU
2	H	170	GLN
2	H	185	SER
2	H	187	ARG
2	H	189	SER
2	H	190	GLU
2	H	195	ASN
2	H	196	VAL
2	H	201	SER
2	H	207	LYS
1	A	1	GLN

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Mol	Chain	Res	Type
1	A	13	THR
1	A	14	SER
1	A	17	GLU
1	A	19	VAL
1	A	24	ARG
1	A	27(C)	ILE
1	A	34	ASN
1	A	36	VAL
1	A	42	HIS
1	A	43	LEU
1	A	51	ASN
1	A	52	ASN
1	A	54	ARG
1	A	70	LYS
1	A	74	THR
1	A	83	GLU
1	A	109	GLN
1	A	111	LYS
1	A	113	SER
1	A	118	LEU
1	A	123	SER
1	A	125	GLU
1	A	127	GLU
1	A	129	ASN
1	A	130	LYS
1	A	137	ILE
1	A	145	VAL
1	A	150	LYS
1	A	156	VAL
1	A	157	THR
1	A	160	MET
1	A	161	GLU
1	A	163	THR
1	A	166	SER
1	A	169	SER
1	A	174	MET
1	A	181	LEU
1	A	184	ARG
1	A	191	SER
1	A	205	LYS
1	A	209	ARG
2	B	5	GLN

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Mol	Chain	Res	Type
2	B	13	LYS
2	B	21	SER
2	B	25	SER
2	B	28	SER
2	B	30	THR
2	B	38	LYS
2	B	45	LEU
2	B	48	ILE
2	B	53	SER
2	B	64	GLN
2	B	70	THR
2	B	82(A)	ASN
2	B	82(B)	SER
2	B	84	SER
2	B	85	GLU
2	B	105	GLN
2	B	111	VAL
2	B	116	THR
2	B	130	GLN
2	B	131	THR
2	B	134	MET
2	B	135	VAL
2	B	149	VAL
2	B	150	THR
2	B	160	SER
2	B	168	VAL
2	B	169	LEU
2	B	185	SER
2	B	187	ARG
2	B	189	SER
2	B	196	VAL
2	B	207	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	1	GLN
1	L	34	ASN
1	L	158	GLN
1	L	168	GLN
1	L	195	GLN
2	H	5	GLN

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Mol	Chain	Res	Type
2	H	40	ASN
2	H	41	HIS
2	H	64	GLN
1	A	1	GLN
1	A	51	ASN
1	A	52	ASN
1	A	109	GLN
1	A	129	ASN
1	A	158	GLN
1	A	168	GLN
1	A	195	GLN
2	B	6	GLN
2	B	41	HIS
2	B	81	HIS
2	B	82(A)	ASN
2	B	132	ASN
2	B	170	GLN

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](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.