



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:11 PM UTC

PDB ID : 1FN4 / pdb_00001fn4
Title : CRYSTAL STRUCTURE OF FAB198, AN EFFICIENT PROTECTOR OF ACETYLCHOLINE RECEPTOR AGAINST MYASTHENOGENIC ANTIBODIES
Authors : Poulas, K.; Eliopoulos, E.; Vatzaki, E.; Navaza, J.; Kontou, M.
Deposited on : 2000-08-21
Resolution : 2.80 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

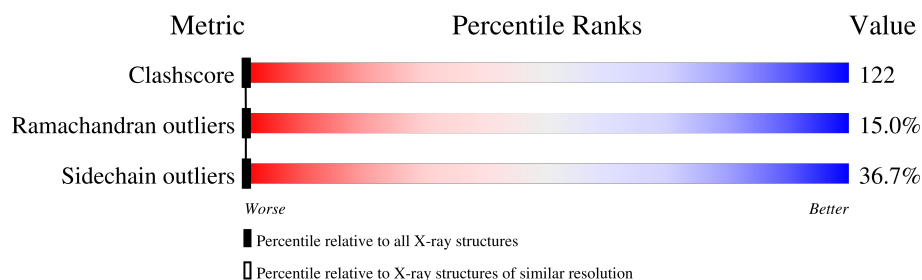
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	211	11% 33% 38% 18%
1	C	211	9% 46% 31% 14%
2	B	218	11% 40% 36% 13%
2	D	218	14% 47% 31% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6714 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 MONOCLONAL ANTIBODY AGAINST ACETYLCHOLINE RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1626	1014	271	334	7			
1	C	211	Total	C	N	O	S	0	0	0
			1626	1014	271	334	7			

- Molecule 2 is a protein called MONOCLONAL ANTIBODY AGAINST ACETYLCHOLINE RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1663	1061	273	319	10			
2	D	218	Total	C	N	O	S	0	0	0
			1663	1061	273	319	10			

- Molecule 3 is water.

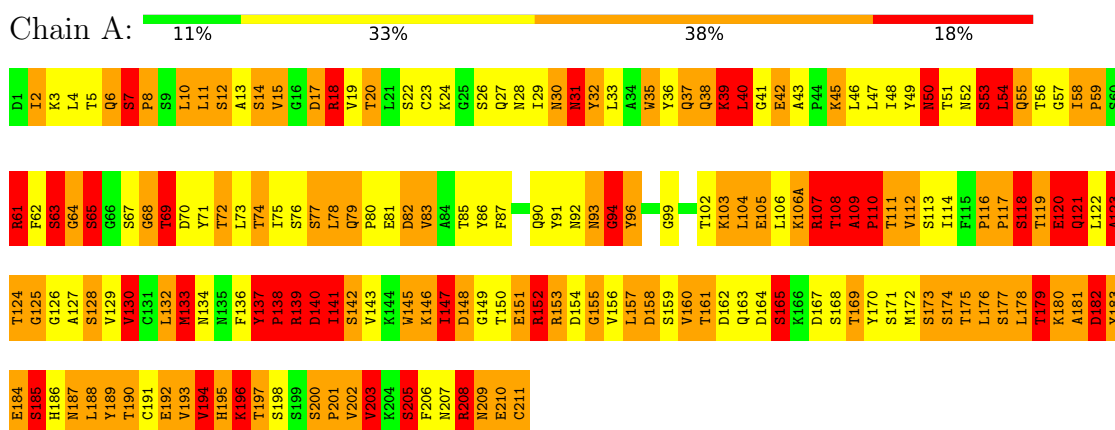
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total	O	0	0
			35	35		
3	B	40	Total	O	0	0
			40	40		
3	C	24	Total	O	0	0
			24	24		
3	D	37	Total	O	0	0
			37	37		

3 Residue-property plots

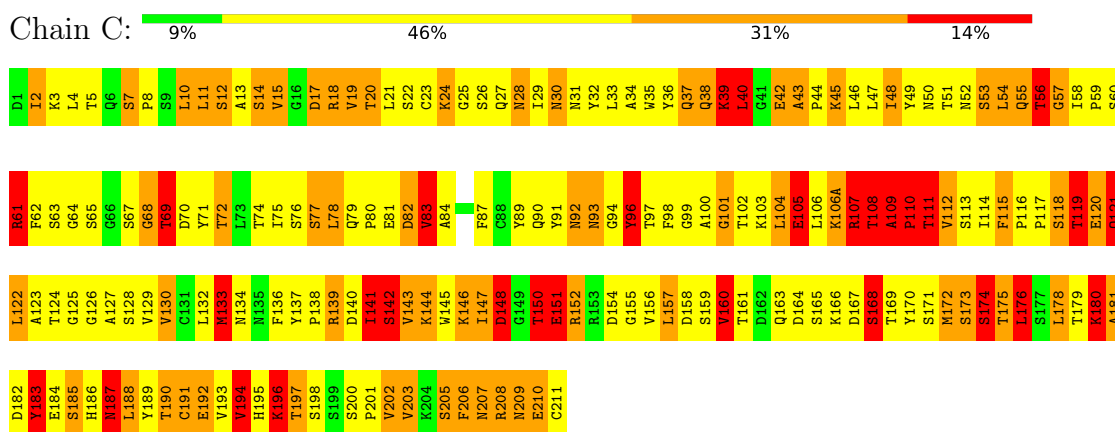
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

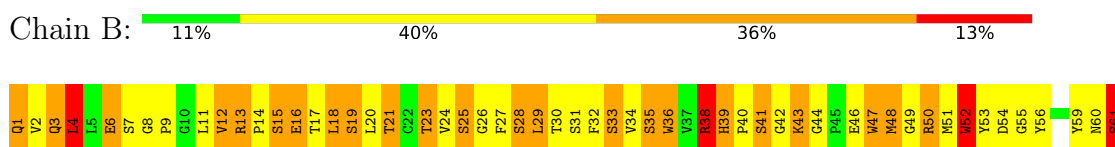
• Molecule 1: MONOCLONAL ANTIBODY AGAINST ACETYLCHOLINE RECEPTOR

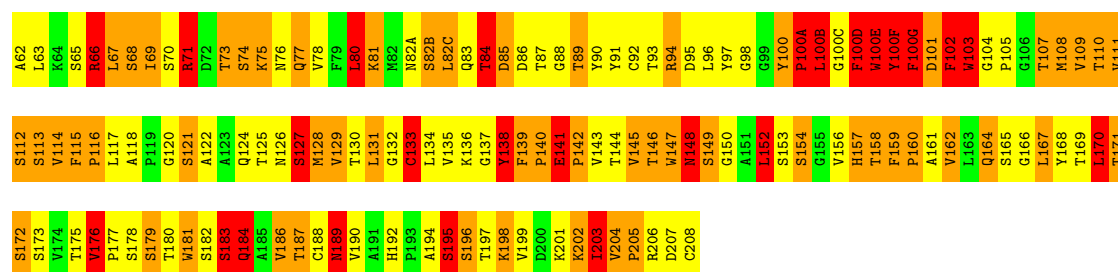


• Molecule 1: MONOCLONAL ANTIBODY AGAINST ACETYLCHOLINE RECEPTOR

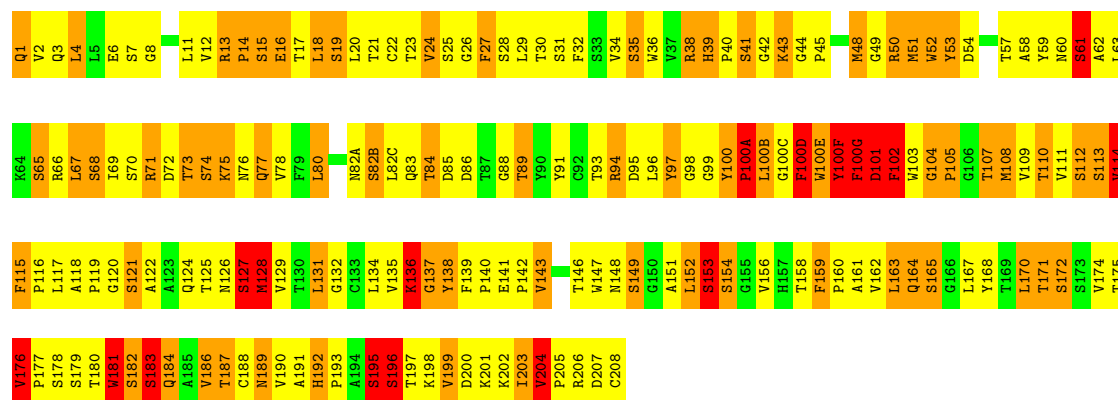
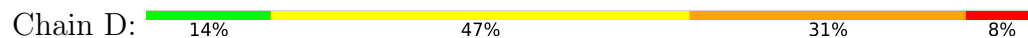


• Molecule 2: MONOCLONAL ANTIBODY AGAINST ACETYLCHOLINE RECEPTOR





● Molecule 2: MONOCLONAL ANTIBODY AGAINST ACETYLCHOLINE RECEPTOR



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.78Å 169.78Å 182.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	98.0 (20.00-2.80)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.198 , 0.294	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6714	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	3.37	42/1648 (2.5%)	2.66	120/2222 (5.4%)
1	C	1.39	14/1658 (0.8%)	1.71	43/2253 (1.9%)
2	B	2.89	29/1706 (1.7%)	2.51	84/2321 (3.6%)
2	D	1.31	6/1712 (0.4%)	1.65	35/2341 (1.5%)
All	All	2.41	91/6724 (1.4%)	2.17	282/9137 (3.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	C	0	2
2	B	0	3
2	D	0	3
All	All	0	12

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	179	SER	C-N	47.51	1.99	1.33
1	A	196	LYS	C-N	46.90	1.97	1.33
2	B	181	TRP	C-N	43.27	1.95	1.33
1	A	183	TYR	C-N	42.43	1.96	1.33
1	A	197	THR	C-N	39.59	1.83	1.33
2	B	85	ASP	C-N	39.54	1.84	1.33
1	A	184	GLU	C-N	37.77	1.85	1.33
2	B	47	TRP	C-N	36.91	1.81	1.33
1	A	189	TYR	C-N	35.41	1.82	1.33
1	A	30	ASN	C-N	35.05	1.82	1.33
2	B	101	ASP	C-N	32.33	1.78	1.33
1	A	205	SER	C-N	31.58	1.77	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	LEU	C-N	31.08	1.77	1.33
2	B	25	SER	C-N	29.45	1.74	1.33
2	B	152	LEU	C-N	28.98	1.74	1.33
1	A	110	PRO	C-N	27.72	1.72	1.33
2	B	127	SER	C-N	26.21	1.70	1.33
1	A	124	THR	C-N	25.18	1.66	1.33
1	A	31	ASN	C-N	21.59	1.69	1.33
1	A	123	ALA	C-N	21.48	1.83	1.34
2	B	102	PHE	C-N	18.25	1.59	1.33
1	A	125	GLY	C-N	-18.04	1.07	1.33
1	A	108	THR	N-CA	15.43	1.66	1.46
1	A	152	ARG	C-N	14.83	1.54	1.33
2	B	146	THR	C-N	-14.77	1.12	1.33
2	B	139	PHE	C-O	13.92	1.42	1.24
1	A	107	ARG	CA-C	13.39	1.70	1.52
1	A	185	SER	N-CA	13.16	1.62	1.46
2	B	138	TYR	C-N	-12.05	1.08	1.33
1	A	107	ARG	C-N	10.91	1.49	1.33
1	A	109	ALA	CA-C	10.71	1.66	1.52
1	A	109	ALA	N-CA	10.58	1.61	1.46
1	A	107	ARG	N-CA	10.24	1.59	1.46
1	A	108	THR	CA-C	9.95	1.66	1.52
1	A	110	PRO	N-CA	9.39	1.59	1.47
1	A	106(A)	LYS	CA-C	9.22	1.63	1.52
1	C	107	ARG	CA-C	8.64	1.64	1.52
1	C	108	THR	CA-CB	8.40	1.67	1.53
1	A	169	THR	C-N	8.22	1.46	1.33
1	C	119	THR	CA-CB	8.15	1.67	1.53
1	C	108	THR	CA-C	7.90	1.63	1.52
1	A	32	TYR	C-N	7.74	1.44	1.33
1	C	108	THR	N-CA	7.48	1.55	1.46
1	A	116	PRO	C-N	7.31	1.42	1.33
2	D	199	VAL	CA-CB	-7.30	1.46	1.54
1	C	111	THR	N-CA	7.13	1.55	1.46
1	A	179	THR	C-N	7.07	1.44	1.33
2	D	108	MET	CG-SD	6.89	1.98	1.80
2	B	100(G)	PHE	N-CA	6.76	1.53	1.46
2	B	194	ALA	N-CA	6.66	1.53	1.46
2	D	48	MET	SD-CE	-6.60	1.63	1.79
2	D	51	MET	CA-C	-6.54	1.43	1.53
1	A	108	THR	C-N	6.37	1.46	1.33
2	B	149	SER	N-CA	-6.35	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	106(A)	LYS	CA-C	6.27	1.60	1.52
1	A	7	SER	N-CA	6.19	1.54	1.46
1	A	64	GLY	N-CA	6.06	1.51	1.44
1	C	133	MET	SD-CE	6.04	1.94	1.79
1	A	110	PRO	CA-C	5.92	1.60	1.52
2	B	140	PRO	CA-CB	-5.91	1.45	1.53
1	A	106(A)	LYS	C-N	5.86	1.41	1.33
1	C	109	ALA	CA-CB	-5.84	1.44	1.53
2	B	154	SER	C-N	5.79	1.40	1.33
1	C	19	VAL	CA-CB	-5.66	1.46	1.54
1	C	111	THR	CA-C	5.62	1.60	1.52
2	B	100(E)	TRP	NE1-CE2	-5.61	1.31	1.37
2	B	103	TRP	NE1-CE2	-5.61	1.31	1.37
2	D	100(G)	PHE	CA-C	5.54	1.58	1.52
1	A	112	VAL	N-CA	5.51	1.53	1.46
1	A	145	TRP	NE1-CE2	-5.50	1.31	1.37
1	C	174	SER	CA-C	-5.43	1.46	1.52
1	A	180	LYS	CA-C	-5.38	1.45	1.52
2	B	101	ASP	N-CA	5.37	1.53	1.45
2	B	147	TRP	NE1-CE2	-5.34	1.31	1.37
1	C	109	ALA	N-CA	5.34	1.53	1.46
1	A	35	TRP	NE1-CE2	-5.33	1.31	1.37
2	D	94	ARG	C-O	-5.27	1.17	1.23
2	B	36	TRP	NE1-CE2	-5.26	1.31	1.37
1	A	109	ALA	C-N	5.26	1.46	1.33
1	A	116	PRO	CA-C	5.25	1.57	1.52
2	B	47	TRP	NE1-CE2	-5.24	1.31	1.37
2	B	81	LYS	N-CA	5.17	1.52	1.46
2	B	118	ALA	N-CA	5.16	1.51	1.46
1	A	94	GLY	C-N	5.12	1.40	1.33
2	B	154	SER	CA-C	-5.11	1.45	1.53
2	B	140	PRO	N-CA	-5.09	1.40	1.47
2	B	100(F)	TYR	N-CA	5.04	1.52	1.46
1	C	107	ARG	N-CA	5.04	1.52	1.46
1	A	184	GLU	C-O	-5.02	1.17	1.24
2	B	181	TRP	NE1-CE2	-5.01	1.31	1.37
1	A	162	ASP	N-CA	5.00	1.51	1.45

All (282) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	127	SER	O-C-N	-36.73	73.74	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	138	TYR	O-C-N	-30.60	81.89	122.59
1	A	205	SER	O-C-N	-27.08	86.58	122.59
1	A	30	ASN	O-C-N	-22.94	94.66	122.87
2	B	181	TRP	O-C-N	-22.19	87.50	123.00
1	A	196	LYS	CA-C-N	-21.84	86.40	122.65
1	A	196	LYS	C-N-CA	-21.84	86.40	122.65
2	B	146	THR	O-C-N	21.45	149.44	123.27
2	B	154	SER	O-C-N	20.12	145.47	122.94
1	A	31	ASN	CA-C-N	-20.04	96.79	122.84
1	A	31	ASN	C-N-CA	-20.04	96.79	122.84
1	A	123	ALA	CA-C-N	-18.66	90.26	122.92
1	A	123	ALA	C-N-CA	-18.66	90.26	122.92
2	B	85	ASP	O-C-N	-18.39	79.45	121.74
1	A	132	LEU	CA-C-N	-16.42	90.17	121.54
1	A	132	LEU	C-N-CA	-16.42	90.17	121.54
2	B	179	SER	CA-C-N	-16.04	92.82	121.70
2	B	179	SER	C-N-CA	-16.04	92.82	121.70
2	B	47	TRP	CA-C-N	-15.77	95.97	122.79
2	B	47	TRP	C-N-CA	-15.77	95.97	122.79
2	B	154	SER	N-CA-C	15.24	133.08	110.52
1	A	180	LYS	O-C-N	15.24	142.04	122.23
2	B	170	LEU	O-C-N	14.26	133.54	120.71
1	A	152	ARG	O-C-N	-13.65	106.24	122.89
2	B	101	ASP	CA-C-N	-13.34	96.07	121.54
2	B	101	ASP	C-N-CA	-13.34	96.07	121.54
1	A	50	ASN	O-C-N	12.79	139.60	122.59
2	B	80	LEU	O-C-N	12.67	137.54	122.84
1	A	201	PRO	O-C-N	12.38	139.36	122.64
2	D	84	THR	N-CA-C	-12.12	98.91	112.72
1	A	140	ASP	O-C-N	12.05	136.89	123.27
2	B	203	ILE	O-C-N	11.93	137.49	122.57
2	B	146	THR	CA-C-N	-11.75	104.70	122.09
2	B	146	THR	C-N-CA	-11.75	104.70	122.09
1	C	180	LYS	N-CA-C	-11.57	98.43	112.54
1	A	39	LYS	O-C-N	11.34	137.68	122.59
2	B	152	LEU	CA-C-N	-11.20	100.15	121.54
2	B	152	LEU	C-N-CA	-11.20	100.15	121.54
1	A	6	GLN	O-C-N	10.82	136.23	121.83
1	A	205	SER	CA-C-N	-10.78	100.96	121.54
1	A	205	SER	C-N-CA	-10.78	100.96	121.54
2	D	104	GLY	CA-C-N	10.72	133.24	119.84
2	D	104	GLY	C-N-CA	10.72	133.24	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	165	SER	N-CA-C	-10.67	99.44	111.71
1	A	50	ASN	CA-CB-CG	10.38	122.98	112.60
1	A	63	SER	CB-CA-C	10.38	131.07	110.42
2	D	114	VAL	N-CA-C	10.33	122.58	106.88
2	D	128	MET	N-CA-C	10.30	125.30	109.96
1	A	7	SER	O-C-N	-10.29	109.49	121.32
2	B	202	LYS	CA-C-N	-10.29	103.45	121.97
2	B	202	LYS	C-N-CA	-10.29	103.45	121.97
1	A	184	GLU	O-C-N	10.24	136.50	122.37
1	A	165	SER	O-C-N	10.17	132.54	122.07
2	B	170	LEU	CB-CA-C	-10.16	94.85	115.28
2	B	145	VAL	CB-CA-C	-10.12	96.61	111.68
2	B	133	CYS	O-C-N	10.04	135.95	122.59
1	A	179	THR	CA-C-N	-10.04	103.42	120.58
1	A	179	THR	C-N-CA	-10.04	103.42	120.58
1	A	132	LEU	O-C-N	-10.01	109.02	121.83
1	A	38	GLN	N-CA-C	-9.90	99.76	112.93
1	A	58	ILE	O-C-N	-9.83	109.89	121.10
1	C	108	THR	N-CA-C	9.80	131.68	110.80
2	B	127	SER	CA-C-N	-9.79	102.85	121.54
2	B	127	SER	C-N-CA	-9.79	102.85	121.54
1	C	109	ALA	CA-C-N	9.72	131.99	119.84
1	C	109	ALA	C-N-CA	9.72	131.99	119.84
1	A	178	LEU	O-C-N	9.64	135.41	122.59
1	C	200	SER	N-CA-C	-9.55	97.51	109.64
1	A	195	HIS	O-C-N	9.51	127.86	120.83
2	D	101	ASP	N-CA-C	9.49	122.08	110.41
1	A	201	PRO	CB-CA-C	-9.22	96.35	111.56
1	A	189	TYR	O-C-N	-9.20	110.74	123.34
2	D	24	VAL	N-CA-C	9.01	121.79	109.80
2	B	202	LYS	O-C-N	-9.01	112.05	122.68
1	C	42	GLU	N-CA-C	-8.98	95.04	108.79
2	B	189	ASN	N-CA-CB	-8.93	95.40	110.49
1	C	134	ASN	N-CA-C	8.88	123.37	109.07
1	A	133	MET	N-CA-C	-8.75	92.16	110.80
2	B	145	VAL	O-C-N	8.72	133.51	122.61
2	B	142	PRO	O-C-N	8.68	133.74	122.89
1	A	83	VAL	O-C-N	8.57	131.41	122.67
1	C	106(A)	LYS	N-CA-C	8.56	122.90	109.81
1	A	119	THR	N-CA-CB	8.55	123.71	109.78
2	D	118	ALA	CA-C-N	8.43	130.38	119.84
2	D	118	ALA	C-N-CA	8.43	130.38	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	138	TYR	CA-C-N	8.37	142.23	121.80
2	B	138	TYR	C-N-CA	8.37	142.23	121.80
1	A	184	GLU	CA-C-O	8.32	129.35	119.28
2	B	203	ILE	CB-CA-C	8.32	124.94	111.29
1	A	137	TYR	O-C-N	-8.18	111.91	121.32
2	B	189	ASN	CB-CA-C	8.18	126.71	110.42
1	A	119	THR	O-C-N	8.12	131.45	122.11
2	D	182	SER	N-CA-C	-8.08	100.10	110.53
1	A	125	GLY	O-C-N	-8.01	113.18	122.31
1	C	183	TYR	N-CA-C	-8.01	102.63	111.36
1	C	190	THR	N-CA-C	7.96	122.07	109.50
1	C	43	ALA	CA-C-N	-7.88	111.85	119.89
1	C	43	ALA	C-N-CA	-7.88	111.85	119.89
1	A	40	LEU	O-C-N	7.88	133.07	122.59
1	A	50	ASN	CA-C-N	7.86	136.54	121.54
1	A	50	ASN	C-N-CA	7.86	136.54	121.54
1	C	112	VAL	N-CA-C	7.77	119.91	108.65
2	B	140	PRO	N-CA-C	-7.75	96.50	112.47
1	A	139	ARG	CA-C-N	-7.73	112.05	122.72
1	A	139	ARG	C-N-CA	-7.73	112.05	122.72
2	D	136	LYS	N-CA-C	7.70	121.46	110.14
1	A	178	LEU	CB-CA-C	-7.70	95.10	110.42
1	A	59	PRO	O-C-N	7.69	133.03	122.64
2	B	139	PHE	CA-C-O	-7.68	109.64	120.16
1	C	82	ASP	N-CA-C	-7.64	103.03	114.64
1	A	133	MET	O-C-N	7.49	132.55	122.59
2	D	204	VAL	CA-C-N	7.46	128.56	120.13
2	D	204	VAL	C-N-CA	7.46	128.56	120.13
1	C	196	LYS	N-CA-C	-7.45	94.93	110.80
2	B	128	MET	O-C-N	7.38	132.41	122.59
1	C	119	THR	N-CA-C	-7.38	102.30	111.75
2	B	25	SER	N-CA-C	-7.37	99.33	109.95
2	B	100(D)	PHE	CA-CB-CG	7.37	121.17	113.80
1	A	39	LYS	CA-C-N	7.34	135.57	121.54
1	A	39	LYS	C-N-CA	7.34	135.57	121.54
1	A	133	MET	CA-C-N	7.33	131.82	120.75
1	A	133	MET	C-N-CA	7.33	131.82	120.75
1	A	146	LYS	O-C-N	7.33	131.52	122.14
2	B	147	TRP	O-C-N	7.33	131.66	123.16
1	A	183	TYR	N-CA-C	-7.30	95.26	110.80
2	B	154	SER	CA-C-N	7.30	132.65	122.29
2	B	154	SER	C-N-CA	7.30	132.65	122.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	142	PRO	CB-CA-C	-7.26	98.92	110.96
1	C	164	ASP	N-CA-C	7.23	120.80	109.96
2	B	100(E)	TRP	N-CA-C	-7.21	103.50	111.36
2	D	151	ALA	N-CA-C	-7.21	104.35	113.72
1	C	187	ASN	CA-C-N	7.19	131.34	121.05
1	C	187	ASN	C-N-CA	7.19	131.34	121.05
1	A	83	VAL	N-CA-CB	7.19	119.77	110.13
1	A	175	THR	O-C-N	7.16	132.70	123.11
2	D	118	ALA	N-CA-C	7.11	114.62	108.22
2	B	154	SER	CB-CA-C	-7.08	97.45	109.83
1	A	82	ASP	N-CA-C	-7.05	103.92	114.64
1	A	180	LYS	N-CA-C	-7.05	103.02	111.69
1	A	190	THR	N-CA-C	7.04	120.14	109.23
2	D	27	PHE	N-CA-C	7.02	117.29	108.45
2	D	102	PHE	N-CA-C	6.99	125.69	110.80
1	C	107	ARG	N-CA-C	6.97	125.65	110.80
1	A	201	PRO	N-CA-C	6.96	126.80	112.47
2	B	108	MET	CB-CA-C	-6.86	96.77	110.42
2	B	100(D)	PHE	CB-CA-C	-6.82	96.86	110.42
2	B	116	PRO	O-C-N	6.79	130.86	122.71
2	B	84	THR	N-CA-C	-6.76	104.91	113.02
2	B	145	VAL	N-CA-CB	6.73	123.47	110.95
1	C	83	VAL	N-CA-C	-6.71	100.31	109.37
1	A	8	PRO	O-C-N	6.64	131.60	122.64
1	C	141	ILE	N-CA-C	-6.64	100.72	108.82
1	C	155	GLY	N-CA-C	-6.62	105.73	115.72
1	A	109	ALA	CA-C-N	6.61	128.10	119.84
1	A	109	ALA	C-N-CA	6.61	128.10	119.84
1	A	110	PRO	CB-CA-C	-6.59	100.68	111.56
2	B	115	PHE	O-C-N	-6.55	115.56	121.39
2	D	30	THR	N-CA-C	-6.54	104.54	113.30
2	B	133	CYS	N-CA-CB	-6.54	99.44	110.49
1	C	110	PRO	N-CA-C	6.47	125.79	112.47
2	D	100(G)	PHE	N-CA-C	6.45	118.71	107.49
1	A	74	THR	CB-CA-C	-6.42	98.65	109.50
2	B	15	SER	O-C-N	6.42	131.13	122.59
1	C	107	ARG	CA-C-N	6.33	133.63	121.54
1	C	107	ARG	C-N-CA	6.33	133.63	121.54
2	B	48	MET	N-CA-C	-6.32	104.53	112.93
2	D	78	VAL	N-CA-C	-6.31	99.03	108.12
2	D	53	TYR	N-CA-C	-6.30	105.42	113.23
2	D	22	CYS	N-CA-C	-6.29	100.26	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	141	GLU	N-CA-C	6.29	123.71	109.81
2	B	3	GLN	CB-CA-C	-6.29	97.91	110.42
2	B	80	LEU	CB-CA-C	-6.28	99.58	110.45
1	A	79	GLN	CB-CA-C	-6.27	97.83	110.17
1	C	22	SER	N-CA-C	6.21	119.77	110.14
2	B	100(B)	LEU	N-CA-CB	6.19	120.95	110.49
2	D	196	SER	CA-C-N	6.19	130.27	121.42
2	D	196	SER	C-N-CA	6.19	130.27	121.42
1	A	201	PRO	CA-C-N	6.17	131.06	123.10
1	A	201	PRO	C-N-CA	6.17	131.06	123.10
1	A	152	ARG	CA-C-N	-6.15	110.62	121.70
1	A	152	ARG	C-N-CA	-6.15	110.62	121.70
1	A	40	LEU	CB-CA-C	-6.13	98.23	110.42
1	A	94	GLY	O-C-N	-6.12	114.75	122.70
2	B	129	VAL	N-CA-CB	6.11	121.31	111.23
1	A	160	VAL	O-C-N	6.10	130.20	122.57
1	C	92	ASN	N-CA-C	-6.09	103.97	111.40
1	A	155	GLY	N-CA-C	-6.08	106.76	115.64
1	A	183	TYR	CA-C-N	-5.95	111.60	122.38
1	A	183	TYR	C-N-CA	-5.95	111.60	122.38
2	D	192	HIS	CA-C-N	5.90	127.22	119.84
2	D	192	HIS	C-N-CA	5.90	127.22	119.84
1	A	160	VAL	CA-C-N	-5.89	110.28	121.54
1	A	160	VAL	C-N-CA	-5.89	110.28	121.54
1	A	118	SER	CA-C-N	-5.84	112.06	120.82
1	A	118	SER	C-N-CA	-5.84	112.06	120.82
1	A	133	MET	CB-CA-C	5.82	122.01	110.42
2	B	15	SER	N-CA-CB	-5.79	100.71	110.49
2	B	205	PRO	CB-CA-C	-5.78	104.47	111.46
1	A	50	ASN	CB-CA-C	5.77	121.90	110.42
1	A	153	ARG	NE-CZ-NH2	5.76	124.39	119.20
2	D	13	ARG	CA-C-N	-5.76	112.64	119.84
2	D	13	ARG	C-N-CA	-5.76	112.64	119.84
2	B	148	ASN	O-C-N	5.76	130.25	122.59
1	C	101	GLY	CA-C-O	-5.76	117.97	122.52
1	C	53	SER	N-CA-C	5.72	118.03	108.02
2	D	115	PHE	CA-C-N	5.71	125.91	120.31
2	D	115	PHE	C-N-CA	5.71	125.91	120.31
1	A	134	ASN	N-CA-C	5.70	118.10	110.35
2	B	140	PRO	N-CA-CB	5.68	109.21	103.25
2	B	48	MET	O-C-N	5.66	129.73	122.03
2	B	176	VAL	N-CA-CB	-5.66	103.29	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	ASP	CB-CA-C	5.63	122.08	110.31
1	C	176	LEU	N-CA-C	-5.63	100.52	109.76
1	C	207	ASN	N-CA-C	5.63	119.47	107.70
1	C	160	VAL	N-CA-C	5.62	121.04	109.34
1	A	180	LYS	CB-CA-C	-5.61	100.43	110.70
1	C	168	SER	N-CA-C	5.61	122.75	110.80
1	A	178	LEU	N-CA-CB	5.56	119.88	110.49
1	C	61	ARG	N-CA-C	-5.55	106.49	113.20
1	A	94	GLY	N-CA-C	5.53	126.29	113.18
2	B	108	MET	O-C-N	5.53	129.94	122.59
1	C	150	THR	N-CA-C	5.53	122.58	110.80
2	D	181	TRP	N-CA-C	-5.52	104.95	110.97
1	A	137	TYR	N-CA-CB	5.51	120.18	110.37
1	A	112	VAL	CB-CA-C	-5.51	101.87	110.52
1	C	105	GLU	N-CA-C	5.51	118.23	110.14
2	D	176	VAL	N-CA-C	5.48	115.20	109.01
1	C	79	GLN	N-CA-C	-5.46	102.06	110.58
2	B	94	ARG	NE-CZ-NH2	5.43	124.09	119.20
1	A	53	SER	N-CA-CB	-5.43	103.34	111.64
1	A	124	THR	O-C-N	5.43	132.32	122.44
2	B	71	ARG	NE-CZ-NH2	5.42	124.07	119.20
1	A	200	SER	N-CA-C	-5.39	99.69	109.44
1	A	82	ASP	CA-C-N	-5.38	113.48	120.63
1	A	82	ASP	C-N-CA	-5.38	113.48	120.63
2	B	142	PRO	N-CA-C	5.37	119.05	110.40
2	B	12	VAL	N-CA-CB	5.37	119.36	111.52
1	A	117	PRO	O-C-N	5.36	129.14	122.71
2	B	66	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	C	115	PHE	CA-C-N	5.34	125.88	120.38
1	C	115	PHE	C-N-CA	5.34	125.88	120.38
1	A	61	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	A	18	ARG	NE-CZ-NH2	5.34	124.00	119.20
2	B	38	ARG	NE-CZ-NH2	5.33	124.00	119.20
2	B	25	SER	O-C-N	-5.31	115.11	122.76
2	B	52	TRP	O-C-N	5.31	129.66	122.59
1	A	134	ASN	O-C-N	5.31	129.34	122.81
1	A	40	LEU	N-CA-C	5.29	122.07	110.80
1	A	208	ARG	NE-CZ-NH2	5.29	123.96	119.20
2	B	13	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	A	148	ASP	N-CA-C	-5.28	96.21	111.00
1	A	108	THR	N-CA-C	5.27	122.03	110.80
2	B	80	LEU	CA-C-N	5.27	131.61	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	80	LEU	C-N-CA	5.27	131.61	121.54
1	A	139	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	A	148	ASP	CB-CA-C	5.25	120.08	110.10
1	A	107	ARG	NE-CZ-NH2	5.25	123.92	119.20
2	B	100(B)	LEU	CB-CA-C	-5.25	99.98	110.42
1	A	130	VAL	O-C-N	5.24	129.12	122.57
2	B	203	ILE	N-CA-CB	-5.23	102.61	111.23
1	A	138	PRO	O-C-N	5.21	129.67	122.64
2	D	143	VAL	N-CA-C	-5.20	101.16	109.17
1	A	140	ASP	N-CA-C	5.20	117.71	109.24
2	B	50	ARG	NE-CZ-NH2	5.19	123.87	119.20
2	D	165	SER	N-CA-C	-5.17	99.53	108.52
1	A	63	SER	N-CA-CB	-5.16	101.76	110.49
2	B	128	MET	CA-C-N	5.14	131.23	121.97
2	B	128	MET	C-N-CA	5.14	131.23	121.97
1	A	116	PRO	O-C-N	-5.13	115.41	121.46
1	A	180	LYS	CA-C-N	5.11	131.30	121.54
1	A	180	LYS	C-N-CA	5.11	131.30	121.54
1	C	7	SER	N-CA-C	5.11	121.10	109.81
1	A	32	TYR	O-C-N	5.09	129.11	123.05
1	A	147	ILE	CB-CA-C	-5.08	102.97	111.29
2	B	129	VAL	CB-CA-C	-5.07	102.97	111.29
1	A	63	SER	O-C-N	5.06	129.32	122.59
1	C	142	SER	N-CA-C	-5.05	101.06	108.99
1	A	165	SER	N-CA-C	-5.04	105.67	111.07
1	A	211	CYS	CA-CB-SG	-5.04	102.80	114.40
2	D	124	GLN	N-CA-C	5.01	121.48	110.80
1	A	106(A)	LYS	O-C-N	-5.01	118.06	123.42
1	A	112	VAL	N-CA-C	5.00	115.90	108.65

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	152	ARG	Peptide,Mainchain
1	A	179	THR	Mainchain
1	A	94	GLY	Mainchain
2	B	102	PHE	Mainchain
2	B	138	TYR	Peptide,Mainchain
1	C	183	TYR	Sidechain
1	C	96	TYR	Sidechain
2	D	100(G)	PHE	Sidechain

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Mol	Chain	Res	Type	Group
2	D	138	TYR	Sidechain
2	D	97	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1626	0	1561	562	0
1	C	1626	0	1579	365	0
2	B	1663	0	1601	447	1
2	D	1663	0	1613	293	4
3	A	35	0	0	0	0
3	B	40	0	0	8	3
3	C	24	0	0	4	0
3	D	37	0	0	5	0
All	All	6714	0	6354	1577	4

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 122.

All (1577) 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:116:PRO:HG3	1:A:206:PHE:CE1	1.17	1.58
1:A:116:PRO:CG	1:A:206:PHE:CE1	1.90	1.53
2:B:127:SER:C	2:B:128:MET:N	1.70	1.49
1:A:31:ASN:C	1:A:32:TYR:N	1.69	1.47
1:A:116:PRO:HB3	1:A:206:PHE:CZ	1.50	1.45
1:A:110:PRO:C	1:A:111:THR:N	1.72	1.44
1:A:40:LEU:C	1:A:40:LEU:HD12	1.26	1.44
2:B:152:LEU:C	2:B:153:SER:N	1.74	1.43
2:B:25:SER:C	2:B:26:GLY:N	1.74	1.42
1:A:205:SER:C	1:A:206:PHE:N	1.77	1.41
2:B:101:ASP:C	2:B:102:PHE:N	1.78	1.40
1:A:180:LYS:CD	1:A:184:GLU:OE2	1.70	1.39
2:B:48:MET:HE1	2:B:90:TYR:CE2	1.55	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LEU:C	1:A:133:MET:N	1.77	1.39
2:B:47:TRP:C	2:B:48:MET:N	1.81	1.38
1:A:30:ASN:C	1:A:31:ASN:N	1.82	1.37
1:A:197:THR:C	1:A:198:SER:N	1.83	1.36
1:A:189:TYR:C	1:A:190:THR:N	1.82	1.36
1:A:123:ALA:C	1:A:124:THR:N	1.83	1.35
1:A:156:VAL:HG12	1:A:176:LEU:CA	1.58	1.34
1:A:40:LEU:C	1:A:40:LEU:CD1	1.90	1.33
2:B:85:ASP:C	2:B:86:ASP:N	1.84	1.33
1:A:184:GLU:C	1:A:185:SER:N	1.85	1.33
2:B:18:LEU:HG	2:B:102:PHE:CZ	1.64	1.31
2:B:101:ASP:O	2:B:102:PHE:HB2	1.16	1.31
1:A:79:GLN:HB3	1:A:80:PRO:CD	1.62	1.30
1:A:116:PRO:HG3	1:A:206:PHE:CD1	1.66	1.29
1:A:171:SER:OG	2:B:157:HIS:HE1	1.16	1.28
2:B:48:MET:HE1	2:B:90:TYR:CD2	1.69	1.27
2:B:175:THR:O	2:B:176:VAL:HG23	1.18	1.26
1:A:180:LYS:CG	1:A:184:GLU:OE2	1.82	1.26
2:B:128:MET:N	2:B:177:PRO:HA	1.48	1.25
1:A:40:LEU:HD12	1:A:40:LEU:O	1.32	1.25
1:A:178:LEU:CD1	1:A:182:ASP:OD1	1.83	1.25
2:B:158:THR:HG21	3:B:211:HOH:O	1.37	1.24
1:A:183:TYR:C	1:A:184:GLU:N	1.96	1.23
1:A:196:LYS:C	1:A:197:THR:N	1.97	1.23
2:B:181:TRP:C	2:B:182:SER:N	1.95	1.22
1:A:116:PRO:CB	1:A:206:PHE:CE1	2.24	1.21
1:A:128:SER:OG	1:A:177:SER:HB3	1.38	1.20
2:B:179:SER:C	2:B:180:THR:N	1.99	1.20
1:A:187:ASN:O	1:A:207:ASN:HA	1.42	1.19
1:A:107:ARG:O	1:A:108:THR:HG22	1.36	1.19
1:A:108:THR:HA	1:A:137:TYR:CB	1.74	1.18
1:A:4:LEU:HD12	1:A:23:CYS:SG	1.83	1.18
2:B:170:LEU:O	2:B:171:THR:HG22	1.42	1.18
1:A:20:THR:OG1	1:A:74:THR:HG22	1.38	1.17
1:A:180:LYS:HG2	1:A:184:GLU:OE2	1.40	1.17
1:C:146:LYS:HG2	1:C:151:GLU:HB2	1.20	1.17
1:A:180:LYS:O	1:A:183:TYR:HB3	1.46	1.16
1:A:150:THR:N	1:A:151:GLU:N	1.93	1.16
1:A:189:TYR:HB2	1:A:206:PHE:CD2	1.80	1.16
1:A:154:ASP:HB2	1:A:155:GLY:N	1.59	1.16
1:A:178:LEU:HD12	1:A:182:ASP:OD1	1.01	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ASP:HA	1:A:149:GLY:N	1.60	1.15
1:A:211:CYS:HA	2:B:120:GLY:C	1.70	1.15
2:D:1:GLN:OE1	3:D:223:HOH:O	1.65	1.15
2:B:18:LEU:CG	2:B:102:PHE:CZ	2.29	1.15
1:A:107:ARG:O	1:A:108:THR:CG2	1.93	1.14
2:B:152:LEU:O	2:B:153:SER:HB3	1.46	1.14
1:A:78:LEU:CD1	1:A:106:LEU:CD2	2.25	1.14
2:B:127:SER:O	2:B:128:MET:N	1.80	1.13
1:A:116:PRO:CG	1:A:206:PHE:HE1	1.43	1.13
2:B:153:SER:C	2:B:154:SER:N	2.05	1.13
2:B:38:ARG:HB3	2:B:48:MET:CE	1.79	1.12
2:B:84:THR:C	2:B:85:ASP:HA	1.74	1.12
2:B:127:SER:O	2:B:178:SER:N	1.83	1.11
1:A:40:LEU:CD1	1:A:40:LEU:O	1.90	1.11
1:A:50:ASN:HB3	1:A:91:TYR:OH	1.48	1.11
1:A:78:LEU:C	1:A:79:GLN:N	2.08	1.11
1:A:108:THR:HA	1:A:137:TYR:HB3	1.26	1.11
1:A:180:LYS:CE	1:A:184:GLU:OE2	1.97	1.11
2:B:153:SER:C	2:B:154:SER:HA	1.75	1.11
2:B:129:VAL:HG21	2:B:181:TRP:CD1	1.84	1.10
2:B:181:TRP:N	2:B:182:SER:N	1.99	1.10
1:A:152:ARG:HA	1:A:152:ARG:HH11	1.08	1.10
1:C:187:ASN:HA	1:C:208:ARG:HB2	1.31	1.10
1:A:116:PRO:HB3	1:A:206:PHE:CE1	1.84	1.10
2:B:180:THR:C	2:B:181:TRP:HA	1.77	1.10
2:B:141:GLU:C	2:B:142:PRO:N	2.10	1.10
2:D:18:LEU:HD21	2:D:102:PHE:CZ	1.85	1.09
1:C:146:LYS:HA	1:C:151:GLU:HA	1.32	1.09
1:C:211:CYS:HB3	2:D:206:ARG:NH1	1.66	1.08
1:A:154:ASP:C	1:A:155:GLY:N	2.10	1.08
2:B:128:MET:H	2:B:177:PRO:CA	1.66	1.08
1:C:148:ASP:HB3	1:C:188:LEU:HD22	1.15	1.08
1:C:152:ARG:HA	1:C:152:ARG:NE	1.67	1.08
1:A:133:MET:HE1	1:A:143:VAL:HG12	1.35	1.07
1:C:141:ILE:H	1:C:141:ILE:HD12	1.03	1.07
1:A:116:PRO:CB	1:A:206:PHE:CZ	2.36	1.07
2:B:101:ASP:O	2:B:102:PHE:CB	2.03	1.07
1:A:171:SER:OG	2:B:157:HIS:CE1	2.06	1.06
1:C:43:ALA:HB1	2:D:100(D):PHE:HB3	1.29	1.06
1:A:156:VAL:HG12	1:A:176:LEU:HA	1.09	1.06
1:A:149:GLY:C	1:A:150:THR:N	2.14	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:THR:HG23	2:B:202:LYS:HA	1.31	1.06
1:A:54:LEU:HD11	1:A:58:ILE:O	1.55	1.05
2:B:14:PRO:O	2:B:15:SER:HB3	1.54	1.05
1:A:79:GLN:CB	1:A:80:PRO:HD2	1.85	1.05
1:A:189:TYR:HB2	1:A:206:PHE:CE2	1.92	1.05
2:B:175:THR:O	2:B:176:VAL:CG2	2.02	1.05
1:A:132:LEU:C	1:A:133:MET:HB2	1.82	1.04
1:C:7:SER:OG	1:C:8:PRO:HD3	1.57	1.04
1:A:200:SER:C	1:A:201:PRO:N	2.15	1.04
1:A:132:LEU:C	1:A:133:MET:CA	2.30	1.04
1:A:154:ASP:CB	1:A:155:GLY:N	2.20	1.04
1:C:178:LEU:HD23	1:C:179:THR:H	1.20	1.04
2:D:1:GLN:CD	3:D:223:HOH:O	1.95	1.04
1:A:211:CYS:HB2	2:B:206:ARG:HB3	1.40	1.04
1:A:173:SER:HB3	2:B:159:PHE:CD1	1.92	1.03
1:A:37:GLN:C	1:A:38:GLN:HA	1.83	1.03
1:A:157:LEU:HG	2:B:162:VAL:HG21	1.35	1.03
2:B:107:THR:C	2:B:108:MET:HA	1.82	1.03
1:C:4:LEU:HD12	1:C:23:CYS:SG	1.98	1.03
1:A:211:CYS:HB3	2:B:206:ARG:NH1	1.72	1.02
1:A:40:LEU:HD12	1:A:41:GLY:N	1.74	1.02
2:B:139:PHE:O	2:B:140:PRO:N	1.90	1.02
1:A:18:ARG:HG3	1:A:18:ARG:O	1.58	1.02
1:A:158:ASP:HB3	1:A:174:SER:HB2	1.41	1.02
1:A:78:LEU:HD13	1:A:106:LEU:CD2	1.89	1.01
2:B:116:PRO:HB3	2:B:203:ILE:HG13	1.40	1.01
1:A:180:LYS:HE2	1:A:184:GLU:OE2	1.59	1.01
1:A:132:LEU:C	1:A:133:MET:CB	2.34	1.00
2:B:12:VAL:HG21	2:B:82(C):LEU:CD1	1.91	1.00
1:A:132:LEU:CD2	1:A:173:SER:HB2	1.91	1.00
2:B:48:MET:CE	2:B:90:TYR:CE2	2.44	1.00
2:B:96:LEU:CD1	2:B:100(A):PRO:HG3	1.90	1.00
1:A:146:LYS:HA	1:A:151:GLU:HA	1.42	1.00
2:B:100(E):TRP:O	2:B:100(F):TYR:HB3	1.58	0.99
1:C:211:CYS:HA	2:D:120:GLY:C	1.86	0.99
1:C:136:PHE:CZ	1:C:141:ILE:HG13	1.96	0.99
1:A:28:ASN:HD22	1:A:68:GLY:HA3	1.27	0.99
1:A:78:LEU:CD1	1:A:106:LEU:HD22	1.90	0.99
1:A:123:ALA:C	1:A:124:THR:CA	2.35	0.99
1:A:182:ASP:HA	1:A:185:SER:HB3	1.42	0.98
1:A:167:ASP:OD1	1:A:167:ASP:O	1.81	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:SER:HB2	1:A:120:GLU:HG2	1.41	0.98
2:B:18:LEU:HG	2:B:102:PHE:HZ	1.21	0.98
1:A:129:VAL:HB	1:A:176:LEU:CD2	1.94	0.98
1:A:133:MET:HE1	1:A:143:VAL:CG1	1.92	0.98
1:A:189:TYR:CB	1:A:206:PHE:CD2	2.46	0.98
1:C:118:SER:OG	1:C:121:GLN:HB3	1.62	0.98
1:A:31:ASN:C	1:A:32:TYR:CA	2.36	0.98
2:B:89:THR:HA	2:B:101:ASP:HA	1.44	0.98
2:B:101:ASP:C	2:B:102:PHE:CB	2.37	0.98
2:B:96:LEU:CG	2:B:100(A):PRO:HG3	1.94	0.97
1:A:156:VAL:CG1	1:A:176:LEU:HA	1.93	0.97
2:B:38:ARG:HB3	2:B:48:MET:HE3	1.43	0.97
1:C:107:ARG:HD2	1:C:168:SER:HB2	1.47	0.97
1:C:129:VAL:HB	1:C:176:LEU:CD2	1.95	0.97
2:B:12:VAL:HG21	2:B:82(C):LEU:HD11	1.42	0.96
1:A:112:VAL:HG21	1:A:193:VAL:HG21	1.47	0.96
1:A:196:LYS:C	1:A:197:THR:CA	2.38	0.96
2:D:183:SER:O	2:D:184:GLN:HB2	1.62	0.96
1:A:118:SER:OG	1:A:121:GLN:HB3	1.65	0.96
1:A:158:ASP:HB3	1:A:174:SER:CB	1.94	0.96
1:C:14:SER:O	1:C:17:ASP:HB2	1.65	0.96
1:C:141:ILE:HD12	1:C:141:ILE:N	1.80	0.96
1:A:117:PRO:HG3	1:A:127:ALA:HB1	1.44	0.96
2:B:48:MET:HE1	2:B:90:TYR:HE2	1.29	0.95
1:C:90:GLN:HE21	1:C:92:ASN:H	1.13	0.95
2:D:187:THR:HG23	2:D:202:LYS:HA	1.45	0.95
1:A:118:SER:OG	2:B:115:PHE:HB3	1.67	0.95
1:A:129:VAL:HB	1:A:176:LEU:HD23	1.48	0.95
2:D:18:LEU:HD22	2:D:19:SER:N	1.82	0.95
1:A:156:VAL:HG12	1:A:176:LEU:CB	1.96	0.95
2:B:152:LEU:C	2:B:153:SER:CB	2.39	0.95
1:A:147:ILE:HG23	1:A:189:TYR:CE2	2.02	0.95
1:A:181:ALA:O	1:A:184:GLU:N	2.00	0.95
2:D:20:LEU:HD21	2:D:102:PHE:HE2	1.31	0.95
2:B:101:ASP:C	2:B:102:PHE:HB2	1.90	0.94
1:A:141:ILE:H	1:A:141:ILE:HD12	1.28	0.94
2:B:153:SER:O	2:B:154:SER:HA	1.67	0.94
1:A:188:LEU:HD12	1:A:188:LEU:H	1.33	0.94
1:A:37:GLN:C	1:A:38:GLN:CA	2.40	0.94
1:A:152:ARG:HA	1:A:152:ARG:NH1	1.83	0.93
2:B:38:ARG:HD2	2:B:48:MET:HE2	1.46	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:VAL:C	1:C:157:LEU:HD23	1.94	0.93
1:C:211:CYS:HB2	2:D:206:ARG:HB3	1.48	0.93
1:A:78:LEU:C	1:A:79:GLN:CA	2.41	0.93
2:B:11:LEU:HG	2:B:140:PRO:HG3	1.49	0.93
1:A:29:ILE:C	1:A:30:ASN:N	2.27	0.92
1:A:156:VAL:CG1	1:A:176:LEU:HB2	1.99	0.92
1:A:193:VAL:O	1:A:194:VAL:HB	1.67	0.92
1:C:18:ARG:HG3	1:C:18:ARG:O	1.70	0.92
1:C:28:ASN:HD22	1:C:68:GLY:HA3	1.34	0.92
1:A:147:ILE:CD1	1:A:152:ARG:H	1.82	0.92
1:A:110:PRO:HB2	1:A:111:THR:N	1.83	0.92
1:A:180:LYS:HD3	1:A:184:GLU:OE2	1.66	0.92
1:A:129:VAL:O	1:A:130:VAL:CG1	2.18	0.92
1:C:118:SER:HB2	1:C:120:GLU:HG2	1.52	0.92
1:A:211:CYS:N	2:B:208:CYS:SG	2.42	0.92
2:B:153:SER:C	2:B:154:SER:CA	2.43	0.92
2:B:183:SER:O	2:B:184:GLN:HB2	1.65	0.92
1:A:78:LEU:C	1:A:79:GLN:HA	1.95	0.91
2:B:4:LEU:CD1	2:B:24:VAL:HG12	2.00	0.91
2:B:128:MET:H	2:B:177:PRO:HA	0.79	0.91
2:B:48:MET:CE	2:B:90:TYR:CD2	2.52	0.91
1:A:78:LEU:CD1	1:A:106:LEU:HD21	1.99	0.91
1:A:132:LEU:O	1:A:133:MET:HB2	1.71	0.91
2:B:12:VAL:CG2	2:B:82(C):LEU:CD1	2.49	0.90
2:B:101:ASP:C	2:B:102:PHE:CA	2.43	0.90
1:A:211:CYS:CB	2:B:206:ARG:HB3	2.02	0.90
1:A:184:GLU:N	1:A:185:SER:N	2.20	0.90
2:B:107:THR:C	2:B:108:MET:CA	2.44	0.90
2:D:14:PRO:O	2:D:16:GLU:N	2.05	0.90
1:A:78:LEU:HD13	1:A:106:LEU:HD21	1.52	0.90
1:A:129:VAL:C	1:A:130:VAL:HG13	1.95	0.90
1:A:10:LEU:HD12	1:A:11:LEU:N	1.87	0.90
1:C:10:LEU:HD12	1:C:11:LEU:N	1.87	0.90
1:C:178:LEU:HD23	1:C:179:THR:HG23	1.52	0.90
1:A:189:TYR:CB	1:A:206:PHE:CE2	2.55	0.89
2:B:84:THR:C	2:B:85:ASP:CA	2.44	0.89
2:B:47:TRP:C	2:B:48:MET:CA	2.45	0.89
2:B:85:ASP:O	2:B:86:ASP:N	2.03	0.89
1:A:182:ASP:O	1:A:183:TYR:C	2.14	0.89
1:A:188:LEU:H	1:A:188:LEU:CD1	1.83	0.89
2:B:38:ARG:HB3	2:B:48:MET:HE2	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:LEU:HG	2:B:102:PHE:CE2	2.06	0.89
1:A:160:VAL:C	1:A:161:THR:HG23	1.95	0.89
2:D:1:GLN:NE2	3:D:223:HOH:O	2.04	0.89
1:A:133:MET:CE	1:A:143:VAL:HG12	2.03	0.89
1:A:94:GLY:C	1:A:96:TYR:CD1	2.51	0.88
1:A:147:ILE:O	1:A:150:THR:OG1	1.92	0.88
2:B:103:TRP:HZ2	2:B:168:TYR:HH	1.16	0.88
2:B:96:LEU:HG	2:B:100(A):PRO:HG3	1.55	0.88
1:A:109:ALA:O	1:A:136:PHE:HA	1.71	0.88
2:B:18:LEU:CD2	2:B:102:PHE:CZ	2.56	0.88
2:D:20:LEU:HD21	2:D:102:PHE:CE2	2.07	0.88
2:D:100(A):PRO:HG2	2:D:100(B):LEU:H	1.37	0.88
1:C:125:GLY:HA2	1:C:180:LYS:HB3	1.53	0.88
2:D:127:SER:O	2:D:178:SER:N	2.05	0.88
1:A:78:LEU:HD11	1:A:106:LEU:CD2	2.00	0.88
1:A:116:PRO:HB3	1:A:206:PHE:HZ	1.15	0.88
2:B:152:LEU:C	2:B:153:SER:CA	2.46	0.88
2:B:181:TRP:CA	2:B:182:SER:N	2.37	0.88
1:A:200:SER:C	1:A:201:PRO:CA	2.47	0.88
2:D:4:LEU:CD1	2:D:24:VAL:HG12	2.03	0.87
1:C:194:VAL:HG12	1:C:194:VAL:O	1.74	0.87
1:C:69:THR:HG23	1:C:70:ASP:OD1	1.75	0.87
1:A:206:PHE:C	1:A:207:ASN:N	2.33	0.87
2:B:198:LYS:HE3	2:D:179:SER:OG	1.74	0.87
2:B:13:ARG:HB2	2:B:16:GLU:CG	2.05	0.86
1:A:79:GLN:HB3	1:A:80:PRO:HD2	0.89	0.86
1:C:54:LEU:HD11	1:C:58:ILE:O	1.75	0.86
1:A:152:ARG:HH11	1:A:152:ARG:CA	1.88	0.86
1:A:210:GLU:C	2:B:208:CYS:SG	2.58	0.86
1:A:160:VAL:HG12	1:A:172:MET:HG3	1.58	0.86
2:B:110:THR:HG21	2:B:167:LEU:HD11	1.57	0.86
1:A:133:MET:HB3	1:A:172:MET:O	1.76	0.86
1:A:110:PRO:HA	1:A:136:PHE:CB	2.06	0.86
2:B:127:SER:C	2:B:128:MET:CA	2.48	0.85
1:C:186:HIS:HB3	1:C:188:LEU:CD1	2.07	0.85
2:D:163:LEU:HD22	2:D:168:TYR:CE2	2.11	0.85
1:A:156:VAL:HB	1:A:175:THR:O	1.75	0.85
2:B:4:LEU:HD11	2:B:24:VAL:HG12	1.55	0.85
2:B:187:THR:HG23	2:B:202:LYS:CA	2.06	0.85
1:A:197:THR:N	1:A:198:SER:N	2.23	0.85
2:B:139:PHE:O	2:B:139:PHE:CD2	2.28	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:LEU:HA	1:A:58:ILE:HG13	1.59	0.85
2:B:85:ASP:CA	2:B:86:ASP:N	2.39	0.85
1:C:90:GLN:HE21	1:C:92:ASN:N	1.74	0.85
2:D:112:SER:HA	2:D:138:TYR:HB3	1.58	0.85
1:A:147:ILE:HD11	1:A:152:ARG:HB2	1.58	0.85
2:B:3:GLN:HG3	3:B:219:HOH:O	1.77	0.85
2:B:100(E):TRP:HA	3:B:221:HOH:O	1.74	0.85
1:A:118:SER:O	1:A:119:THR:C	2.18	0.85
1:A:205:SER:O	1:A:206:PHE:N	2.10	0.85
1:A:211:CYS:HA	2:B:120:GLY:CA	2.07	0.85
1:C:211:CYS:CB	2:D:206:ARG:HB3	2.07	0.85
1:A:192:GLU:HA	1:A:203:VAL:HB	1.58	0.84
2:B:114:VAL:CG2	2:B:190:VAL:HG21	2.05	0.84
2:D:111:VAL:HG13	2:D:197:THR:OG1	1.78	0.84
1:A:30:ASN:CA	1:A:31:ASN:N	2.40	0.84
2:B:139:PHE:C	2:B:140:PRO:N	2.34	0.84
1:C:43:ALA:HB1	2:D:100(D):PHE:CB	2.06	0.84
2:B:18:LEU:HD21	2:B:102:PHE:CE1	2.13	0.84
1:A:14:SER:O	1:A:17:ASP:HB2	1.76	0.84
2:D:11:LEU:HD21	2:D:139:PHE:HE2	1.42	0.84
1:A:156:VAL:CG1	1:A:176:LEU:CB	2.55	0.84
2:B:141:GLU:C	2:B:142:PRO:CA	2.50	0.84
1:A:62:PHE:O	1:A:63:SER:HB3	1.73	0.84
1:A:206:PHE:HA	1:A:207:ASN:N	1.92	0.84
2:B:13:ARG:HB2	2:B:16:GLU:HG3	1.60	0.84
1:A:20:THR:OG1	1:A:74:THR:CG2	2.24	0.84
2:B:73:THR:O	2:B:76:ASN:N	2.11	0.84
1:A:180:LYS:O	1:A:183:TYR:CB	2.27	0.83
1:A:180:LYS:O	1:A:184:GLU:HG3	1.78	0.83
1:C:147:ILE:HD11	1:C:152:ARG:HB2	1.58	0.83
2:B:152:LEU:C	2:B:153:SER:HB3	2.00	0.83
1:C:148:ASP:HB3	1:C:188:LEU:CD2	2.06	0.83
1:A:7:SER:OG	1:A:8:PRO:HD2	1.77	0.83
2:D:100(A):PRO:CG	2:D:100(B):LEU:H	1.91	0.83
1:C:118:SER:OG	2:D:115:PHE:HB3	1.79	0.83
1:A:122:LEU:CD1	1:A:127:ALA:HB2	2.08	0.83
2:D:103:TRP:HZ2	2:D:168:TYR:HH	1.25	0.83
1:A:205:SER:C	1:A:206:PHE:CB	2.51	0.82
1:A:28:ASN:HD22	1:A:68:GLY:CA	1.92	0.82
1:A:197:THR:CA	1:A:198:SER:N	2.42	0.82
1:A:205:SER:C	1:A:206:PHE:CA	2.51	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:GLY:O	2:B:203:ILE:HD11	1.79	0.82
1:A:110:PRO:CD	1:A:197:THR:OG1	2.28	0.82
1:A:128:SER:HG	1:A:177:SER:HB3	1.42	0.82
1:C:109:ALA:O	1:C:136:PHE:HA	1.80	0.82
2:D:38:ARG:HG2	2:D:40:PRO:HD3	1.61	0.82
1:A:40:LEU:O	1:A:40:LEU:HD13	1.79	0.82
1:A:108:THR:CA	1:A:137:TYR:HB3	2.09	0.82
2:B:42:GLY:O	2:B:43:LYS:HG3	1.79	0.82
2:B:96:LEU:HD11	2:B:100(A):PRO:HG3	1.60	0.81
1:A:107:ARG:O	1:A:108:THR:HG23	1.80	0.81
1:A:148:ASP:CA	1:A:149:GLY:N	2.44	0.81
1:A:196:LYS:C	1:A:197:THR:HA	2.05	0.81
1:A:211:CYS:HB2	2:B:206:ARG:CB	2.10	0.81
1:A:43:ALA:HB1	2:B:100(D):PHE:HB3	1.59	0.81
1:A:112:VAL:CG2	1:A:193:VAL:HG21	2.10	0.81
2:B:179:SER:C	2:B:180:THR:CA	2.53	0.81
1:A:28:ASN:ND2	1:A:68:GLY:HA3	1.95	0.81
1:A:154:ASP:CA	1:A:155:GLY:N	2.44	0.81
1:A:189:TYR:CB	1:A:206:PHE:HD2	1.91	0.81
1:C:107:ARG:CD	1:C:168:SER:HB2	2.11	0.81
2:D:163:LEU:HD12	2:D:164:GLN:H	1.44	0.81
1:A:167:ASP:O	1:A:169:THR:N	2.13	0.80
2:D:187:THR:HG23	2:D:202:LYS:CA	2.11	0.80
1:A:29:ILE:C	1:A:30:ASN:CA	2.54	0.80
1:A:129:VAL:HG12	1:A:145:TRP:HH2	1.45	0.80
1:A:205:SER:C	1:A:206:PHE:HB3	2.05	0.80
2:B:89:THR:CA	2:B:101:ASP:HA	2.11	0.80
2:B:25:SER:CA	2:B:26:GLY:N	2.43	0.80
1:C:28:ASN:HD22	1:C:68:GLY:CA	1.95	0.80
1:C:152:ARG:HA	1:C:152:ARG:HE	1.45	0.80
2:D:4:LEU:HD12	2:D:24:VAL:HG12	1.62	0.80
2:B:48:MET:HB3	2:B:63:LEU:HD23	1.62	0.80
1:A:108:THR:CA	1:A:137:TYR:CB	2.59	0.80
1:A:160:VAL:O	1:A:171:SER:O	1.97	0.80
2:B:159:PHE:H	2:B:159:PHE:HD2	1.29	0.80
1:C:112:VAL:HG12	1:C:113:SER:N	1.94	0.80
1:A:147:ILE:HB	1:A:150:THR:OG1	1.80	0.79
2:D:18:LEU:HD21	2:D:102:PHE:HZ	1.46	0.79
2:D:164:GLN:HA	2:D:164:GLN:NE2	1.96	0.79
1:A:69:THR:CG2	1:A:70:ASP:N	2.46	0.79
1:A:187:ASN:O	1:A:207:ASN:CA	2.28	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ALA:C	1:A:124:THR:HA	2.06	0.79
1:A:147:ILE:HD11	1:A:152:ARG:H	1.46	0.79
1:C:158:ASP:HB3	1:C:174:SER:HA	1.62	0.79
2:B:146:THR:O	2:B:189:ASN:HB3	1.83	0.79
1:A:11:LEU:C	1:A:11:LEU:HD12	2.08	0.79
1:A:29:ILE:HG12	1:A:71:TYR:CE1	2.18	0.79
1:A:160:VAL:O	1:A:161:THR:HG23	1.83	0.79
1:A:62:PHE:O	1:A:63:SER:CB	2.30	0.78
1:A:187:ASN:HA	1:A:208:ARG:HB2	1.65	0.78
1:A:108:THR:HA	1:A:137:TYR:CG	2.18	0.78
1:A:186:HIS:HB3	1:A:188:LEU:CD1	2.13	0.78
2:B:143:VAL:O	2:B:144:THR:HG23	1.83	0.78
2:B:40:PRO:HB2	2:B:43:LYS:HD3	1.65	0.78
1:A:149:GLY:C	1:A:150:THR:CA	2.56	0.78
2:B:96:LEU:O	2:B:98:GLY:N	2.17	0.78
1:A:69:THR:HG23	1:A:70:ASP:OD1	1.84	0.78
1:C:76:SER:O	1:C:77:SER:HB2	1.82	0.78
1:C:107:ARG:HG3	1:C:107:ARG:HH11	1.47	0.78
2:D:158:THR:HG22	2:D:172:SER:HB2	1.63	0.78
2:B:18:LEU:HD22	2:B:19:SER:N	1.99	0.78
1:C:211:CYS:SG	2:D:206:ARG:HB3	2.23	0.78
1:A:189:TYR:CA	1:A:190:THR:N	2.46	0.78
2:B:66:ARG:NH2	2:B:86:ASP:OD1	2.17	0.78
1:A:117:PRO:HG3	1:A:127:ALA:CB	2.13	0.78
1:C:147:ILE:CD1	1:C:152:ARG:H	1.96	0.78
2:B:129:VAL:CG2	2:B:181:TRP:CD1	2.67	0.78
2:B:70:SER:HB2	3:B:242:HOH:O	1.85	0.77
1:C:112:VAL:HG21	1:C:193:VAL:HG21	1.66	0.77
1:A:37:GLN:O	1:A:38:GLN:HA	1.85	0.77
1:A:184:GLU:CA	1:A:185:SER:N	2.47	0.77
1:A:117:PRO:HG2	1:A:122:LEU:HD13	1.66	0.77
2:B:14:PRO:O	2:B:15:SER:CB	2.30	0.77
2:B:100(C):GLY:O	2:B:100(D):PHE:HB2	1.85	0.77
2:B:147:TRP:CD1	2:B:156:VAL:HG13	2.19	0.77
1:C:178:LEU:CD2	1:C:179:THR:H	1.97	0.77
1:C:180:LYS:NZ	1:C:184:GLU:HB2	1.99	0.77
1:A:109:ALA:HA	1:A:197:THR:HG21	1.66	0.77
1:A:5:THR:O	1:A:23:CYS:HA	1.85	0.76
1:A:207:ASN:O	1:A:210:GLU:HB2	1.84	0.76
2:B:107:THR:O	2:B:108:MET:HA	1.84	0.76
1:A:121:GLN:HA	2:B:115:PHE:CE2	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:ILE:HD13	1:C:48:ILE:C	2.11	0.76
1:A:133:MET:HE3	1:A:193:VAL:HG13	1.66	0.76
2:B:82(B):SER:O	2:B:82(B):SER:OG	2.02	0.76
2:D:18:LEU:CD2	2:D:19:SER:N	2.48	0.76
1:A:200:SER:C	1:A:201:PRO:HA	2.11	0.76
2:D:105:PRO:HG3	2:D:139:PHE:HZ	1.50	0.76
1:A:206:PHE:CA	1:A:207:ASN:N	2.48	0.76
1:C:211:CYS:HB2	2:D:206:ARG:CB	2.15	0.76
1:A:188:LEU:HD12	1:A:188:LEU:N	2.00	0.76
1:C:105:GLU:C	1:C:106:LEU:HD12	2.11	0.76
1:A:129:VAL:C	1:A:130:VAL:CG1	2.57	0.75
1:A:37:GLN:C	1:A:38:GLN:N	2.44	0.75
2:B:36:TRP:CD1	2:B:69:ILE:HG12	2.22	0.75
2:D:38:ARG:HD2	2:D:48:MET:SD	2.26	0.75
1:A:78:LEU:HD13	1:A:106:LEU:HD22	1.59	0.75
1:C:122:LEU:HA	1:C:126:GLY:O	1.86	0.75
2:D:138:TYR:CE1	2:D:143:VAL:HG13	2.22	0.75
1:C:182:ASP:HA	1:C:185:SER:HB3	1.66	0.75
1:A:40:LEU:CG	1:A:41:GLY:N	2.48	0.75
1:A:183:TYR:HD2	1:A:184:GLU:HA	1.50	0.75
1:A:173:SER:HB3	2:B:159:PHE:CE1	2.21	0.75
2:B:1:GLN:HA	2:B:1:GLN:OE1	1.87	0.75
2:B:128:MET:HE1	2:B:175:THR:HG21	1.69	0.75
1:A:132:LEU:HD21	1:A:173:SER:HB2	1.68	0.74
1:A:150:THR:CA	1:A:151:GLU:N	2.50	0.74
2:B:114:VAL:HG21	2:B:190:VAL:HG21	1.67	0.74
2:D:18:LEU:CD2	2:D:19:SER:H	1.99	0.74
2:D:159:PHE:H	2:D:159:PHE:HD2	1.35	0.74
1:C:196:LYS:HG3	1:C:197:THR:N	2.01	0.74
1:A:67:SER:O	1:A:68:GLY:C	2.31	0.74
2:B:35:SER:HB3	2:B:50:ARG:HA	1.68	0.74
1:C:25:GLY:HA3	1:C:29:ILE:HD11	1.69	0.74
1:C:167:ASP:O	1:C:169:THR:N	2.21	0.74
2:B:170:LEU:C	2:B:171:THR:HG22	2.12	0.73
2:D:188:CYS:C	2:D:189:ASN:HD22	1.96	0.73
1:A:46:LEU:HD23	1:A:55:GLN:HG3	1.69	0.73
2:B:96:LEU:HG	2:B:100(A):PRO:CG	2.17	0.73
2:D:114:VAL:HG12	2:D:114:VAL:O	1.87	0.73
1:A:76:SER:O	1:A:77:SER:HB2	1.88	0.73
1:A:94:GLY:C	1:A:96:TYR:HD1	1.95	0.73
1:A:129:VAL:O	1:A:130:VAL:HG13	1.83	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:GLU:CA	1:A:165:SER:O	2.36	0.73
1:A:180:LYS:HG2	1:A:184:GLU:CD	2.13	0.73
2:B:161:ALA:HB2	2:B:170:LEU:CD2	2.18	0.73
2:D:103:TRP:HB2	2:D:140:PRO:HB2	1.69	0.73
2:D:153:SER:HB3	3:D:221:HOH:O	1.88	0.73
1:A:48:ILE:CD1	1:A:64:GLY:HA3	2.19	0.73
1:A:110:PRO:HA	1:A:136:PHE:HB3	1.71	0.73
2:B:111:VAL:HG12	2:B:197:THR:OG1	1.89	0.73
1:A:211:CYS:SG	2:B:206:ARG:HB3	2.28	0.73
1:C:147:ILE:N	1:C:147:ILE:HD12	2.04	0.73
1:A:90:GLN:HE21	1:A:92:ASN:N	1.87	0.72
2:B:164:GLN:HA	2:B:164:GLN:NE2	2.04	0.72
1:C:192:GLU:HA	1:C:203:VAL:HB	1.71	0.72
2:D:103:TRP:NE1	2:D:168:TYR:HE1	1.87	0.72
1:A:122:LEU:HA	1:A:126:GLY:O	1.88	0.72
2:B:182:SER:O	2:B:183:SER:O	2.06	0.72
2:D:73:THR:O	2:D:75:LYS:N	2.22	0.72
2:B:107:THR:C	2:B:108:MET:N	2.48	0.72
2:B:143:VAL:HG12	2:B:192:HIS:HD2	1.54	0.72
2:B:104:GLY:N	2:B:105:PRO:CD	2.52	0.72
2:D:100(C):GLY:O	2:D:100(D):PHE:HB2	1.89	0.72
2:D:163:LEU:HD12	2:D:164:GLN:N	2.04	0.72
1:C:192:GLU:HG3	1:C:203:VAL:HB	1.72	0.72
2:D:59:TYR:CE2	2:D:68:SER:HA	2.23	0.72
2:B:82(A):ASN:O	2:B:82(B):SER:HB3	1.90	0.72
2:B:132:GLY:O	2:B:133:CYS:HB2	1.89	0.72
1:C:94:GLY:C	1:C:96:TYR:CD1	2.68	0.72
1:A:29:ILE:C	1:A:30:ASN:C	2.58	0.71
2:B:195:SER:O	2:B:197:THR:N	2.23	0.71
1:A:120:GLU:CD	1:A:120:GLU:H	1.96	0.71
2:B:103:TRP:CD1	2:B:139:PHE:HE1	2.07	0.71
2:B:100(C):GLY:O	2:B:100(D):PHE:CD2	2.44	0.71
1:A:121:GLN:HB2	2:B:115:PHE:CG	2.26	0.71
2:B:89:THR:CB	2:B:100(G):PHE:O	2.38	0.71
1:C:150:THR:O	1:C:151:GLU:HB3	1.90	0.71
1:C:122:LEU:HD12	1:C:180:LYS:HD2	1.71	0.71
1:A:129:VAL:O	1:A:130:VAL:HG12	1.90	0.71
2:D:35:SER:HB3	2:D:50:ARG:HA	1.73	0.71
1:A:81:GLU:HA	1:A:165:SER:O	1.90	0.71
1:A:196:LYS:H	1:A:197:THR:N	1.87	0.71
2:B:178:SER:O	2:B:181:TRP:N	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:40:PRO:HB2	2:D:43:LYS:HD3	1.73	0.71
2:D:42:GLY:O	2:D:43:LYS:HG3	1.91	0.71
2:B:12:VAL:CG2	2:B:82(C):LEU:HD13	2.20	0.71
1:A:46:LEU:HD23	1:A:55:GLN:CG	2.21	0.71
1:A:112:VAL:HG12	1:A:113:SER:N	2.06	0.71
1:A:153:ARG:O	1:A:153:ARG:HG2	1.91	0.71
2:B:52:TRP:HB2	2:B:56:TYR:O	1.91	0.71
2:B:83:GLN:HB2	2:B:85:ASP:N	2.05	0.71
1:A:69:THR:HG22	1:A:70:ASP:H	1.56	0.70
2:D:36:TRP:CD1	2:D:69:ILE:HG12	2.26	0.70
2:D:73:THR:O	2:D:76:ASN:N	2.21	0.70
2:B:59:TYR:CE2	2:B:68:SER:HA	2.26	0.70
1:C:108:THR:HB	1:C:138:PRO:HD3	1.72	0.70
2:B:18:LEU:HD21	2:B:102:PHE:CZ	2.25	0.70
2:D:18:LEU:CD2	2:D:102:PHE:CZ	2.72	0.70
2:B:66:ARG:HH22	2:B:86:ASP:CG	2.00	0.70
1:A:29:ILE:O	1:A:30:ASN:C	2.35	0.70
1:C:196:LYS:O	1:C:198:SER:N	2.24	0.70
1:A:132:LEU:O	1:A:133:MET:CA	2.39	0.70
1:C:28:ASN:ND2	1:C:68:GLY:HA3	2.05	0.70
1:C:98:PHE:CG	2:D:45:PRO:HB2	2.27	0.70
2:B:182:SER:O	2:B:183:SER:C	2.33	0.70
1:C:110:PRO:HD3	1:C:197:THR:HG21	1.73	0.70
1:A:192:GLU:HG3	1:A:203:VAL:HB	1.74	0.70
1:A:7:SER:OG	1:A:8:PRO:CD	2.40	0.69
2:D:4:LEU:HD11	2:D:24:VAL:HG12	1.73	0.69
1:A:31:ASN:N	1:A:71:TYR:HH	1.89	0.69
1:A:94:GLY:O	1:A:96:TYR:HB2	1.90	0.69
1:C:112:VAL:HG12	1:C:113:SER:H	1.56	0.69
1:C:129:VAL:HB	1:C:176:LEU:HD21	1.73	0.69
1:A:40:LEU:CD1	1:A:41:GLY:N	2.42	0.69
1:A:211:CYS:CB	2:B:120:GLY:HA2	2.22	0.69
1:C:178:LEU:CD2	1:C:179:THR:HG23	2.22	0.69
2:D:114:VAL:HG21	2:D:190:VAL:HG21	1.73	0.69
1:C:47:LEU:HA	1:C:58:ILE:HG13	1.73	0.69
2:D:103:TRP:NE1	2:D:168:TYR:CE1	2.61	0.69
2:D:203:ILE:HD13	2:D:203:ILE:H	1.57	0.69
2:B:111:VAL:HG22	3:B:226:HOH:O	1.91	0.69
2:B:175:THR:HG22	2:B:176:VAL:N	2.07	0.69
1:A:54:LEU:CD1	1:A:58:ILE:O	2.37	0.69
2:D:164:GLN:NE2	2:D:164:GLN:CA	2.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LEU:O	1:A:133:MET:CB	2.37	0.69
2:B:153:SER:N	2:B:156:VAL:HG23	2.07	0.69
1:C:145:TRP:CD1	1:C:156:VAL:HG21	2.28	0.69
2:B:100(C):GLY:O	2:B:100(D):PHE:CB	2.40	0.68
2:B:103:TRP:HZ2	2:B:168:TYR:OH	1.75	0.68
2:D:100(C):GLY:O	2:D:100(D):PHE:CD2	2.46	0.68
1:A:80:PRO:HA	1:A:106:LEU:HD11	1.73	0.68
1:A:122:LEU:O	1:A:124:THR:N	2.26	0.68
1:C:187:ASN:O	1:C:208:ARG:N	2.20	0.68
1:A:43:ALA:CB	2:B:100(D):PHE:HB3	2.22	0.68
1:A:76:SER:O	1:A:77:SER:CB	2.40	0.68
2:B:11:LEU:HG	2:B:140:PRO:CG	2.23	0.68
1:C:121:GLN:HB2	2:D:115:PHE:CG	2.28	0.68
2:D:14:PRO:O	2:D:16:GLU:HG2	1.93	0.68
1:A:116:PRO:CB	1:A:206:PHE:HE1	1.88	0.68
1:A:147:ILE:HD12	1:A:152:ARG:H	1.59	0.68
2:B:175:THR:CG2	2:B:176:VAL:N	2.57	0.68
1:C:69:THR:CG2	1:C:70:ASP:N	2.55	0.68
2:D:158:THR:CG2	2:D:172:SER:HB2	2.24	0.68
1:A:79:GLN:CB	1:A:80:PRO:CD	2.44	0.68
1:A:90:GLN:NE2	1:A:93:ASN:H	1.90	0.68
1:A:137:TYR:O	1:A:139:ARG:N	2.27	0.68
1:A:178:LEU:CD1	1:A:182:ASP:CG	2.66	0.68
2:D:32:PHE:CD2	2:D:94:ARG:HD3	2.29	0.68
2:B:145:VAL:O	3:B:211:HOH:O	2.10	0.68
2:D:170:LEU:HD12	2:D:171:THR:N	2.09	0.68
1:C:179:THR:OG1	1:C:181:ALA:HB3	1.94	0.68
2:D:183:SER:O	2:D:184:GLN:CB	2.38	0.68
2:B:181:TRP:O	2:B:182:SER:N	2.27	0.68
2:D:105:PRO:HG2	2:D:107:THR:HG23	1.75	0.68
1:C:160:VAL:O	1:C:171:SER:O	2.12	0.68
1:A:112:VAL:HG12	1:A:113:SER:H	1.58	0.67
2:B:180:THR:C	2:B:181:TRP:CA	2.62	0.67
2:D:59:TYR:HE2	2:D:68:SER:HA	1.59	0.67
2:B:60:ASN:O	2:B:62:ALA:N	2.27	0.67
2:B:67:LEU:HD12	2:B:80:LEU:CD2	2.23	0.67
1:C:11:LEU:C	1:C:11:LEU:HD12	2.20	0.67
1:C:122:LEU:C	1:C:124:THR:H	2.01	0.67
1:A:4:LEU:HD21	1:A:90:GLN:CB	2.24	0.67
1:A:31:ASN:C	1:A:32:TYR:HA	2.17	0.67
1:A:145:TRP:CZ3	1:A:176:LEU:HD22	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:LEU:O	2:B:171:THR:CG2	2.34	0.67
1:C:179:THR:CB	1:C:181:ALA:HB3	2.24	0.67
2:D:50:ARG:NH2	2:D:95:ASP:OD2	2.22	0.67
2:B:4:LEU:HD12	2:B:24:VAL:HG12	1.74	0.67
1:A:147:ILE:O	1:A:148:ASP:C	2.38	0.67
2:B:183:SER:O	2:B:184:GLN:CB	2.41	0.67
1:A:118:SER:OG	1:A:121:GLN:CB	2.43	0.67
1:A:194:VAL:HG12	1:A:194:VAL:O	1.93	0.67
1:C:118:SER:H	1:C:121:GLN:HB3	1.59	0.67
2:D:199:VAL:CG1	2:D:200:ASP:N	2.57	0.67
1:A:160:VAL:O	1:A:161:THR:OG1	2.13	0.67
2:B:89:THR:HA	2:B:101:ASP:CA	2.24	0.67
1:C:50:ASN:ND2	1:C:91:TYR:OH	2.27	0.67
1:C:148:ASP:CB	1:C:188:LEU:HD22	2.09	0.67
2:D:199:VAL:HG12	2:D:200:ASP:N	2.07	0.67
1:A:122:LEU:HD11	1:A:127:ALA:HB2	1.76	0.67
1:A:123:ALA:O	1:A:124:THR:HA	1.94	0.67
2:B:18:LEU:CD2	2:B:19:SER:H	2.08	0.67
1:C:130:VAL:HG12	1:C:175:THR:HB	1.75	0.67
1:A:196:LYS:C	1:A:198:SER:N	2.53	0.66
1:C:196:LYS:HG3	1:C:197:THR:H	1.59	0.66
1:A:11:LEU:O	1:A:104:LEU:HA	1.95	0.66
1:C:137:TYR:CD2	1:C:138:PRO:HA	2.30	0.66
2:B:13:ARG:O	2:B:16:GLU:HG3	1.96	0.66
2:B:89:THR:CA	2:B:100(G):PHE:O	2.43	0.66
1:C:158:ASP:HB3	1:C:174:SER:HB2	1.77	0.66
1:C:159:SER:HB2	2:D:160:PRO:HG2	1.77	0.66
1:C:182:ASP:HA	1:C:185:SER:CB	2.25	0.66
2:B:117:LEU:HB2	2:B:132:GLY:C	2.21	0.66
2:B:153:SER:N	2:B:156:VAL:CG2	2.58	0.66
2:B:177:PRO:O	2:B:180:THR:N	2.28	0.66
1:C:31:ASN:ND2	3:C:234:HOH:O	2.28	0.66
1:A:110:PRO:HD2	1:A:197:THR:OG1	1.95	0.66
1:A:156:VAL:CB	1:A:175:THR:O	2.44	0.66
1:C:33:LEU:HD22	1:C:71:TYR:CB	2.25	0.66
2:D:15:SER:O	2:D:16:GLU:O	2.13	0.66
2:D:60:ASN:O	2:D:61:SER:C	2.37	0.66
2:B:38:ARG:HG2	2:B:40:PRO:HD3	1.78	0.66
1:C:133:MET:CE	1:C:193:VAL:HG13	2.25	0.66
1:A:147:ILE:HD11	1:A:152:ARG:CB	2.25	0.66
1:C:107:ARG:HH11	1:C:107:ARG:CG	2.07	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:VAL:HB	1:C:176:LEU:HD23	1.76	0.66
2:D:164:GLN:HE21	2:D:164:GLN:C	2.04	0.66
1:A:39:LYS:O	1:A:42:GLU:HB2	1.95	0.66
2:B:14:PRO:C	2:B:16:GLU:H	2.03	0.66
1:C:26:SER:O	1:C:27:GLN:HG3	1.95	0.66
1:C:122:LEU:CD1	1:C:180:LYS:HD2	2.26	0.66
1:A:90:GLN:HE21	1:A:92:ASN:H	1.44	0.65
1:C:107:ARG:HB2	1:C:107:ARG:NH1	2.12	0.65
1:A:129:VAL:HG12	1:A:145:TRP:CH2	2.29	0.65
1:C:121:GLN:NE2	2:D:115:PHE:CE1	2.64	0.65
1:A:69:THR:HG23	1:A:70:ASP:N	2.11	0.65
1:C:11:LEU:O	1:C:104:LEU:HA	1.96	0.65
1:A:128:SER:OG	1:A:177:SER:CB	2.30	0.65
2:B:112:SER:HA	2:B:138:TYR:HB3	1.79	0.65
2:D:126:ASN:O	2:D:127:SER:C	2.36	0.65
1:C:173:SER:HB3	2:D:159:PHE:CD1	2.31	0.65
2:B:147:TRP:CZ3	2:B:188:CYS:HB3	2.32	0.65
2:D:100(C):GLY:O	2:D:100(D):PHE:CB	2.45	0.65
1:A:137:TYR:CD2	1:A:138:PRO:HD3	2.32	0.65
1:C:141:ILE:H	1:C:141:ILE:CD1	1.92	0.65
1:C:44:PRO:HD2	2:D:100(D):PHE:CD1	2.31	0.65
1:C:117:PRO:HB3	1:C:127:ALA:HA	1.79	0.65
1:C:196:LYS:C	1:C:198:SER:N	2.50	0.65
1:C:211:CYS:HB3	2:D:206:ARG:HH11	1.60	0.65
1:A:107:ARG:C	1:A:108:THR:CG2	2.70	0.65
1:A:196:LYS:O	1:A:198:SER:N	2.30	0.65
1:C:122:LEU:O	1:C:124:THR:N	2.29	0.65
1:A:147:ILE:CD1	1:A:152:ARG:N	2.59	0.64
2:B:113:SER:N	2:B:136:LYS:O	2.30	0.64
1:A:110:PRO:HD3	1:A:197:THR:OG1	1.97	0.64
1:A:149:GLY:C	1:A:150:THR:HA	2.21	0.64
2:B:94:ARG:O	2:B:100:TYR:HB3	1.98	0.64
1:C:117:PRO:HG2	1:C:127:ALA:HB1	1.79	0.64
1:A:10:LEU:HD13	1:A:103:LYS:HB3	1.79	0.64
1:A:78:LEU:O	1:A:79:GLN:HA	1.96	0.64
2:B:12:VAL:O	2:B:104:GLY:O	2.15	0.64
1:C:188:LEU:HD12	1:C:188:LEU:N	2.13	0.64
2:D:13:ARG:HB2	2:D:16:GLU:HG3	1.80	0.64
2:D:20:LEU:CD2	2:D:100(G):PHE:HE2	2.10	0.64
2:D:66:ARG:HH22	2:D:86:ASP:CG	2.04	0.64
2:B:132:GLY:HA2	2:B:173:SER:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:TYR:HD1	2:B:139:PHE:N	1.95	0.64
2:D:8:GLY:HA3	2:D:20:LEU:HD23	1.80	0.64
2:D:158:THR:CB	2:D:172:SER:HB2	2.28	0.64
2:B:14:PRO:O	2:B:16:GLU:HG2	1.98	0.64
2:B:60:ASN:O	2:B:61:SER:C	2.41	0.64
2:D:100(C):GLY:O	2:D:100(D):PHE:HD2	1.79	0.64
1:A:132:LEU:HD22	2:B:159:PHE:CZ	2.31	0.64
2:B:12:VAL:HG23	2:B:82(C):LEU:HD13	1.80	0.64
2:B:103:TRP:CD1	2:B:139:PHE:CE1	2.86	0.64
2:B:31:SER:O	2:B:32:PHE:CD1	2.51	0.64
2:B:47:TRP:C	2:B:48:MET:HA	2.23	0.64
1:C:194:VAL:H	1:C:202:VAL:HG23	1.63	0.64
1:A:4:LEU:CD1	1:A:23:CYS:SG	2.76	0.63
1:C:29:ILE:HG22	1:C:29:ILE:O	1.96	0.63
1:C:163:GLN:HG3	1:C:170:TYR:OH	1.99	0.63
1:A:30:ASN:O	1:A:31:ASN:N	2.30	0.63
1:A:187:ASN:O	1:A:208:ARG:N	2.30	0.63
1:A:211:CYS:HB3	2:B:206:ARG:HH11	1.60	0.63
1:C:211:CYS:HA	2:D:120:GLY:CA	2.27	0.63
1:A:117:PRO:CG	1:A:127:ALA:HB1	2.25	0.63
1:C:160:VAL:C	1:C:161:THR:HG23	2.22	0.63
2:B:67:LEU:CD1	2:B:80:LEU:HD21	2.28	0.63
1:A:121:GLN:O	1:A:126:GLY:O	2.16	0.63
1:A:186:HIS:HB3	1:A:188:LEU:HD12	1.78	0.63
2:B:139:PHE:O	2:B:139:PHE:CG	2.50	0.63
2:D:1:GLN:OE1	2:D:1:GLN:HA	1.97	0.63
2:B:141:GLU:C	2:B:142:PRO:HA	2.22	0.63
2:B:159:PHE:N	2:B:159:PHE:CD2	2.66	0.63
2:B:175:THR:CG2	2:B:176:VAL:H	2.12	0.63
1:C:90:GLN:NE2	1:C:93:ASN:H	1.96	0.63
1:C:118:SER:OG	1:C:121:GLN:CB	2.42	0.63
1:A:69:THR:CG2	1:A:70:ASP:H	2.10	0.63
1:A:209:ASN:O	2:B:208:CYS:HB2	1.99	0.63
2:B:6:GLU:O	2:B:100(G):PHE:CE1	2.52	0.63
2:B:18:LEU:CD2	2:B:19:SER:N	2.62	0.63
2:D:75:LYS:HD3	2:D:77:GLN:CD	2.24	0.63
2:B:8:GLY:HA3	2:B:20:LEU:HD23	1.80	0.62
1:C:195:HIS:ND1	1:C:197:THR:HG23	2.14	0.62
1:A:189:TYR:HB3	1:A:206:PHE:CD2	2.33	0.62
2:B:12:VAL:HG23	2:B:82(C):LEU:CD1	2.28	0.62
2:D:66:ARG:NH2	2:D:86:ASP:OD1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:SER:O	1:A:27:GLN:HG3	2.00	0.62
1:A:110:PRO:CB	1:A:111:THR:N	2.60	0.62
1:A:147:ILE:C	1:A:150:THR:HG1	2.01	0.62
2:B:147:TRP:HD1	2:B:156:VAL:HG13	1.62	0.62
1:A:147:ILE:HG23	1:A:189:TYR:HE2	1.59	0.62
2:B:161:ALA:HB2	2:B:170:LEU:HD22	1.80	0.62
1:C:5:THR:O	1:C:23:CYS:HA	1.99	0.62
1:A:31:ASN:O	1:A:32:TYR:HA	2.00	0.62
2:B:87:THR:HG23	2:B:103:TRP:HA	1.81	0.62
1:C:194:VAL:O	1:C:194:VAL:CG1	2.45	0.62
2:D:100(A):PRO:CG	2:D:100(B):LEU:N	2.60	0.62
2:D:136:LYS:HG2	2:D:137:GLY:H	1.63	0.62
1:A:151:GLU:HG3	1:A:151:GLU:O	2.00	0.62
1:A:160:VAL:O	1:A:161:THR:CG2	2.47	0.62
2:B:13:ARG:O	2:B:16:GLU:CG	2.47	0.62
1:C:121:GLN:HA	2:D:115:PHE:CE2	2.34	0.62
1:C:31:ASN:HA	1:C:71:TYR:HE2	1.63	0.62
2:D:204:VAL:HB	2:D:205:PRO:HD2	1.80	0.62
1:A:38:GLN:N	1:A:85:THR:O	2.33	0.62
1:A:160:VAL:O	1:A:161:THR:CB	2.46	0.62
1:C:159:SER:HB2	2:D:160:PRO:CG	2.30	0.62
2:D:96:LEU:O	2:D:98:GLY:N	2.33	0.62
1:A:67:SER:O	1:A:68:GLY:O	2.17	0.61
1:A:133:MET:O	1:A:136:PHE:HD2	1.83	0.61
1:A:211:CYS:CA	2:B:120:GLY:HA2	2.30	0.61
2:B:11:LEU:CG	2:B:140:PRO:HG3	2.26	0.61
2:B:180:THR:O	2:B:184:GLN:HB3	2.00	0.61
2:D:20:LEU:HD22	2:D:100(G):PHE:CE2	2.35	0.61
1:C:112:VAL:CG1	1:C:113:SER:N	2.64	0.61
2:B:60:ASN:O	2:B:63:LEU:N	2.33	0.61
2:B:138:TYR:CD1	2:B:139:PHE:N	2.68	0.61
1:C:158:ASP:HB3	1:C:174:SER:CA	2.29	0.61
2:D:164:GLN:HG3	2:D:165:SER:H	1.63	0.61
1:A:158:ASP:CB	1:A:174:SER:HB2	2.24	0.61
2:B:96:LEU:HG	2:B:100(A):PRO:HD3	1.81	0.61
1:C:147:ILE:HD12	1:C:147:ILE:H	1.63	0.61
2:B:91:TYR:CD2	2:B:100(F):TYR:HA	2.35	0.61
2:B:100(E):TRP:O	2:B:100(F):TYR:CB	2.41	0.61
1:C:187:ASN:O	1:C:207:ASN:HA	2.00	0.61
2:B:161:ALA:HB2	2:B:170:LEU:HD23	1.81	0.61
1:C:133:MET:HE2	1:C:193:VAL:HG13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:60:ASN:O	2:D:62:ALA:N	2.34	0.61
2:D:143:VAL:HG21	2:D:170:LEU:CD2	2.31	0.61
1:A:146:LYS:O	1:A:147:ILE:HG13	2.00	0.61
1:C:125:GLY:CA	1:C:180:LYS:HB3	2.26	0.61
1:A:189:TYR:CB	1:A:206:PHE:HE2	2.10	0.61
1:A:195:HIS:HB3	1:A:197:THR:N	2.16	0.61
2:B:103:TRP:HD1	2:B:139:PHE:CE1	2.19	0.61
1:A:50:ASN:HB3	1:A:91:TYR:HH	1.61	0.60
2:B:83:GLN:CB	2:B:85:ASP:N	2.63	0.60
1:C:76:SER:O	1:C:77:SER:CB	2.49	0.60
2:D:143:VAL:HG21	2:D:170:LEU:HD23	1.83	0.60
1:A:29:ILE:HD11	1:A:33:LEU:HD13	1.83	0.60
1:A:122:LEU:C	1:A:124:THR:N	2.59	0.60
2:B:135:VAL:HG22	2:B:190:VAL:HG21	1.82	0.60
2:B:145:VAL:CG1	2:B:190:VAL:HG22	2.31	0.60
1:C:147:ILE:O	1:C:148:ASP:C	2.44	0.60
2:D:13:ARG:HB2	2:D:16:GLU:CG	2.30	0.60
2:D:111:VAL:HG12	2:D:112:SER:N	2.16	0.60
1:A:138:PRO:O	1:A:140:ASP:N	2.34	0.60
1:C:137:TYR:CD2	1:C:138:PRO:N	2.69	0.60
1:C:142:SER:O	1:C:193:VAL:O	2.18	0.60
1:C:207:ASN:O	1:C:210:GLU:HB2	2.01	0.60
2:D:159:PHE:CD2	2:D:159:PHE:N	2.69	0.60
1:A:107:ARG:C	1:A:108:THR:HG22	2.20	0.60
1:A:210:GLU:CA	2:B:208:CYS:SG	2.90	0.60
2:B:100(C):GLY:O	2:B:100(D):PHE:HD2	1.84	0.60
1:C:132:LEU:HD22	1:C:173:SER:HB2	1.82	0.60
2:B:134:LEU:HD13	2:B:171:THR:HB	1.84	0.60
1:A:137:TYR:HD2	1:A:138:PRO:HD3	1.65	0.60
1:A:141:ILE:O	1:A:142:SER:HB3	2.00	0.60
2:B:73:THR:O	2:B:75:LYS:N	2.34	0.60
2:D:182:SER:O	2:D:183:SER:O	2.20	0.60
2:B:38:ARG:CB	2:B:48:MET:HE2	2.30	0.60
2:B:96:LEU:HG	2:B:100(A):PRO:CD	2.30	0.60
2:B:103:TRP:HD1	2:B:139:PHE:HE1	1.47	0.60
2:B:36:TRP:HD1	2:B:69:ILE:HG12	1.64	0.60
1:C:36:TYR:OH	2:D:100:TYR:CD1	2.54	0.60
1:C:67:SER:O	1:C:68:GLY:C	2.44	0.60
1:C:107:ARG:HB2	1:C:107:ARG:CZ	2.31	0.60
1:C:112:VAL:CG2	1:C:193:VAL:HG21	2.30	0.60
2:D:8:GLY:HA3	2:D:20:LEU:CD2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:107:THR:OG1	2:D:108:MET:N	2.35	0.60
2:B:143:VAL:HG12	2:B:192:HIS:CD2	2.37	0.59
1:C:147:ILE:HD11	1:C:152:ARG:H	1.67	0.59
2:D:103:TRP:C	2:D:105:PRO:HD3	2.27	0.59
2:D:161:ALA:HB2	2:D:170:LEU:HB3	1.84	0.59
1:A:137:TYR:O	1:A:138:PRO:C	2.38	0.59
1:C:136:PHE:HZ	1:C:141:ILE:HG13	1.64	0.59
1:A:47:LEU:CA	1:A:58:ILE:HG13	2.32	0.59
1:A:71:TYR:C	1:A:72:THR:HG22	2.27	0.59
2:B:51:MET:HE2	2:B:71:ARG:HG2	1.83	0.59
1:C:193:VAL:O	1:C:194:VAL:HB	2.02	0.59
2:D:112:SER:CA	2:D:138:TYR:HB3	2.31	0.59
2:D:192:HIS:HB3	2:D:197:THR:HB	1.84	0.59
2:B:18:LEU:CG	2:B:102:PHE:CE2	2.78	0.59
1:C:90:GLN:NE2	1:C:92:ASN:N	2.47	0.59
1:A:30:ASN:HA	1:A:31:ASN:N	2.16	0.59
1:A:121:GLN:N	2:B:115:PHE:CD2	2.71	0.59
1:C:4:LEU:HD21	1:C:90:GLN:CB	2.32	0.59
1:C:151:GLU:O	1:C:151:GLU:HG3	2.03	0.59
2:D:51:MET:SD	2:D:71:ARG:HG2	2.42	0.59
1:A:108:THR:HA	1:A:137:TYR:CD2	2.36	0.59
1:A:133:MET:HE1	1:A:143:VAL:HG13	1.82	0.59
1:C:7:SER:OG	1:C:8:PRO:CD	2.42	0.59
1:C:46:LEU:HD23	1:C:55:GLN:CG	2.33	0.59
1:C:137:TYR:CD2	1:C:138:PRO:CA	2.86	0.59
2:D:20:LEU:HD22	2:D:100(G):PHE:HE2	1.66	0.59
2:B:143:VAL:CG2	2:B:170:LEU:HD11	2.33	0.59
1:C:178:LEU:HD23	1:C:179:THR:N	2.03	0.59
2:D:158:THR:HA	2:D:172:SER:HA	1.85	0.59
1:A:142:SER:O	1:A:193:VAL:O	2.20	0.58
1:A:189:TYR:HA	1:A:190:THR:N	2.18	0.58
2:B:32:PHE:CD2	2:B:94:ARG:HD3	2.38	0.58
1:C:36:TYR:CZ	2:D:100:TYR:HD1	2.21	0.58
1:C:159:SER:O	1:C:172:MET:HG2	2.03	0.58
2:D:91:TYR:CD2	2:D:100(F):TYR:HA	2.38	0.58
2:D:143:VAL:CG2	2:D:170:LEU:CD2	2.82	0.58
2:B:110:THR:O	2:B:138:TYR:HA	2.04	0.58
1:C:196:LYS:C	1:C:198:SER:H	2.10	0.58
1:A:33:LEU:HD22	1:A:71:TYR:CB	2.34	0.58
1:C:118:SER:C	1:C:120:GLU:N	2.57	0.58
2:B:126:ASN:O	2:B:127:SER:C	2.45	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ASN:HA	1:A:71:TYR:HE2	1.69	0.58
2:B:164:GLN:NE2	2:B:164:GLN:CA	2.67	0.58
2:D:186:VAL:HG22	2:D:203:ILE:HD11	1.85	0.58
1:C:108:THR:HA	1:C:137:TYR:HB3	1.85	0.58
1:A:187:ASN:HD22	1:A:207:ASN:HB3	1.69	0.58
2:D:18:LEU:HD22	2:D:19:SER:H	1.55	0.58
2:D:132:GLY:HA2	2:D:147:TRP:CZ2	2.38	0.58
2:B:11:LEU:HD11	2:B:108:MET:O	2.03	0.58
1:C:160:VAL:O	1:C:161:THR:HG23	2.03	0.58
2:B:100(E):TRP:CD1	3:B:221:HOH:O	2.57	0.58
1:A:40:LEU:HD12	1:A:41:GLY:CA	2.34	0.57
1:A:147:ILE:HG23	1:A:189:TYR:CD2	2.38	0.57
2:B:139:PHE:HA	2:B:140:PRO:O	2.04	0.57
1:C:36:TYR:HA	1:C:45:LYS:O	2.03	0.57
1:A:37:GLN:HB2	1:A:86:TYR:CE2	2.39	0.57
1:A:121:GLN:CA	2:B:115:PHE:CE2	2.87	0.57
2:D:129:VAL:HG21	2:D:181:TRP:CD1	2.39	0.57
1:A:11:LEU:HD12	1:A:12:SER:N	2.19	0.57
1:C:180:LYS:HZ2	1:C:184:GLU:HB2	1.69	0.57
2:D:195:SER:O	2:D:197:THR:N	2.37	0.57
1:A:160:VAL:C	1:A:161:THR:CG2	2.63	0.57
2:D:182:SER:O	2:D:183:SER:C	2.47	0.57
1:A:80:PRO:HA	1:A:106:LEU:CD1	2.35	0.57
2:B:38:ARG:CD	2:B:48:MET:HE2	2.28	0.57
2:B:48:MET:HE1	2:B:90:TYR:HD2	1.56	0.57
2:B:161:ALA:HB1	2:B:169:THR:O	2.04	0.57
1:C:157:LEU:HD23	1:C:157:LEU:N	2.19	0.57
1:C:211:CYS:HB3	2:D:206:ARG:CZ	2.32	0.57
2:D:19:SER:HA	2:D:80:LEU:O	2.05	0.57
1:A:52:ASN:HA	1:A:64:GLY:HA3	1.85	0.57
2:B:143:VAL:CG1	2:B:192:HIS:HD2	2.18	0.57
2:B:175:THR:O	2:B:176:VAL:CB	2.52	0.57
1:C:147:ILE:HD11	1:C:152:ARG:CB	2.32	0.57
2:D:89:THR:HA	2:D:101:ASP:HA	1.86	0.57
2:D:105:PRO:HG3	2:D:139:PHE:CZ	2.37	0.57
2:D:203:ILE:HD13	2:D:203:ILE:N	2.19	0.57
1:A:10:LEU:HD12	1:A:10:LEU:C	2.30	0.57
1:A:13:ALA:O	1:A:106:LEU:HA	2.03	0.57
1:A:121:GLN:CA	2:B:115:PHE:CD2	2.88	0.57
2:B:158:THR:HA	2:B:172:SER:HA	1.87	0.57
1:C:179:THR:O	1:C:183:TYR:HB3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:ALA:HA	1:C:197:THR:HG21	1.87	0.57
1:C:158:ASP:HB3	1:C:174:SER:CB	2.34	0.57
2:B:52:TRP:NE1	2:B:56:TYR:HD2	2.03	0.56
2:D:51:MET:HG3	2:D:51:MET:O	2.03	0.56
2:D:114:VAL:CG2	2:D:190:VAL:HG21	2.34	0.56
1:C:54:LEU:HD21	1:C:59:PRO:O	2.05	0.56
2:D:89:THR:HG21	2:D:100(F):TYR:CE1	2.40	0.56
1:A:14:SER:O	1:A:15:VAL:C	2.45	0.56
1:A:127:ALA:HB1	1:A:183:TYR:CD1	2.40	0.56
1:A:132:LEU:HD23	1:A:173:SER:HB2	1.82	0.56
1:A:176:LEU:HD23	1:A:176:LEU:O	2.04	0.56
2:B:18:LEU:CG	2:B:102:PHE:HZ	1.90	0.56
2:B:48:MET:CB	2:B:63:LEU:HD23	2.33	0.56
1:C:38:GLN:HG3	1:C:87:PHE:HE1	1.70	0.56
1:C:46:LEU:HD23	1:C:55:GLN:HG3	1.86	0.56
1:C:55:GLN:HB3	3:C:215:HOH:O	2.05	0.56
1:C:137:TYR:CD2	1:C:137:TYR:C	2.83	0.56
1:C:152:ARG:NE	1:C:152:ARG:CA	2.57	0.56
1:C:193:VAL:N	1:C:202:VAL:O	2.29	0.56
1:A:94:GLY:O	1:A:96:TYR:CB	2.53	0.56
1:A:110:PRO:C	1:A:111:THR:CA	2.73	0.56
2:B:104:GLY:N	2:B:105:PRO:HD3	2.20	0.56
1:C:211:CYS:N	2:D:208:CYS:SG	2.79	0.56
2:D:103:TRP:HD1	2:D:139:PHE:CE1	2.22	0.56
2:D:152:LEU:O	2:D:153:SER:CB	2.51	0.56
1:A:149:GLY:O	1:A:150:THR:N	2.35	0.56
1:A:185:SER:O	1:A:186:HIS:ND1	2.39	0.56
2:B:90:TYR:N	2:B:100(G):PHE:O	2.39	0.56
2:B:133:CYS:HB2	2:B:203:ILE:HD11	1.88	0.56
2:B:188:CYS:O	2:B:189:ASN:HB2	2.03	0.56
1:C:67:SER:O	1:C:68:GLY:O	2.24	0.56
1:C:69:THR:HG23	1:C:70:ASP:N	2.19	0.56
1:A:78:LEU:HD11	1:A:106:LEU:HD21	1.76	0.56
2:B:3:GLN:O	2:B:4:LEU:HB2	2.05	0.56
1:C:36:TYR:OH	2:D:100:TYR:HD1	1.88	0.56
1:A:182:ASP:HA	1:A:185:SER:CB	2.28	0.56
1:C:11:LEU:HD12	1:C:12:SER:N	2.21	0.56
2:D:114:VAL:O	2:D:114:VAL:CG1	2.54	0.56
1:A:47:LEU:HA	1:A:58:ILE:CG1	2.35	0.55
1:A:110:PRO:HD3	1:A:197:THR:CG2	2.35	0.55
1:A:138:PRO:C	1:A:140:ASP:N	2.62	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:CYS:HB3	2:B:206:ARG:CZ	2.33	0.55
2:B:75:LYS:HD3	2:B:77:GLN:CD	2.31	0.55
2:B:109:VAL:O	2:B:110:THR:OG1	2.18	0.55
2:D:105:PRO:HG2	2:D:107:THR:CG2	2.34	0.55
2:D:147:TRP:HZ3	2:D:203:ILE:HD12	1.71	0.55
1:A:6:GLN:HE22	1:A:87:PHE:HA	1.70	0.55
1:C:196:LYS:O	1:C:197:THR:C	2.49	0.55
2:D:39:HIS:HE1	2:D:44:GLY:HA2	1.71	0.55
2:D:51:MET:HE2	2:D:71:ARG:HG2	1.88	0.55
1:A:173:SER:HB3	2:B:159:PHE:CG	2.39	0.55
1:A:193:VAL:HG12	1:A:194:VAL:N	2.21	0.55
1:C:163:GLN:HG3	1:C:170:TYR:CZ	2.41	0.55
1:C:117:PRO:HB2	1:C:122:LEU:HD23	1.87	0.55
1:C:120:GLU:O	1:C:122:LEU:N	2.39	0.55
1:A:49:TYR:HE2	1:A:55:GLN:HE21	1.53	0.55
1:A:147:ILE:O	1:A:150:THR:N	2.40	0.55
1:C:167:ASP:O	1:C:167:ASP:OD1	2.25	0.55
2:D:147:TRP:HZ3	2:D:203:ILE:CD1	2.19	0.55
2:B:67:LEU:HD12	2:B:80:LEU:HD21	1.87	0.55
2:B:113:SER:O	2:B:136:LYS:N	2.31	0.55
1:A:152:ARG:N	1:A:152:ARG:HD2	2.13	0.55
1:A:190:THR:HB	1:A:205:SER:OG	2.05	0.55
1:C:118:SER:HB3	2:D:116:PRO:HD2	1.88	0.55
1:C:190:THR:HB	1:C:205:SER:OG	2.06	0.55
2:D:104:GLY:N	2:D:105:PRO:HD3	2.22	0.55
2:B:25:SER:C	2:B:26:GLY:CA	2.74	0.55
1:C:112:VAL:CG1	1:C:113:SER:H	2.18	0.55
1:A:117:PRO:CG	1:A:122:LEU:HD13	2.35	0.55
1:A:150:THR:C	1:A:151:GLU:N	2.65	0.55
1:A:54:LEU:HD21	1:A:59:PRO:O	2.07	0.55
1:C:19:VAL:HG12	1:C:20:THR:N	2.21	0.55
1:A:147:ILE:CG2	1:A:189:TYR:CE2	2.83	0.54
2:B:109:VAL:O	2:B:110:THR:CB	2.55	0.54
1:C:38:GLN:O	1:C:39:LYS:HB2	2.07	0.54
1:C:43:ALA:CB	2:D:100(D):PHE:HB3	2.21	0.54
1:C:133:MET:CE	1:C:143:VAL:HG13	2.37	0.54
2:D:51:MET:CE	2:D:71:ARG:HG2	2.37	0.54
2:B:89:THR:HB	2:B:101:ASP:HA	1.89	0.54
2:B:147:TRP:O	2:B:150:GLY:N	2.39	0.54
2:B:195:SER:C	2:B:197:THR:N	2.65	0.54
1:C:176:LEU:HD23	1:C:176:LEU:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:100(B):LEU:CD1	2:D:100(C):GLY:H	2.20	0.54
1:A:117:PRO:HG3	1:A:127:ALA:CA	2.38	0.54
1:A:211:CYS:O	2:B:121:SER:OG	2.22	0.54
2:B:18:LEU:CD1	2:B:102:PHE:CE2	2.89	0.54
1:A:10:LEU:HD12	1:A:11:LEU:H	1.67	0.54
1:C:71:TYR:CD1	1:C:71:TYR:N	2.76	0.54
1:A:200:SER:O	1:A:201:PRO:HA	2.07	0.54
1:A:70:ASP:C	1:A:71:TYR:CD1	2.85	0.54
1:A:137:TYR:HB3	1:A:138:PRO:HD3	1.88	0.54
1:A:137:TYR:CD2	1:A:138:PRO:CD	2.90	0.54
1:A:167:ASP:OD1	1:A:167:ASP:C	2.51	0.54
2:B:114:VAL:HG12	2:B:201:LYS:HG3	1.90	0.54
2:B:133:CYS:HB2	2:B:203:ILE:CD1	2.38	0.54
1:A:68:GLY:O	1:A:69:THR:HG22	2.08	0.54
1:C:19:VAL:CG1	1:C:20:THR:N	2.71	0.54
2:D:73:THR:O	2:D:74:SER:C	2.50	0.54
2:D:83:GLN:C	2:D:85:ASP:H	2.15	0.54
2:D:135:VAL:HG22	2:D:190:VAL:HG21	1.89	0.54
1:A:138:PRO:HG3	1:A:196:LYS:HE3	1.90	0.54
2:B:18:LEU:HD22	2:B:19:SER:H	1.63	0.54
1:C:118:SER:O	1:C:119:THR:C	2.49	0.54
2:D:13:ARG:O	2:D:16:GLU:HG3	2.08	0.54
1:A:47:LEU:HD23	1:A:58:ILE:HD12	1.89	0.54
1:A:94:GLY:HA2	1:A:96:TYR:CD1	2.43	0.54
1:C:80:PRO:HD2	1:C:81:GLU:OE2	2.08	0.54
2:B:131:LEU:HD23	2:B:186:VAL:HG11	1.90	0.53
1:C:14:SER:O	1:C:15:VAL:C	2.50	0.53
1:C:71:TYR:C	1:C:72:THR:HG22	2.32	0.53
1:A:12:SER:HA	1:A:105:GLU:O	2.08	0.53
1:A:71:TYR:CD1	1:A:71:TYR:N	2.76	0.53
2:B:137:GLY:C	2:B:167:LEU:HD13	2.33	0.53
1:C:106(A):LYS:O	1:C:107:ARG:HB3	2.07	0.53
1:C:43:ALA:CB	2:D:100(D):PHE:O	2.56	0.53
1:C:210:GLU:C	2:D:208:CYS:SG	2.91	0.53
2:D:139:PHE:CE2	2:D:140:PRO:HB3	2.44	0.53
1:A:61:ARG:O	1:A:75:ILE:HA	2.09	0.53
2:B:84:THR:O	2:B:85:ASP:HA	2.04	0.53
2:B:84:THR:C	2:B:85:ASP:N	2.66	0.53
1:C:13:ALA:O	1:C:106:LEU:HA	2.09	0.53
1:C:106(A):LYS:C	1:C:107:ARG:HG2	2.32	0.53
1:C:146:LYS:HG2	1:C:151:GLU:CB	2.13	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:103:TRP:HD1	2:D:139:PHE:CZ	2.27	0.53
1:A:49:TYR:O	1:A:50:ASN:C	2.51	0.53
1:A:110:PRO:C	1:A:111:THR:CB	2.82	0.53
2:B:136:LYS:HG2	2:B:137:GLY:N	2.22	0.53
1:C:122:LEU:HD21	1:C:183:TYR:CD1	2.43	0.53
2:D:117:LEU:HB2	2:D:132:GLY:C	2.34	0.53
1:A:150:THR:HB	1:A:151:GLU:N	2.23	0.53
2:B:8:GLY:HA3	2:B:20:LEU:CD2	2.39	0.53
2:D:60:ASN:O	2:D:63:LEU:N	2.40	0.53
2:D:154:SER:N	3:D:221:HOH:O	2.41	0.53
1:A:33:LEU:HD22	1:A:71:TYR:HB3	1.91	0.53
1:A:36:TYR:OH	2:B:100:TYR:CD1	2.56	0.53
1:A:48:ILE:HD12	1:A:52:ASN:HA	1.91	0.53
1:A:110:PRO:HA	1:A:136:PHE:CA	2.39	0.53
1:C:151:GLU:O	1:C:151:GLU:CG	2.56	0.53
1:A:133:MET:CE	1:A:143:VAL:CG1	2.74	0.53
1:C:31:ASN:HA	1:C:71:TYR:CE2	2.43	0.53
1:A:29:ILE:HG12	1:A:71:TYR:CZ	2.43	0.53
1:A:61:ARG:HH21	1:A:82:ASP:CG	2.16	0.53
1:A:141:ILE:HD12	1:A:141:ILE:N	2.08	0.53
1:A:147:ILE:HD11	1:A:152:ARG:N	2.20	0.53
2:B:139:PHE:HB3	2:B:167:LEU:HD22	1.90	0.53
1:A:50:ASN:CB	1:A:91:TYR:OH	2.40	0.52
2:B:29:LEU:HD21	2:B:78:VAL:CG2	2.39	0.52
2:B:113:SER:HB2	2:B:136:LYS:O	2.09	0.52
2:D:103:TRP:NE1	2:D:168:TYR:HH	2.07	0.52
1:A:29:ILE:CD1	1:A:33:LEU:HD13	2.38	0.52
2:B:14:PRO:O	2:B:16:GLU:N	2.40	0.52
1:C:121:GLN:OE1	1:C:128:SER:N	2.42	0.52
1:C:116:PRO:HB3	1:C:206:PHE:CZ	2.43	0.52
1:C:117:PRO:HB2	1:C:122:LEU:CD2	2.39	0.52
1:A:117:PRO:HD2	1:A:183:TYR:CE1	2.44	0.52
1:A:189:TYR:HB3	1:A:206:PHE:CE2	2.44	0.52
2:B:34:VAL:HA	2:B:93:THR:O	2.09	0.52
1:C:10:LEU:HD12	1:C:10:LEU:C	2.34	0.52
1:C:118:SER:CB	2:D:116:PRO:HD2	2.39	0.52
2:D:164:GLN:HE21	2:D:165:SER:N	2.07	0.52
2:B:85:ASP:O	2:B:86:ASP:CA	2.58	0.52
1:C:173:SER:N	2:D:159:PHE:CE1	2.77	0.52
1:C:179:THR:HB	1:C:181:ALA:HB3	1.92	0.52
1:A:109:ALA:H	1:A:137:TYR:HB3	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:TRP:O	2:B:48:MET:N	2.43	0.52
2:B:186:VAL:O	2:B:203:ILE:HG22	2.10	0.52
1:C:146:LYS:HA	1:C:151:GLU:CA	2.22	0.52
1:A:48:ILE:CD1	1:A:64:GLY:CA	2.87	0.52
1:A:112:VAL:HG21	1:A:193:VAL:CG2	2.32	0.52
1:A:146:LYS:C	1:A:147:ILE:HG13	2.35	0.52
2:B:40:PRO:O	2:B:41:SER:C	2.52	0.52
2:B:138:TYR:CD1	2:B:138:TYR:C	2.88	0.52
2:B:143:VAL:O	2:B:144:THR:CG2	2.55	0.52
2:B:152:LEU:CB	2:B:153:SER:N	2.73	0.52
1:C:186:HIS:HB3	1:C:188:LEU:HD11	1.88	0.52
2:D:31:SER:O	2:D:32:PHE:CD1	2.62	0.52
2:D:114:VAL:CG1	2:D:201:LYS:HB2	2.39	0.52
1:A:193:VAL:N	1:A:202:VAL:O	2.35	0.52
2:B:38:ARG:HD2	2:B:48:MET:CE	2.31	0.52
1:C:36:TYR:OH	2:D:100:TYR:N	2.41	0.52
2:D:50:ARG:HG2	2:D:52:TRP:CD1	2.44	0.52
2:D:143:VAL:CG2	2:D:170:LEU:HD23	2.40	0.52
2:D:164:GLN:CG	2:D:165:SER:H	2.22	0.52
1:A:137:TYR:CD2	1:A:138:PRO:N	2.78	0.52
2:B:114:VAL:HG21	2:B:190:VAL:CG2	2.38	0.52
1:C:178:LEU:HD22	1:C:182:ASP:CG	2.35	0.52
1:A:189:TYR:O	1:A:206:PHE:HD2	1.93	0.52
2:B:18:LEU:CD1	2:B:102:PHE:CZ	2.93	0.52
2:B:132:GLY:O	2:B:203:ILE:CD1	2.56	0.52
1:A:29:ILE:CG1	1:A:71:TYR:CE1	2.92	0.51
1:A:118:SER:CB	1:A:121:GLN:HB3	2.40	0.51
2:B:6:GLU:O	2:B:100(G):PHE:CD1	2.64	0.51
2:B:91:TYR:HD2	2:B:100(F):TYR:HA	1.75	0.51
1:C:2:ILE:HB	1:C:90:GLN:OE1	2.10	0.51
1:C:35:TRP:HD1	1:C:48:ILE:HD12	1.76	0.51
1:C:69:THR:HG23	1:C:70:ASP:CG	2.35	0.51
1:C:83:VAL:HG11	1:C:163:GLN:HB3	1.92	0.51
1:C:129:VAL:HG13	1:C:206:PHE:HE1	1.76	0.51
2:D:148:ASN:HB2	2:D:152:LEU:CD2	2.40	0.51
2:B:96:LEU:C	2:B:98:GLY:H	2.17	0.51
1:C:116:PRO:HG3	1:C:206:PHE:CD1	2.45	0.51
2:D:13:ARG:O	2:D:14:PRO:O	2.29	0.51
1:A:123:ALA:O	1:A:124:THR:HG22	2.10	0.51
1:C:37:GLN:N	1:C:45:LYS:O	2.40	0.51
2:D:100(G):PHE:CD1	2:D:100(G):PHE:C	2.86	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:ARG:HD3	2:B:46:GLU:HG2	1.93	0.51
1:C:68:GLY:O	1:C:69:THR:HG22	2.11	0.51
1:C:106(A):LYS:O	1:C:107:ARG:CB	2.58	0.51
2:D:13:ARG:CB	2:D:16:GLU:HG3	2.40	0.51
1:A:129:VAL:CG1	1:A:145:TRP:CH2	2.94	0.51
1:A:171:SER:CB	2:B:157:HIS:CE1	2.94	0.51
1:C:187:ASN:HD22	1:C:207:ASN:C	2.19	0.51
2:B:89:THR:CB	2:B:101:ASP:HA	2.41	0.51
2:D:100(E):TRP:O	2:D:100(F):TYR:CB	2.59	0.51
1:A:102:THR:HG22	1:A:103:LYS:O	2.10	0.51
1:A:117:PRO:HD2	1:A:183:TYR:HE1	1.75	0.51
1:A:122:LEU:CD1	1:A:127:ALA:CB	2.86	0.51
1:A:138:PRO:HG2	1:A:196:LYS:HG2	1.92	0.51
1:A:173:SER:CB	2:B:159:PHE:CE1	2.92	0.51
2:B:88:GLY:O	2:B:102:PHE:HB3	2.11	0.51
1:C:43:ALA:HB2	2:D:100(D):PHE:O	2.11	0.51
1:C:179:THR:C	1:C:181:ALA:N	2.66	0.51
1:A:27:GLN:O	1:A:28:ASN:C	2.54	0.51
2:B:114:VAL:HG12	2:B:114:VAL:O	2.11	0.51
1:C:54:LEU:CD1	1:C:58:ILE:O	2.54	0.51
2:D:100(A):PRO:HG2	2:D:100(B):LEU:N	2.17	0.51
2:D:132:GLY:HA2	2:D:147:TRP:CH2	2.46	0.51
1:A:36:TYR:HA	1:A:45:LYS:O	2.10	0.50
2:D:164:GLN:NE2	2:D:164:GLN:C	2.69	0.50
2:D:174:VAL:HG22	2:D:175:THR:N	2.26	0.50
1:A:127:ALA:CB	1:A:183:TYR:CD1	2.94	0.50
1:C:186:HIS:HB3	1:C:188:LEU:HD12	1.91	0.50
2:D:189:ASN:HD22	2:D:189:ASN:N	2.09	0.50
1:A:2:ILE:HB	1:A:90:GLN:OE1	2.11	0.50
1:A:29:ILE:O	1:A:32:TYR:N	2.44	0.50
1:A:183:TYR:CA	1:A:184:GLU:N	2.74	0.50
2:B:18:LEU:CD2	2:B:102:PHE:CE1	2.85	0.50
2:B:13:ARG:CB	2:B:16:GLU:HG3	2.35	0.50
2:B:101:ASP:OD2	2:B:102:PHE:N	2.44	0.50
2:B:157:HIS:O	2:B:159:PHE:CE2	2.64	0.50
1:C:137:TYR:CG	1:C:138:PRO:HA	2.46	0.50
1:C:141:ILE:N	1:C:141:ILE:CD1	2.55	0.50
2:D:204:VAL:CB	2:D:205:PRO:HD2	2.41	0.50
1:C:38:GLN:O	1:C:39:LYS:CB	2.58	0.50
1:C:156:VAL:HG23	1:C:175:THR:C	2.36	0.50
1:C:159:SER:HB2	2:D:160:PRO:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ASN:CA	1:A:32:TYR:N	2.67	0.50
2:D:117:LEU:HB2	2:D:132:GLY:O	2.11	0.50
1:A:180:LYS:HE2	1:A:184:GLU:CD	2.33	0.50
1:C:133:MET:HE3	1:C:193:VAL:HG22	1.94	0.50
2:D:100(E):TRP:O	2:D:100(F):TYR:HB2	2.12	0.50
1:A:7:SER:OG	1:A:22:SER:HB3	2.11	0.49
1:A:11:LEU:HD21	1:A:19:VAL:CG1	2.42	0.49
1:A:133:MET:O	1:A:136:PHE:CD2	2.63	0.49
2:B:202:LYS:O	2:B:203:ILE:HB	2.05	0.49
2:D:13:ARG:C	2:D:14:PRO:O	2.55	0.49
1:A:78:LEU:HD12	1:A:106:LEU:HD22	1.88	0.49
2:B:11:LEU:HA	2:B:103:TRP:O	2.12	0.49
1:A:30:ASN:C	1:A:32:TYR:H	2.21	0.49
1:A:94:GLY:CA	1:A:96:TYR:CD1	2.95	0.49
2:B:148:ASN:O	2:B:149:SER:C	2.55	0.49
1:C:148:ASP:C	1:C:150:THR:H	2.20	0.49
2:D:16:GLU:HB2	2:D:82(C):LEU:HD11	1.93	0.49
1:A:17:ASP:O	1:A:78:LEU:HB2	2.11	0.49
1:A:123:ALA:O	1:A:124:THR:CA	2.56	0.49
2:B:52:TRP:NE1	2:B:56:TYR:CD2	2.81	0.49
1:C:28:ASN:ND2	1:C:30:ASN:H	2.11	0.49
1:C:133:MET:HE3	1:C:193:VAL:HG13	1.94	0.49
1:C:179:THR:OG1	1:C:182:ASP:N	2.46	0.49
1:A:48:ILE:HD13	1:A:64:GLY:CA	2.43	0.49
1:A:153:ARG:H	1:A:154:ASP:N	2.10	0.49
2:B:120:GLY:O	2:B:121:SER:CB	2.60	0.49
1:C:140:ASP:O	1:C:195:HIS:CD2	2.66	0.49
2:D:11:LEU:HG	2:D:140:PRO:HG3	1.94	0.49
2:B:114:VAL:CG1	2:B:201:LYS:HB2	2.42	0.49
1:C:10:LEU:HD11	1:C:105:GLU:HG3	1.94	0.49
1:A:208:ARG:C	1:A:210:GLU:H	2.20	0.49
1:A:211:CYS:C	2:B:121:SER:OG	2.56	0.49
1:C:115:PHE:HB2	1:C:130:VAL:HG22	1.94	0.49
2:D:36:TRP:HD1	2:D:69:ILE:HG12	1.73	0.49
1:A:7:SER:O	1:A:8:PRO:C	2.48	0.49
1:A:183:TYR:CD2	1:A:184:GLU:HA	2.39	0.49
2:B:148:ASN:C	2:B:150:GLY:N	2.69	0.49
2:D:111:VAL:CG1	2:D:112:SER:N	2.75	0.49
2:D:126:ASN:O	2:D:127:SER:O	2.31	0.49
2:D:139:PHE:CD2	2:D:140:PRO:N	2.81	0.49
1:C:194:VAL:HG23	1:C:201:PRO:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:SER:N	2:B:159:PHE:CE1	2.80	0.48
2:B:48:MET:O	2:B:60:ASN:N	2.39	0.48
2:B:73:THR:O	2:B:74:SER:C	2.56	0.48
2:D:66:ARG:HB2	2:D:82(A):ASN:O	2.13	0.48
2:D:134:LEU:HD13	2:D:171:THR:HB	1.94	0.48
1:A:192:GLU:HG3	1:A:203:VAL:CB	2.41	0.48
2:B:63:LEU:O	2:B:67:LEU:HB3	2.13	0.48
1:C:120:GLU:N	1:C:120:GLU:CD	2.72	0.48
2:D:18:LEU:HD23	2:D:19:SER:H	1.75	0.48
1:A:106:LEU:C	1:A:106(A):LYS:HG3	2.38	0.48
1:A:110:PRO:HA	1:A:136:PHE:HA	1.95	0.48
2:B:89:THR:HA	2:B:100(G):PHE:O	2.11	0.48
1:C:69:THR:HG22	1:C:70:ASP:H	1.78	0.48
1:C:109:ALA:HA	1:C:197:THR:CG2	2.43	0.48
1:C:193:VAL:HG12	1:C:194:VAL:N	2.27	0.48
1:C:196:LYS:CG	1:C:197:THR:N	2.75	0.48
1:A:4:LEU:HD21	1:A:90:GLN:HB2	1.95	0.48
1:A:32:TYR:HB3	1:A:91:TYR:CE1	2.48	0.48
2:B:152:LEU:HD23	2:B:152:LEU:N	2.29	0.48
1:C:56:THR:N	3:C:215:HOH:O	2.46	0.48
1:C:211:CYS:CB	2:D:120:GLY:HA2	2.43	0.48
2:D:48:MET:SD	2:D:63:LEU:HD21	2.53	0.48
2:D:111:VAL:HG12	2:D:112:SER:O	2.13	0.48
1:A:141:ILE:O	1:A:142:SER:CB	2.62	0.48
1:A:151:GLU:O	1:A:151:GLU:CG	2.60	0.48
1:A:211:CYS:CA	2:B:120:GLY:C	2.64	0.48
2:B:52:TRP:HB3	2:B:54:ASP:OD1	2.13	0.48
2:B:76:ASN:C	2:B:77:GLN:HG2	2.37	0.48
2:B:131:LEU:HD21	2:B:181:TRP:CD2	2.48	0.48
2:B:141:GLU:O	2:B:142:PRO:CA	2.61	0.48
1:C:29:ILE:O	1:C:29:ILE:CG2	2.59	0.48
1:C:33:LEU:HD22	1:C:71:TYR:HB3	1.96	0.48
1:C:147:ILE:HD13	1:C:150:THR:CG2	2.44	0.48
2:D:82(C):LEU:HA	2:D:86:ASP:OD1	2.13	0.48
2:D:89:THR:HG21	2:D:100(F):TYR:CZ	2.48	0.48
1:A:32:TYR:HB3	1:A:91:TYR:CZ	2.48	0.48
1:C:178:LEU:HD22	1:C:182:ASP:OD1	2.13	0.48
1:A:117:PRO:CD	1:A:183:TYR:HE1	2.26	0.48
2:B:59:TYR:HE2	2:B:68:SER:HA	1.75	0.48
2:D:100(G):PHE:CE2	2:D:102:PHE:CE2	3.02	0.48
1:A:117:PRO:CD	1:A:183:TYR:CE1	2.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:TYR:C	1:A:184:GLU:CA	2.85	0.48
2:B:143:VAL:HG21	2:B:170:LEU:HD11	1.95	0.48
1:C:107:ARG:CZ	1:C:107:ARG:CB	2.91	0.48
2:D:158:THR:HB	2:D:172:SER:HB2	1.95	0.48
2:B:21:THR:O	2:B:21:THR:HG22	2.14	0.48
2:B:52:TRP:CD1	2:B:56:TYR:HD2	2.32	0.48
1:C:159:SER:CB	2:D:160:PRO:HG2	2.43	0.48
1:C:160:VAL:O	1:C:161:THR:CB	2.61	0.48
1:A:185:SER:O	1:A:186:HIS:CG	2.67	0.47
1:A:129:VAL:CG1	1:A:145:TRP:HH2	2.22	0.47
1:A:139:ARG:O	1:A:139:ARG:HD3	2.15	0.47
2:B:112:SER:CA	2:B:138:TYR:HB3	2.43	0.47
2:D:139:PHE:CD2	2:D:139:PHE:C	2.92	0.47
1:A:81:GLU:HB3	1:A:165:SER:O	2.14	0.47
1:A:118:SER:H	1:A:121:GLN:HB3	1.79	0.47
2:B:147:TRP:CH2	2:B:188:CYS:HB3	2.48	0.47
1:C:192:GLU:HA	1:C:203:VAL:CB	2.42	0.47
1:C:206:PHE:C	1:C:206:PHE:CD2	2.92	0.47
2:D:11:LEU:HD21	2:D:139:PHE:CE2	2.33	0.47
1:A:122:LEU:HG	1:A:180:LYS:HE3	1.96	0.47
2:B:13:ARG:HB2	2:B:16:GLU:CD	2.39	0.47
1:C:107:ARG:CG	1:C:107:ARG:NH1	2.68	0.47
1:C:152:ARG:HA	1:C:152:ARG:CZ	2.42	0.47
2:D:4:LEU:HD22	2:D:100(C):GLY:HA3	1.97	0.47
1:A:40:LEU:HG	1:A:41:GLY:N	2.27	0.47
2:B:39:HIS:HE1	2:B:44:GLY:HA2	1.79	0.47
1:C:49:TYR:O	1:C:50:ASN:C	2.58	0.47
1:C:148:ASP:OD2	1:C:188:LEU:HD13	2.14	0.47
1:A:148:ASP:OD1	1:A:148:ASP:O	2.31	0.47
1:A:194:VAL:H	1:A:202:VAL:HG23	1.79	0.47
2:B:51:MET:CE	2:B:71:ARG:HG2	2.44	0.47
2:B:127:SER:C	2:B:128:MET:CB	2.87	0.47
2:B:129:VAL:HG21	2:B:181:TRP:NE1	2.25	0.47
1:C:99:GLY:O	1:C:100:ALA:C	2.56	0.47
1:C:147:ILE:HD13	1:C:150:THR:HG21	1.96	0.47
2:D:187:THR:HA	2:D:203:ILE:HD13	1.97	0.47
1:A:10:LEU:HD11	1:A:105:GLU:HG3	1.96	0.47
1:A:28:ASN:HD21	1:A:30:ASN:HB3	1.80	0.47
1:A:87:PHE:HD2	1:A:99:GLY:O	1.98	0.47
1:A:211:CYS:HB2	2:B:206:ARG:HD3	1.95	0.47
2:B:89:THR:OG1	2:B:100(G):PHE:O	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:GLY:N	2:B:105:PRO:HD2	2.30	0.47
2:B:202:LYS:O	2:B:203:ILE:CB	2.55	0.47
1:C:57:GLY:N	3:C:215:HOH:O	2.47	0.47
2:D:82(C):LEU:H	2:D:82(C):LEU:HG	1.19	0.47
2:D:102:PHE:O	2:D:103:TRP:C	2.57	0.47
1:C:188:LEU:CD1	1:C:188:LEU:N	2.61	0.47
1:A:7:SER:CB	1:A:8:PRO:CD	2.93	0.47
1:A:37:GLN:HB2	1:A:86:TYR:CD2	2.49	0.47
1:A:121:GLN:N	2:B:115:PHE:CE2	2.82	0.47
1:A:180:LYS:C	1:A:184:GLU:HG3	2.40	0.47
2:B:138:TYR:CE1	2:B:168:TYR:HB2	2.50	0.47
1:A:30:ASN:C	1:A:32:TYR:N	2.73	0.46
1:A:109:ALA:N	1:A:137:TYR:HB3	2.30	0.46
1:A:208:ARG:O	1:A:210:GLU:N	2.42	0.46
2:D:53:TYR:O	2:D:71:ARG:NH2	2.48	0.46
1:A:137:TYR:HB3	1:A:138:PRO:CD	2.45	0.46
1:A:179:THR:O	1:A:180:LYS:C	2.56	0.46
2:B:18:LEU:HD23	2:B:19:SER:H	1.80	0.46
1:C:29:ILE:HG12	1:C:90:GLN:HG3	1.97	0.46
1:C:36:TYR:OH	2:D:100:TYR:O	2.24	0.46
2:D:20:LEU:HD21	2:D:100(G):PHE:HE2	1.80	0.46
2:D:100(G):PHE:HE2	2:D:102:PHE:HE2	1.63	0.46
2:B:50:ARG:NH2	2:B:95:ASP:OD2	2.41	0.46
2:B:139:PHE:CA	2:B:140:PRO:N	2.77	0.46
1:C:10:LEU:HD12	1:C:11:LEU:H	1.71	0.46
1:C:37:GLN:NE2	1:C:84:ALA:CB	2.79	0.46
1:C:90:GLN:NE2	1:C:93:ASN:N	2.62	0.46
1:C:182:ASP:HA	1:C:185:SER:OG	2.16	0.46
1:A:121:GLN:HA	2:B:115:PHE:CZ	2.50	0.46
2:B:82(C):LEU:HA	2:B:86:ASP:OD1	2.15	0.46
2:D:72:ASP:O	2:D:73:THR:O	2.33	0.46
1:A:152:ARG:HA	1:A:152:ARG:CZ	2.44	0.46
2:B:52:TRP:CD1	2:B:56:TYR:CD2	3.03	0.46
2:B:114:VAL:HB	2:B:199:VAL:HG11	1.98	0.46
1:C:4:LEU:HD21	1:C:90:GLN:HB3	1.98	0.46
1:C:69:THR:CG2	1:C:70:ASP:H	2.28	0.46
1:C:145:TRP:NE1	1:C:156:VAL:HG21	2.30	0.46
2:D:12:VAL:HG11	2:D:82(C):LEU:HD22	1.97	0.46
2:D:127:SER:O	2:D:178:SER:CB	2.64	0.46
1:A:91:TYR:N	1:A:91:TYR:CD2	2.83	0.46
1:A:118:SER:C	1:A:120:GLU:N	2.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ILE:CG2	1:A:189:TYR:HE2	2.23	0.46
2:B:35:SER:O	2:B:92:CYS:HA	2.16	0.46
1:C:39:LYS:O	1:C:40:LEU:C	2.59	0.46
1:C:120:GLU:O	1:C:121:GLN:C	2.58	0.46
1:C:189:TYR:N	1:C:206:PHE:O	2.48	0.46
1:A:160:VAL:HG23	1:A:161:THR:O	2.15	0.46
1:A:167:ASP:O	1:A:167:ASP:CG	2.50	0.46
2:B:152:LEU:N	2:B:152:LEU:CD2	2.79	0.46
2:D:94:ARG:O	2:D:100:TYR:HB3	2.16	0.46
2:D:103:TRP:NE1	2:D:168:TYR:OH	2.48	0.46
2:D:119:PRO:C	2:D:121:SER:H	2.21	0.46
1:A:180:LYS:HG2	1:A:184:GLU:CG	2.45	0.46
2:B:158:THR:O	2:B:158:THR:OG1	2.27	0.46
1:C:38:GLN:HG3	1:C:87:PHE:CE1	2.50	0.46
1:C:187:ASN:H	1:C:188:LEU:CD1	2.29	0.46
2:B:28:SER:C	2:B:30:THR:H	2.24	0.46
2:B:110:THR:HG21	2:B:167:LEU:CD1	2.37	0.46
1:C:47:LEU:HD23	1:C:58:ILE:HD12	1.97	0.46
1:C:124:THR:C	1:C:126:GLY:H	2.22	0.46
2:D:113:SER:N	2:D:136:LYS:O	2.49	0.46
2:B:51:MET:O	2:B:52:TRP:O	2.33	0.46
1:C:8:PRO:O	1:C:102:THR:HG23	2.15	0.46
1:C:107:ARG:NH1	1:C:107:ARG:CB	2.78	0.46
1:A:197:THR:C	1:A:198:SER:CA	2.83	0.45
1:C:188:LEU:H	1:C:188:LEU:HG	1.03	0.45
1:A:90:GLN:HE22	1:A:93:ASN:H	1.64	0.45
1:A:187:ASN:ND2	1:A:207:ASN:HB3	2.32	0.45
1:A:211:CYS:HB2	2:B:120:GLY:HA2	1.98	0.45
2:B:9:PRO:O	2:B:102:PHE:CD1	2.69	0.45
2:B:48:MET:CE	2:B:90:TYR:HE2	2.05	0.45
2:B:51:MET:C	2:B:52:TRP:O	2.59	0.45
1:C:122:LEU:CD1	1:C:180:LYS:HB2	2.46	0.45
2:D:53:TYR:CD2	2:D:53:TYR:N	2.80	0.45
1:A:150:THR:CB	1:A:151:GLU:N	2.80	0.45
1:A:189:TYR:CD1	1:A:206:PHE:HE2	2.35	0.45
1:C:61:ARG:HH21	1:C:82:ASP:CG	2.25	0.45
1:C:195:HIS:ND1	1:C:197:THR:CG2	2.80	0.45
2:D:14:PRO:C	2:D:16:GLU:N	2.74	0.45
2:D:114:VAL:HG21	2:D:190:VAL:CG2	2.44	0.45
2:B:51:MET:SD	2:B:71:ARG:HG2	2.56	0.45
2:B:152:LEU:CA	2:B:153:SER:N	2.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:SER:N	2:B:156:VAL:HG21	2.32	0.45
1:C:37:GLN:HE21	1:C:84:ALA:CB	2.28	0.45
2:D:139:PHE:CD2	2:D:140:PRO:CA	2.99	0.45
2:D:147:TRP:CZ3	2:D:203:ILE:HD12	2.51	0.45
2:D:179:SER:O	2:D:182:SER:O	2.34	0.45
1:A:90:GLN:C	1:A:90:GLN:CD	2.84	0.45
1:A:125:GLY:HA2	1:A:180:LYS:HB2	1.99	0.45
1:A:191:CYS:O	1:A:203:VAL:HA	2.17	0.45
1:C:118:SER:CB	1:C:121:GLN:HB3	2.43	0.45
1:C:148:ASP:OD1	1:C:148:ASP:N	2.49	0.45
2:D:15:SER:OG	2:D:16:GLU:N	2.49	0.45
2:D:18:LEU:HB2	2:D:82(C):LEU:CD2	2.47	0.45
2:D:146:THR:O	2:D:189:ASN:HB2	2.17	0.45
1:A:48:ILE:HB	1:A:53:SER:H	1.82	0.45
2:B:11:LEU:CD1	2:B:108:MET:O	2.64	0.45
1:C:52:ASN:HA	1:C:64:GLY:HA3	1.98	0.45
1:C:139:ARG:HD3	1:C:139:ARG:O	2.17	0.45
1:A:139:ARG:HB2	1:A:170:TYR:CE1	2.51	0.45
2:B:108:MET:HB2	2:B:109:VAL:H	1.16	0.45
2:B:164:GLN:C	2:B:166:GLY:N	2.75	0.45
1:C:29:ILE:O	1:C:30:ASN:C	2.60	0.45
1:C:148:ASP:OD2	1:C:186:HIS:ND1	2.50	0.45
2:D:48:MET:HB3	2:D:63:LEU:HD23	1.98	0.45
1:A:140:ASP:O	1:A:140:ASP:OD1	2.35	0.45
1:A:209:ASN:OD1	1:A:209:ASN:N	2.48	0.45
2:D:110:THR:HG21	2:D:167:LEU:HD11	1.98	0.45
2:D:138:TYR:CD1	2:D:143:VAL:HG13	2.51	0.45
2:B:136:LYS:CG	2:B:137:GLY:N	2.80	0.45
2:B:157:HIS:O	2:B:159:PHE:CD2	2.70	0.45
2:B:164:GLN:C	2:B:166:GLY:H	2.21	0.45
1:C:147:ILE:O	1:C:150:THR:N	2.50	0.45
1:A:48:ILE:HD12	1:A:64:GLY:HA3	1.95	0.45
2:B:127:SER:O	2:B:177:PRO:HA	2.15	0.45
2:B:139:PHE:CE1	2:B:140:PRO:HA	2.52	0.45
1:C:24:LYS:HA	1:C:69:THR:O	2.16	0.45
1:C:61:ARG:O	1:C:75:ILE:HA	2.17	0.45
1:C:147:ILE:HD12	1:C:152:ARG:H	1.78	0.45
1:A:10:LEU:HD11	1:A:105:GLU:CG	2.47	0.44
1:A:52:ASN:OD1	1:A:52:ASN:C	2.58	0.44
2:B:39:HIS:CE1	2:B:43:LYS:O	2.70	0.44
1:C:90:GLN:HE22	1:C:93:ASN:N	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:PRO:HA	1:C:136:PHE:CB	2.47	0.44
2:D:128:MET:SD	2:D:177:PRO:HA	2.58	0.44
1:A:182:ASP:C	1:A:184:GLU:N	2.75	0.44
1:C:150:THR:CG2	1:C:152:ARG:HD2	2.47	0.44
1:C:159:SER:OG	2:D:159:PHE:HB3	2.16	0.44
2:D:152:LEU:O	2:D:153:SER:HB2	2.16	0.44
1:A:78:LEU:HD23	1:A:78:LEU:HA	1.76	0.44
1:A:81:GLU:N	1:A:165:SER:O	2.50	0.44
1:A:153:ARG:O	1:A:153:ARG:CG	2.62	0.44
1:A:187:ASN:HD22	1:A:207:ASN:CB	2.30	0.44
2:B:116:PRO:HG3	2:B:201:LYS:HD2	1.99	0.44
2:B:179:SER:C	2:B:180:THR:HA	2.37	0.44
1:C:106:LEU:HD12	1:C:106:LEU:N	2.30	0.44
1:C:159:SER:HB2	2:D:160:PRO:CD	2.47	0.44
2:D:53:TYR:H	2:D:53:TYR:HD2	1.57	0.44
2:D:139:PHE:HB2	2:D:167:LEU:HD23	1.99	0.44
1:A:31:ASN:HA	1:A:71:TYR:CE2	2.49	0.44
1:A:177:SER:O	1:A:178:LEU:HD23	2.16	0.44
2:B:13:ARG:C	2:B:16:GLU:HG3	2.42	0.44
2:B:47:TRP:O	2:B:48:MET:HA	2.17	0.44
2:B:161:ALA:CB	2:B:170:LEU:HD23	2.46	0.44
2:B:165:SER:O	2:B:165:SER:OG	2.33	0.44
1:C:120:GLU:C	1:C:122:LEU:N	2.74	0.44
2:B:145:VAL:HG13	2:B:190:VAL:HG22	2.00	0.44
2:B:148:ASN:HD22	2:B:148:ASN:HA	1.43	0.44
1:A:117:PRO:HB3	1:A:121:GLN:HG3	2.00	0.44
2:B:53:TYR:O	2:B:71:ARG:NH2	2.50	0.44
1:C:21:LEU:HD12	1:C:21:LEU:N	2.32	0.44
2:D:82(A):ASN:O	2:D:82(B):SER:HB3	2.17	0.44
2:B:170:LEU:C	2:B:171:THR:CG2	2.84	0.44
1:C:118:SER:N	1:C:121:GLN:HB3	2.30	0.44
1:A:156:VAL:HG12	1:A:176:LEU:N	2.24	0.44
1:A:205:SER:O	1:A:206:PHE:CB	2.65	0.44
2:B:38:ARG:CB	2:B:48:MET:CE	2.71	0.44
2:B:38:ARG:HH11	2:B:48:MET:HE2	1.83	0.44
2:B:128:MET:CE	2:B:175:THR:HG21	2.45	0.44
1:C:159:SER:O	1:C:172:MET:CG	2.65	0.44
2:D:88:GLY:O	2:D:102:PHE:HB2	2.17	0.44
2:D:163:LEU:HD13	2:D:168:TYR:CD2	2.53	0.44
1:A:35:TRP:CD2	1:A:73:LEU:HB2	2.53	0.44
1:A:91:TYR:CD1	2:B:98:GLY:HA3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:VAL:CG1	1:A:113:SER:H	2.27	0.44
1:A:120:GLU:N	1:A:120:GLU:OE2	2.51	0.44
1:A:147:ILE:HD13	1:A:152:ARG:HG2	2.00	0.44
2:D:18:LEU:HB2	2:D:82(C):LEU:HD23	2.00	0.44
1:A:120:GLU:O	1:A:122:LEU:N	2.52	0.43
1:A:208:ARG:HB3	1:A:209:ASN:H	1.49	0.43
2:B:23:THR:HG23	2:B:77:GLN:NE2	2.32	0.43
1:C:11:LEU:C	1:C:11:LEU:CD1	2.88	0.43
1:C:39:LYS:O	1:C:40:LEU:O	2.36	0.43
1:C:52:ASN:OD1	1:C:52:ASN:C	2.61	0.43
1:C:181:ALA:O	1:C:184:GLU:HB3	2.17	0.43
2:D:34:VAL:HA	2:D:93:THR:O	2.17	0.43
2:D:147:TRP:HA	2:D:188:CYS:HA	2.00	0.43
1:A:71:TYR:C	1:A:72:THR:CG2	2.91	0.43
1:A:120:GLU:O	1:A:121:GLN:C	2.61	0.43
2:B:67:LEU:HD12	2:B:80:LEU:HD22	1.97	0.43
1:C:187:ASN:HD22	1:C:207:ASN:HB3	1.83	0.43
2:D:2:VAL:HB	2:D:100(B):LEU:HG	1.99	0.43
2:D:187:THR:HA	2:D:203:ILE:CD1	2.48	0.43
1:C:189:TYR:HB2	1:C:206:PHE:CE2	2.54	0.43
1:C:211:CYS:HA	2:D:120:GLY:HA2	1.98	0.43
2:D:103:TRP:CB	2:D:140:PRO:HB2	2.43	0.43
1:A:120:GLU:C	1:A:122:LEU:N	2.73	0.43
2:B:159:PHE:C	2:B:160:PRO:O	2.56	0.43
1:C:117:PRO:CG	1:C:127:ALA:HB1	2.48	0.43
2:B:3:GLN:HB2	2:B:25:SER:HB2	2.01	0.43
2:B:100(C):GLY:O	2:B:100(D):PHE:CG	2.71	0.43
2:B:103:TRP:C	2:B:105:PRO:HD2	2.43	0.43
1:C:102:THR:HG22	1:C:103:LYS:O	2.19	0.43
2:D:18:LEU:HD23	2:D:18:LEU:HA	1.70	0.43
2:D:141:GLU:HG2	2:D:168:TYR:CD1	2.54	0.43
1:A:68:GLY:O	1:A:69:THR:CB	2.66	0.43
1:C:187:ASN:N	1:C:188:LEU:CD1	2.81	0.43
1:A:160:VAL:C	1:A:171:SER:O	2.62	0.43
1:A:211:CYS:HA	2:B:121:SER:N	2.27	0.43
2:B:52:TRP:CE2	2:B:56:TYR:HD2	2.37	0.43
2:B:96:LEU:C	2:B:98:GLY:N	2.75	0.43
2:B:158:THR:CB	2:B:172:SER:HB2	2.49	0.43
2:B:164:GLN:CG	2:B:165:SER:H	2.31	0.43
2:D:49:GLY:HA2	2:D:58:ALA:O	2.19	0.43
1:A:36:TYR:HH	2:B:100:TYR:H	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:PHE:O	2:B:140:PRO:CD	2.63	0.43
1:C:89:TYR:HE2	2:D:99:GLY:HA2	1.84	0.43
1:C:145:TRP:CZ3	1:C:176:LEU:HD22	2.53	0.43
2:D:134:LEU:C	2:D:134:LEU:HD12	2.43	0.43
1:A:138:PRO:O	1:A:139:ARG:C	2.62	0.43
1:A:145:TRP:CH2	1:A:176:LEU:HD22	2.54	0.43
1:A:189:TYR:C	1:A:190:THR:CA	2.81	0.43
1:A:192:GLU:HA	1:A:203:VAL:CB	2.38	0.43
2:B:114:VAL:CG2	2:B:135:VAL:HG22	2.49	0.43
2:B:139:PHE:HB3	2:B:167:LEU:CD2	2.49	0.43
2:B:145:VAL:CG1	2:B:190:VAL:CG2	2.97	0.43
2:B:195:SER:C	2:B:197:THR:H	2.25	0.43
1:C:122:LEU:C	1:C:122:LEU:CD1	2.92	0.43
2:D:40:PRO:O	2:D:41:SER:C	2.61	0.43
2:D:103:TRP:HZ2	2:D:168:TYR:OH	1.96	0.43
1:A:68:GLY:HA2	1:A:71:TYR:OH	2.18	0.43
2:B:109:VAL:HG23	2:B:110:THR:N	2.34	0.43
1:C:29:ILE:H	1:C:69:THR:H	1.67	0.43
1:C:33:LEU:HG	1:C:34:ALA:N	2.34	0.43
1:C:209:ASN:OD1	1:C:209:ASN:N	2.52	0.43
2:D:13:ARG:C	2:D:16:GLU:HG3	2.43	0.43
1:A:4:LEU:HD21	1:A:90:GLN:HB3	2.00	0.42
1:A:211:CYS:SG	2:B:208:CYS:N	2.92	0.42
1:C:78:LEU:HD23	1:C:78:LEU:HA	1.69	0.42
1:C:144:LYS:O	1:C:191:CYS:HA	2.19	0.42
2:D:69:ILE:CG2	2:D:70:SER:N	2.82	0.42
2:B:14:PRO:C	2:B:16:GLU:N	2.76	0.42
2:B:51:MET:CE	2:B:55:GLY:HA2	2.49	0.42
2:B:138:TYR:OH	2:B:170:LEU:HD21	2.19	0.42
1:C:25:GLY:CA	1:C:29:ILE:HD11	2.44	0.42
1:C:118:SER:CB	1:C:120:GLU:HG2	2.37	0.42
1:C:148:ASP:OD2	1:C:188:LEU:CD1	2.67	0.42
2:D:18:LEU:HG	2:D:102:PHE:CE1	2.54	0.42
2:B:120:GLY:O	2:B:121:SER:HB2	2.19	0.42
2:B:164:GLN:HE21	2:B:165:SER:N	2.18	0.42
1:C:48:ILE:HD13	1:C:48:ILE:O	2.17	0.42
1:A:28:ASN:ND2	1:A:68:GLY:CA	2.69	0.42
2:B:158:THR:HB	2:B:172:SER:HB2	2.01	0.42
2:D:16:GLU:HG2	2:D:16:GLU:H	1.60	0.42
1:A:58:ILE:O	1:A:59:PRO:C	2.61	0.42
1:A:139:ARG:NH2	1:A:160:VAL:HG21	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:13:ARG:O	2:D:16:GLU:CG	2.67	0.42
2:D:163:LEU:HD22	2:D:168:TYR:CZ	2.53	0.42
1:A:47:LEU:O	1:A:58:ILE:HG13	2.19	0.42
1:C:80:PRO:HA	1:C:106:LEU:CD2	2.50	0.42
1:C:211:CYS:HA	2:D:120:GLY:O	2.16	0.42
2:D:32:PHE:CE2	2:D:94:ARG:NH1	2.87	0.42
2:D:91:TYR:CE2	2:D:100(F):TYR:HA	2.55	0.42
1:A:7:SER:HG	1:A:8:PRO:HD2	1.81	0.42
1:A:40:LEU:C	1:A:40:LEU:HD13	2.16	0.42
1:A:196:LYS:N	1:A:197:THR:N	2.62	0.42
2:B:38:ARG:CG	2:B:40:PRO:HD3	2.48	0.42
2:B:130:THR:HG23	2:B:130:THR:O	2.19	0.42
2:B:141:GLU:O	2:B:142:PRO:C	2.62	0.42
2:B:152:LEU:O	2:B:153:SER:CB	2.29	0.42
1:C:49:TYR:HD1	1:C:50:ASN:HB2	1.85	0.42
2:D:13:ARG:NH2	2:D:108:MET:SD	2.85	0.42
2:D:190:VAL:CG1	2:D:191:ALA:N	2.81	0.42
1:A:94:GLY:CA	1:A:96:TYR:HD1	2.32	0.42
2:D:14:PRO:O	2:D:16:GLU:CG	2.64	0.42
2:D:129:VAL:O	2:D:129:VAL:HG13	2.18	0.42
1:A:29:ILE:CG1	1:A:71:TYR:CZ	3.02	0.42
2:B:69:ILE:CG2	2:B:70:SER:N	2.82	0.42
2:B:89:THR:HB	2:B:100(G):PHE:O	2.20	0.42
2:B:111:VAL:O	2:B:137:GLY:O	2.38	0.42
1:C:110:PRO:HB2	1:C:111:THR:H	1.52	0.42
1:C:158:ASP:HB2	1:C:173:SER:O	2.20	0.42
2:D:39:HIS:O	2:D:40:PRO:C	2.62	0.42
2:D:100(G):PHE:CZ	2:D:101:ASP:O	2.72	0.42
2:D:120:GLY:O	2:D:121:SER:CB	2.68	0.42
2:D:143:VAL:HG21	2:D:170:LEU:HD21	2.02	0.42
1:A:38:GLN:O	1:A:39:LYS:CB	2.66	0.42
1:A:112:VAL:CG1	1:A:113:SER:N	2.76	0.42
1:A:117:PRO:HB3	1:A:121:GLN:CG	2.50	0.42
1:A:123:ALA:O	1:A:124:THR:CG2	2.68	0.42
1:C:54:LEU:HD13	1:C:55:GLN:O	2.19	0.42
1:C:208:ARG:HB3	1:C:209:ASN:H	1.63	0.42
1:C:211:CYS:HB2	2:D:206:ARG:HD3	2.02	0.42
1:A:90:GLN:CD	1:A:90:GLN:O	2.63	0.41
1:C:60:SER:C	1:C:62:PHE:H	2.27	0.41
2:D:179:SER:OG	2:D:180:THR:N	2.52	0.41
1:A:81:GLU:CB	1:A:165:SER:O	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:MET:CE	2:B:90:TYR:HD2	2.22	0.41
2:B:104:GLY:H	2:B:105:PRO:HD3	1.83	0.41
1:C:158:ASP:CB	1:C:173:SER:O	2.69	0.41
2:D:67:LEU:HD12	2:D:80:LEU:HD12	2.02	0.41
2:D:72:ASP:O	2:D:73:THR:C	2.61	0.41
1:A:90:GLN:NE2	1:A:93:ASN:N	2.65	0.41
2:B:35:SER:HB3	2:B:49:GLY:O	2.20	0.41
1:C:107:ARG:HD3	1:C:168:SER:C	2.45	0.41
1:C:147:ILE:CD1	1:C:152:ARG:N	2.74	0.41
1:A:64:GLY:O	1:A:65:SER:HB2	2.19	0.41
1:A:189:TYR:O	1:A:206:PHE:HB3	2.20	0.41
2:B:51:MET:HB2	2:B:69:ILE:HG21	2.02	0.41
1:C:10:LEU:HD11	1:C:105:GLU:CG	2.49	0.41
1:C:118:SER:H	1:C:121:GLN:CB	2.30	0.41
1:A:81:GLU:CD	1:A:81:GLU:H	2.28	0.41
1:C:91:TYR:CD2	1:C:91:TYR:N	2.88	0.41
1:C:106:LEU:N	1:C:163:GLN:OE1	2.52	0.41
2:D:146:THR:O	2:D:146:THR:OG1	2.33	0.41
1:A:12:SER:CA	1:A:105:GLU:O	2.68	0.41
1:A:36:TYR:CE2	1:A:46:LEU:HB2	2.55	0.41
1:A:132:LEU:CD2	1:A:173:SER:CB	2.81	0.41
2:B:195:SER:O	2:B:196:SER:C	2.63	0.41
1:C:96:TYR:CD1	1:C:96:TYR:N	2.89	0.41
1:C:133:MET:HE1	1:C:143:VAL:HG13	2.01	0.41
2:D:103:TRP:HB2	2:D:140:PRO:CB	2.46	0.41
2:D:147:TRP:O	2:D:148:ASN:C	2.64	0.41
2:D:153:SER:H	2:D:156:VAL:HG21	1.85	0.41
1:A:120:GLU:CD	1:A:120:GLU:N	2.73	0.41
1:A:138:PRO:CG	1:A:196:LYS:HE3	2.51	0.41
1:A:173:SER:N	2:B:159:PHE:CD1	2.88	0.41
2:B:11:LEU:HG	2:B:140:PRO:CB	2.50	0.41
2:B:158:THR:HG22	2:B:172:SER:HB2	2.01	0.41
1:C:32:TYR:HB2	1:C:92:ASN:HB2	2.03	0.41
2:D:100(C):GLY:O	2:D:100(D):PHE:CG	2.74	0.41
1:A:78:LEU:HD22	1:A:79:GLN:O	2.21	0.41
1:A:207:ASN:O	1:A:208:ARG:C	2.63	0.41
2:B:181:TRP:O	2:B:184:GLN:O	2.39	0.41
1:C:99:GLY:C	1:C:101:GLY:N	2.75	0.41
1:C:129:VAL:CG1	1:C:206:PHE:HE1	2.33	0.41
1:A:65:SER:O	1:A:72:THR:HG23	2.21	0.41
1:A:94:GLY:HA2	1:A:96:TYR:HD1	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ARG:CZ	1:A:160:VAL:HG21	2.51	0.41
2:B:13:ARG:HH11	2:B:13:ARG:HG2	1.86	0.41
2:B:139:PHE:CD1	2:B:140:PRO:HA	2.56	0.41
2:B:147:TRP:HD1	2:B:156:VAL:CG1	2.31	0.41
1:C:148:ASP:CG	1:C:188:LEU:HD13	2.46	0.41
1:C:179:THR:HB	1:C:181:ALA:H	1.86	0.41
1:C:181:ALA:O	1:C:184:GLU:N	2.53	0.41
2:D:18:LEU:HD22	2:D:18:LEU:C	2.37	0.41
2:D:100(B):LEU:HD12	2:D:100(C):GLY:H	1.85	0.41
2:D:131:LEU:HD23	2:D:186:VAL:HG11	2.02	0.41
2:D:176:VAL:HB	2:D:177:PRO:HD2	2.03	0.41
1:A:48:ILE:HD13	1:A:64:GLY:HA3	2.00	0.41
1:A:83:VAL:HG11	1:A:163:GLN:OE1	2.21	0.41
1:A:121:GLN:HA	2:B:115:PHE:CD2	2.54	0.41
2:B:127:SER:C	2:B:128:MET:HB2	2.45	0.41
1:C:144:LYS:HB3	1:C:192:GLU:HB2	2.02	0.41
2:B:2:VAL:HG13	2:B:27:PHE:CE1	2.56	0.40
2:B:117:LEU:HB2	2:B:132:GLY:O	2.22	0.40
2:B:139:PHE:HA	2:B:140:PRO:N	2.36	0.40
1:C:156:VAL:O	1:C:157:LEU:HD23	2.16	0.40
1:C:189:TYR:HB2	1:C:206:PHE:CD2	2.56	0.40
2:B:131:LEU:HD21	2:B:181:TRP:CE3	2.56	0.40
1:C:10:LEU:HD13	1:C:103:LYS:HB3	2.02	0.40
1:C:140:ASP:O	1:C:195:HIS:HD2	2.04	0.40
1:C:187:ASN:H	1:C:188:LEU:HD11	1.85	0.40
2:D:190:VAL:HG12	2:D:191:ALA:N	2.35	0.40
1:A:46:LEU:O	1:A:58:ILE:HD11	2.20	0.40
1:A:61:ARG:NH2	1:A:82:ASP:OD1	2.54	0.40
1:A:118:SER:O	1:A:120:GLU:N	2.54	0.40
1:A:127:ALA:HB1	1:A:183:TYR:HD1	1.85	0.40
2:B:33:SER:OG	2:B:52:TRP:HA	2.21	0.40
2:B:129:VAL:O	2:B:129:VAL:HG23	2.21	0.40
2:B:148:ASN:O	2:B:150:GLY:N	2.54	0.40
2:B:204:VAL:HB	2:B:205:PRO:HD2	2.02	0.40
2:D:13:ARG:CA	2:D:16:GLU:HG3	2.52	0.40
2:D:129:VAL:HG12	2:D:176:VAL:HG22	2.01	0.40
1:A:159:SER:O	1:A:172:MET:CG	2.68	0.40
2:B:3:GLN:CG	3:B:219:HOH:O	2.49	0.40
2:B:164:GLN:HG3	2:B:165:SER:H	1.86	0.40
2:D:20:LEU:CD2	2:D:102:PHE:HE2	2.17	0.40
2:B:80:LEU:HD23	2:B:80:LEU:HA	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:VAL:HG11	2:B:201:LYS:HB2	2.04	0.40
1:C:120:GLU:N	1:C:120:GLU:OE2	2.54	0.40
1:C:137:TYR:HA	1:C:138:PRO:C	2.46	0.40
1:C:148:ASP:C	1:C:150:THR:N	2.80	0.40
1:C:150:THR:HG22	1:C:151:GLU:N	2.36	0.40
2:D:136:LYS:HG2	2:D:137:GLY:N	2.32	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:28:SER:N	3:B:234:HOH:O[5_555]	2.12	0.08
2:B:28:SER:OG	2:D:54:ASP:OD2[3_655]	2.14	0.06
2:D:27:PHE:N	3:B:232:HOH:O[5_555]	2.18	0.02
2:D:26:GLY:C	3:B:232:HOH:O[5_555]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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	192/211 (91%)	120 (62%)	35 (18%)	37 (19%)	0	0
1	C	209/211 (99%)	151 (72%)	31 (15%)	27 (13%)	0	0
2	B	204/218 (94%)	137 (67%)	35 (17%)	32 (16%)	0	0
2	D	216/218 (99%)	164 (76%)	25 (12%)	27 (12%)	0	0
All	All	821/858 (96%)	572 (70%)	126 (15%)	123 (15%)	0	0

All (123) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	SER

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Mol	Chain	Res	Type
1	A	31	ASN
1	A	40	LEU
1	A	50	ASN
1	A	77	SER
1	A	96	TYR
1	A	107	ARG
1	A	108	THR
1	A	109	ALA
1	A	111	THR
1	A	133	MET
1	A	139	ARG
1	A	142	SER
1	A	168	SER
1	A	181	ALA
1	A	208	ARG
2	B	4	LEU
2	B	52	TRP
2	B	61	SER
2	B	65	SER
2	B	74	SER
2	B	97	TYR
2	B	100(A)	PRO
2	B	100(D)	PHE
2	B	100(F)	TYR
2	B	102	PHE
2	B	110	THR
2	B	122	ALA
2	B	127	SER
2	B	171	THR
2	B	183	SER
2	B	196	SER
1	C	30	ASN
1	C	40	LEU
1	C	77	SER
1	C	107	ARG
1	C	108	THR
1	C	109	ALA
1	C	110	PRO
1	C	111	THR
1	C	123	ALA
1	C	148	ASP
1	C	150	THR

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Mol	Chain	Res	Type
1	C	151	GLU
1	C	168	SER
1	C	181	ALA
2	D	16	GLU
2	D	52	TRP
2	D	61	SER
2	D	65	SER
2	D	73	THR
2	D	74	SER
2	D	97	TYR
2	D	100(D)	PHE
2	D	122	ALA
2	D	196	SER
1	A	68	GLY
1	A	69	THR
1	A	110	PRO
1	A	123	ALA
1	A	137	TYR
1	A	194	VAL
1	A	196	LYS
1	A	209	ASN
2	B	16	GLU
2	B	82(B)	SER
2	B	121	SER
2	B	184	GLN
2	B	203	ILE
1	C	39	LYS
1	C	68	GLY
1	C	121	GLN
1	C	185	SER
1	C	194	VAL
1	C	196	LYS
1	C	197	THR
1	C	209	ASN
2	D	82(B)	SER
2	D	100(A)	PRO
2	D	100(F)	TYR
2	D	110	THR
2	D	121	SER
2	D	149	SER
2	D	183	SER
2	D	184	GLN

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Mol	Chain	Res	Type
2	D	195	SER
1	A	39	LYS
1	A	54	LEU
1	A	57	GLY
1	A	63	SER
1	A	65	SER
2	B	73	THR
2	B	82(C)	LEU
2	B	133	CYS
2	B	152	LEU
1	C	56	THR
1	C	208	ARG
2	D	14	PRO
2	D	15	SER
2	D	109	VAL
2	D	153	SER
2	B	148	ASN
1	C	57	GLY
1	C	96	TYR
2	D	127	SER
1	A	121	GLN
1	A	130	VAL
1	A	141	ILE
2	B	81	LYS
2	B	109	VAL
2	B	195	SER
1	C	69	THR
2	D	193	PRO
1	A	120	GLU
2	B	100(B)	LEU
1	A	138	PRO
2	B	176	VAL
1	A	147	ILE
2	B	160	PRO
1	A	193	VAL
1	A	203	VAL
2	D	137	GLY
2	D	142	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	188/188 (100%)	126 (67%)	62 (33%)	0	1
1	C	188/188 (100%)	109 (58%)	79 (42%)	0	0
2	B	189/189 (100%)	124 (66%)	65 (34%)	0	0
2	D	189/189 (100%)	118 (62%)	71 (38%)	0	0
All	All	754/754 (100%)	477 (63%)	277 (37%)	0	0

All (277) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	3	LYS
1	A	10	LEU
1	A	11	LEU
1	A	12	SER
1	A	14	SER
1	A	15	VAL
1	A	17	ASP
1	A	18	ARG
1	A	20	THR
1	A	24	LYS
1	A	37	GLN
1	A	40	LEU
1	A	42	GLU
1	A	45	LYS
1	A	51	THR
1	A	53	SER
1	A	54	LEU
1	A	55	GLN
1	A	56	THR
1	A	61	ARG
1	A	63	SER
1	A	65	SER
1	A	69	THR

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Mol	Chain	Res	Type
1	A	72	THR
1	A	78	LEU
1	A	93	ASN
1	A	103	LYS
1	A	104	LEU
1	A	105	GLU
1	A	108	THR
1	A	114	ILE
1	A	118	SER
1	A	120	GLU
1	A	121	GLN
1	A	128	SER
1	A	139	ARG
1	A	140	ASP
1	A	141	ILE
1	A	147	ILE
1	A	151	GLU
1	A	152	ARG
1	A	157	LEU
1	A	158	ASP
1	A	161	THR
1	A	164	ASP
1	A	165	SER
1	A	173	SER
1	A	174	SER
1	A	176	LEU
1	A	177	SER
1	A	182	ASP
1	A	185	SER
1	A	187	ASN
1	A	188	LEU
1	A	192	GLU
1	A	194	VAL
1	A	196	LYS
1	A	202	VAL
1	A	203	VAL
1	A	205	SER
1	A	210	GLU
2	B	1	GLN
2	B	4	LEU
2	B	6	GLU
2	B	7	SER

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Mol	Chain	Res	Type
2	B	17	THR
2	B	18	LEU
2	B	19	SER
2	B	21	THR
2	B	23	THR
2	B	28	SER
2	B	29	LEU
2	B	33	SER
2	B	35	SER
2	B	38	ARG
2	B	39	HIS
2	B	41	SER
2	B	43	LYS
2	B	61	SER
2	B	66	ARG
2	B	67	LEU
2	B	68	SER
2	B	69	ILE
2	B	71	ARG
2	B	75	LYS
2	B	77	GLN
2	B	80	LEU
2	B	84	THR
2	B	89	THR
2	B	100	TYR
2	B	100(A)	PRO
2	B	100(B)	LEU
2	B	100(D)	PHE
2	B	100(E)	TRP
2	B	100(F)	TYR
2	B	100(G)	PHE
2	B	103	TRP
2	B	107	THR
2	B	111	VAL
2	B	112	SER
2	B	113	SER
2	B	114	VAL
2	B	124	GLN
2	B	125	THR
2	B	127	SER
2	B	131	LEU
2	B	141	GLU

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Mol	Chain	Res	Type
2	B	148	ASN
2	B	152	LEU
2	B	157	HIS
2	B	158	THR
2	B	159	PHE
2	B	162	VAL
2	B	164	GLN
2	B	167	LEU
2	B	170	LEU
2	B	172	SER
2	B	183	SER
2	B	184	GLN
2	B	186	VAL
2	B	187	THR
2	B	189	ASN
2	B	195	SER
2	B	198	LYS
2	B	204	VAL
2	B	207	ASP
1	C	2	ILE
1	C	3	LYS
1	C	10	LEU
1	C	11	LEU
1	C	12	SER
1	C	14	SER
1	C	15	VAL
1	C	17	ASP
1	C	18	ARG
1	C	20	THR
1	C	24	LYS
1	C	28	ASN
1	C	37	GLN
1	C	38	GLN
1	C	39	LYS
1	C	40	LEU
1	C	42	GLU
1	C	45	LYS
1	C	48	ILE
1	C	51	THR
1	C	53	SER
1	C	54	LEU
1	C	55	GLN

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Mol	Chain	Res	Type
1	C	56	THR
1	C	61	ARG
1	C	63	SER
1	C	65	SER
1	C	69	THR
1	C	72	THR
1	C	74	THR
1	C	78	LEU
1	C	83	VAL
1	C	93	ASN
1	C	96	TYR
1	C	97	THR
1	C	104	LEU
1	C	105	GLU
1	C	107	ARG
1	C	108	THR
1	C	114	ILE
1	C	118	SER
1	C	119	THR
1	C	120	GLU
1	C	121	GLN
1	C	122	LEU
1	C	130	VAL
1	C	133	MET
1	C	139	ARG
1	C	141	ILE
1	C	142	SER
1	C	143	VAL
1	C	144	LYS
1	C	146	LYS
1	C	147	ILE
1	C	148	ASP
1	C	151	GLU
1	C	152	ARG
1	C	154	ASP
1	C	157	LEU
1	C	160	VAL
1	C	166	LYS
1	C	172	MET
1	C	173	SER
1	C	174	SER
1	C	175	THR

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Mol	Chain	Res	Type
1	C	176	LEU
1	C	178	LEU
1	C	180	LYS
1	C	187	ASN
1	C	188	LEU
1	C	191	CYS
1	C	192	GLU
1	C	194	VAL
1	C	196	LYS
1	C	202	VAL
1	C	203	VAL
1	C	205	SER
1	C	206	PHE
1	C	210	GLU
2	D	1	GLN
2	D	3	GLN
2	D	4	LEU
2	D	6	GLU
2	D	7	SER
2	D	17	THR
2	D	18	LEU
2	D	19	SER
2	D	21	THR
2	D	23	THR
2	D	25	SER
2	D	29	LEU
2	D	35	SER
2	D	38	ARG
2	D	39	HIS
2	D	41	SER
2	D	43	LYS
2	D	50	ARG
2	D	57	THR
2	D	61	SER
2	D	65	SER
2	D	67	LEU
2	D	68	SER
2	D	71	ARG
2	D	75	LYS
2	D	77	GLN
2	D	80	LEU
2	D	84	THR

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Mol	Chain	Res	Type
2	D	89	THR
2	D	100	TYR
2	D	100(A)	PRO
2	D	100(B)	LEU
2	D	100(D)	PHE
2	D	100(E)	TRP
2	D	100(F)	TYR
2	D	100(G)	PHE
2	D	101	ASP
2	D	102	PHE
2	D	105	PRO
2	D	107	THR
2	D	112	SER
2	D	113	SER
2	D	114	VAL
2	D	125	THR
2	D	127	SER
2	D	128	MET
2	D	131	LEU
2	D	136	LYS
2	D	149	SER
2	D	152	LEU
2	D	153	SER
2	D	154	SER
2	D	159	PHE
2	D	162	VAL
2	D	163	LEU
2	D	164	GLN
2	D	170	LEU
2	D	171	THR
2	D	172	SER
2	D	176	VAL
2	D	181	TRP
2	D	183	SER
2	D	186	VAL
2	D	187	THR
2	D	189	ASN
2	D	195	SER
2	D	196	SER
2	D	198	LYS
2	D	203	ILE
2	D	204	VAL

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Mol	Chain	Res	Type
2	D	207	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	31	ASN
1	A	37	GLN
1	A	50	ASN
1	A	55	GLN
1	A	90	GLN
1	A	135	ASN
1	A	187	ASN
2	B	39	HIS
2	B	60	ASN
2	B	77	GLN
2	B	82(A)	ASN
2	B	148	ASN
2	B	157	HIS
2	B	164	GLN
1	C	28	ASN
1	C	30	ASN
1	C	31	ASN
1	C	37	GLN
1	C	50	ASN
1	C	55	GLN
1	C	90	GLN
1	C	93	ASN
1	C	135	ASN
1	C	187	ASN
2	D	39	HIS
2	D	60	ASN
2	D	77	GLN
2	D	164	GLN
2	D	189	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	23
2	B	16

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	148:ASP	C	149:GLY	N	3.30
1	A	153:ARG	C	154:ASP	N	3.05
1	B	180:THR	C	181:TRP	N	3.02
1	B	84:THR	C	85:ASP	N	2.66
1	A	150:THR	C	151:GLU	N	2.65
1	B	107:THR	C	108:MET	N	2.48
1	A	37:GLN	C	38:GLN	N	2.44
1	B	139:PHE	C	140:PRO	N	2.34
1	A	206:PHE	C	207:ASN	N	2.33
1	A	29:ILE	C	30:ASN	N	2.27
1	A	200:SER	C	201:PRO	N	2.15
1	A	149:GLY	C	150:THR	N	2.14
1	A	154:ASP	C	155:GLY	N	2.10
1	B	141:GLU	C	142:PRO	N	2.10
1	A	78:LEU	C	79:GLN	N	2.08

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	153:SER	C	154:SER	N	2.05
1	B	179:SER	C	180:THR	N	1.99
1	A	196:LYS	C	197:THR	N	1.97
1	A	183:TYR	C	184:GLU	N	1.96
1	B	181:TRP	C	182:SER	N	1.95
1	A	184:GLU	C	185:SER	N	1.85
1	B	85:ASP	C	86:ASP	N	1.84
1	A	123:ALA	C	124:THR	N	1.83
1	A	197:THR	C	198:SER	N	1.83
1	A	30:ASN	C	31:ASN	N	1.82
1	A	189:TYR	C	190:THR	N	1.82
1	B	47:TRP	C	48:MET	N	1.81
1	B	101:ASP	C	102:PHE	N	1.78
1	A	132:LEU	C	133:MET	N	1.77
1	A	205:SER	C	206:PHE	N	1.77
1	B	25:SER	C	26:GLY	N	1.74
1	B	152:LEU	C	153:SER	N	1.74
1	A	110:PRO	C	111:THR	N	1.72
1	B	127:SER	C	128:MET	N	1.70
1	A	31:ASN	C	32:TYR	N	1.69
1	A	124:THR	C	125:GLY	N	1.66
1	B	146:THR	C	147:TRP	N	1.12
1	B	138:TYR	C	139:PHE	N	1.08
1	A	125:GLY	C	126:GLY	N	1.07

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.