



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:15 PM UTC

PDB ID : 2G33 / pdb_00002g33
Title : Human Hepatitis B Virus T=4 capsid, strain adyw
Authors : Bourne, C.R.; Zlotnick, A.
Deposited on : 2006-02-17
Resolution : 3.96 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

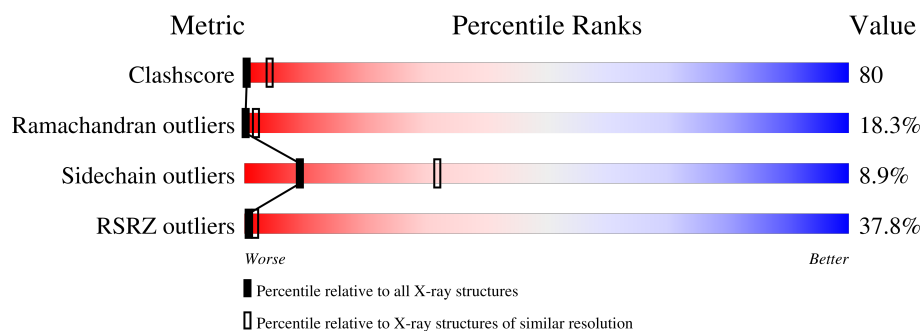
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.96 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1019 (4.14-3.78)
Ramachandran outliers	187476	1031 (4.16-3.76)
Sidechain outliers	187428	1024 (4.16-3.76)
RSRZ outliers	180081	1046 (4.16-3.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	150	39% 21% 50% 23% ..
1	B	150	29% 21% 50% 24% ..
1	C	150	41% 21% 47% 27% ..
1	D	150	40% 19% 51% 25% ..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4658 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 Core antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	147	Total	C	N	O	S	0	0	0
			1167	759	191	215	2			
1	D	146	Total	C	N	O	S	0	0	0
			1160	755	190	213	2			
1	B	147	Total	C	N	O	S	0	0	0
			1167	759	191	215	2			
1	A	148	Total	C	N	O	S	0	0	0
			1164	758	192	212	2			

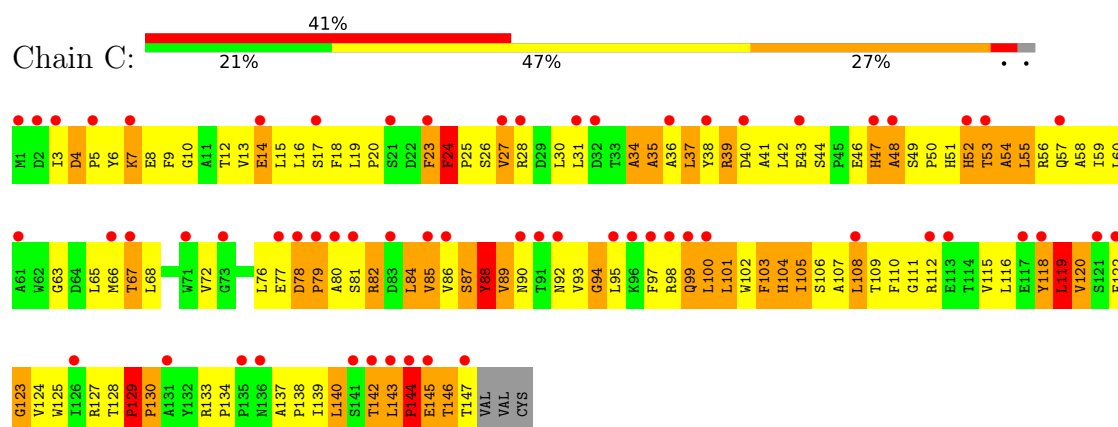
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	48	ALA	CYS	engineered mutation	UNP P03147
C	61	ALA	CYS	engineered mutation	UNP P03147
C	107	ALA	CYS	engineered mutation	UNP P03147
C	150	CYS	-	insertion	UNP P03147
D	48	ALA	CYS	engineered mutation	UNP P03147
D	61	ALA	CYS	engineered mutation	UNP P03147
D	107	ALA	CYS	engineered mutation	UNP P03147
D	150	CYS	-	insertion	UNP P03147
B	48	ALA	CYS	engineered mutation	UNP P03147
B	61	ALA	CYS	engineered mutation	UNP P03147
B	107	ALA	CYS	engineered mutation	UNP P03147
B	150	CYS	-	insertion	UNP P03147
A	48	ALA	CYS	engineered mutation	UNP P03147
A	61	ALA	CYS	engineered mutation	UNP P03147
A	107	ALA	CYS	engineered mutation	UNP P03147
A	150	CYS	-	insertion	UNP P03147

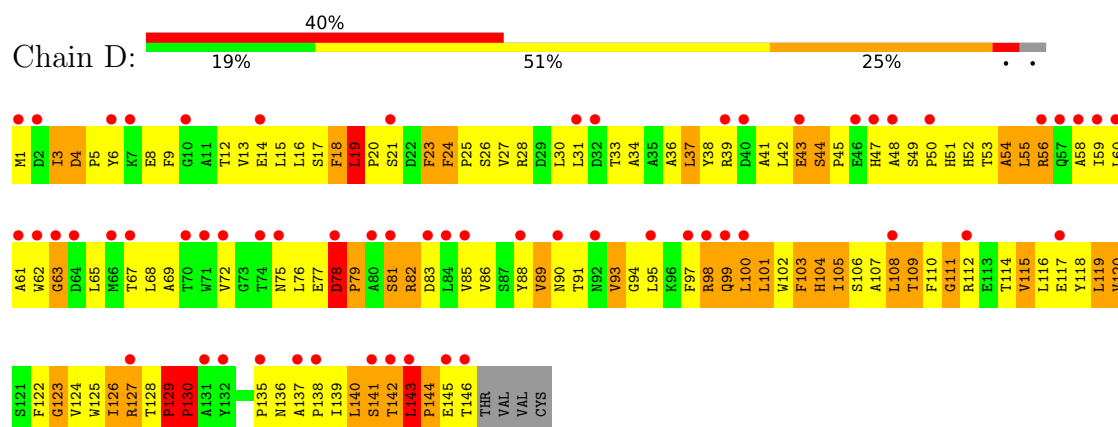
3 Residue-property plots [i](#)

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

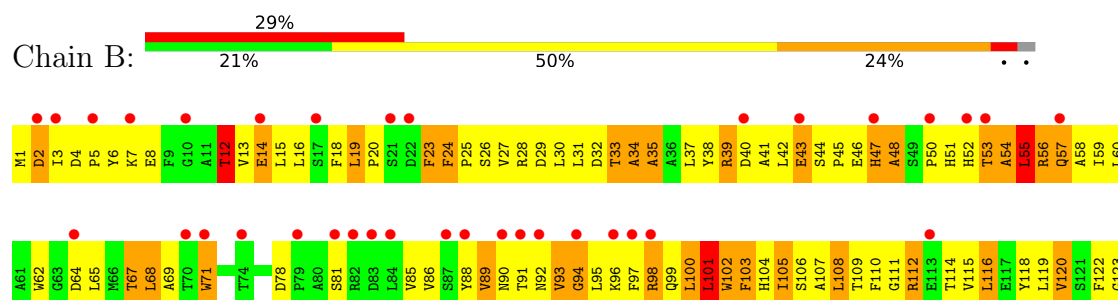
• Molecule 1: Core antigen

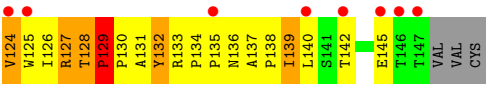


• Molecule 1: Core antigen

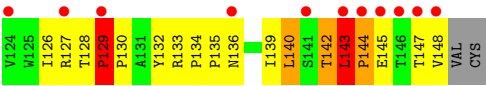
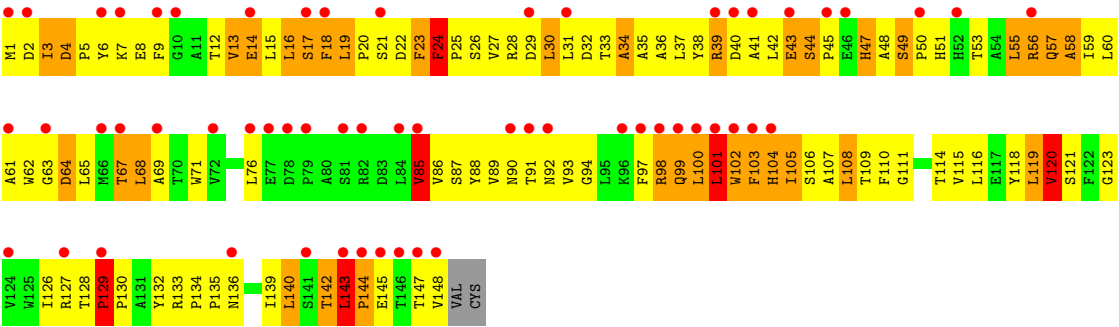
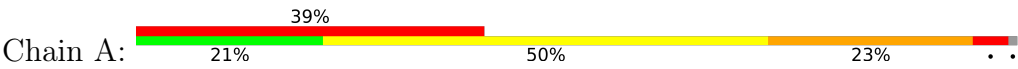


• Molecule 1: Core antigen





● Molecule 1: Core antigen



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	558.40Å 327.14Å 562.24Å 90.00° 109.12° 90.00°	Depositor
Resolution (Å)	40.00 – 3.96 40.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	79.2 (40.00-3.96) 81.4 (40.00-4.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 4.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.360 , 0.372 0.337 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	133.8	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 103.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h-1/2*k-l 0.000 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h+1/2*k-l	Xtriage
F_o, F_c correlation	0.51	EDS
Total number of atoms	4658	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.74	0/1200	1.35	24/1648 (1.5%)
1	B	0.73	0/1203	1.34	22/1652 (1.3%)
1	C	0.78	0/1203	1.46	24/1652 (1.5%)
1	D	0.81	1/1196 (0.1%)	1.45	29/1642 (1.8%)
All	All	0.77	1/4802 (0.0%)	1.40	99/6594 (1.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	144	PRO	CA-C	5.33	1.58	1.52

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	145	GLU	N-CA-C	16.37	136.58	109.24
1	D	82	ARG	N-CA-C	-11.06	99.81	113.20
1	C	85	VAL	N-CA-C	-10.96	103.02	111.90
1	C	140	LEU	N-CA-C	10.69	126.46	110.64
1	D	17	SER	N-CA-C	-10.47	99.60	112.38
1	A	64	ASP	N-CA-C	-10.28	101.24	113.88
1	A	142	THR	N-CA-C	-10.16	97.91	110.41
1	A	43	GLU	N-CA-C	-9.58	100.18	113.20
1	C	144	PRO	N-CA-C	9.41	131.85	112.47
1	A	144	PRO	N-CA-C	-9.36	102.51	114.03
1	D	143	LEU	N-CA-C	9.18	130.09	109.81
1	D	98	ARG	N-CA-C	-9.02	100.60	111.69
1	B	71	TRP	N-CA-C	-8.93	103.22	114.56
1	D	88	TYR	N-CA-C	-8.79	102.35	113.43
1	A	44	SER	CA-C-N	8.61	128.26	119.82
1	A	44	SER	C-N-CA	8.61	128.26	119.82
1	B	24	PHE	N-CA-C	8.40	121.68	110.08
1	D	67	THR	N-CA-C	-8.34	103.12	113.38
1	C	82	ARG	N-CA-C	-8.18	93.37	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	43	GLU	N-CA-C	-8.10	102.19	113.37
1	A	140	LEU	N-CA-C	7.85	122.93	112.25
1	D	129	PRO	CA-C-N	7.74	129.51	119.84
1	D	129	PRO	C-N-CA	7.74	129.51	119.84
1	B	14	GLU	N-CA-C	-7.68	102.36	112.34
1	A	94	GLY	N-CA-C	-7.64	103.64	112.50
1	C	144	PRO	CA-C-N	-7.54	110.52	122.73
1	C	144	PRO	C-N-CA	-7.54	110.52	122.73
1	C	4	ASP	CA-C-N	7.47	128.41	120.12
1	C	4	ASP	C-N-CA	7.47	128.41	120.12
1	B	24	PHE	CA-C-N	7.47	127.23	119.76
1	B	24	PHE	C-N-CA	7.47	127.23	119.76
1	C	24	PHE	CA-C-N	7.43	127.47	119.89
1	C	24	PHE	C-N-CA	7.43	127.47	119.89
1	B	142	THR	N-CA-C	-7.39	99.09	110.10
1	A	13	VAL	N-CA-C	-7.32	103.32	110.72
1	D	142	THR	N-CA-C	-7.24	101.38	111.81
1	D	140	LEU	N-CA-C	7.20	120.62	108.23
1	B	139	ILE	N-CA-C	7.18	120.33	109.20
1	C	67	THR	N-CA-C	-7.12	104.16	112.92
1	B	112	ARG	N-CA-C	-6.98	102.12	111.96
1	B	94	GLY	N-CA-C	-6.90	104.09	113.27
1	D	4	ASP	CA-C-N	6.85	128.40	119.84
1	D	4	ASP	C-N-CA	6.85	128.40	119.84
1	D	44	SER	CA-C-N	6.73	127.31	120.04
1	D	44	SER	C-N-CA	6.73	127.31	120.04
1	D	24	PHE	CA-C-N	6.55	126.58	119.89
1	D	24	PHE	C-N-CA	6.55	126.58	119.89
1	C	36	ALA	N-CA-C	-6.47	105.34	112.72
1	B	67	THR	N-CA-C	-6.38	104.81	112.59
1	D	141	SER	N-CA-C	6.36	119.59	107.75
1	A	24	PHE	CA-C-N	6.21	126.16	119.76
1	A	24	PHE	C-N-CA	6.21	126.16	119.76
1	A	98	ARG	N-CA-C	-6.14	103.74	111.11
1	C	129	PRO	N-CA-C	6.11	118.16	110.70
1	A	67	THR	N-CA-C	-6.11	104.73	111.82
1	C	128	THR	CA-C-N	6.05	126.61	120.38
1	C	128	THR	C-N-CA	6.05	126.61	120.38
1	B	98	ARG	N-CA-C	-6.01	104.65	111.14
1	C	17	SER	N-CA-C	-5.94	105.74	112.87
1	C	24	PHE	N-CA-C	5.92	117.16	109.64
1	D	19	LEU	N-CA-C	5.87	116.79	109.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	12	THR	N-CA-C	5.86	117.75	108.79
1	C	80	ALA	N-CA-C	-5.79	106.38	113.50
1	A	129	PRO	N-CA-C	5.79	117.77	110.70
1	A	143	LEU	CA-C-N	-5.79	113.85	119.87
1	A	143	LEU	C-N-CA	-5.79	113.85	119.87
1	B	128	THR	CA-C-N	5.76	126.31	120.38
1	B	128	THR	C-N-CA	5.76	126.31	120.38
1	D	78	ASP	CA-C-N	-5.75	112.65	119.84
1	D	78	ASP	C-N-CA	-5.75	112.65	119.84
1	A	93	VAL	N-CA-C	-5.70	106.75	113.42
1	D	81	SER	N-CA-C	5.69	120.03	112.30
1	D	115	VAL	CB-CA-C	-5.63	104.50	111.94
1	C	94	GLY	N-CA-C	-5.60	105.99	112.83
1	D	129	PRO	N-CA-C	5.49	117.40	110.70
1	D	72	VAL	N-CA-C	-5.47	106.51	112.80
1	C	66	MET	N-CA-C	-5.46	106.58	113.18
1	D	115	VAL	N-CA-C	5.46	115.71	110.74
1	A	30	LEU	N-CA-C	5.43	116.88	111.07
1	A	36	ALA	N-CA-C	-5.42	107.22	112.97
1	A	143	LEU	N-CA-C	5.38	121.69	109.81
1	A	4	ASP	CA-C-N	5.37	126.08	120.12
1	A	4	ASP	C-N-CA	5.37	126.08	120.12
1	B	78	ASP	CA-C-N	5.30	124.97	119.56
1	B	78	ASP	C-N-CA	5.30	124.97	119.56
1	C	129	PRO	CA-C-N	5.26	126.42	119.84
1	C	129	PRO	C-N-CA	5.26	126.42	119.84
1	B	57	GLN	N-CA-C	-5.24	105.25	110.97
1	B	132	TYR	N-CA-C	5.24	120.68	113.97
1	D	36	ALA	N-CA-C	-5.24	106.65	112.57
1	C	142	THR	N-CA-C	5.20	121.87	110.80
1	B	129	PRO	CA-C-N	5.14	126.26	119.84
1	B	129	PRO	C-N-CA	5.14	126.26	119.84
1	B	124	VAL	N-CA-C	5.13	115.35	110.42
1	A	44	SER	N-CA-C	5.12	117.87	110.14
1	D	63	GLY	N-CA-C	-5.11	107.97	114.16
1	B	128	THR	N-CA-C	5.06	119.88	109.11
1	A	63	GLY	N-CA-C	-5.05	107.44	115.66
1	D	93	VAL	CB-CA-C	-5.03	106.58	111.05

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	1164	0	1136	198	0
1	B	1167	0	1148	181	0
1	C	1167	0	1148	212	0
1	D	1160	0	1141	205	0
All	All	4658	0	4573	743	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 80.

All (743) 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:139:ILE:HG22	1:A:140:LEU:H	0.93	1.07
1:C:78:ASP:HB3	1:C:79:PRO:CD	1.80	1.06
1:D:139:ILE:HG22	1:D:140:LEU:H	1.18	1.04
1:C:78:ASP:HB3	1:C:79:PRO:HD3	1.10	1.04
1:D:55:LEU:H	1:D:55:LEU:HD12	1.25	1.01
1:D:12:THR:HG23	1:D:15:LEU:HB2	1.41	1.00
1:A:139:ILE:CG2	1:A:140:LEU:H	1.74	0.98
1:C:3:ILE:HG22	1:D:43:GLU:HG2	1.46	0.97
1:C:129:PRO:HG2	1:B:23:PHE:O	1.63	0.97
1:A:139:ILE:HG22	1:A:140:LEU:N	1.74	0.96
1:D:119:LEU:HD12	1:D:119:LEU:H	1.31	0.96
1:A:119:LEU:HD12	1:A:119:LEU:H	1.27	0.96
1:B:55:LEU:HG	1:B:59:ILE:HD11	1.48	0.95
1:D:116:LEU:O	1:D:120:VAL:HG23	1.64	0.95
1:C:12:THR:HG23	1:C:15:LEU:HB2	1.48	0.94
1:B:119:LEU:HD12	1:B:119:LEU:H	1.30	0.93
1:C:119:LEU:H	1:C:119:LEU:HD12	1.30	0.93
1:B:110:PHE:O	1:B:114:THR:HB	1.68	0.92
1:B:59:ILE:H	1:B:59:ILE:HD12	1.34	0.92
1:C:100:LEU:O	1:C:103:PHE:HB3	1.71	0.90
1:A:15:LEU:HD22	1:A:16:LEU:HD23	1.51	0.89
1:C:24:PHE:H	1:C:24:PHE:HD2	1.16	0.89
1:D:15:LEU:HD21	1:D:119:LEU:HD23	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:TYR:HD1	1:C:140:LEU:HD21	1.36	0.88
1:B:60:LEU:HD12	1:A:5:PRO:HG3	1.56	0.87
1:C:116:LEU:O	1:C:120:VAL:HG23	1.75	0.87
1:C:51:HIS:HB3	1:C:108:LEU:HD11	1.57	0.87
1:C:15:LEU:HD21	1:C:119:LEU:HD23	1.54	0.87
1:D:42:LEU:C	1:D:44:SER:H	1.82	0.87
1:C:118:TYR:CD1	1:C:140:LEU:HD21	2.09	0.86
1:B:42:LEU:C	1:B:44:SER:H	1.78	0.86
1:B:116:LEU:O	1:B:120:VAL:HG23	1.75	0.86
1:D:23:PHE:C	1:D:23:PHE:HD2	1.82	0.85
1:D:12:THR:O	1:D:15:LEU:HB3	1.76	0.85
1:A:100:LEU:HD23	1:A:101:LEU:N	1.90	0.85
1:C:18:PHE:HE1	1:B:33:THR:HA	1.40	0.85
1:A:12:THR:O	1:A:15:LEU:HB3	1.77	0.85
1:D:139:ILE:HG22	1:D:140:LEU:N	1.92	0.83
1:C:18:PHE:HE2	1:C:123:GLY:HA3	1.44	0.83
1:A:100:LEU:O	1:A:103:PHE:HB3	1.78	0.83
1:D:119:LEU:H	1:D:119:LEU:CD1	1.92	0.83
1:B:23:PHE:C	1:B:23:PHE:HD2	1.87	0.82
1:C:13:VAL:HG13	1:C:14:GLU:H	1.45	0.82
1:C:59:ILE:HD12	1:C:59:ILE:H	1.45	0.82
1:B:12:THR:HG23	1:B:15:LEU:HB2	1.60	0.82
1:D:110:PHE:O	1:D:114:THR:HB	1.80	0.81
1:C:60:LEU:HD11	1:D:3:ILE:HD11	1.61	0.81
1:C:89:VAL:HA	1:C:93:VAL:HG12	1.62	0.81
1:A:119:LEU:HD12	1:A:119:LEU:N	1.94	0.81
1:B:100:LEU:O	1:B:103:PHE:HB3	1.80	0.81
1:C:15:LEU:C	1:C:15:LEU:HD23	2.07	0.80
1:D:78:ASP:HB2	1:D:79:PRO:CD	2.10	0.80
1:D:97:PHE:O	1:D:101:LEU:HB2	1.82	0.80
1:A:42:LEU:C	1:A:44:SER:H	1.89	0.80
1:D:100:LEU:HD23	1:D:101:LEU:N	1.96	0.80
1:C:47:HIS:HB3	1:D:8:GLU:OE2	1.82	0.80
1:C:23:PHE:CD1	1:C:23:PHE:C	2.60	0.79
1:C:55:LEU:HD23	1:C:56:ARG:N	1.96	0.79
1:A:89:VAL:C	1:A:91:THR:H	1.90	0.79
1:C:24:PHE:HD2	1:C:24:PHE:N	1.78	0.78
1:D:139:ILE:CG2	1:D:140:LEU:H	1.95	0.78
1:D:89:VAL:HA	1:D:93:VAL:HG12	1.66	0.78
1:B:62:TRP:HB2	1:B:97:PHE:CE2	2.19	0.78
1:D:145:GLU:HG3	1:D:146:THR:H	1.47	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:PRO:C	1:D:139:ILE:HG13	2.07	0.77
1:C:13:VAL:HG13	1:C:14:GLU:N	2.00	0.76
1:C:110:PHE:CE2	1:C:140:LEU:HB3	2.21	0.76
1:D:23:PHE:C	1:D:23:PHE:CD2	2.56	0.76
1:B:35:ALA:O	1:B:39:ARG:HB2	1.86	0.76
1:C:27:VAL:HG12	1:C:31:LEU:HD11	1.68	0.76
1:C:8:GLU:HG3	1:D:47:HIS:HB3	1.68	0.75
1:D:51:HIS:HB3	1:D:108:LEU:HD11	1.69	0.75
1:D:59:ILE:HD12	1:D:59:ILE:H	1.51	0.75
1:D:126:ILE:C	1:D:128:THR:H	1.92	0.75
1:B:39:ARG:NH2	1:A:1:MET:HB2	2.01	0.75
1:A:23:PHE:C	1:A:23:PHE:CD2	2.64	0.75
1:C:18:PHE:CE2	1:C:123:GLY:HA3	2.20	0.75
1:C:24:PHE:N	1:C:24:PHE:CD2	2.52	0.74
1:B:23:PHE:C	1:B:23:PHE:CD2	2.60	0.74
1:D:55:LEU:H	1:D:55:LEU:CD1	2.00	0.74
1:D:77:GLU:HA	1:D:82:ARG:HD3	1.70	0.74
1:A:47:HIS:O	1:A:49:SER:N	2.21	0.73
1:A:126:ILE:HG23	1:A:127:ARG:H	1.54	0.73
1:B:12:THR:O	1:B:15:LEU:HB3	1.88	0.73
1:D:15:LEU:CD2	1:D:119:LEU:HD23	2.19	0.73
1:C:95:LEU:O	1:C:99:GLN:HB2	1.89	0.72
1:B:56:ARG:HA	1:B:59:ILE:HD13	1.69	0.72
1:B:81:SER:HB2	1:A:76:LEU:HD21	1.71	0.72
1:C:60:LEU:HD13	1:D:5:PRO:HG3	1.71	0.72
1:C:109:THR:HB	1:C:110:PHE:CD1	2.25	0.72
1:B:19:LEU:N	1:B:19:LEU:HD23	2.03	0.71
1:A:51:HIS:HB3	1:A:108:LEU:HD11	1.71	0.71
1:B:59:ILE:HD12	1:B:59:ILE:N	2.06	0.71
1:D:21:SER:HB3	1:D:95:LEU:HD11	1.71	0.71
1:A:123:GLY:O	1:A:127:ARG:HG2	1.91	0.71
1:A:55:LEU:HB3	1:A:59:ILE:HD11	1.73	0.70
1:D:102:TRP:O	1:D:103:PHE:C	2.34	0.70
1:D:78:ASP:HB2	1:D:79:PRO:HD2	1.72	0.70
1:D:122:PHE:C	1:D:124:VAL:H	1.99	0.70
1:C:42:LEU:C	1:C:44:SER:H	1.98	0.70
1:A:4:ASP:OD2	1:A:13:VAL:HG12	1.91	0.70
1:A:109:THR:HB	1:A:110:PHE:CD2	2.26	0.70
1:C:23:PHE:C	1:C:23:PHE:HD1	1.99	0.69
1:C:109:THR:HB	1:C:110:PHE:CE1	2.27	0.69
1:B:100:LEU:C	1:B:100:LEU:HD23	2.18	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:PRO:HG3	1:D:60:LEU:HD12	1.72	0.69
1:A:13:VAL:C	1:A:15:LEU:N	2.47	0.69
1:A:142:THR:O	1:A:144:PRO:HD3	1.91	0.69
1:C:47:HIS:O	1:C:49:SER:N	2.25	0.69
1:C:120:VAL:O	1:C:124:VAL:HG23	1.93	0.69
1:D:75:ASN:O	1:D:76:LEU:HG	1.92	0.69
1:C:12:THR:O	1:C:15:LEU:HB3	1.92	0.69
1:B:39:ARG:HH21	1:A:1:MET:HB2	1.56	0.69
1:C:81:SER:OG	1:D:76:LEU:HD21	1.91	0.69
1:D:16:LEU:C	1:D:18:PHE:N	2.47	0.69
1:C:78:ASP:CB	1:C:79:PRO:CD	2.65	0.68
1:C:122:PHE:O	1:C:125:TRP:N	2.24	0.68
1:A:118:TYR:O	1:A:119:LEU:C	2.35	0.68
1:B:62:TRP:HB2	1:B:97:PHE:HE2	1.58	0.68
1:B:5:PRO:HB3	1:A:60:LEU:HD12	1.74	0.68
1:C:79:PRO:HG2	1:D:78:ASP:CG	2.19	0.68
1:C:15:LEU:O	1:C:18:PHE:HB2	1.94	0.67
1:C:85:VAL:O	1:C:89:VAL:HG23	1.94	0.67
1:B:42:LEU:HA	1:B:56:ARG:HH21	1.59	0.67
1:A:55:LEU:C	1:A:59:ILE:HD12	2.19	0.67
1:B:25:PRO:O	1:B:98:ARG:HD2	1.94	0.67
1:D:3:ILE:C	1:D:3:ILE:HD12	2.19	0.67
1:B:42:LEU:C	1:B:44:SER:N	2.48	0.67
1:C:38:TYR:O	1:C:39:ARG:C	2.37	0.67
1:A:15:LEU:HD23	1:A:15:LEU:C	2.20	0.67
1:B:13:VAL:C	1:B:15:LEU:N	2.48	0.67
1:A:13:VAL:C	1:A:15:LEU:H	2.01	0.67
1:B:119:LEU:H	1:B:119:LEU:CD1	2.07	0.67
1:B:107:ALA:C	1:B:109:THR:H	2.03	0.66
1:A:143:LEU:C	1:A:145:GLU:H	2.03	0.66
1:B:60:LEU:HG	1:A:3:ILE:HD11	1.77	0.66
1:B:60:LEU:CD1	1:A:5:PRO:HG3	2.23	0.66
1:A:1:MET:HG3	1:A:3:ILE:HG23	1.77	0.66
1:C:23:PHE:HD1	1:C:24:PHE:N	1.94	0.66
1:D:141:SER:C	1:D:143:LEU:H	2.04	0.66
1:A:33:THR:HG22	1:A:34:ALA:N	2.09	0.66
1:C:100:LEU:C	1:C:100:LEU:HD23	2.21	0.66
1:A:102:TRP:O	1:A:103:PHE:C	2.39	0.66
1:C:3:ILE:HD12	1:C:3:ILE:C	2.20	0.66
1:C:18:PHE:HE2	1:C:123:GLY:CA	2.08	0.66
1:C:25:PRO:HB2	1:C:30:LEU:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:HIS:HD2	1:A:50:PRO:HG2	1.59	0.66
1:A:55:LEU:HD11	1:A:104:HIS:HB3	1.78	0.66
1:C:24:PHE:CD1	1:C:99:GLN:HA	2.31	0.65
1:B:85:VAL:HG23	1:B:86:VAL:N	2.10	0.65
1:C:72:VAL:HG12	1:C:72:VAL:O	1.96	0.65
1:B:15:LEU:HD22	1:B:16:LEU:HD23	1.79	0.65
1:A:20:PRO:C	1:A:22:ASP:H	2.03	0.65
1:A:109:THR:HB	1:A:110:PHE:CE2	2.31	0.65
1:D:12:THR:CG2	1:D:15:LEU:HB2	2.22	0.65
1:A:143:LEU:C	1:A:145:GLU:N	2.52	0.65
1:D:59:ILE:HD12	1:D:59:ILE:N	2.10	0.65
1:C:38:TYR:O	1:C:41:ALA:N	2.30	0.64
1:D:126:ILE:O	1:D:128:THR:N	2.31	0.64
1:A:23:PHE:C	1:A:23:PHE:HD2	2.04	0.64
1:A:89:VAL:C	1:A:91:THR:N	2.55	0.64
1:A:107:ALA:C	1:A:109:THR:H	2.06	0.64
1:C:146:THR:O	1:C:147:THR:O	2.15	0.64
1:B:47:HIS:HB3	1:A:8:GLU:OE1	1.96	0.64
1:B:3:ILE:HG22	1:A:43:GLU:HG2	1.80	0.64
1:B:115:VAL:O	1:B:118:TYR:HB3	1.98	0.64
1:A:111:GLY:O	1:A:115:VAL:HG23	1.98	0.64
1:D:126:ILE:HG23	1:D:127:ARG:H	1.61	0.64
1:A:116:LEU:O	1:A:120:VAL:HG23	1.97	0.64
1:B:100:LEU:CD2	1:B:101:LEU:N	2.61	0.64
1:D:4:ASP:OD2	1:D:13:VAL:HG12	1.98	0.63
1:C:139:ILE:HG22	1:C:140:LEU:N	2.13	0.63
1:D:85:VAL:O	1:D:89:VAL:HG23	1.99	0.63
1:C:13:VAL:CG1	1:C:14:GLU:H	2.10	0.63
1:D:100:LEU:HD23	1:D:100:LEU:C	2.24	0.63
1:B:55:LEU:HG	1:B:59:ILE:CD1	2.25	0.63
1:C:59:ILE:HD12	1:C:59:ILE:N	2.13	0.63
1:C:15:LEU:O	1:C:18:PHE:CB	2.47	0.63
1:D:18:PHE:CE1	1:D:123:GLY:HA3	2.34	0.63
1:D:135:PRO:HG2	1:D:136:ASN:H	1.62	0.63
1:A:132:TYR:O	1:A:134:PRO:HD3	1.98	0.63
1:C:107:ALA:C	1:C:109:THR:H	2.07	0.62
1:A:126:ILE:HG23	1:A:127:ARG:N	2.13	0.62
1:C:60:LEU:CD1	1:D:5:PRO:HG3	2.30	0.62
1:B:59:ILE:H	1:B:59:ILE:CD1	2.09	0.62
1:C:122:PHE:O	1:C:124:VAL:N	2.33	0.62
1:A:119:LEU:O	1:A:120:VAL:C	2.43	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:LEU:HD23	1:D:15:LEU:O	1.99	0.62
1:A:12:THR:HG23	1:A:15:LEU:HB2	1.80	0.62
1:D:78:ASP:CB	1:D:79:PRO:CD	2.77	0.62
1:D:93:VAL:C	1:D:95:LEU:N	2.55	0.62
1:B:139:ILE:HG22	1:B:140:LEU:H	1.64	0.62
1:B:53:THR:HG23	1:A:8:GLU:OE1	2.00	0.62
1:C:4:ASP:OD2	1:C:13:VAL:HG12	2.00	0.61
1:D:116:LEU:N	1:D:116:LEU:HD23	2.14	0.61
1:D:12:THR:HG23	1:D:15:LEU:CB	2.26	0.61
1:D:16:LEU:C	1:D:18:PHE:H	2.07	0.61
1:C:12:THR:HG23	1:C:15:LEU:CB	2.26	0.61
1:C:103:PHE:CD2	1:C:104:HIS:N	2.68	0.61
1:D:145:GLU:HG3	1:D:146:THR:N	2.15	0.61
1:B:23:PHE:O	1:B:23:PHE:HD2	1.81	0.61
1:D:47:HIS:O	1:D:49:SER:N	2.34	0.61
1:D:145:GLU:CG	1:D:146:THR:N	2.64	0.61
1:C:15:LEU:HD22	1:C:16:LEU:HD23	1.83	0.61
1:C:15:LEU:CD2	1:C:16:LEU:HD23	2.30	0.61
1:B:115:VAL:O	1:B:118:TYR:N	2.30	0.60
1:A:13:VAL:O	1:A:15:LEU:N	2.33	0.60
1:A:101:LEU:O	1:A:102:TRP:C	2.42	0.60
1:B:13:VAL:C	1:B:15:LEU:H	2.09	0.60
1:B:67:THR:HG22	1:B:67:THR:O	2.01	0.60
1:D:42:LEU:C	1:D:44:SER:N	2.51	0.60
1:D:81:SER:C	1:D:83:ASP:H	2.07	0.60
1:D:93:VAL:HG13	1:D:94:GLY:N	2.16	0.60
1:A:13:VAL:HG13	1:A:14:GLU:N	2.17	0.60
1:A:15:LEU:CD2	1:A:16:LEU:N	2.64	0.60
1:D:55:LEU:HD12	1:D:55:LEU:N	2.03	0.60
1:D:6:TYR:C	1:D:8:GLU:N	2.57	0.60
1:D:51:HIS:CB	1:D:108:LEU:HD11	2.32	0.60
1:D:119:LEU:HD12	1:D:119:LEU:N	2.08	0.60
1:B:56:ARG:CA	1:B:59:ILE:HD13	2.32	0.60
1:D:15:LEU:HD21	1:D:119:LEU:CD2	2.28	0.60
1:D:51:HIS:HB3	1:D:108:LEU:CD1	2.32	0.60
1:B:106:SER:O	1:B:110:PHE:HD2	1.82	0.60
1:C:76:LEU:O	1:C:82:ARG:HD3	2.02	0.60
1:C:119:LEU:HD12	1:C:119:LEU:N	2.11	0.60
1:D:13:VAL:C	1:D:15:LEU:H	2.09	0.60
1:D:112:ARG:O	1:D:115:VAL:HB	2.02	0.60
1:B:35:ALA:CB	1:A:1:MET:HE1	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:PHE:O	1:B:123:GLY:C	2.44	0.60
1:D:13:VAL:HG13	1:D:14:GLU:N	2.17	0.59
1:B:5:PRO:HB3	1:A:60:LEU:CD1	2.32	0.59
1:A:100:LEU:O	1:A:101:LEU:C	2.44	0.59
1:A:118:TYR:CE2	1:A:140:LEU:HG	2.37	0.59
1:C:16:LEU:C	1:C:18:PHE:H	2.09	0.59
1:C:139:ILE:CG2	1:C:140:LEU:N	2.65	0.59
1:B:43:GLU:HG2	1:A:3:ILE:HG22	1.84	0.59
1:C:24:PHE:CE1	1:C:99:GLN:HG3	2.37	0.59
1:D:59:ILE:H	1:D:59:ILE:CD1	2.15	0.59
1:C:59:ILE:H	1:C:59:ILE:CD1	2.13	0.59
1:D:15:LEU:O	1:D:16:LEU:HD23	2.02	0.59
1:B:100:LEU:HD23	1:B:101:LEU:N	2.18	0.59
1:A:87:SER:O	1:A:91:THR:HB	2.02	0.59
1:A:115:VAL:O	1:A:118:TYR:N	2.31	0.59
1:A:119:LEU:N	1:A:119:LEU:CD1	2.65	0.59
1:A:55:LEU:HB3	1:A:59:ILE:CD1	2.33	0.59
1:C:16:LEU:C	1:C:18:PHE:N	2.60	0.59
1:C:12:THR:CG2	1:C:15:LEU:HB2	2.28	0.58
1:C:88:TYR:O	1:C:92:ASN:HB3	2.03	0.58
1:D:99:GLN:O	1:D:100:LEU:C	2.45	0.58
1:C:6:TYR:C	1:C:8:GLU:N	2.57	0.58
1:D:137:ALA:HB1	1:D:138:PRO:HD2	1.85	0.58
1:C:15:LEU:C	1:C:15:LEU:CD2	2.76	0.58
1:D:13:VAL:C	1:D:15:LEU:N	2.57	0.58
1:C:24:PHE:CE1	1:C:99:GLN:HA	2.38	0.58
1:B:103:PHE:CD2	1:B:104:HIS:N	2.71	0.58
1:A:23:PHE:HD2	1:A:23:PHE:O	1.87	0.58
1:C:139:ILE:HG23	1:C:140:LEU:HG	1.85	0.58
1:D:59:ILE:O	1:D:63:GLY:N	2.34	0.58
1:A:16:LEU:O	1:A:18:PHE:N	2.36	0.58
1:A:26:SER:O	1:A:29:ASP:HB2	2.04	0.58
1:A:89:VAL:O	1:A:91:THR:N	2.37	0.58
1:C:4:ASP:OD1	1:C:6:TYR:HD2	1.87	0.58
1:B:89:VAL:C	1:B:91:THR:H	2.12	0.58
1:D:126:ILE:C	1:D:128:THR:N	2.59	0.57
1:B:68:LEU:HD13	1:A:88:TYR:CE2	2.38	0.57
1:B:139:ILE:HG22	1:B:140:LEU:N	2.19	0.57
1:A:55:LEU:O	1:A:56:ARG:C	2.46	0.57
1:C:51:HIS:CB	1:C:108:LEU:HD11	2.33	0.57
1:C:100:LEU:HD23	1:C:101:LEU:N	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:PHE:CD1	1:A:24:PHE:N	2.66	0.57
1:C:5:PRO:HG3	1:D:60:LEU:CD1	2.35	0.57
1:C:122:PHE:C	1:C:124:VAL:N	2.62	0.57
1:A:15:LEU:HD22	1:A:16:LEU:CD2	2.31	0.57
1:C:37:LEU:O	1:C:37:LEU:HD12	2.05	0.57
1:C:127:ARG:HD2	1:B:29:ASP:HB3	1.87	0.57
1:D:109:THR:HB	1:D:110:PHE:CE1	2.39	0.57
1:D:116:LEU:C	1:D:118:TYR:H	2.13	0.57
1:C:119:LEU:H	1:C:119:LEU:CD1	2.09	0.57
1:D:23:PHE:HD2	1:D:23:PHE:O	1.86	0.57
1:D:19:LEU:HD23	1:D:19:LEU:N	2.20	0.57
1:B:98:ARG:O	1:B:99:GLN:C	2.48	0.57
1:D:126:ILE:HG23	1:D:127:ARG:N	2.19	0.57
1:B:106:SER:O	1:B:110:PHE:CD2	2.57	0.57
1:D:30:LEU:O	1:D:33:THR:HB	2.05	0.57
1:B:38:TYR:HB2	1:B:42:LEU:HD11	1.86	0.57
1:C:88:TYR:O	1:C:92:ASN:N	2.31	0.56
1:C:55:LEU:O	1:C:58:ALA:HB3	2.05	0.56
1:C:118:TYR:HB3	1:C:119:LEU:HD12	1.86	0.56
1:C:130:PRO:O	1:C:133:ARG:HG2	2.06	0.56
1:B:31:LEU:O	1:B:32:ASP:C	2.48	0.56
1:B:85:VAL:CG2	1:B:86:VAL:N	2.67	0.56
1:D:85:VAL:HG23	1:D:86:VAL:HG23	1.88	0.56
1:A:100:LEU:CD2	1:A:101:LEU:N	2.66	0.56
1:C:53:THR:HG23	1:D:8:GLU:OE2	2.06	0.56
1:D:89:VAL:C	1:D:91:THR:H	2.13	0.56
1:D:55:LEU:O	1:D:58:ALA:N	2.39	0.56
1:B:15:LEU:O	1:B:15:LEU:HD23	2.04	0.56
1:A:116:LEU:O	1:A:120:VAL:CG2	2.53	0.56
1:B:128:THR:O	1:B:133:ARG:NH1	2.38	0.56
1:A:142:THR:HG22	1:A:143:LEU:N	2.21	0.55
1:C:8:GLU:CG	1:D:47:HIS:HB3	2.35	0.55
1:B:4:ASP:OD2	1:B:13:VAL:HG12	2.07	0.55
1:D:93:VAL:C	1:D:95:LEU:H	2.14	0.55
1:B:54:ALA:O	1:B:55:LEU:C	2.49	0.55
1:B:89:VAL:O	1:B:91:THR:N	2.39	0.55
1:A:128:THR:O	1:A:129:PRO:C	2.50	0.55
1:C:100:LEU:CD2	1:C:101:LEU:N	2.69	0.55
1:C:122:PHE:C	1:C:122:PHE:CD1	2.84	0.55
1:D:6:TYR:C	1:D:8:GLU:H	2.14	0.55
1:A:20:PRO:C	1:A:22:ASP:N	2.59	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:TYR:O	1:C:8:GLU:N	2.40	0.55
1:C:115:VAL:O	1:C:118:TYR:N	2.39	0.55
1:D:86:VAL:HA	1:D:89:VAL:HB	1.88	0.55
1:A:56:ARG:HB2	1:A:57:GLN:NE2	2.21	0.55
1:C:129:PRO:HB3	1:C:130:PRO:HD2	1.89	0.55
1:A:42:LEU:C	1:A:44:SER:N	2.55	0.55
1:B:81:SER:CB	1:A:76:LEU:HD21	2.36	0.55
1:A:34:ALA:O	1:A:37:LEU:HB3	2.07	0.55
1:D:104:HIS:O	1:D:105:ILE:C	2.50	0.54
1:D:122:PHE:O	1:D:124:VAL:N	2.40	0.54
1:D:122:PHE:O	1:D:126:ILE:HG22	2.07	0.54
1:C:35:ALA:CB	1:D:1:MET:HE1	2.37	0.54
1:D:15:LEU:HD23	1:D:16:LEU:CD2	2.37	0.54
1:C:82:ARG:HH11	1:C:82:ARG:HB2	1.72	0.54
1:D:30:LEU:HD23	1:D:101:LEU:HD22	1.89	0.54
1:D:115:VAL:O	1:D:118:TYR:CB	2.56	0.54
1:A:61:ALA:O	1:A:64:ASP:HB2	2.07	0.54
1:D:110:PHE:CE2	1:D:140:LEU:HB3	2.42	0.54
1:B:38:TYR:O	1:B:41:ALA:N	2.40	0.54
1:A:12:THR:CG2	1:A:15:LEU:HB2	2.36	0.54
1:A:57:GLN:O	1:A:58:ALA:C	2.50	0.54
1:C:60:LEU:HD11	1:D:3:ILE:CD1	2.36	0.54
1:D:18:PHE:CD1	1:D:123:GLY:HA3	2.42	0.54
1:C:6:TYR:C	1:C:8:GLU:H	2.16	0.54
1:C:15:LEU:HD21	1:C:119:LEU:CD2	2.32	0.54
1:D:61:ALA:O	1:D:65:LEU:HG	2.08	0.54
1:D:100:LEU:O	1:D:101:LEU:C	2.51	0.54
1:B:112:ARG:O	1:B:115:VAL:HB	2.07	0.54
1:A:107:ALA:O	1:A:109:THR:N	2.39	0.54
1:B:94:GLY:O	1:B:98:ARG:HG3	2.07	0.54
1:C:41:ALA:O	1:C:44:SER:HB3	2.08	0.53
1:D:13:VAL:HG13	1:D:14:GLU:H	1.72	0.53
1:B:38:TYR:O	1:B:39:ARG:C	2.51	0.53
1:C:101:LEU:O	1:C:102:TRP:C	2.52	0.53
1:D:100:LEU:CD2	1:D:101:LEU:N	2.70	0.53
1:D:118:TYR:HE1	1:D:140:LEU:HG	1.73	0.53
1:A:103:PHE:CD2	1:A:104:HIS:N	2.76	0.53
1:C:79:PRO:HG2	1:D:78:ASP:OD1	2.08	0.53
1:D:27:VAL:HG12	1:D:31:LEU:HG	1.91	0.53
1:A:106:SER:O	1:A:110:PHE:HD2	1.91	0.53
1:C:67:THR:O	1:C:67:THR:HG22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:ALA:O	1:C:39:ARG:HB2	2.08	0.53
1:A:15:LEU:C	1:A:15:LEU:CD2	2.82	0.53
1:A:61:ALA:O	1:A:65:LEU:HG	2.09	0.53
1:D:21:SER:HB3	1:D:95:LEU:CD1	2.37	0.53
1:C:87:SER:O	1:C:88:TYR:C	2.52	0.52
1:C:139:ILE:CG2	1:C:140:LEU:H	2.21	0.52
1:D:106:SER:O	1:D:110:PHE:HD1	1.92	0.52
1:B:115:VAL:O	1:B:118:TYR:CB	2.57	0.52
1:C:27:VAL:CG1	1:C:31:LEU:HD11	2.37	0.52
1:C:3:ILE:CD1	1:D:60:LEU:HD11	2.39	0.52
1:D:115:VAL:O	1:D:118:TYR:HB3	2.09	0.52
1:D:118:TYR:HB3	1:D:119:LEU:HD12	1.91	0.52
1:C:106:SER:O	1:C:110:PHE:HD1	1.91	0.52
1:C:6:TYR:OH	1:C:100:LEU:HB2	2.09	0.52
1:B:5:PRO:HG2	1:B:6:TYR:CD2	2.44	0.52
1:B:68:LEU:HG	1:B:69:ALA:N	2.24	0.52
1:B:88:TYR:O	1:B:92:ASN:N	2.42	0.52
1:A:118:TYR:HB3	1:A:119:LEU:HD12	1.92	0.52
1:C:42:LEU:C	1:C:44:SER:N	2.67	0.52
1:C:3:ILE:HD12	1:C:3:ILE:O	2.10	0.52
1:B:93:VAL:C	1:B:95:LEU:N	2.64	0.52
1:B:100:LEU:O	1:B:101:LEU:C	2.52	0.52
1:C:77:GLU:HA	1:C:82:ARG:CZ	2.39	0.52
1:D:39:ARG:O	1:D:43:GLU:HG3	2.10	0.52
1:C:50:PRO:O	1:C:51:HIS:C	2.53	0.51
1:B:19:LEU:HD13	1:B:23:PHE:CD1	2.45	0.51
1:C:23:PHE:CD1	1:C:24:PHE:N	2.76	0.51
1:D:38:TYR:O	1:D:42:LEU:HD12	2.10	0.51
1:C:15:LEU:HD22	1:C:16:LEU:CD2	2.40	0.51
1:C:97:PHE:O	1:C:101:LEU:HB2	2.10	0.51
1:C:102:TRP:O	1:C:103:PHE:C	2.53	0.51
1:B:1:MET:HG2	1:B:3:ILE:HG23	1.92	0.51
1:C:86:VAL:HG12	1:C:90:ASN:HD22	1.76	0.51
1:D:1:MET:HG3	1:D:3:ILE:HG23	1.92	0.51
1:B:47:HIS:HB3	1:A:8:GLU:CD	2.36	0.51
1:B:126:ILE:C	1:B:128:THR:H	2.19	0.51
1:A:85:VAL:HG23	1:A:86:VAL:N	2.26	0.51
1:C:15:LEU:HD23	1:C:15:LEU:O	2.11	0.51
1:C:23:PHE:HD1	1:C:24:PHE:HA	1.75	0.51
1:B:15:LEU:O	1:B:18:PHE:CD2	2.64	0.51
1:B:116:LEU:N	1:B:116:LEU:HD23	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LEU:C	1:A:18:PHE:N	2.65	0.51
1:B:68:LEU:HD13	1:A:88:TYR:HE2	1.75	0.51
1:A:38:TYR:O	1:A:41:ALA:HB3	2.11	0.51
1:A:118:TYR:CD2	1:A:140:LEU:HD21	2.46	0.51
1:D:116:LEU:C	1:D:118:TYR:N	2.68	0.51
1:A:65:LEU:O	1:A:68:LEU:HB3	2.11	0.51
1:C:122:PHE:C	1:C:124:VAL:H	2.18	0.51
1:B:37:LEU:HD12	1:B:37:LEU:O	2.11	0.51
1:B:109:THR:HB	1:B:110:PHE:CD2	2.46	0.50
1:A:53:THR:HA	1:A:56:ARG:HG3	1.93	0.50
1:C:54:ALA:O	1:C:55:LEU:C	2.53	0.50
1:C:84:LEU:O	1:C:84:LEU:HG	2.10	0.50
1:B:119:LEU:O	1:B:120:VAL:C	2.55	0.50
1:A:100:LEU:HD23	1:A:101:LEU:CA	2.40	0.50
1:C:118:TYR:O	1:C:119:LEU:C	2.54	0.50
1:B:93:VAL:O	1:B:94:GLY:C	2.53	0.50
1:B:118:TYR:HE1	1:B:140:LEU:N	2.09	0.50
1:D:55:LEU:O	1:D:56:ARG:C	2.53	0.50
1:A:39:ARG:HG3	1:A:40:ASP:H	1.76	0.50
1:D:81:SER:C	1:D:83:ASP:N	2.66	0.50
1:B:52:HIS:O	1:B:55:LEU:HB3	2.12	0.50
1:D:38:TYR:HB2	1:D:42:LEU:CD1	2.42	0.50
1:A:27:VAL:HG22	1:A:98:ARG:HG2	1.93	0.50
1:B:13:VAL:HG13	1:B:14:GLU:N	2.26	0.50
1:B:100:LEU:C	1:B:100:LEU:CD2	2.84	0.50
1:D:50:PRO:O	1:D:51:HIS:C	2.55	0.50
1:C:18:PHE:HE2	1:C:123:GLY:C	2.19	0.49
1:D:85:VAL:CG2	1:D:86:VAL:HG23	2.42	0.49
1:A:68:LEU:HG	1:A:69:ALA:N	2.27	0.49
1:C:110:PHE:CD2	1:C:140:LEU:HB3	2.47	0.49
1:B:68:LEU:O	1:B:71:TRP:N	2.45	0.49
1:B:118:TYR:O	1:B:119:LEU:C	2.54	0.49
1:A:55:LEU:HD11	1:A:104:HIS:CB	2.42	0.49
1:A:20:PRO:O	1:A:22:ASP:N	2.44	0.49
1:C:43:GLU:HG2	1:D:3:ILE:HG22	1.94	0.49
1:C:52:HIS:O	1:C:53:THR:C	2.55	0.49
1:D:138:PRO:O	1:D:139:ILE:HG13	2.12	0.49
1:B:25:PRO:O	1:B:30:LEU:CD1	2.61	0.49
1:B:30:LEU:HD23	1:B:105:ILE:HD12	1.93	0.49
1:A:15:LEU:O	1:A:17:SER:N	2.46	0.49
1:B:137:ALA:HB1	1:B:138:PRO:HD2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:LEU:HD23	1:B:15:LEU:C	2.38	0.49
1:A:56:ARG:HB2	1:A:57:GLN:HE21	1.76	0.49
1:C:100:LEU:C	1:C:100:LEU:CD2	2.86	0.49
1:B:47:HIS:HB3	1:A:8:GLU:CG	2.42	0.49
1:A:27:VAL:O	1:A:28:ARG:C	2.55	0.49
1:A:103:PHE:CG	1:A:104:HIS:N	2.78	0.49
1:A:100:LEU:HD23	1:A:100:LEU:C	2.37	0.49
1:D:116:LEU:O	1:D:118:TYR:N	2.46	0.49
1:B:25:PRO:O	1:B:26:SER:C	2.56	0.49
1:B:134:PRO:C	1:B:136:ASN:N	2.71	0.49
1:A:31:LEU:C	1:A:33:THR:N	2.70	0.49
1:C:119:LEU:O	1:C:120:VAL:C	2.56	0.49
1:C:119:LEU:O	1:C:123:GLY:N	2.39	0.49
1:A:68:LEU:O	1:A:71:TRP:HB3	2.12	0.49
1:C:25:PRO:HB2	1:C:30:LEU:CD1	2.43	0.48
1:D:4:ASP:OD1	1:D:6:TYR:HD2	1.95	0.48
1:B:112:ARG:O	1:B:115:VAL:N	2.38	0.48
1:B:65:LEU:HA	1:B:68:LEU:HB3	1.95	0.48
1:A:6:TYR:CD1	1:A:6:TYR:N	2.80	0.48
1:B:55:LEU:O	1:B:58:ALA:N	2.46	0.48
1:A:62:TRP:C	1:A:64:ASP:H	2.21	0.48
1:A:103:PHE:O	1:A:104:HIS:C	2.55	0.48
1:A:147:THR:O	1:A:148:VAL:O	2.31	0.48
1:C:13:VAL:C	1:C:15:LEU:N	2.69	0.48
1:B:18:PHE:O	1:B:20:PRO:HD3	2.13	0.48
1:C:116:LEU:HA	1:C:119:LEU:HD13	1.96	0.48
1:D:9:PHE:CD1	1:D:9:PHE:N	2.82	0.48
1:B:134:PRO:C	1:B:136:ASN:H	2.21	0.48
1:A:115:VAL:O	1:A:116:LEU:C	2.57	0.48
1:C:55:LEU:O	1:C:56:ARG:C	2.55	0.48
1:C:127:ARG:HD2	1:B:29:ASP:CB	2.43	0.48
1:B:62:TRP:HB2	1:B:97:PHE:CD2	2.49	0.48
1:B:101:LEU:HD23	1:B:105:ILE:HD11	1.95	0.48
1:C:65:LEU:HA	1:C:68:LEU:HB3	1.94	0.48
1:D:54:ALA:O	1:D:55:LEU:C	2.56	0.48
1:B:24:PHE:HA	1:B:25:PRO:HD3	1.63	0.48
1:A:107:ALA:C	1:A:109:THR:N	2.71	0.48
1:C:3:ILE:CG2	1:D:43:GLU:HG2	2.30	0.48
1:D:100:LEU:O	1:D:103:PHE:HB3	2.14	0.48
1:A:4:ASP:OD1	1:A:6:TYR:HD1	1.95	0.48
1:D:37:LEU:HG	1:D:38:TYR:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:VAL:HG12	1:C:31:LEU:CD1	2.41	0.48
1:C:112:ARG:O	1:C:115:VAL:HB	2.14	0.48
1:D:129:PRO:HA	1:D:130:PRO:HD3	1.78	0.48
1:A:128:THR:O	1:A:133:ARG:HG3	2.14	0.48
1:B:39:ARG:NH2	1:A:1:MET:CB	2.76	0.47
1:A:33:THR:O	1:A:34:ALA:C	2.57	0.47
1:A:44:SER:HA	1:A:45:PRO:HD3	1.70	0.47
1:C:30:LEU:HD12	1:C:30:LEU:H	1.79	0.47
1:B:134:PRO:O	1:B:136:ASN:N	2.47	0.47
1:D:109:THR:HB	1:D:110:PHE:CD1	2.48	0.47
1:B:47:HIS:O	1:B:48:ALA:C	2.58	0.47
1:C:85:VAL:HG23	1:C:86:VAL:N	2.30	0.47
1:B:20:PRO:O	1:B:23:PHE:HB3	2.13	0.47
1:A:62:TRP:HB2	1:A:97:PHE:CE2	2.49	0.47
1:C:16:LEU:CB	1:C:99:GLN:HE21	2.28	0.47
1:D:93:VAL:CG1	1:D:94:GLY:N	2.78	0.47
1:A:15:LEU:HD23	1:A:16:LEU:N	2.28	0.47
1:C:8:GLU:CD	1:D:47:HIS:HB3	2.40	0.47
1:D:25:PRO:O	1:D:30:LEU:HD13	2.15	0.47
1:B:131:ALA:C	1:B:132:TYR:HD2	2.22	0.47
1:A:123:GLY:C	1:A:127:ARG:HE	2.23	0.47
1:B:6:TYR:C	1:B:8:GLU:N	2.71	0.47
1:B:51:HIS:O	1:B:52:HIS:C	2.58	0.47
1:A:31:LEU:O	1:A:32:ASP:C	2.58	0.47
1:C:123:GLY:O	1:C:127:ARG:HB2	2.15	0.47
1:B:42:LEU:O	1:B:44:SER:N	2.47	0.47
1:A:34:ALA:O	1:A:37:LEU:N	2.48	0.47
1:C:118:TYR:OH	1:C:139:ILE:HG12	2.14	0.47
1:C:144:PRO:O	1:C:145:GLU:HG2	2.14	0.47
1:D:44:SER:HA	1:D:45:PRO:HD3	1.69	0.47
1:A:139:ILE:CG2	1:A:140:LEU:N	2.46	0.46
1:C:144:PRO:C	1:C:145:GLU:CG	2.88	0.46
1:B:47:HIS:HB3	1:A:8:GLU:HG3	1.97	0.46
1:D:62:TRP:HA	1:D:65:LEU:HD12	1.97	0.46
1:D:119:LEU:CD1	1:D:119:LEU:N	2.67	0.46
1:A:88:TYR:O	1:A:92:ASN:HB2	2.14	0.46
1:C:34:ALA:O	1:C:37:LEU:N	2.47	0.46
1:B:13:VAL:O	1:B:16:LEU:N	2.48	0.46
1:B:95:LEU:O	1:B:96:LYS:C	2.56	0.46
1:B:23:PHE:O	1:B:23:PHE:CD2	2.67	0.46
1:B:60:LEU:HA	1:B:60:LEU:HD23	1.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:LEU:O	1:B:102:TRP:C	2.58	0.46
1:B:122:PHE:C	1:B:122:PHE:CD2	2.93	0.46
1:A:12:THR:HG23	1:A:15:LEU:N	2.31	0.46
1:A:16:LEU:C	1:A:18:PHE:H	2.24	0.46
1:C:27:VAL:O	1:C:28:ARG:C	2.58	0.46
1:C:6:TYR:O	1:C:7:LYS:C	2.59	0.46
1:C:106:SER:O	1:C:107:ALA:C	2.59	0.46
1:D:6:TYR:O	1:D:8:GLU:N	2.48	0.46
1:D:119:LEU:O	1:D:120:VAL:C	2.59	0.46
1:B:3:ILE:O	1:B:3:ILE:HD12	2.16	0.46
1:A:116:LEU:HA	1:A:119:LEU:HD13	1.98	0.46
1:C:3:ILE:HD11	1:D:60:LEU:HD11	1.97	0.46
1:C:111:GLY:O	1:C:115:VAL:HG23	2.16	0.46
1:D:38:TYR:HB3	1:D:41:ALA:HB3	1.98	0.46
1:B:62:TRP:C	1:B:64:ASP:N	2.73	0.46
1:B:116:LEU:HA	1:B:119:LEU:HD13	1.98	0.46
1:A:35:ALA:O	1:A:39:ARG:HB3	2.16	0.46
1:A:134:PRO:O	1:A:136:ASN:N	2.49	0.46
1:C:49:SER:HB2	1:C:50:PRO:HD2	1.98	0.45
1:C:59:ILE:O	1:C:63:GLY:N	2.40	0.45
1:C:115:VAL:O	1:C:116:LEU:C	2.57	0.45
1:D:30:LEU:CD2	1:D:101:LEU:HD22	2.46	0.45
1:A:6:TYR:O	1:A:9:PHE:N	2.48	0.45
1:A:15:LEU:O	1:A:16:LEU:C	2.59	0.45
1:A:98:ARG:O	1:A:99:GLN:C	2.59	0.45
1:A:115:VAL:O	1:A:119:LEU:CD1	2.64	0.45
1:C:115:VAL:O	1:C:118:TYR:CB	2.64	0.45
1:B:46:GLU:C	1:B:48:ALA:H	2.24	0.45
1:A:19:LEU:HA	1:A:20:PRO:HD3	1.89	0.45
1:D:115:VAL:O	1:D:118:TYR:N	2.42	0.45
1:C:8:GLU:OE2	1:D:53:THR:HG23	2.16	0.45
1:D:124:VAL:O	1:D:125:TRP:C	2.60	0.45
1:D:25:PRO:HB2	1:D:30:LEU:CD1	2.46	0.45
1:D:27:VAL:O	1:D:28:ARG:C	2.59	0.45
1:D:55:LEU:O	1:D:58:ALA:HB3	2.16	0.45
1:D:86:VAL:HG12	1:D:86:VAL:O	2.16	0.45
1:D:89:VAL:O	1:D:91:THR:N	2.49	0.45
1:A:88:TYR:O	1:A:88:TYR:CG	2.70	0.45
1:D:25:PRO:HB2	1:D:30:LEU:HD12	1.98	0.45
1:D:77:GLU:HA	1:D:82:ARG:CD	2.44	0.45
1:A:110:PHE:HB3	1:A:114:THR:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ILE:O	1:A:3:ILE:CG1	2.65	0.45
1:A:115:VAL:O	1:A:118:TYR:HB3	2.16	0.45
1:A:2:ASP:C	1:A:3:ILE:HG23	2.42	0.45
1:D:25:PRO:O	1:D:26:SER:C	2.60	0.45
1:D:122:PHE:C	1:D:124:VAL:N	2.69	0.45
1:B:5:PRO:HG2	1:B:6:TYR:CE2	2.52	0.45
1:C:110:PHE:CD1	1:C:110:PHE:N	2.84	0.45
1:B:15:LEU:HD22	1:B:16:LEU:CD2	2.45	0.45
1:C:23:PHE:HD1	1:C:24:PHE:CA	2.30	0.44
1:C:86:VAL:HG12	1:C:90:ASN:ND2	2.31	0.44
1:C:122:PHE:O	1:C:123:GLY:C	2.58	0.44
1:D:89:VAL:HA	1:D:93:VAL:CG1	2.41	0.44
1:B:30:LEU:O	1:B:33:THR:HB	2.17	0.44
1:B:65:LEU:N	1:B:65:LEU:HD23	2.31	0.44
1:B:111:GLY:O	1:B:115:VAL:HG23	2.17	0.44
1:A:55:LEU:O	1:A:58:ALA:HB3	2.16	0.44
1:A:104:HIS:O	1:A:105:ILE:C	2.59	0.44
1:D:107:ALA:HB2	1:D:115:VAL:HG21	1.99	0.44
1:A:3:ILE:O	1:A:3:ILE:HG13	2.17	0.44
1:A:47:HIS:C	1:A:49:SER:N	2.75	0.44
1:B:89:VAL:C	1:B:91:THR:N	2.73	0.44
1:C:26:SER:O	1:C:27:VAL:C	2.60	0.44
1:C:100:LEU:O	1:C:101:LEU:C	2.61	0.44
1:D:13:VAL:O	1:D:16:LEU:N	2.43	0.44
1:D:76:LEU:O	1:D:82:ARG:HD3	2.18	0.44
1:A:27:VAL:O	1:A:30:LEU:N	2.50	0.44
1:C:104:HIS:O	1:C:105:ILE:C	2.60	0.44
1:D:27:VAL:HG12	1:D:31:LEU:CG	2.46	0.44
1:D:51:HIS:O	1:D:54:ALA:HB3	2.17	0.44
1:B:44:SER:HA	1:B:45:PRO:HD3	1.69	0.44
1:B:85:VAL:CG2	1:B:86:VAL:H	2.29	0.44
1:A:25:PRO:O	1:A:30:LEU:CD1	2.66	0.44
1:A:85:VAL:CG2	1:A:86:VAL:N	2.79	0.44
1:C:57:GLN:O	1:C:58:ALA:C	2.59	0.44
1:C:95:LEU:HA	1:C:98:ARG:HG2	2.00	0.44
1:C:107:ALA:C	1:C:109:THR:N	2.73	0.44
1:B:20:PRO:HG3	1:B:126:ILE:HD12	2.00	0.44
1:B:119:LEU:HD12	1:B:119:LEU:N	2.12	0.44
1:C:88:TYR:CE2	1:D:68:LEU:HD13	2.52	0.44
1:D:115:VAL:O	1:D:116:LEU:C	2.61	0.44
1:B:116:LEU:HD23	1:B:116:LEU:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:ASP:C	1:B:3:ILE:HG23	2.43	0.44
1:A:57:GLN:NE2	1:A:57:GLN:H	2.15	0.44
1:C:13:VAL:O	1:C:15:LEU:N	2.51	0.44
1:C:103:PHE:O	1:C:104:HIS:C	2.61	0.44
1:C:115:VAL:O	1:C:118:TYR:HB3	2.17	0.44
1:C:143:LEU:CB	1:C:144:PRO:CD	2.96	0.44
1:D:4:ASP:HA	1:D:5:PRO:HD3	1.65	0.44
1:A:13:VAL:CG1	1:A:14:GLU:N	2.80	0.44
1:A:142:THR:O	1:A:144:PRO:CD	2.62	0.44
1:D:52:HIS:O	1:D:56:ARG:HG3	2.17	0.43
1:D:100:LEU:HD23	1:D:101:LEU:CA	2.48	0.43
1:A:106:SER:O	1:A:107:ALA:C	2.60	0.43
1:C:46:GLU:C	1:C:48:ALA:H	2.26	0.43
1:D:13:VAL:O	1:D:15:LEU:N	2.51	0.43
1:B:6:TYR:HB2	1:B:12:THR:HA	2.00	0.43
1:A:57:GLN:O	1:A:60:LEU:N	2.51	0.43
1:A:6:TYR:O	1:A:7:LYS:C	2.61	0.43
1:C:107:ALA:O	1:C:109:THR:N	2.50	0.43
1:D:141:SER:C	1:D:143:LEU:N	2.73	0.43
1:A:129:PRO:HA	1:A:130:PRO:HD3	1.66	0.43
1:A:142:THR:CG2	1:A:143:LEU:N	2.82	0.43
1:D:19:LEU:HA	1:D:20:PRO:HD3	1.86	0.43
1:C:86:VAL:O	1:C:89:VAL:HB	2.18	0.43
1:C:111:GLY:O	1:C:112:ARG:C	2.61	0.43
1:B:6:TYR:O	1:B:7:LYS:C	2.61	0.43
1:B:103:PHE:O	1:B:104:HIS:C	2.62	0.43
1:A:31:LEU:O	1:A:33:THR:N	2.52	0.43
1:A:120:VAL:HB	1:A:121:SER:H	1.44	0.43
1:D:51:HIS:O	1:D:55:LEU:HD13	2.18	0.43
1:D:116:LEU:C	1:D:120:VAL:HG23	2.41	0.43
1:A:1:MET:HG3	1:A:3:ILE:CG2	2.48	0.43
1:A:30:LEU:N	1:A:30:LEU:HD12	2.34	0.43
1:D:27:VAL:HG12	1:D:31:LEU:HD11	2.00	0.42
1:D:106:SER:C	1:D:108:LEU:N	2.76	0.42
1:C:3:ILE:HD12	1:D:60:LEU:HD11	2.02	0.42
1:C:47:HIS:HB3	1:D:8:GLU:CD	2.43	0.42
1:C:119:LEU:N	1:C:119:LEU:CD1	2.77	0.42
1:D:15:LEU:HD23	1:D:16:LEU:HD21	2.00	0.42
1:D:118:TYR:O	1:D:119:LEU:C	2.61	0.42
1:B:109:THR:HB	1:B:110:PHE:CE2	2.54	0.42
1:A:97:PHE:O	1:A:101:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:PHE:CE1	1:A:140:LEU:O	2.72	0.42
1:A:116:LEU:C	1:A:118:TYR:H	2.26	0.42
1:C:19:LEU:HA	1:C:20:PRO:HD3	1.79	0.42
1:D:3:ILE:C	1:D:3:ILE:CD1	2.87	0.42
1:B:13:VAL:O	1:B:15:LEU:N	2.52	0.42
1:A:47:HIS:C	1:A:49:SER:H	2.26	0.42
1:A:115:VAL:HG12	1:A:119:LEU:HD11	2.01	0.42
1:C:67:THR:O	1:C:67:THR:CG2	2.68	0.42
1:D:24:PHE:HA	1:D:25:PRO:HD3	1.82	0.42
1:D:38:TYR:HB2	1:D:42:LEU:HD12	2.01	0.42
1:B:95:LEU:O	1:B:97:PHE:N	2.53	0.42
1:C:38:TYR:HB2	1:C:42:LEU:HD11	2.00	0.42
1:C:119:LEU:O	1:C:120:VAL:O	2.38	0.42
1:A:25:PRO:O	1:A:26:SER:C	2.63	0.42
1:A:99:GLN:O	1:A:100:LEU:C	2.62	0.42
1:D:89:VAL:C	1:D:91:THR:N	2.77	0.42
1:B:3:ILE:O	1:B:3:ILE:CG1	2.67	0.42
1:B:34:ALA:O	1:B:37:LEU:N	2.36	0.42
1:B:115:VAL:O	1:B:116:LEU:C	2.62	0.42
1:A:4:ASP:OD1	1:A:6:TYR:CD1	2.72	0.42
1:D:19:LEU:H	1:D:19:LEU:HG	1.40	0.42
1:D:77:GLU:O	1:D:77:GLU:HG2	2.18	0.42
1:B:57:GLN:O	1:B:58:ALA:C	2.61	0.42
1:A:13:VAL:HG13	1:A:14:GLU:H	1.84	0.42
1:A:24:PHE:HA	1:A:25:PRO:HD3	1.72	0.42
1:A:115:VAL:O	1:A:119:LEU:HD12	2.20	0.42
1:C:18:PHE:CE1	1:B:33:THR:HA	2.33	0.42
1:D:20:PRO:O	1:D:23:PHE:HB3	2.19	0.42
1:B:39:ARG:O	1:B:40:ASP:C	2.62	0.42
1:A:4:ASP:HA	1:A:5:PRO:HD3	1.78	0.42
1:A:15:LEU:HD21	1:A:119:LEU:HD23	2.01	0.42
1:B:55:LEU:O	1:B:58:ALA:HB3	2.20	0.42
1:C:34:ALA:O	1:C:37:LEU:HB3	2.20	0.41
1:D:111:GLY:O	1:D:112:ARG:C	2.62	0.41
1:B:104:HIS:O	1:B:107:ALA:HB3	2.20	0.41
1:C:9:PHE:O	1:C:10:GLY:C	2.63	0.41
1:D:4:ASP:OD1	1:D:5:PRO:HD2	2.20	0.41
1:B:26:SER:O	1:B:29:ASP:HB2	2.20	0.41
1:C:137:ALA:HA	1:C:138:PRO:HD3	1.94	0.41
1:D:37:LEU:HG	1:D:38:TYR:CZ	2.55	0.41
1:D:79:PRO:HG2	1:D:81:SER:OG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:SER:O	1:B:27:VAL:C	2.64	0.41
1:D:62:TRP:HB2	1:D:97:PHE:CE1	2.55	0.41
1:B:50:PRO:HG2	1:A:47:HIS:HD2	1.85	0.41
1:C:140:LEU:N	1:C:140:LEU:HD23	2.35	0.41
1:C:143:LEU:HB2	1:C:144:PRO:CD	2.50	0.41
1:D:79:PRO:C	1:D:81:SER:H	2.28	0.41
1:B:15:LEU:CD2	1:B:16:LEU:HD23	2.49	0.41
1:B:100:LEU:HD22	1:B:101:LEU:N	2.35	0.41
1:B:124:VAL:O	1:B:125:TRP:C	2.63	0.41
1:B:126:ILE:C	1:B:128:THR:N	2.78	0.41
1:A:115:VAL:O	1:A:118:TYR:CB	2.69	0.41
1:A:118:TYR:HD1	1:A:119:LEU:N	2.18	0.41
1:B:131:ALA:C	1:B:132:TYR:CD2	2.98	0.41
1:A:24:PHE:CD2	1:A:99:GLN:HA	2.56	0.41
1:A:100:LEU:HD23	1:A:101:LEU:HA	2.03	0.41
1:C:93:VAL:O	1:C:94:GLY:C	2.62	0.41
1:D:98:ARG:O	1:D:99:GLN:O	2.39	0.41
1:D:104:HIS:O	1:D:106:SER:N	2.54	0.41
1:B:3:ILE:O	1:B:3:ILE:HG13	2.21	0.41
1:B:13:VAL:O	1:B:14:GLU:C	2.64	0.41
1:C:13:VAL:O	1:C:16:LEU:N	2.54	0.41
1:C:79:PRO:CG	1:D:78:ASP:CG	2.92	0.41
1:C:87:SER:O	1:C:89:VAL:N	2.54	0.41
1:C:146:THR:O	1:C:147:THR:C	2.64	0.41
1:D:25:PRO:O	1:D:30:LEU:CD1	2.69	0.41
1:D:116:LEU:HA	1:D:119:LEU:HD13	2.02	0.41
1:D:126:ILE:HG23	1:D:127:ARG:HG2	2.02	0.41
1:B:19:LEU:HD13	1:B:23:PHE:CE1	2.55	0.41
1:B:28:ARG:O	1:B:32:ASP:OD2	2.39	0.41
1:B:53:THR:O	1:B:54:ALA:C	2.64	0.41
1:B:105:ILE:HG22	1:B:106:SER:N	2.34	0.41
1:B:126:ILE:HG23	1:B:127:ARG:N	2.35	0.41
1:A:118:TYR:CD2	1:A:140:LEU:CD2	3.04	0.41
1:D:38:TYR:HB2	1:D:42:LEU:HD11	2.03	0.41
1:B:134:PRO:HA	1:B:135:PRO:HD3	1.96	0.41
1:A:12:THR:HG23	1:A:15:LEU:CB	2.50	0.41
1:A:30:LEU:O	1:A:33:THR:HB	2.21	0.41
1:A:57:GLN:HB2	1:A:58:ALA:H	1.63	0.41
1:C:93:VAL:HG13	1:C:94:GLY:N	2.35	0.40
1:C:55:LEU:HD23	1:C:56:ARG:CA	2.51	0.40
1:C:103:PHE:CG	1:C:104:HIS:N	2.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:LEU:O	1:C:119:LEU:HD13	2.20	0.40
1:C:143:LEU:CB	1:C:144:PRO:HD3	2.52	0.40
1:D:76:LEU:O	1:D:82:ARG:CD	2.69	0.40
1:B:95:LEU:C	1:B:97:PHE:N	2.79	0.40
1:A:37:LEU:O	1:A:37:LEU:HD12	2.21	0.40
1:C:39:ARG:O	1:C:40:ASP:C	2.64	0.40
1:C:52:HIS:O	1:C:56:ARG:HG3	2.22	0.40
1:B:116:LEU:C	1:B:118:TYR:N	2.78	0.40
1:A:38:TYR:O	1:A:39:ARG:C	2.64	0.40
1:A:127:ARG:H	1:A:127:ARG:HG2	1.68	0.40
1:C:35:ALA:HB1	1:D:1:MET:HE1	2.03	0.40
1:D:27:VAL:HG12	1:D:31:LEU:CD1	2.51	0.40
1:B:52:HIS:HB3	1:B:56:ARG:NH1	2.37	0.40
1:B:128:THR:HA	1:B:129:PRO:HD2	1.61	0.40
1:A:15:LEU:HD22	1:A:16:LEU:N	2.33	0.40
1:A:76:LEU:HD23	1:A:76:LEU:HA	1.93	0.40
1:A:127:ARG:O	1:A:127:ARG:HG3	2.21	0.40
1:C:124:VAL:O	1:C:125:TRP:C	2.64	0.40
1:B:52:HIS:O	1:B:53:THR:C	2.63	0.40
1:B:62:TRP:HA	1:B:65:LEU:HG	2.03	0.40
1:A:50:PRO:O	1:A:51:HIS:C	2.64	0.40
1:A:62:TRP:O	1:A:65:LEU:HB2	2.22	0.40
1:A:134:PRO:C	1:A:136:ASN:N	2.78	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	146/150 (97%)	78 (53%)	41 (28%)	27 (18%)	0 2
1	B	145/150 (97%)	86 (59%)	36 (25%)	23 (16%)	0 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	145/150 (97%)	76 (52%)	37 (26%)	32 (22%)	0	1
1	D	144/150 (96%)	80 (56%)	40 (28%)	24 (17%)	0	3
All	All	580/600 (97%)	320 (55%)	154 (27%)	106 (18%)	0	2

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	34	ALA
1	C	39	ARG
1	C	48	ALA
1	C	54	ALA
1	C	78	ASP
1	C	79	PRO
1	C	120	VAL
1	C	130	PRO
1	D	48	ALA
1	D	78	ASP
1	D	99	GLN
1	D	103	PHE
1	D	127	ARG
1	D	143	LEU
1	B	34	ALA
1	B	56	ARG
1	B	89	VAL
1	B	101	LEU
1	B	105	ILE
1	B	120	VAL
1	A	34	ALA
1	A	48	ALA
1	A	56	ARG
1	A	99	GLN
1	A	103	PHE
1	A	119	LEU
1	A	120	VAL
1	C	7	LYS
1	C	52	HIS
1	C	89	VAL
1	C	99	GLN
1	C	103	PHE
1	C	105	ILE
1	C	118	TYR

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Mol	Chain	Res	Type
1	C	123	GLY
1	C	142	THR
1	D	55	LEU
1	D	89	VAL
1	D	90	ASN
1	D	104	HIS
1	D	105	ILE
1	D	111	GLY
1	B	2	ASP
1	B	39	ARG
1	B	53	THR
1	B	55	LEU
1	B	90	ASN
1	B	100	LEU
1	B	103	PHE
1	A	14	GLU
1	A	16	LEU
1	A	17	SER
1	A	18	PHE
1	A	90	ASN
1	A	101	LEU
1	A	104	HIS
1	A	105	ILE
1	C	35	ALA
1	C	53	THR
1	C	55	LEU
1	C	88	TYR
1	C	104	HIS
1	C	108	LEU
1	C	134	PRO
1	D	18	PHE
1	D	37	LEU
1	D	54	ALA
1	D	117	GLU
1	B	129	PRO
1	A	39	ARG
1	A	55	LEU
1	A	57	GLN
1	A	58	ALA
1	A	100	LEU
1	A	102	TRP
1	A	108	LEU

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Mol	Chain	Res	Type
1	A	129	PRO
1	C	84	LEU
1	C	119	LEU
1	D	34	ALA
1	D	69	ALA
1	D	100	LEU
1	D	130	PRO
1	B	35	ALA
1	B	48	ALA
1	A	21	SER
1	A	85	VAL
1	C	14	GLU
1	C	87	SER
1	D	56	ARG
1	D	123	GLY
1	B	33	THR
1	B	102	TRP
1	A	143	LEU
1	C	27	VAL
1	C	146	THR
1	B	43	GLU
1	B	54	ALA
1	B	108	LEU
1	B	127	ARG
1	B	130	PRO
1	C	129	PRO
1	D	120	VAL
1	C	143	LEU
1	D	79	PRO
1	A	135	PRO

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	124/130 (95%)	112 (90%)	12 (10%)	8 28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	127/130 (98%)	116 (91%)	11 (9%)	9	33
1	C	127/130 (98%)	117 (92%)	10 (8%)	11	35
1	D	126/130 (97%)	114 (90%)	12 (10%)	8	28
All	All	504/520 (97%)	459 (91%)	45 (9%)	9	32

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	23	PHE
1	C	24	PHE
1	C	37	LEU
1	C	47	HIS
1	C	88	TYR
1	C	100	LEU
1	C	101	LEU
1	C	119	LEU
1	C	129	PRO
1	C	144	PRO
1	D	3	ILE
1	D	19	LEU
1	D	23	PHE
1	D	101	LEU
1	D	108	LEU
1	D	109	THR
1	D	119	LEU
1	D	126	ILE
1	D	129	PRO
1	D	130	PRO
1	D	142	THR
1	D	144	PRO
1	B	12	THR
1	B	19	LEU
1	B	23	PHE
1	B	47	HIS
1	B	55	LEU
1	B	68	LEU
1	B	93	VAL
1	B	101	LEU
1	B	108	LEU
1	B	116	LEU
1	B	145	GLU

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Mol	Chain	Res	Type
1	A	3	ILE
1	A	19	LEU
1	A	23	PHE
1	A	24	PHE
1	A	47	HIS
1	A	49	SER
1	A	67	THR
1	A	68	LEU
1	A	85	VAL
1	A	101	LEU
1	A	120	VAL
1	A	129	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	90	ASN
1	C	99	GLN
1	B	90	ASN
1	A	57	GLN
1	A	75	ASN
1	A	90	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	148/150 (98%)	1.97	58 (39%) 1 1	44, 95, 160, 196	0
1	B	147/150 (98%)	1.64	43 (29%) 1 3	43, 94, 159, 200	0
1	C	147/150 (98%)	2.00	61 (41%) 0 1	35, 105, 176, 200	0
1	D	146/150 (97%)	1.97	60 (41%) 0 1	40, 106, 171, 194	0
All	All	588/600 (98%)	1.90	222 (37%) 1 2	35, 100, 172, 200	0

All (222) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	145	GLU	10.1
1	A	148	VAL	8.9
1	B	147	THR	8.8
1	B	40	ASP	8.3
1	D	141	SER	7.6
1	D	80	ALA	7.6
1	A	14	GLU	6.9
1	D	146	THR	6.7
1	A	90	ASN	6.5
1	B	84	LEU	6.4
1	D	97	PHE	6.3
1	B	146	THR	6.2
1	A	21	SER	6.2
1	D	2	ASP	6.1
1	A	146	THR	6.1
1	C	17	SER	5.8
1	A	99	GLN	5.8
1	A	7	LYS	5.7
1	D	83	ASP	5.6
1	A	96	LYS	5.5
1	C	1	MET	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	46	GLU	5.3
1	C	144	PRO	5.3
1	C	80	ALA	5.2
1	B	14	GLU	5.2
1	D	145	GLU	5.2
1	C	43	GLU	5.1
1	C	99	GLN	5.0
1	D	78	ASP	5.0
1	C	141	SER	4.8
1	C	57	GLN	4.8
1	C	121	SER	4.7
1	C	90	ASN	4.7
1	A	66	MET	4.6
1	A	17	SER	4.6
1	D	135	PRO	4.5
1	B	17	SER	4.5
1	D	40	ASP	4.5
1	D	92	ASN	4.5
1	D	127	ARG	4.5
1	B	98	ARG	4.5
1	A	147	THR	4.5
1	C	5	PRO	4.5
1	D	74	THR	4.4
1	B	140	LEU	4.4
1	D	43	GLU	4.4
1	C	7	LYS	4.4
1	C	47	HIS	4.4
1	C	147	THR	4.4
1	D	88	TYR	4.4
1	D	57	GLN	4.4
1	A	9	PHE	4.4
1	B	91	THR	4.4
1	A	143	LEU	4.3
1	C	32	ASP	4.3
1	A	1	MET	4.2
1	D	70	THR	4.2
1	A	2	ASP	4.1
1	C	48	ALA	4.1
1	D	1	MET	4.1
1	D	99	GLN	4.1
1	D	60	LEU	4.1
1	B	43	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	58	ALA	4.0
1	C	142	THR	3.9
1	C	95	LEU	3.8
1	A	77	GLU	3.8
1	A	50	PRO	3.8
1	B	92	ASN	3.8
1	D	48	ALA	3.8
1	C	131	ALA	3.8
1	B	83	ASP	3.7
1	D	131	ALA	3.7
1	D	84	LEU	3.7
1	C	91	THR	3.7
1	A	40	ASP	3.7
1	D	63	GLY	3.6
1	B	57	GLN	3.6
1	C	96	LYS	3.6
1	A	76	LEU	3.6
1	D	143	LEU	3.5
1	D	72	VAL	3.5
1	D	47	HIS	3.5
1	A	82	ARG	3.5
1	C	79	PRO	3.5
1	C	98	ARG	3.5
1	C	36	ALA	3.5
1	C	23	PHE	3.4
1	D	67	THR	3.4
1	D	100	LEU	3.4
1	A	84	LEU	3.4
1	D	39	ARG	3.4
1	A	127	ARG	3.4
1	A	6	TYR	3.4
1	C	52	HIS	3.3
1	C	143	LEU	3.3
1	D	66	MET	3.3
1	D	21	SER	3.2
1	A	79	PRO	3.2
1	C	117	GLU	3.2
1	C	21	SER	3.2
1	C	112	ARG	3.2
1	B	64	ASP	3.2
1	D	71	TRP	3.1
1	A	52	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	98	ARG	3.1
1	A	101	LEU	3.1
1	A	136	ASN	3.1
1	C	118	TYR	3.1
1	B	21	SER	3.1
1	C	135	PRO	3.1
1	A	92	ASN	3.1
1	C	28	ARG	3.0
1	C	2	ASP	3.0
1	C	78	ASP	3.0
1	D	138	PRO	3.0
1	D	142	THR	3.0
1	C	81	SER	3.0
1	C	92	ASN	3.0
1	B	22	ASP	3.0
1	D	46	GLU	2.9
1	B	82	ARG	2.9
1	B	7	LYS	2.9
1	D	14	GLU	2.9
1	D	64	ASP	2.9
1	A	129	PRO	2.9
1	D	62	TRP	2.9
1	A	31	LEU	2.9
1	C	61	ALA	2.8
1	C	71	TRP	2.8
1	B	88	TYR	2.8
1	B	145	GLU	2.8
1	B	74	THR	2.8
1	A	45	PRO	2.8
1	A	81	SER	2.8
1	B	90	ASN	2.8
1	A	124	VAL	2.8
1	A	97	PHE	2.7
1	A	67	THR	2.7
1	D	81	SER	2.7
1	B	52	HIS	2.7
1	D	132	TYR	2.7
1	D	75	ASN	2.7
1	C	122	PHE	2.7
1	B	71	TRP	2.6
1	D	32	ASP	2.6
1	B	142	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	144	PRO	2.6
1	C	38	TYR	2.6
1	C	97	PHE	2.6
1	C	27	VAL	2.6
1	D	61	ALA	2.6
1	B	87	SER	2.6
1	B	94	GLY	2.6
1	B	125	TRP	2.5
1	D	117	GLU	2.5
1	A	145	GLU	2.5
1	A	39	ARG	2.5
1	B	124	VAL	2.5
1	A	103	PHE	2.5
1	C	40	ASP	2.5
1	D	31	LEU	2.5
1	D	85	VAL	2.5
1	A	10	GLY	2.5
1	C	66	MET	2.5
1	B	50	PRO	2.4
1	A	100	LEU	2.4
1	D	112	ARG	2.4
1	C	77	GLU	2.4
1	A	141	SER	2.4
1	C	31	LEU	2.4
1	A	104	HIS	2.4
1	D	10	GLY	2.4
1	C	85	VAL	2.4
1	C	83	ASP	2.4
1	B	2	ASP	2.4
1	B	5	PRO	2.4
1	D	98	ARG	2.4
1	D	50	PRO	2.3
1	A	41	ALA	2.3
1	C	3	ILE	2.3
1	D	59	ILE	2.3
1	C	53	THR	2.3
1	A	72	VAL	2.3
1	C	14	GLU	2.3
1	D	7	LYS	2.3
1	D	6	TYR	2.3
1	B	81	SER	2.3
1	B	10	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	108	LEU	2.3
1	C	113	GLU	2.3
1	A	63	GLY	2.3
1	B	97	PHE	2.2
1	B	113	GLU	2.2
1	A	43	GLU	2.2
1	D	56	ARG	2.2
1	A	69	ALA	2.2
1	C	126	ILE	2.2
1	A	18	PHE	2.2
1	C	108	LEU	2.2
1	B	135	PRO	2.2
1	C	100	LEU	2.2
1	A	29	ASP	2.1
1	C	73	GLY	2.1
1	C	136	ASN	2.1
1	B	47	HIS	2.1
1	C	86	VAL	2.1
1	C	67	THR	2.1
1	A	61	ALA	2.1
1	B	79	PRO	2.1
1	A	78	ASP	2.1
1	B	53	THR	2.1
1	A	56	ARG	2.1
1	B	96	LYS	2.1
1	A	91	THR	2.0
1	D	137	ALA	2.0
1	D	90	ASN	2.0
1	B	3	ILE	2.0
1	D	95	LEU	2.0
1	B	70	THR	2.0
1	A	102	TRP	2.0
1	A	85	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.