Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:04 pm BST

PDB ID	:	1FN4
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.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

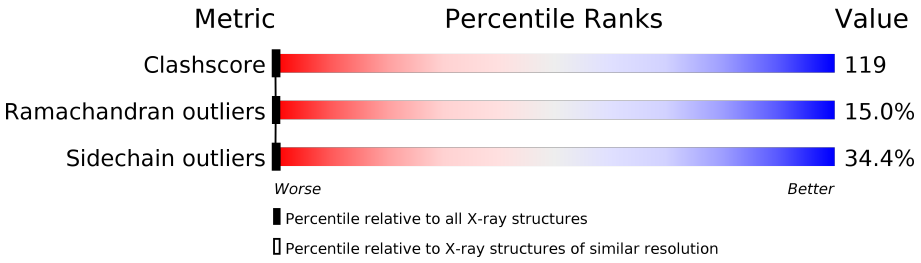
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	211	12% 39% 34% 16%
1	C	211	12% 49% 31% 8%
2	B	218	12% 45% 33% 9%
2	D	218	18% 47% 28% 6%

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		

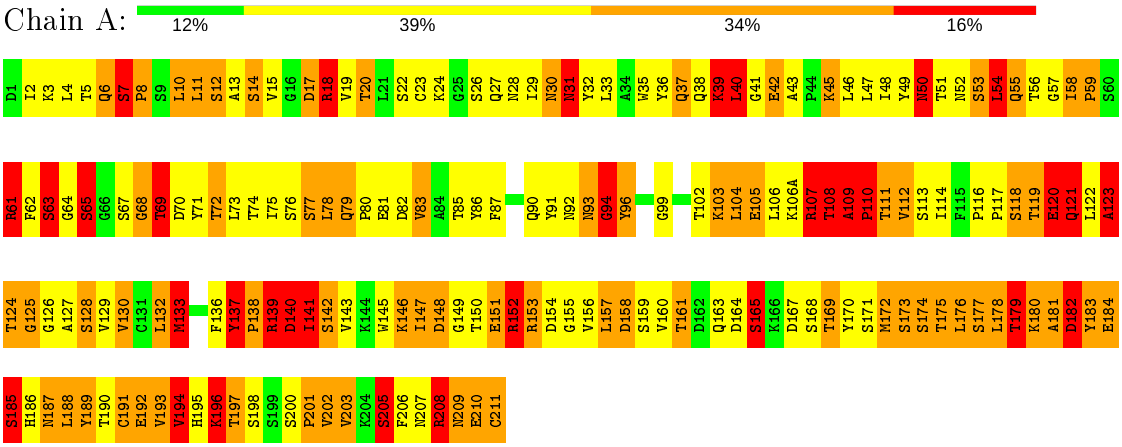
3 Residue-property plots (i)

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

Note EDS was not executed.

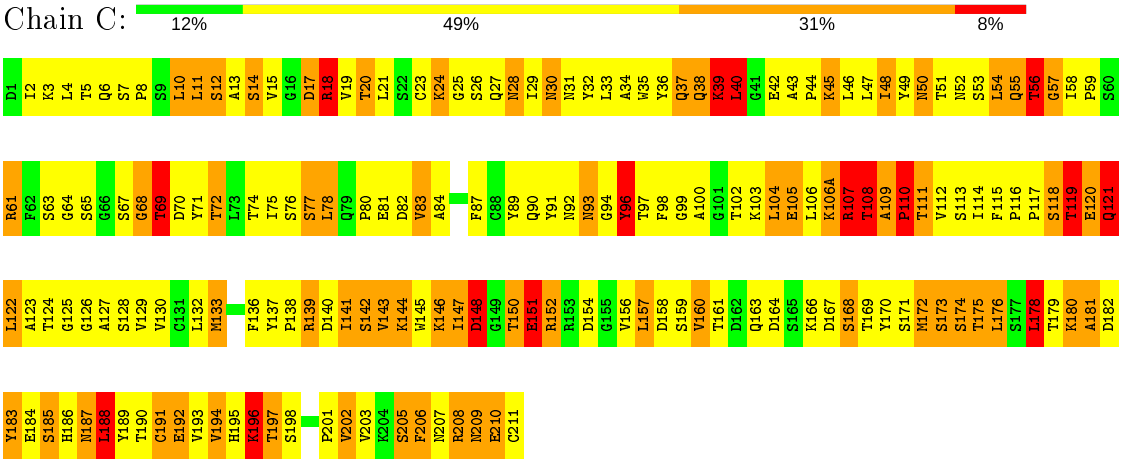
- Molecule 1: MONOCLONAL ANTIBODY AGAINST ACETYLCHOLINE RECEPTOR

Chain A:



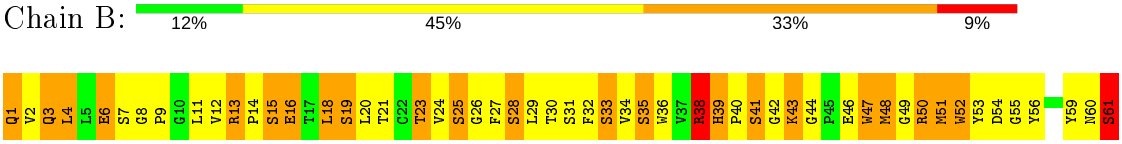
- Molecule 1: MONOCLONAL ANTIBODY AGAINST ACETYLCHOLINE RECEPTOR

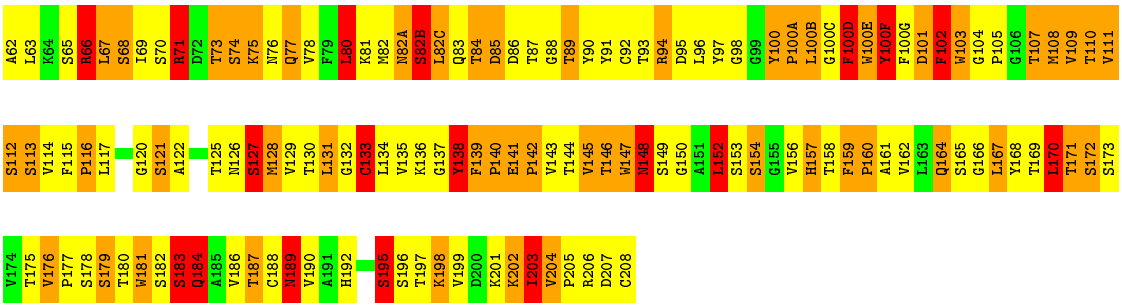
Chain C:



- Molecule 2: MONOCLONAL ANTIBODY AGAINST ACETYLCHOLINE RECEPTOR

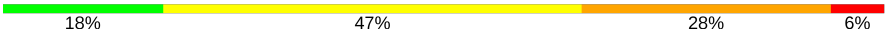
Chain B:

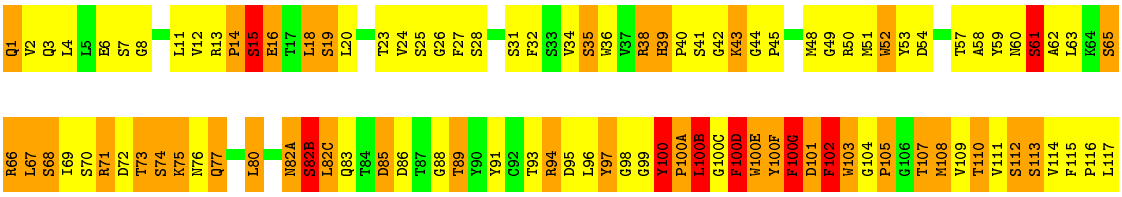




• Molecule 2: MONOCLONAL ANTIBODY AGAINST ACETYLCHOLINE RECEPTOR

Chain D:





4 Data and refinement statistics (i)

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	2.19	26/1648 (1.6%)	2.09	75/2222 (3.4%)
1	C	1.09	2/1658 (0.1%)	1.19	9/2253 (0.4%)
2	B	1.90	12/1706 (0.7%)	2.18	65/2321 (2.8%)
2	D	1.12	5/1712 (0.3%)	1.15	4/2341 (0.2%)
All	All	1.65	45/6724 (0.7%)	1.72	153/9137 (1.7%)

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 (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	179	SER	C-N	28.62	1.99	1.34
1	A	196	LYS	C-N	27.59	1.97	1.34
1	A	183	TYR	C-N	27.07	1.96	1.34
2	B	181	TRP	C-N	26.77	1.95	1.34
2	B	25	SER	C-N	22.79	1.74	1.33
1	A	184	GLU	C-N	22.20	1.85	1.34
2	B	85	ASP	C-N	22.02	1.84	1.34
1	A	197	THR	C-N	21.47	1.83	1.34
1	A	123	ALA	C-N	21.33	1.83	1.34
1	A	30	ASN	C-N	21.18	1.82	1.34
1	A	189	TYR	C-N	20.89	1.82	1.34
2	B	47	TRP	C-N	20.52	1.81	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	101	ASP	C-N	19.52	1.78	1.34
1	A	205	SER	C-N	19.07	1.77	1.34
1	A	132	LEU	C-N	18.76	1.77	1.34
1	A	124	THR	C-N	18.46	1.66	1.33
2	B	152	LEU	C-N	17.48	1.74	1.34
1	A	110	PRO	C-N	16.72	1.72	1.34
2	B	127	SER	C-N	15.80	1.70	1.34
1	A	31	ASN	C-N	15.27	1.69	1.34
1	A	125	GLY	C-N	-14.38	1.07	1.33
2	B	138	TYR	C-N	-11.06	1.08	1.34
2	B	102	PHE	C-N	10.94	1.59	1.34
1	A	108	THR	N-CA	9.88	1.66	1.46
2	B	139	PHE	C-O	9.84	1.42	1.23
2	B	146	THR	C-N	-9.57	1.12	1.34
1	A	152	ARG	C-N	8.72	1.54	1.34
1	A	185	SER	N-CA	8.04	1.62	1.46
1	A	109	ALA	N-CA	7.35	1.61	1.46
1	A	110	PRO	N-CA	7.11	1.59	1.47
1	A	107	ARG	CA-C	6.83	1.70	1.52
1	A	107	ARG	N-CA	6.52	1.59	1.46
1	A	107	ARG	C-N	6.48	1.49	1.34
2	D	108	MET	CG-SD	6.47	1.98	1.81
1	A	109	ALA	C-N	6.26	1.46	1.34
2	D	100(D)	PHE	CB-CG	5.56	1.60	1.51
1	A	108	THR	C-N	5.52	1.46	1.34
1	C	108	THR	CA-CB	5.51	1.67	1.53
2	D	100(G)	PHE	CB-CG	-5.43	1.42	1.51
1	C	119	THR	CA-CB	5.32	1.67	1.53
2	D	100	TYR	CD1-CE1	-5.30	1.31	1.39
1	A	169	THR	C-N	5.19	1.46	1.34
1	A	109	ALA	CA-C	5.14	1.66	1.52
2	D	147	TRP	CB-CG	-5.10	1.41	1.50
1	A	108	THR	CA-C	5.06	1.66	1.52

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	127	SER	O-C-N	-30.60	73.74	122.70
2	B	85	ASP	O-C-N	-27.03	79.45	122.70
2	B	138	TYR	O-C-N	-25.51	81.89	122.70
1	A	205	SER	O-C-N	-22.58	86.58	122.70
2	B	181	TRP	O-C-N	-22.00	87.50	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	30	ASN	O-C-N	-17.53	94.66	122.70
2	B	146	THR	O-C-N	16.71	149.44	122.70
2	B	181	TRP	CA-C-N	-14.63	85.02	117.20
1	A	196	LYS	C-N-CA	-14.12	86.40	121.70
2	B	138	TYR	CA-C-N	14.12	148.27	117.20
2	B	127	SER	CA-C-N	13.34	146.55	117.20
2	B	154	SER	O-C-N	13.10	145.47	123.20
1	A	132	LEU	C-N-CA	-12.61	90.17	121.70
2	B	146	THR	CA-C-N	-12.58	89.53	117.20
1	A	123	ALA	C-N-CA	-12.58	90.26	121.70
2	B	85	ASP	CA-C-N	-12.37	90.00	117.20
1	A	180	LYS	O-C-N	12.09	142.04	122.70
1	A	30	ASN	CA-C-N	-11.78	91.29	117.20
1	A	197	THR	CA-C-N	-11.70	91.47	117.20
2	B	179	SER	C-N-CA	-11.55	92.82	121.70
1	A	124	THR	CA-C-N	-11.05	94.10	116.20
1	A	63	SER	CB-CA-C	11.04	131.07	110.10
1	A	184	GLU	CA-C-N	-10.79	93.47	117.20
1	A	50	ASN	O-C-N	10.56	139.60	122.70
1	A	189	TYR	CA-C-N	-10.53	94.03	117.20
1	A	201	PRO	O-C-N	10.41	139.36	122.70
2	B	47	TRP	C-N-CA	-10.29	95.97	121.70
1	A	152	ARG	O-C-N	-10.29	106.24	122.70
2	B	101	ASP	C-N-CA	-10.25	96.07	121.70
2	B	154	SER	CA-C-N	-10.09	96.03	116.20
2	B	25	SER	CA-C-N	-9.98	96.24	116.20
1	A	31	ASN	C-N-CA	-9.96	96.79	121.70
1	A	39	LYS	O-C-N	9.36	137.68	122.70
2	B	80	LEU	O-C-N	9.27	137.54	122.70
2	B	203	ILE	O-C-N	9.24	137.49	122.70
1	A	205	SER	CA-C-N	9.00	136.99	117.20
1	A	140	ASP	O-C-N	8.87	136.89	122.70
1	A	184	GLU	O-C-N	8.62	136.50	122.70
2	B	152	LEU	C-N-CA	-8.62	100.15	121.70
1	A	132	LEU	O-C-N	-8.55	109.02	122.70
1	A	180	LYS	CA-C-N	-8.53	98.44	117.20
1	A	6	GLN	O-C-N	8.46	136.23	122.70
2	B	189	ASN	N-CA-CB	-8.45	95.40	110.60
1	A	205	SER	C-N-CA	-8.30	100.96	121.70
2	B	133	CYS	O-C-N	8.28	135.95	122.70
2	B	138	TYR	C-N-CA	8.21	142.23	121.70
2	B	154	SER	N-CA-C	8.18	133.08	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	153	ARG	NE-CZ-NH2	8.17	124.39	120.30
2	B	189	ASN	CB-CA-C	8.15	126.71	110.40
2	B	170	LEU	CB-CA-C	-8.08	94.85	110.20
1	A	178	LEU	O-C-N	7.95	135.41	122.70
1	A	178	LEU	CB-CA-C	-7.95	95.10	110.20
2	B	145	VAL	CB-CA-C	-7.79	96.61	111.40
1	C	108	THR	N-CA-C	7.66	131.68	111.00
1	A	50	ASN	CA-C-N	-7.62	100.45	117.20
2	B	94	ARG	NE-CZ-NH2	7.58	124.09	120.30
2	B	71	ARG	NE-CZ-NH2	7.55	124.07	120.30
2	B	127	SER	C-N-CA	-7.54	102.85	121.70
1	A	189	TYR	O-C-N	-7.48	110.74	122.70
2	B	66	ARG	NE-CZ-NH2	7.42	124.01	120.30
1	A	61	ARG	NE-CZ-NH2	7.41	124.01	120.30
1	A	18	ARG	NE-CZ-NH2	7.41	124.00	120.30
2	B	38	ARG	NE-CZ-NH2	7.39	124.00	120.30
1	A	208	ARG	NE-CZ-NH2	7.32	123.96	120.30
2	B	13	ARG	NE-CZ-NH2	7.32	123.96	120.30
1	A	179	THR	C-N-CA	-7.31	103.42	121.70
2	B	202	LYS	C-N-CA	-7.30	103.45	121.70
1	A	139	ARG	NE-CZ-NH2	7.28	123.94	120.30
1	A	107	ARG	NE-CZ-NH2	7.24	123.92	120.30
2	B	50	ARG	NE-CZ-NH2	7.15	123.87	120.30
1	A	201	PRO	CA-C-N	-7.09	101.59	117.20
1	A	119	THR	N-CA-CB	7.06	123.71	110.30
1	A	133	MET	N-CA-C	-6.98	92.16	111.00
2	B	142	PRO	O-C-N	6.90	133.74	122.70
2	B	108	MET	CB-CA-C	-6.82	96.77	110.40
2	B	146	THR	C-N-CA	-6.80	104.70	121.70
2	B	170	LEU	O-C-N	6.78	133.54	122.70
2	B	100(D)	PHE	CB-CA-C	-6.77	96.86	110.40
2	B	145	VAL	O-C-N	6.76	133.51	122.70
1	A	140	ASP	CA-C-N	-6.71	102.44	117.20
2	B	203	ILE	CB-CA-C	6.67	124.94	111.60
2	B	154	SER	CB-CA-C	-6.66	97.45	110.10
2	B	202	LYS	O-C-N	-6.66	112.05	122.70
2	B	102	PHE	CA-C-N	-6.66	102.56	117.20
1	A	183	TYR	CA-C-N	-6.57	102.75	117.20
2	B	15	SER	N-CA-CB	-6.53	100.71	110.50
1	A	59	PRO	O-C-N	6.45	133.03	122.70
1	C	40	LEU	CA-CB-CG	6.43	130.09	115.30
1	A	40	LEU	CB-CA-C	-6.30	98.23	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	79	GLN	CB-CA-C	-6.29	97.83	110.40
1	A	201	PRO	CB-CA-C	-6.26	96.35	112.00
1	A	175	THR	O-C-N	6.25	132.70	122.70
2	B	3	GLN	CB-CA-C	-6.25	97.91	110.40
1	A	211	CYS	CA-CB-SG	-6.22	102.80	114.00
2	B	133	CYS	N-CA-CB	-6.20	99.44	110.60
1	A	133	MET	O-C-N	6.16	132.55	122.70
1	A	165	SER	O-C-N	6.15	132.54	122.70
2	B	203	ILE	CA-C-N	-6.14	103.68	117.20
1	A	133	MET	CG-SD-CE	6.13	110.00	100.20
2	B	108	MET	CG-SD-CE	6.13	110.00	100.20
1	A	172	MET	CG-SD-CE	6.12	110.00	100.20
2	B	128	MET	CG-SD-CE	6.11	109.98	100.20
1	A	7	SER	O-C-N	-6.11	109.49	121.10
2	B	82	MET	CG-SD-CE	6.10	109.95	100.20
2	B	51	MET	CG-SD-CE	6.09	109.94	100.20
2	B	48	MET	CG-SD-CE	6.09	109.94	100.20
2	B	128	MET	O-C-N	6.07	132.41	122.70
2	B	140	PRO	N-CA-C	-6.00	96.50	112.10
1	C	196	LYS	N-CA-C	-5.95	94.93	111.00
1	A	50	ASN	C-N-CA	5.94	136.54	121.70
1	C	42	GLU	N-CA-C	-5.91	95.04	111.00
1	A	178	LEU	CA-C-N	-5.90	104.22	117.20
1	A	58	ILE	O-C-N	-5.90	109.89	121.10
1	A	125	GLY	O-C-N	-5.90	113.18	123.20
1	C	178	LEU	CA-CB-CG	-5.85	101.86	115.30
1	A	182	ASP	CB-CA-C	5.84	122.08	110.40
1	A	183	TYR	N-CA-C	-5.83	95.26	111.00
1	A	63	SER	N-CA-CB	-5.82	101.76	110.50
1	A	40	LEU	O-C-N	5.81	133.07	123.20
1	A	133	MET	CB-CA-C	5.80	122.01	110.40
1	A	39	LYS	CA-C-N	-5.79	104.45	117.20
1	A	50	ASN	CB-CA-C	5.75	121.90	110.40
2	D	100(B)	LEU	CA-CB-CG	5.70	128.40	115.30
1	A	201	PRO	N-CA-C	5.65	126.80	112.10
2	B	147	TRP	O-C-N	5.60	131.66	122.70
2	B	80	LEU	CB-CA-C	-5.59	99.58	110.20
1	A	8	PRO	O-C-N	5.57	131.60	122.70
1	A	39	LYS	C-N-CA	5.55	135.57	121.70
1	A	146	LYS	O-C-N	5.51	131.52	122.70
1	A	148	ASP	N-CA-C	-5.48	96.21	111.00
1	A	119	THR	O-C-N	5.47	131.45	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	83	VAL	O-C-N	5.44	131.41	122.70
2	B	145	VAL	N-CA-CB	5.44	123.47	111.50
2	D	102	PHE	N-CA-C	5.44	125.69	111.00
1	C	107	ARG	N-CA-C	5.43	125.65	111.00
1	A	152	ARG	NE-CZ-NH2	5.40	123.00	120.30
2	B	133	CYS	CA-C-N	-5.39	105.33	117.20
2	B	100(B)	LEU	CB-CA-C	-5.38	99.98	110.20
1	A	124	THR	O-C-N	5.36	132.32	123.20
1	C	18	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	137	TYR	N-CA-CB	5.32	120.18	110.60
2	D	128	MET	N-CA-C	5.30	125.30	111.00
1	A	94	GLY	N-CA-C	5.28	126.29	113.10
2	B	100(B)	LEU	N-CA-CB	5.28	120.95	110.40
2	B	15	SER	O-C-N	5.27	131.13	122.70
1	C	110	PRO	N-CA-C	5.27	125.79	112.10
2	B	142	PRO	CB-CA-C	-5.23	98.92	112.00
2	B	116	PRO	O-C-N	5.10	130.86	122.70
1	A	133	MET	CA-C-N	-5.05	106.09	117.20
1	C	188	LEU	CA-CB-CG	-5.05	103.69	115.30
1	A	112	VAL	CB-CA-C	-5.01	101.87	111.40
2	B	80	LEU	CA-C-N	-5.00	106.20	117.20
2	D	206	ARG	NE-CZ-NH1	-5.00	117.80	120.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	152	ARG	Mainchain,Peptide
1	A	179	THR	Mainchain
1	A	94	GLY	Mainchain
2	B	102	PHE	Mainchain
2	B	138	TYR	Mainchain,Peptide
1	C	183	TYR	Sidechain
1	C	96	TYR	Sidechain
2	D	100(G)	PHE	Sidechain
2	D	138	TYR	Sidechain
2	D	97	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1626	0	1561	547	0
1	C	1626	0	1579	358	0
2	B	1663	0	1600	436	1
2	D	1663	0	1613	285	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	6353	1536	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 119.

All (1536) 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
1:A:116:PRO:HB3	1:A:206:PHE:CZ	1.50	1.45
2:B:127:SER:C	2:B:128:MET:N	1.70	1.45
1:A:31:ASN:C	1:A:32:TYR:N	1.69	1.44
1:A:110:PRO:C	1:A:111:THR:N	1.72	1.39
1:A:180:LYS:CD	1:A:184:GLU:OE2	1.70	1.39
1:A:40:LEU:C	1:A:40:LEU:HD12	1.26	1.39
2:B:152:LEU:C	2:B:153:SER:N	1.74	1.38
2:B:25:SER:C	2:B:26:GLY:N	1.74	1.37
1:A:205:SER:C	1:A:206:PHE:N	1.77	1.37
2:B:101:ASP:C	2:B:102:PHE:N	1.78	1.35
1:A:132:LEU:C	1:A:133:MET:N	1.77	1.34
1:A:156:VAL:HG12	1:A:176:LEU:CA	1.58	1.34
1:A:30:ASN:C	1:A:31:ASN:N	1.82	1.32
1:A:189:TYR:C	1:A:190:THR:N	1.82	1.32
2:B:47:TRP:C	2:B:48:MET:N	1.81	1.31
2:B:18:LEU:HG	2:B:102:PHE:CZ	1.64	1.31
1:A:123:ALA:C	1:A:124:THR:N	1.83	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:197:THR:C	1:A:198:SER:N	1.83	1.30
1:A:116:PRO:HG3	1:A:206:PHE:CD1	1.66	1.29
2:B:85:ASP:C	2:B:86:ASP:N	1.84	1.29
1:A:184:GLU:C	1:A:185:SER:N	1.85	1.29
1:A:171:SER:OG	2:B:157:HIS:HE1	1.16	1.28
1:A:40:LEU:CD1	1:A:40:LEU:C	1.90	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:48:MET:HE3	2:B:90:TYR:CD2	1.71	1.26
2:B:128:MET:N	2:B:177:PRO:HA	1.48	1.25
1:A:178:LEU:CD1	1:A:182:ASP:OD1	1.83	1.25
1:A:40:LEU:O	1:A:40:LEU:HD12	1.32	1.25
2:B:158:THR:HG21	3:B:211:HOH:O	1.37	1.24
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
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:183:TYR:C	1:A:184:GLU:N	1.96	1.18
1:A:196:LYS:C	1:A:197:THR:N	1.97	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
2:B:181:TRP:C	2:B:182:SER:N	1.95	1.18
1:A:20:THR:OG1	1:A:74:THR:HG22	1.38	1.17
1:C:146:LYS:HG2	1:C:151:GLU:HB2	1.20	1.17
1:A:180:LYS:HG2	1:A:184:GLU:OE2	1.40	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:178:LEU:HD12	1:A:182:ASP:OD1	1.01	1.16
1:A:154:ASP:HB2	1:A:155:GLY:N	1.59	1.16
1:A:40:LEU:CD1	1:A:40:LEU:O	1.90	1.16
2:B:179:SER:C	2:B:180:THR:N	1.99	1.16
1:A:148:ASP:HA	1:A:149:GLY:N	1.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:38:ARG:HB3	2:B:48:MET:CE	1.79	1.12
2:B:127:SER:O	2:B:178:SER:N	1.83	1.11
1:A:108:THR:HA	1:A:137:TYR:HB3	1.26	1.11
1:A:50:ASN:HB3	1:A:91:TYR:OH	1.48	1.11
1:A:180:LYS:CE	1:A:184:GLU:OE2	1.97	1.11
1:A:211:CYS:HA	2:B:120:GLY:C	1.70	1.10
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: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
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
2:B:153:SER:C	2:B:154:SER:N	2.05	1.08
1:C:152:ARG:HA	1:C:152:ARG:NE	1.67	1.08
2:B:153:SER:C	2:B:154:SER:HA	1.75	1.07
2:B:84:THR:C	2:B:85:ASP:HA	1.74	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
2:B:38:ARG:HB3	2:B:48:MET:HE2	1.07	1.06
2:B:187:THR:HG23	2:B:202:LYS:HA	1.31	1.06
1:A:78:LEU:C	1:A:79:GLN:N	2.08	1.06
1:A:54:LEU:HD11	1:A:58:ILE:O	1.55	1.05
2:B:180:THR:C	2:B:181:TRP:HA	1.77	1.05
2:B:141:GLU:C	2:B:142:PRO:N	2.10	1.05
2:B:14:PRO:O	2:B:15:SER:HB3	1.54	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:79:GLN:CB	1:A:80:PRO:HD2	1.85	1.05
1:C:7:SER:OG	1:C:8:PRO:HD3	1.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:157:LEU:HG	2:B:162:VAL:HG21	1.35	1.03
1:A:154:ASP:C	1:A:155:GLY:N	2.10	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
2:B:116:PRO:HB3	2:B:203:ILE:HG13	1.40	1.01
1:A:78:LEU:HD13	1:A:106:LEU:CD2	1.89	1.01
1:A:149:GLY:C	1:A:150:THR:N	2.14	1.01
1:A:180:LYS:HE2	1:A:184:GLU:OE2	1.59	1.01
2:B:12:VAL:HG21	2:B:82(C):LEU:CD1	1.91	1.00
1:A:200:SER:C	1:A:201:PRO:N	2.15	1.00
2:B:96:LEU:CD1	2:B:100(A):PRO:HG3	1.90	1.00
2:B:48:MET:CE	2:B:90:TYR:CE2	2.44	1.00
1:A:132:LEU:C	1:A:133:MET:HB2	1.82	1.00
1:A:132:LEU:CD2	1:A:173:SER:HB2	1.91	1.00
1:A:146:LYS:HA	1:A:151:GLU:HA	1.42	1.00
2:D:1:GLN:CD	3:D:223:HOH:O	1.95	1.00
2:B:100(E):TRP:O	2:B:100(F):TYR:HB3	1.58	0.99
1:A:132:LEU:C	1:A:133:MET:CA	2.30	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:37:GLN:C	1:A:38:GLN:HA	1.83	0.99
1:A:78:LEU:CD1	1:A:106:LEU:HD22	1.90	0.99
2:B:107:THR:C	2:B:108:MET:HA	1.82	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
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: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
2:B:89:THR:HA	2:B:101:ASP:HA	1.44	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
1:C:107:ARG:HD2	1:C:168:SER:HB2	1.47	0.97
2:B:48:MET:HE1	2:B:90:TYR:CE2	2.00	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:132:LEU:C	1:A:133:MET:CB	2.34	0.96
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
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
1:C:211:CYS:HA	2:D:120:GLY:C	1.86	0.95
2:D:20:LEU:HD21	2:D:102:PHE:HE2	1.31	0.95
1:A:141:ILE:HD12	1:A:141:ILE:H	1.28	0.94
2:B:153:SER:O	2:B:154:SER:HA	1.67	0.94
1:A:188:LEU:H	1:A:188:LEU:HD12	1.33	0.94
2:B:48:MET:HE3	2:B:90:TYR:HD2	1.25	0.94
1:A:123:ALA:C	1:A:124:THR:CA	2.35	0.94
1:A:152:ARG:NH1	1:A:152:ARG:HA	1.83	0.93
1:A:31:ASN:C	1:A:32:TYR:CA	2.36	0.93
2:B:101:ASP:C	2:B:102:PHE:CB	2.37	0.93
1:C:211:CYS:HB2	2:D:206:ARG:HB3	1.48	0.93
2:B:11:LEU:HG	2:B:140:PRO:HG3	1.49	0.93
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:O	1:C:18:ARG:HG3	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:196:LYS:C	1:A:197:THR:CA	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:183:SER:O	2:B:184:GLN:HB2	1.65	0.92
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
1:A:211:CYS:CB	2:B:206:ARG:HB3	2.02	0.90
2:B:152:LEU:C	2:B:153:SER:CB	2.39	0.90
1:A:184:GLU:N	1:A:185:SER:N	2.20	0.90
2:B:101:ASP:C	2:B:102:PHE:HB2	1.90	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:133:MET:HE3	1:A:143:VAL:HG12	1.54	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
1:A:37:GLN:C	1:A:38:GLN:CA	2.40	0.89
2:B:85:ASP:O	2:B:86:ASP:N	2.03	0.89
1:A:188:LEU:H	1:A:188:LEU:CD1	1.83	0.89
2:B:18:LEU:HG	2:B:102:PHE:CE2	2.06	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:147:ILE:O	1:A:150:THR:OG1	1.92	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
1:A:78:LEU:C	1:A:79:GLN:CA	2.41	0.88
1:C:156:VAL:C	1:C:157:LEU:HD23	1.94	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
1:A:29:ILE:C	1:A:30:ASN:N	2.27	0.88
2:B:181:TRP:CA	2:B:182:SER:N	2.37	0.88
2:D:4:LEU:CD1	2:D:24:VAL:HG12	2.03	0.87
2:B:48:MET:HE3	2:B:90:TYR:CE2	2.08	0.87
1:C:194:VAL:HG12	1:C:194:VAL:O	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:THR:HG23	1:C:70:ASP:OD1	1.75	0.87
2:B:198:LYS:HE3	2:D:179:SER:OG	1.74	0.87
1:A:78:LEU:C	1:A:79:GLN:HA	1.95	0.87
1:A:129:VAL:C	1:A:130:VAL:HG13	1.95	0.86
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:CA	1:A:152:ARG:HH11	1.88	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
2:B:153:SER:C	2:B:154:SER:CA	2.43	0.86
1:A:133:MET:HB3	1:A:172:MET:O	1.76	0.86
2:B:101:ASP:C	2:B:102:PHE:CA	2.43	0.86
1:A:110:PRO:HA	1:A:136:PHE:CB	2.06	0.86
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:187:THR:HG23	2:B:202:LYS:CA	2.06	0.85
2:B:4:LEU:HD11	2:B:24:VAL:HG12	1.55	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
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:107:THR:C	2:B:108:MET:CA	2.44	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
2:B:47:TRP:C	2:B:48:MET:CA	2.45	0.85
2:B:84:THR:C	2:B:85:ASP:CA	2.44	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:182:ASP:O	1:A:183:TYR:C	2.14	0.84
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
1:C:43:ALA:HB1	2:D:100(D):PHE:CB	2.06	0.84
1:A:160:VAL:C	1:A:161:THR:HG23	1.95	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:206:PHE:HA	1:A:207:ASN:N	1.92	0.84
1:A:62:PHE:O	1:A:63:SER:HB3	1.73	0.84
1:A:94:GLY:C	1:A:96:TYR:CD1	2.51	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:200:SER:C	1:A:201:PRO:CA	2.47	0.83
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
1:C:148:ASP:HB3	1:C:188:LEU:CD2	2.06	0.83
2:B:152:LEU:C	2:B:153:SER:CA	2.46	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
1:A:197:THR:CA	1:A:198:SER:N	2.42	0.82
1:A:28:ASN:HD22	1:A:68:GLY:CA	1.92	0.82
1:A:206:PHE:C	1:A:207:ASN:N	2.33	0.82
2:B:132:GLY:O	2:B:203:ILE:HD11	1.79	0.82
1:A:128:SER:HG	1:A:177:SER:HB3	1.42	0.82
1:A:110:PRO:CD	1:A:197:THR:OG1	2.28	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:108:THR:CA	1:A:137:TYR:HB3	2.09	0.82
1:A:40:LEU:O	1:A:40:LEU:HD13	1.79	0.82
2:B:42:GLY:O	2:B:43:LYS:HG3	1.79	0.82
1:A:210:GLU:C	2:B:208:CYS:SG	2.58	0.81
2:B:96:LEU:HD11	2:B:100(A):PRO:HG3	1.60	0.81
1:A:148:ASP:CA	1:A:149:GLY:N	2.44	0.81
1:A:211:CYS:HB2	2:B:206:ARG:CB	2.10	0.81
1:A:107:ARG:O	1:A:108:THR:HG23	1.80	0.81
1:A:112:VAL:CG2	1:A:193:VAL:HG21	2.10	0.81
1:A:43:ALA:HB1	2:B:100(D):PHE:HB3	1.59	0.81
2:B:127:SER:C	2:B:128:MET:CA	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ASN:ND2	1:A:68:GLY:HA3	1.95	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:129:VAL:HG12	1:A:145:TRP:HH2	1.45	0.80
1:A:118:SER:O	1:A:119:THR:C	2.18	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:139:PHE:C	2:B:140:PRO:N	2.34	0.80
2:B:159:PHE:HD2	2:B:159:PHE:H	1.29	0.80
1:C:112:VAL:HG12	1:C:113:SER:N	1.94	0.80
2:B:141:GLU:C	2:B:142:PRO:CA	2.50	0.79
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:187:ASN:O	1:A:207:ASN:CA	2.28	0.79
1:A:69:THR:CG2	1:A:70:ASP:N	2.46	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
1:A:205:SER:C	1:A:206:PHE:CB	2.51	0.79
2:B:146:THR:O	2:B:189:ASN:HB3	1.83	0.79
1:A:29:ILE:HG12	1:A:71:TYR:CE1	2.18	0.79
2:B:152:LEU:C	2:B:153:SER:HB3	2.00	0.79
1:A:160:VAL:O	1:A:161:THR:HG23	1.83	0.79
2:B:103:TRP:HZ2	2:B:168:TYR:HH	1.31	0.79
1:A:187:ASN:HA	1:A:208:ARG:HB2	1.65	0.78
1:A:62:PHE:O	1:A:63:SER:CB	2.30	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
2:B:96:LEU:O	2:B:98:GLY:N	2.17	0.78
1:A:129:VAL:O	1:A:130:VAL:HG13	1.83	0.78
1:A:69:THR:HG23	1:A:70:ASP:OD1	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:ARG:HH11	1:C:107:ARG:HG3	1.47	0.78
1:C:76:SER:O	1:C:77:SER:HB2	1.82	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
1:A:205:SER:C	1:A:206:PHE:CA	2.51	0.77
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:184:GLU:CA	1:A:185:SER:N	2.47	0.77
1:A:37:GLN:O	1:A:38:GLN:HA	1.85	0.77
1:A:117:PRO:HG2	1:A:122:LEU:HD13	1.66	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
2:B:14:PRO:O	2:B:15:SER:CB	2.30	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:196:LYS:C	1:A:197:THR:HA	2.05	0.77
1:A:109:ALA:HA	1:A:197:THR:HG21	1.66	0.77
1:A:207:ASN:O	1:A:210:GLU:HB2	1.84	0.76
1:A:5:THR:O	1:A:23:CYS:HA	1.85	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
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:205:SER:C	1:A:206:PHE:HB3	2.05	0.76
2:B:179:SER:C	2:B:180:THR:CA	2.53	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:N	1:A:188:LEU:HD12	2.00	0.76
1:A:29:ILE:C	1:A:30:ASN:CA	2.54	0.76
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:ASP:HA	1:C:185:SER:HB3	1.66	0.75
1:A:183:TYR:HD2	1:A:184:GLU:HA	1.50	0.75
1:A:40:LEU:CG	1:A:41:GLY:N	2.48	0.75
1:C:196:LYS:HG3	1:C:197:THR:N	2.01	0.75
1:A:173:SER:HB3	2:B:159:PHE:CE1	2.21	0.75
2:B:1:GLN:OE1	2:B:1:GLN:HA	1.87	0.75
1:A:123:ALA:C	1:A:124:THR:HA	2.06	0.74
1:A:150:THR:CA	1:A:151:GLU:N	2.50	0.74
1:A:132:LEU:HD21	1:A:173:SER:HB2	1.68	0.74
2:B:114:VAL:HG21	2:B:190:VAL:HG21	1.67	0.74
1:A:11:LEU:HD12	1:A:11:LEU:C	2.08	0.74
2:D:18:LEU:CD2	2:D:19:SER:H	1.99	0.74
1:A:149:GLY:C	1:A:150:THR:CA	2.56	0.74
2:D:159:PHE:HD2	2:D:159:PHE:H	1.35	0.74
2:B:38:ARG:CB	2:B:48:MET:HE2	2.03	0.74
2:B:35:SER:HB3	2:B:50:ARG:HA	1.68	0.74
1:C:167:ASP:O	1:C:169:THR:N	2.21	0.74
1:C:25:GLY:HA3	1:C:29:ILE:HD11	1.69	0.74
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:81:GLU:CA	1:A:165:SER:O	2.36	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:110:PRO:HA	1:A:136:PHE:HB3	1.71	0.73
1:A:48:ILE:CD1	1:A:64:GLY:HA3	2.19	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:HD12	1:C:147:ILE:N	2.04	0.73
1:A:90:GLN:HE21	1:A:92:ASN:N	1.87	0.72
2:B:164:GLN:NE2	2:B:164:GLN:HA	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:132:GLY:O	2:B:133:CYS:HB2	1.89	0.72
2:B:82(A):ASN:O	2:B:82(B):SER:HB3	1.90	0.72
2:B:195:SER:O	2:B:197:THR:N	2.23	0.71
1:C:48:ILE:C	1:C:48:ILE:HD13	2.11	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
1:A:200:SER:C	1:A:201:PRO:HA	2.11	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:196:LYS:H	1:A:197:THR:N	1.87	0.71
1:A:81:GLU:HA	1:A:165:SER:O	1.90	0.71
2:B:178:SER:O	2:B:181:TRP:N	2.24	0.71
1:C:105:GLU:C	1:C:106:LEU:HD12	2.11	0.71
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
1:A:37:GLN:C	1:A:38:GLN:N	2.44	0.71
2:B:12:VAL:CG2	2:B:82(C):LEU:HD13	2.20	0.71
1:A:112:VAL:HG12	1:A:113:SER:N	2.06	0.71
1:A:153:ARG:HG2	1:A:153:ARG:O	1.91	0.71
1:A:46:LEU:HD23	1:A:55:GLN:CG	2.21	0.71
2:B:48:MET:HE1	2:B:90:TYR:HE2	1.50	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:211:CYS:CB	2:B:120:GLY:HA2	2.22	0.69
1:A:40:LEU:CD1	1:A:41:GLY:N	2.42	0.69
1:C:133:MET:HE2	1:C:193:VAL:HG13	1.74	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
1:A:67:SER:O	1:A:68:GLY:C	2.31	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
2:B:170:LEU:C	2:B:171:THR:HG22	2.12	0.69
1:A:54:LEU:CD1	1:A:58:ILE:O	2.37	0.69
1:A:94:GLY:C	1:A:96:TYR:HD1	1.95	0.69
2:D:164:GLN:CA	2:D:164:GLN:NE2	2.56	0.69
2:D:188:CYS:C	2:D:189:ASN:HD22	1.96	0.69
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:122:LEU:O	1:A:124:THR:N	2.26	0.68
1:A:80:PRO:HA	1:A:106:LEU:HD11	1.73	0.68
1:C:187:ASN:O	1:C:208:ARG:N	2.20	0.68
1:A:180:LYS:HG2	1:A:184:GLU:CD	2.13	0.68
1:A:76:SER:O	1:A:77:SER:CB	2.40	0.68
1:A:43:ALA:CB	2:B:100(D):PHE:HB3	2.22	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:147:ILE:HD12	1:A:152:ARG:H	1.59	0.68
1:A:116:PRO:CB	1:A:206:PHE:HE1	1.88	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:137:TYR:O	1:A:139:ARG:N	2.27	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
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:107:THR:C	2:B:108:MET:N	2.48	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:A:120:GLU:H	1:A:120:GLU:CD	1.96	0.67
1:A:145:TRP:CZ3	1:A:176:LEU:HD22	2.28	0.67
1:A:4:LEU:HD21	1:A:90:GLN:CB	2.24	0.67
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
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:O	1:A:194:VAL:HG12	1.93	0.67
1:C:118:SER:H	1:C:121:GLN:HB3	1.59	0.67
1:C:94:GLY:C	1:C:96:TYR:CD1	2.68	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:148:ASP:CB	1:C:188:LEU:HD22	2.09	0.67
1:C:50:ASN:ND2	1:C:91:TYR:OH	2.27	0.67
2:D:199:VAL:HG12	2:D:200:ASP:N	2.07	0.67
1:A:123:ALA:O	1:A:124:THR:HA	1.94	0.67
1:A:122:LEU:HD11	1:A:127:ALA:HB2	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:89:THR:CA	2:B:100(G):PHE:O	2.43	0.66
2:B:13:ARG:O	2:B:16:GLU:HG3	1.96	0.66
1:C:158:ASP:HB3	1:C:174:SER:HB2	1.77	0.66
1:C:182:ASP:HA	1:C:185:SER:CB	2.25	0.66
1:C:159:SER:HB2	2:D:160:PRO:HG2	1.77	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:B:38:ARG:HG2	2:B:40:PRO:HD3	1.78	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
1:C:129:VAL:HB	1:C:176:LEU:HD23	1.76	0.66
1:A:39:LYS:O	1:A:42:GLU:HB2	1.95	0.66
1:C:133:MET:CE	1:C:193:VAL:HG13	2.25	0.66
1:C:122:LEU:CD1	1:C:180:LYS:HD2	2.26	0.66
1:C:26:SER:O	1:C:27:GLN:HG3	1.95	0.66
1:A:90:GLN:HE21	1:A:92:ASN:H	1.44	0.65
2:B:66:ARG:HH22	2:B:86:ASP:CG	2.00	0.65
1:C:107:ARG:HB2	1:C:107:ARG:NH1	2.12	0.65
1:A:133:MET:CE	1:A:143:VAL:CG1	2.74	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
2:B:182:SER:O	2:B:183:SER:C	2.33	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:103:TRP:HZ2	2:D:168:TYR:HH	1.38	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:A:29:ILE:O	1:A:30:ASN:C	2.35	0.65
1:C:141:ILE:H	1:C:141:ILE:CD1	1.92	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:PRO:HB3	1:C:127:ALA:HA	1.79	0.65
1:C:211:CYS:HB3	2:D:206:ARG:HH11	1.60	0.65
1:C:44:PRO:HD2	2:D:100(D):PHE:CD1	2.31	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
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:N	1:C:188:LEU:HD12	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:B:138:TYR:HD1	2:B:139:PHE:N	1.95	0.64
2:B:132:GLY:HA2	2:B:173:SER:HA	1.79	0.64
2:D:158:THR:CB	2:D:172:SER:HB2	2.28	0.64
2:D:8:GLY:HA3	2:D:20:LEU:HD23	1.80	0.64
2:B:180:THR:C	2:B:181:TRP:CA	2.62	0.64
2:B:14:PRO:O	2:B:16:GLU:HG2	1.98	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:103:TRP:CD1	2:B:139:PHE:CE1	2.86	0.64
2:B:12:VAL:HG23	2:B:82(C):LEU:HD13	1.80	0.64
2:B:31:SER:O	2:B:32:PHE:CD1	2.51	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:163:GLN:HG3	1:C:170:TYR:OH	1.99	0.63
1:C:29:ILE:O	1:C:29:ILE:HG22	1.96	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:A:30:ASN:O	1:A:31:ASN:N	2.30	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:A:178:LEU:CD1	1:A:182:ASP:CG	2.66	0.63
2:B:103:TRP:CZ2	2:B:168:TYR:OH	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ASN:C	1:A:32:TYR:HA	2.17	0.63
2:B:139:PHE:CG	2:B:139:PHE:O	2.50	0.63
2:D:1:GLN:HA	2:D:1:GLN:OE1	1.97	0.63
2:B:159:PHE:CD2	2:B:159:PHE:N	2.66	0.63
2:B:175:THR:CG2	2:B:176:VAL:H	2.12	0.63
1:C:118:SER:OG	1:C:121:GLN:CB	2.42	0.63
1:C:90:GLN:NE2	1:C:93:ASN:H	1.96	0.63
1:A:209:ASN:O	2:B:208:CYS:HB2	1.99	0.63
1:A:69:THR:CG2	1:A:70:ASP:H	2.10	0.63
2:B:18:LEU:CD2	2:B:19:SER:N	2.62	0.63
2:B:6:GLU:O	2:B:100(G):PHE:CE1	2.52	0.63
1:C:11:LEU:HD12	1:C:11:LEU:C	2.20	0.63
2:B:8:GLY:HA3	2:B:20:LEU:HD23	1.80	0.62
1:C:122:LEU:C	1:C:124:THR:H	2.01	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
1:A:110:PRO:CB	1:A:111:THR:N	2.60	0.62
1:A:26:SER:O	1:A:27:GLN:HG3	2.00	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
1:A:147:ILE:O	1:A:148:ASP:C	2.38	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:CG1	1:C:194:VAL:O	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
1:A:29:ILE:C	1:A:30:ASN:C	2.58	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:160:VAL:O	1:A:161:THR:CB	2.46	0.62
1:A:38:GLN:N	1:A:85:THR:O	2.33	0.62
2:B:38:ARG:HH11	2:B:48:MET:HE1	1.65	0.62
1:A:196:LYS:C	1:A:198:SER:N	2.53	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:133:MET:O	1:A:136:PHE:HD2	1.83	0.61
1:A:67:SER:O	1:A:68:GLY:O	2.17	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:117:LEU:HB2	2:B:132:GLY:C	2.21	0.61
2:B:138:TYR:CD1	2:B:139:PHE:N	2.68	0.61
2:B:60:ASN:O	2:B:63:LEU:N	2.33	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
2:D:60:ASN:O	2:D:61:SER:C	2.37	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:D:164:GLN:C	2:D:164:GLN:HE21	2.04	0.61
2:B:100(E):TRP:O	2:B:100(F):TYR:CB	2.41	0.61
2:B:91:TYR:CD2	2:B:100(F):TYR:HA	2.35	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
2:B:14:PRO:C	2:B:16:GLU:H	2.03	0.61
2:D:143:VAL:HG21	2:D:170:LEU:CD2	2.31	0.61
2:D:60:ASN:O	2:D:62:ALA:N	2.34	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
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
2:B:135:VAL:HG22	2:B:190:VAL:HG21	1.82	0.60
2:B:152:LEU:O	2:B:153:SER:CB	2.29	0.60
2:B:145:VAL:CG1	2:B:190:VAL:HG22	2.31	0.60
2:D:111:VAL:HG12	2:D:112:SER:N	2.16	0.60
2:D:13:ARG:HB2	2:D:16:GLU:CG	2.30	0.60
1:A:138:PRO:O	1:A:140:ASP:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:100(C):GLY:O	2:B:100(D):PHE:HD2	1.84	0.60
1:A:210:GLU:CA	2:B:208:CYS:SG	2.90	0.60
1:C:132:LEU:HD22	1:C:173:SER:HB2	1.82	0.60
2:D:126:ASN:O	2:D:127:SER:C	2.36	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:103:TRP:HD1	2:B:139:PHE:HE1	1.47	0.60
2:B:96:LEU:HG	2:B:100(A):PRO:CD	2.30	0.60
1:C:196:LYS:C	1:C:198:SER:N	2.50	0.60
1:A:107:ARG:C	1:A:108:THR:CG2	2.70	0.60
2:B:36:TRP:HD1	2:B:69:ILE:HG12	1.64	0.60
1:C:107:ARG:CZ	1:C:107:ARG:HB2	2.31	0.60
1:C:112:VAL:CG2	1:C:193:VAL:HG21	2.30	0.60
1:C:36:TYR:OH	2:D:100:TYR:CD1	2.54	0.60
2:D:8:GLY:HA3	2:D:20:LEU:CD2	2.31	0.60
1:A:149:GLY:C	1:A:150:THR:HA	2.21	0.60
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:161:ALA:HB2	2:D:170:LEU:HB3	1.84	0.59
2:B:38:ARG:HD2	2:B:48:MET:CE	2.31	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: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
2:D:66:ARG:HH22	2:D:86:ASP:CG	2.04	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
2:B:60:ASN:O	2:B:61:SER:C	2.41	0.59
1:C:151:GLU:HG3	1:C:151:GLU:O	2.03	0.59
1:C:4:LEU:HD21	1:C:90:GLN:CB	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:TRP:C	2:B:48:MET:HA	2.23	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:149:GLY:O	1:A:150:THR:N	2.35	0.59
1:C:137:TYR:CD2	1:C:138:PRO:CA	2.86	0.59
1:C:160:VAL:C	1:C:161:THR:HG23	2.22	0.59
1:C:46:LEU:HD23	1:C:55:GLN:CG	2.33	0.59
1:C:7:SER:OG	1:C:8:PRO:CD	2.42	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:189:TYR:HA	1:A:190:THR:N	2.18	0.58
1:A:142:SER:O	1:A:193:VAL:O	2.20	0.58
2:B:32:PHE:CD2	2:B:94:ARG:HD3	2.38	0.58
1:C:159:SER:O	1:C:172:MET:HG2	2.03	0.58
1:C:36:TYR:CZ	2:D:100:TYR:HD1	2.21	0.58
2:D:143:VAL:CG2	2:D:170:LEU:CD2	2.82	0.58
2:D:91:TYR:CD2	2:D:100(F):TYR:HA	2.38	0.58
2:B:110:THR:O	2:B:138:TYR:HA	2.04	0.58
1:A:33:LEU:HD22	1:A:71:TYR:CB	2.34	0.58
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
2:B:141:GLU:C	2:B:142:PRO:HA	2.22	0.58
1:C:108:THR:HA	1:C:137:TYR:HB3	1.85	0.58
2:D:75:LYS:HD3	2:D:77:GLN:CD	2.24	0.58
1:A:187:ASN:HD22	1:A:207:ASN:HB3	1.69	0.58
2:D:132:GLY:HA2	2:D:147:TRP:CZ2	2.38	0.58
2:D:18:LEU:HD22	2:D:19:SER:H	1.55	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:51:MET:HE2	2:B:71:ARG:HG2	1.85	0.58
1:A:147:ILE:HG23	1:A:189:TYR:CD2	2.38	0.57
1:A:40:LEU:HD12	1:A:41:GLY:CA	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:195:SER:O	2:D:197:THR:N	2.37	0.57
1:A:80:PRO:HA	1:A:106:LEU:CD1	2.35	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: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
2:D:89:THR:HA	2:D:101:ASP:HA	1.86	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
1:C:158:ASP:HB3	1:C:174:SER:CB	2.34	0.57
1:C:109:ALA:HA	1:C:197:THR:HG21	1.87	0.57
1:A:137:TYR:O	1:A:138:PRO:C	2.38	0.56
2:B:52:TRP:NE1	2:B:56:TYR:HD2	2.03	0.56
2:D:114:VAL:CG2	2:D:190:VAL:HG21	2.34	0.56
2:D:51:MET:O	2:D:51:MET:HG3	2.03	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:176:LEU:O	1:A:176:LEU:HD23	2.04	0.56
2:B:48:MET:CB	2:B:63:LEU:HD23	2.33	0.56
1:C:118:SER:C	1:C:120:GLU:N	2.57	0.56
1:A:132:LEU:HD23	1:A:173:SER:HB2	1.82	0.56
1:A:127:ALA:HB1	1:A:183:TYR:CD1	2.40	0.56
2:B:18:LEU:CG	2:B:102:PHE:HZ	1.90	0.56
2:B:109:VAL:O	2:B:110:THR:OG1	2.18	0.56
1:C:152:ARG:CA	1:C:152:ARG:NE	2.57	0.56
1:C:193:VAL:N	1:C:202:VAL:O	2.29	0.56
1:C:38:GLN:HG3	1:C:87:PHE:HE1	1.70	0.56
1:C:55:GLN:HB3	3:C:215:HOH:O	2.05	0.56
1:C:46:LEU:HD23	1:C:55:GLN:HG3	1.86	0.56
1:A:94:GLY:O	1:A:96:TYR:CB	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:152:LEU:O	2:D:153:SER:CB	2.51	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:188:CYS:O	2:B:189:ASN:HB2	2.03	0.56
2:B:133:CYS:HB2	2:B:203:ILE:HD11	1.88	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
2:B:48:MET:CE	2:B:90:TYR:HE2	2.05	0.56
1:C:36:TYR:OH	2:D:100:TYR:HD1	1.88	0.56
1:A:122:LEU:C	1:A:124:THR:N	2.59	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
1:C:147:ILE:O	1:C:148:ASP:C	2.44	0.56
2:D:114:VAL:O	2:D:114:VAL:CG1	2.54	0.56
1:A:107:ARG:C	1:A:108:THR:HG22	2.20	0.56
1:A:110:PRO:C	1:A:111:THR:CA	2.73	0.55
1:A:110:PRO:HD3	1:A:197:THR:CG2	2.35	0.55
1:A:211:CYS:HB3	2:B:206:ARG:CZ	2.33	0.55
1:A:47:LEU:HA	1:A:58:ILE:CG1	2.35	0.55
1:A:20:THR:HG1	1:A:74:THR:HG22	1.65	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
2:D:39:HIS:HE1	2:D:44:GLY:HA2	1.71	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:120:GLU:O	1:C:122:LEU:N	2.39	0.55
1:C:117:PRO:HB2	1:C:122:LEU:HD23	1.87	0.55
1:A:147:ILE:O	1:A:150:THR:N	2.40	0.55
1:A:49:TYR:HE2	1:A:55:GLN:HE21	1.53	0.55
1:A:71:TYR:C	1:A:72:THR:HG22	2.27	0.55
1:C:167:ASP:O	1:C:167:ASP:OD1	2.25	0.55
1:C:67:SER:O	1:C:68:GLY:C	2.44	0.55
2:D:147:TRP:HZ3	2:D:203:ILE:CD1	2.19	0.55
2:B:113:SER:O	2:B:136:LYS:N	2.31	0.55
2:B:67:LEU:HD12	2:B:80:LEU:HD21	1.87	0.55
1:A:152:ARG:HD2	1:A:152:ARG:N	2.13	0.55
1:A:190:THR:HB	1:A:205:SER:OG	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:107:THR:HG1	2:B:108:MET:N	2.05	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: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:133:MET:CE	1:C:143:VAL:HG13	2.37	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
2:D:51:MET:CE	2:D:71:ARG:HG2	2.37	0.54
2:B:147:TRP:O	2:B:150:GLY:N	2.39	0.54
2:B:89:THR:HB	2:B:101:ASP:HA	1.89	0.54
1:C:176:LEU:O	1:C:176:LEU:HD23	2.06	0.54
2:D:100(B):LEU:CD1	2:D:100(C):GLY:H	2.20	0.54
2:D:103:TRP:C	2:D:105:PRO:HD3	2.27	0.54
1:A:117:PRO:HG3	1:A:127:ALA:CA	2.38	0.54
2:B:18:LEU:CD1	2:B:102:PHE:CE2	2.89	0.54
1:A:211:CYS:O	2:B:121:SER:OG	2.22	0.54
2:B:38:ARG:CB	2:B:48:MET:CE	2.71	0.54
1:A:10:LEU:HD12	1:A:11:LEU:H	1.67	0.54
1:C:71:TYR:N	1:C:71:TYR:CD1	2.76	0.54
1:A:200:SER:O	1:A:201:PRO:HA	2.07	0.54
1:C:180:LYS:HZ2	1:C:184:GLU:HB2	1.70	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
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:C:196:LYS:C	1:C:198:SER:H	2.10	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:ASN:O	2:B:127:SER:C	2.45	0.53
2:B:131:LEU:HD23	2:B:186:VAL:HG11	1.90	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
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
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
1:C:13:ALA:O	1:C:106:LEU:HA	2.09	0.53
1:C:146:LYS:HG2	1:C:151:GLU:CB	2.13	0.53
2:D:103:TRP:HD1	2:D:139:PHE:CZ	2.27	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
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:154:SER:N	3:D:221:HOH:O	2.41	0.53
2:D:60:ASN:O	2:D:63:LEU:N	2.40	0.53
1:A:110:PRO:HA	1:A:136:PHE:CA	2.39	0.53
1:A:48:ILE:HD12	1:A:52:ASN:HA	1.91	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:C:151:GLU:CG	1:C:151:GLU:O	2.56	0.53
1:C:31:ASN:HA	1:C:71:TYR:CE2	2.43	0.53
1:A:141:ILE:N	1:A:141:ILE:HD12	2.08	0.53
1:A:147:ILE:HD11	1:A:152:ARG:N	2.20	0.53
1:A:29:ILE:HG12	1:A:71:TYR:CZ	2.43	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:113:SER:HB2	2:B:136:LYS:O	2.09	0.52
2:B:29:LEU:HD21	2:B:78:VAL:CG2	2.39	0.52
2:D:164:GLN:HE21	2:D:165:SER:N	2.07	0.52
2:D:182:SER:O	2:D:183:SER:C	2.47	0.52
1:A:160:VAL:C	1:A:161:THR:CG2	2.63	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:117:PRO:HB2	1:C:122:LEU:CD2	2.39	0.52
1:C:116:PRO:HB3	1:C:206:PHE:CZ	2.43	0.52
1:A:10:LEU:C	1:A:10:LEU:HD12	2.30	0.52
1:A:117:PRO:HD2	1:A:183:TYR:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:SER:O	1:A:15:VAL:C	2.45	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:118:SER:CB	2:D:116:PRO:HD2	2.39	0.52
2:B:85:ASP:O	2:B:86:ASP:CA	2.58	0.52
1:C:179:THR:HB	1:C:181:ALA:HB3	1.92	0.52
1:C:173:SER:N	2:D:159:PHE:CE1	2.77	0.52
1:A:109:ALA:H	1:A:137:TYR:HB3	1.73	0.52
2:B:186:VAL:O	2:B:203:ILE:HG22	2.10	0.52
2:B:36:TRP:O	2:B:48:MET:N	2.43	0.52
1:C:146:LYS:HA	1:C:151:GLU:CA	2.22	0.52
1:A:112:VAL:HG21	1:A:193:VAL:CG2	2.32	0.52
1:A:48:ILE:CD1	1:A:64:GLY:CA	2.87	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:114:VAL:CG1	2:D:201:LYS:HB2	2.39	0.52
2:D:31:SER:O	2:D:32:PHE:CD1	2.62	0.52
1:A:193:VAL:N	1:A:202:VAL:O	2.35	0.52
1:C:36:TYR:OH	2:D:100:TYR:N	2.41	0.52
2:D:164:GLN:CG	2:D:165:SER:H	2.22	0.52
2:D:143:VAL:CG2	2:D:170:LEU:HD23	2.40	0.52
2:D:50:ARG:HG2	2:D:52:TRP:CD1	2.44	0.52
2:D:82(B):SER:OG	2:D:82(B):SER:O	2.28	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:137:TYR:CD2	1:C:137:TYR:C	2.83	0.52
1:A:189:TYR:O	1:A:206:PHE:HD2	1.93	0.52
2:B:132:GLY:O	2:B:203:ILE:CD1	2.56	0.52
2:B:18:LEU:CD1	2:B:102:PHE:CZ	2.93	0.52
1:A:118:SER:CB	1:A:121:GLN:HB3	2.40	0.51
1:A:29:ILE:CG1	1:A:71:TYR:CE1	2.92	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:A:138:PRO:C	1:A:140:ASP:N	2.62	0.51
1:C:129:VAL:HG13	1:C:206:PHE:HE1	1.76	0.51
1:C:83:VAL:HG11	1:C:163:GLN:HB3	1.92	0.51
1:C:35:TRP:HD1	1:C:48:ILE:HD12	1.76	0.51
2:D:148:ASN:HB2	2:D:152:LEU:CD2	2.40	0.51
1:C:116:PRO:HG3	1:C:206:PHE:CD1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:38:ARG:HD3	2:B:46:GLU:HG2	1.93	0.51
1:C:106(A):LYS:O	1:C:107:ARG:CB	2.58	0.51
1:C:68:GLY:O	1:C:69:THR:HG22	2.11	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
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:196:LYS:O	1:C:197:THR:C	2.49	0.51
1:C:43:ALA:HB2	2:D:100(D):PHE:O	2.11	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: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:183:TYR:CA	1:A:184:GLU:N	2.74	0.50
1:A:29:ILE:O	1:A:32:TYR:N	2.44	0.50
1:A:2:ILE:HB	1:A:90:GLN:OE1	2.11	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:75:LYS:HD3	2:B:77:GLN:CD	2.31	0.50
1:C:71:TYR:C	1:C:72:THR:HG22	2.32	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:CD1	1:C:141:ILE:N	2.55	0.50
2:D:204:VAL:CB	2:D:205:PRO:HD2	2.41	0.50
2:D:73:THR:O	2:D:74:SER:C	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:SER:HB2	2:D:160:PRO:HD2	1.94	0.50
1:C:38:GLN:O	1:C:39:LYS:CB	2.58	0.50
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:150:THR:C	1:A:151:GLU:N	2.65	0.50
2:B:195:SER:C	2:B:197:THR:N	2.65	0.50
2:D:100(E):TRP:O	2:D:100(F):TYR:HB2	2.12	0.50
1:A:11:LEU:HD21	1:A:19:VAL:CG1	2.42	0.49
1:A:7:SER:OG	1:A:22:SER:HB3	2.11	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
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
2:D:83:GLN:C	2:D:85:ASP:H	2.15	0.49
1:A:70:ASP:C	1:A:71:TYR:CD1	2.85	0.49
1:A:94:GLY:CA	1:A:96:TYR:CD1	2.95	0.49
2:D:16:GLU:HB2	2:D:82(C):LEU:HD11	1.93	0.49
1:A:123:ALA:O	1:A:124:THR:CA	2.56	0.49
1:A:167:ASP:OD1	1:A:167:ASP:C	2.51	0.49
1:A:17:ASP:O	1:A:78:LEU:HB2	2.11	0.49
2:B:52:TRP:NE1	2:B:56:TYR:CD2	2.81	0.49
1:C:179:THR:OG1	1:C:182:ASP:N	2.46	0.49
1:C:28:ASN:ND2	1:C:30:ASN:H	2.11	0.49
1:A:153:ARG:H	1:A:154:ASP:N	2.10	0.49
1:A:48:ILE:HD13	1:A:64:GLY:CA	2.43	0.49
1:A:7:SER:O	1:A:8:PRO:C	2.48	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:C:118:SER:O	1:C:119:THR:C	2.49	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:183:TYR:CD2	1:A:184:GLU:HA	2.39	0.49
1:C:14:SER:O	1:C:15:VAL:C	2.50	0.49
1:C:193:VAL:HG12	1:C:194:VAL:N	2.27	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
2:B:137:GLY:C	2:B:167:LEU:HD13	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:VAL:HG23	1:C:201:PRO:HB3	1.94	0.49
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
1:C:210:GLU:C	2:D:208:CYS:SG	2.91	0.48
2:D:134:LEU:HD13	2:D:171:THR:HB	1.94	0.48
2:D:66:ARG:HB2	2:D:82(A):ASN:O	2.13	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
2:B:84:THR:C	2:B:85:ASP:N	2.66	0.48
2:D:18:LEU:HD23	2:D:19:SER:H	1.75	0.48
1:A:110:PRO:HA	1:A:136:PHE:HA	1.95	0.48
2:B:25:SER:C	2:B:26:GLY:CA	2.74	0.48
2:B:89:THR:HA	2:B:100(G):PHE:O	2.11	0.48
1:C:109:ALA:HA	1:C:197:THR:CG2	2.43	0.48
1:C:196:LYS:CG	1:C:197:THR:N	2.75	0.48
1:C:69:THR:HG22	1:C:70:ASP:H	1.78	0.48
1:A:110:PRO:C	1:A:111:THR:CB	2.82	0.48
1:A:133:MET:HE2	1:A:193:VAL:HG13	1.94	0.48
1:A:32:TYR:HB3	1:A:91:TYR:CE1	2.48	0.48
1:A:49:TYR:O	1:A:50:ASN:C	2.51	0.48
1:A:4:LEU:HD21	1:A:90:GLN:HB2	1.95	0.48
2:D:117:LEU:HB2	2:D:132:GLY:C	2.34	0.48
2:B:152:LEU:N	2:B:152:LEU:HD23	2.29	0.48
1:C:106(A):LYS:C	1:C:107:ARG:HG2	2.32	0.48
1:C:211:CYS:CB	2:D:120:GLY:HA2	2.43	0.48
1:C:56:THR:N	3:C:215:HOH:O	2.46	0.48
2:D:111:VAL:HG12	2:D:112:SER:O	2.13	0.48
2:D:48:MET:SD	2:D:63:LEU:HD21	2.53	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
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
2:B:52:TRP:HB3	2:B:54:ASP:OD1	2.13	0.48
1:C:147:ILE:HD13	1:C:150:THR:CG2	2.44	0.48
1:C:29:ILE:CG2	1:C:29:ILE:O	2.59	0.48
1:C:33:LEU:HD22	1:C:71:TYR:HB3	1.96	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:61:ARG:HH21	1:A:82:ASP:CG	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HG22	2:B:21:THR:O	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:139:ARG:HD3	1:A:139:ARG:O	2.15	0.47
1:A:129:VAL:CG1	1:A:145:TRP:HH2	2.22	0.47
2:B:112:SER:CA	2:B:138:TYR:HB3	2.43	0.47
1:A:118:SER:H	1:A:121:GLN:HB3	1.79	0.47
1:A:81:GLU:HB3	1:A:165:SER:O	2.14	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
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:138:TYR:CD1	2:B:138:TYR:C	2.88	0.47
2:B:40:PRO:O	2:B:41:SER:C	2.52	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:148:ASP:OD2	1:C:188:LEU:HD13	2.14	0.47
2:B:128:MET:CE	2:B:175:THR:HG21	2.45	0.47
2:B:129:VAL:HG21	2:B:181:TRP:NE1	2.25	0.47
1:C:178:LEU:HD22	1:C:182:ASP:CG	2.35	0.47
2:D:187:THR:HA	2:D:203:ILE:HD13	1.97	0.47
1:A:148:ASP:O	1:A:148:ASP:OD1	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
1:C:147:ILE:HD13	1:C:150:THR:HG21	1.96	0.47
1:A:10:LEU:HD11	1:A:105:GLU:HG3	1.96	0.47
1:A:211:CYS:HB2	2:B:206:ARG:HD3	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:89:THR:OG1	2:B:100(G):PHE:O	2.33	0.47
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:HG	2:D:82(C):LEU:H	1.19	0.47
1:C:188:LEU:N	1:C:188:LEU:CD1	2.61	0.47
1:A:121:GLN:N	2:B:115:PHE:CE2	2.82	0.47
1:A:37:GLN:HB2	1:A:86:TYR:CD2	2.49	0.47
1:A:7:SER:CB	1:A:8:PRO:CD	2.93	0.47
2:B:138:TYR:CE1	2:B:168:TYR:HB2	2.50	0.47
1:C:69:THR:HG23	1:C:70:ASP:CG	2.35	0.47
2:D:103:TRP:HZ2	2:D:168:TYR:OH	1.96	0.47
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:B:96:LEU:C	2:B:98:GLY:H	2.17	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:146:LYS:C	1:A:147:ILE:HG13	2.35	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
2:D:100(G):PHE:CD1	2:D:100(G):PHE:C	2.86	0.46
2:D:20:LEU:HD21	2:D:100(G):PHE:HE2	1.80	0.46
1:C:36:TYR:OH	2:D:100:TYR:O	2.24	0.46
2:D:100(G):PHE:HE2	2:D:102:PHE:HE2	1.63	0.46
2:B:139:PHE:CA	2:B:140:PRO:N	2.77	0.46
2:B:50:ARG:NH2	2:B:95:ASP:OD2	2.41	0.46
1:C:10:LEU:HD12	1:C:11:LEU:H	1.71	0.46
1:C:182:ASP:HA	1:C:185:SER:OG	2.16	0.46
1:C:187:ASN:HD22	1:C:207:ASN:C	2.19	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: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
1:C:179:THR:C	1:C:181:ALA:N	2.66	0.46
2:D:72:ASP:O	2:D:73:THR:O	2.33	0.46
1:A:152:ARG:CZ	1:A:152:ARG:HA	2.44	0.46
2:B:114:VAL:HB	2:B:199:VAL:HG11	1.98	0.46
2:B:52:TRP:CD1	2:B:56:TYR:CD2	3.03	0.46
1:C:10:LEU:HD12	1:C:10:LEU:C	2.34	0.46
1:C:145:TRP:NE1	1:C:156:VAL:HG21	2.30	0.46
1:C:4:LEU:HD21	1:C:90:GLN:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:THR:CG2	1:C:70:ASP:H	2.28	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:147:ILE:CG2	1:A:189:TYR:HE2	2.23	0.46
1:A:91:TYR:CD2	1:A:91:TYR:N	2.83	0.46
2:B:35:SER:O	2:B:92:CYS:HA	2.16	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:27:GLN:O	1:A:28:ASN:C	2.54	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
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:156:VAL:O	1:C:157:LEU:HD23	2.16	0.46
1:C:187:ASN:H	1:C:188:LEU:CD1	2.29	0.46
1:C:38:GLN:HG3	1:C:87:PHE:CE1	2.50	0.46
2:B:110:THR:HG21	2:B:167:LEU:CD1	2.37	0.46
1:C:156:VAL:HG23	1:C:175:THR:C	2.36	0.46
1:C:47:LEU:HD23	1:C:58:ILE:HD12	1.97	0.46
2:D:113:SER:N	2:D:136:LYS:O	2.49	0.46
2:B:38:ARG:HD2	2:B:48:MET:HE2	1.96	0.46
2:B:51:MET:O	2:B:52:TRP:O	2.33	0.46
1:C:107:ARG:NH1	1:C:107:ARG:CB	2.78	0.46
1:C:8:PRO:O	1:C:102:THR:HG23	2.15	0.46
1:C:188:LEU:H	1:C:188:LEU:HG	1.03	0.45
1:A:187:ASN:ND2	1:A:207:ASN:HB3	2.32	0.45
1:A:90:GLN:HE22	1:A:93:ASN:H	1.64	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
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:195:HIS:ND1	1:C:197:THR:CG2	2.80	0.45
2:D:114:VAL:HG21	2:D:190:VAL:CG2	2.44	0.45
2:B:152:LEU:CA	2:B:153:SER:N	2.71	0.45
2:B:153:SER:N	2:B:156:VAL:HG21	2.32	0.45
2:B:51:MET:SD	2:B:71:ARG:HG2	2.56	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:179:SER:O	2:D:182:SER:O	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:147:TRP:CZ3	2:D:203:ILE:HD12	2.51	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:N	1:C:148:ASP:OD1	2.49	0.45
2:D:146:THR:O	2:D:189:ASN:HB2	2.17	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
1:A:180:LYS:HE2	1:A:184:GLU:CD	2.33	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:139:ARG:O	1:C:139:ARG:HD3	2.17	0.45
1:C:52:ASN:HA	1:C:64:GLY:HA3	1.98	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:76:ASN:C	2:B:77:GLN:HG2	2.37	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:OD1	1:A:140:ASP:O	2.35	0.45
1:A:209:ASN:N	1:A:209:ASN:OD1	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:D:13:ARG:C	2:D:14:PRO:O	2.55	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
1:C:147:ILE:O	1:C:150:THR:N	2.50	0.45
1:A:211:CYS:HA	2:B:121:SER:N	2.27	0.45
1:A:48:ILE:HD12	1:A:64:GLY:HA3	1.95	0.45
2:B:139:PHE:CE1	2:B:140:PRO:HA	2.52	0.45
2:B:148:ASN:O	2:B:149:SER:C	2.55	0.45
2:B:127:SER:O	2:B:177:PRO:HA	2.15	0.45
1:C:148:ASP:C	1:C:150:THR:H	2.20	0.45
1:C:147:ILE:HD12	1:C:152:ARG:H	1.78	0.45
1:C:61:ARG:O	1:C:75:ILE:HA	2.17	0.45
1:C:24:LYS:HA	1:C:69:THR:O	2.16	0.45
1:A:10:LEU:HD11	1:A:105:GLU:CG	2.47	0.44
1:A:30:ASN:C	1:A:32:TYR:H	2.21	0.44
2:B:39:HIS:CE1	2:B:43:LYS:O	2.70	0.44
1:C:110:PRO:HA	1:C:136:PHE:CB	2.47	0.44
1:C:90:GLN:HE22	1:C:93:ASN:N	2.15	0.44
2:D:128:MET:SD	2:D:177:PRO:HA	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:153:ARG:CG	1:A:153:ARG:O	2.62	0.44
1:A:81:GLU:N	1:A:165:SER:O	2.50	0.44
1:A:187:ASN:HD22	1:A:207:ASN:CB	2.30	0.44
1:A:78:LEU:HA	1:A:78:LEU:HD23	1.76	0.44
2:B:116:PRO:HG3	2:B:201:LYS:HD2	1.99	0.44
1:C:106:LEU:N	1:C:106:LEU:HD12	2.30	0.44
2:D:139:PHE:HB2	2:D:167:LEU:HD23	1.99	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
1:A:177:SER:O	1:A:178:LEU:HD23	2.16	0.44
1:A:31:ASN:HA	1:A:71:TYR:CE2	2.49	0.44
1:A:211:CYS:C	2:B:121:SER:OG	2.56	0.44
2:B:165:SER:O	2:B:165:SER:OG	2.33	0.44
2:B:161:ALA:CB	2:B:170:LEU:HD23	2.46	0.44
2:B:47:TRP:O	2:B:48:MET:HA	2.17	0.44
1:A:208:ARG:C	1:A:210:GLU:H	2.20	0.44
2:B:148:ASN:C	2:B:150:GLY:N	2.69	0.44
2:B:148:ASN:HA	2:B:148:ASN:HD22	1.43	0.44
2:B:145:VAL:HG13	2:B:190:VAL:HG22	2.00	0.44
1:C:133:MET:HE3	1:C:193:VAL:HG22	2.00	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:N	1:C:21:LEU:HD12	2.32	0.44
2:D:82(A):ASN:O	2:D:82(B):SER:HB3	2.17	0.44
1:A:137:TYR:CG	1:A:138:PRO:N	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:73:THR:O	2:B:74:SER:C	2.56	0.44
1:C:159:SER:O	1:C:172:MET:CG	2.65	0.44
2:D:163:LEU:HD13	2:D:168:TYR:CD2	2.53	0.44
2:D:88:GLY:O	2:D:102:PHE:HB2	2.17	0.44
1:A:106:LEU:C	1:A:106(A):LYS:HG3	2.38	0.44
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:133:MET:HE1	1:A:143:VAL:CG1	2.46	0.44
1:A:147:ILE:HD13	1:A:152:ARG:HG2	2.00	0.44
1:A:35:TRP:CD2	1:A:73:LEU:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLN:O	1:A:39:LYS:CB	2.66	0.44
1:A:91:TYR:CD1	2:B:98:GLY:HA3	2.53	0.44
1:C:133:MET:HE3	1:C:143:VAL:HG13	1.99	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:181:ALA:O	1:C:184:GLU:HB3	2.17	0.43
1:C:39:LYS:O	1:C:40:LEU:O	2.36	0.43
2:D:147:TRP:HA	2:D:188:CYS:HA	2.00	0.43
2:D:34:VAL:HA	2:D:93:THR:O	2.17	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:187:THR:HA	2:D:203:ILE:CD1	2.48	0.43
2:D:2:VAL:HB	2:D:100(B):LEU:HG	1.99	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:C:117:PRO:CG	1:C:127:ALA:HB1	2.48	0.43
1:A:183:TYR:C	1:A:184:GLU:CA	2.85	0.43
2:B:100(C):GLY:O	2:B:100(D):PHE:CG	2.71	0.43
2:B:3:GLN:HB2	2:B:25:SER:HB2	2.01	0.43
1:C:102:THR:HG22	1:C:103:LYS:O	2.19	0.43
1:C:180:LYS:HZ1	1:C:184:GLU:HB2	1.83	0.43
2:D:141:GLU:HG2	2:D:168:TYR:CD1	2.54	0.43
2:D:18:LEU:HD23	2:D:18:LEU:HA	1.70	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
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:B:52:TRP:CE2	2:B:56:TYR:HD2	2.37	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
2:B:139:PHE:O	2:B:140:PRO:CD	2.63	0.43
1:C:120:GLU:N	1:C:120:GLU:CD	2.72	0.43
1:C:145:TRP:CZ3	1:C:176:LEU:HD22	2.53	0.43
1:C:89:TYR:HE2	2:D:99:GLY:HA2	1.84	0.43
1:A:145:TRP:CH2	1:A:176:LEU:HD22	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:VAL:CG1	2:B:190:VAL:CG2	2.97	0.43
2:D:139:PHE:C	2:D:139:PHE:CD2	2.92	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:122:LEU:C	1:C:124:THR:N	2.70	0.43
1:C:206:PHE:C	1:C:206:PHE:CD2	2.92	0.43
1:C:209:ASN:N	1:C:209:ASN:OD1	2.52	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: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:144:LYS:O	1:C:191:CYS:HA	2.19	0.42
1:C:78:LEU:HD23	1:C:78:LEU:HA	1.69	0.42
2:D:69:ILE:CG2	2:D:70:SER:N	2.82	0.42
2:B:138:TYR:OH	2:B:170:LEU:HD21	2.19	0.42
2:B:13:ARG:HB2	2:B:16:GLU:CD	2.39	0.42
1:A:171:SER:HG	2:B:157:HIS:HE1	1.50	0.42
2:B:51:MET:CE	2:B:55:GLY:HA2	2.49	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
1:C:25:GLY:CA	1:C:29:ILE:HD11	2.44	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:127:SER:C	2:B:128:MET:CB	2.87	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:C:49:TYR:O	1:C:50:ASN:C	2.58	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:H	2:D:16:GLU:HG2	1.60	0.42
1:A:139:ARG:NH2	1:A:160:VAL:HG21	2.34	0.42
1:C:99:GLY:O	1:C:100:ALA:C	2.56	0.42
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:211:CYS:HA	2:D:120:GLY:O	2.16	0.42
1:C:80:PRO:HA	1:C:106:LEU:CD2	2.50	0.42
2:D:91:TYR:CE2	2:D:100(F):TYR:HA	2.55	0.42
2:D:32:PHE:CE2	2:D:94:ARG:NH1	2.87	0.42
1:A:196:LYS:N	1:A:197:THR:N	2.62	0.42
2:B:130:THR:HG23	2:B:130:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:ARG:CG	2:B:40:PRO:HD3	2.48	0.42
1:C:49:TYR:HD1	1:C:50:ASN:HB2	1.85	0.42
2:D:102:PHE:O	2:D:103:TRP:C	2.57	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:133:MET:CE	1:A:193:VAL:HG13	2.49	0.42
1:A:179:THR:O	1:A:180:LYS:C	2.56	0.42
1:A:180:LYS:C	1:A:184:GLU:HG3	2.40	0.42
1:A:94:GLY:CA	1:A:96:TYR:HD1	2.32	0.42
2:D:129:VAL:O	2:D:129:VAL:HG13	2.18	0.42
2:D:14:PRO:O	2:D:16:GLU:CG	2.64	0.42
1:A:29:ILE:CG1	1:A:71:TYR:CZ	3.02	0.42
1:A:30:ASN:C	1:A:32:TYR:N	2.73	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
2:B:69:ILE:CG2	2:B:70:SER:N	2.82	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
1:C:133:MET:HE3	1:C:193:VAL:HG13	2.02	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: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:A:52:ASN:C	1:A:52:ASN:OD1	2.58	0.42
1:C:124:THR:C	1:C:126:GLY:H	2.22	0.42
1:C:208:ARG:HB3	1:C:209:ASN:H	1.63	0.42
1:C:54:LEU:HD13	1:C:55:GLN:O	2.19	0.42
1:C:211:CYS:HB2	2:D:206:ARG:HD3	2.02	0.42
2:D:158:THR:O	2:D:158:THR:OG1	2.38	0.41
2:D:179:SER:OG	2:D:180:THR:N	2.52	0.41
1:A:120:GLU:C	1:A:122:LEU:N	2.73	0.41
1:A:81:GLU:CB	1:A:165:SER:O	2.67	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
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:147:ILE:CD1	1:C:152:ARG:N	2.74	0.41
1:A:118:SER:C	1:A:120:GLU:N	2.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:TYR:O	1:A:206:PHE:HB3	2.20	0.41
1:A:64:GLY:O	1:A:65:SER:HB2	2.19	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:C:120:GLU:O	1:C:121:GLN:C	2.58	0.41
1:C:39:LYS:O	1:C:40:LEU:C	2.59	0.41
1:A:167:ASP:O	1:A:167:ASP:CG	2.50	0.41
1:C:106:LEU:N	1:C:163:GLN:OE1	2.52	0.41
1:C:48:ILE:HG12	1:C:49:TYR:N	2.36	0.41
1:C:91:TYR:N	1:C:91:TYR:CD2	2.88	0.41
2:D:119:PRO:C	2:D:121:SER:H	2.21	0.41
2:D:146:THR:OG1	2:D:146:THR:O	2.33	0.41
1:A:12:SER:CA	1:A:105:GLU:O	2.68	0.41
1:A:132:LEU:CD2	1:A:173:SER:CB	2.81	0.41
1:A:36:TYR:CE2	1:A:46:LEU:HB2	2.55	0.41
1:C:96:TYR:CD1	1:C:96:TYR:N	2.89	0.41
2:D:103:TRP:HB2	2:D:140:PRO:CB	2.46	0.41
2:D:153:SER:H	2:D:156:VAL:HG21	1.85	0.41
1:A:173:SER:N	2:B:159:PHE:CD1	2.88	0.41
1:A:138:PRO:CG	1:A:196:LYS:HE3	2.51	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
2:B:181:TRP:O	2:B:184:GLN:O	2.39	0.41
1:C:129:VAL:CG1	1:C:206:PHE:HE1	2.33	0.41
1:A:139:ARG:CZ	1:A:160:VAL:HG21	2.51	0.41
1:A:7:SER:HG	1:A:8:PRO:HD2	1.82	0.41
1:A:94:GLY:HA2	1:A:96:TYR:HD1	1.83	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: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: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
1:A:65:SER:O	1:A:72:THR:HG23	2.21	0.41
2:B:179:SER:C	2:B:180:THR:HA	2.37	0.41
2:D:103:TRP:NE1	2:D:168:TYR:OH	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:176:VAL:HB	2:D:177:PRO:HD2	2.03	0.41
1:A:121:GLN:HA	2:B:115:PHE:CD2	2.54	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
2:B:51:MET:C	2:B:52:TRP:O	2.59	0.41
1:C:150:THR:HG22	1:C:151:GLU:N	2.36	0.41
1:C:144:LYS:HB3	1:C:192:GLU:HB2	2.02	0.41
1:C:61:ARG:HH21	1:C:82:ASP:CG	2.25	0.41
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
2:B:28:SER:C	2:B:30:THR:H	2.24	0.40
2:B:2:VAL:HG13	2:B:27:PHE:CE1	2.56	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
2:B:159:PHE:C	2:B:160:PRO:O	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: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
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
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:B:33:SER:OG	2:B:52:TRP:HA	2.21	0.40
2:D:129:VAL:HG12	2:D:176:VAL:HG22	2.01	0.40
2:D:13:ARG:CA	2:D:16:GLU:HG3	2.52	0.40
1:A:159:SER:O	1:A:172:MET:CG	2.68	0.40
2:B:100(E):TRP:CD1	3:B:221:HOH:O	2.57	0.40
2:B:164:GLN:HG3	2:B:165:SER:H	1.86	0.40
2:B:164:GLN:C	2:B:166:GLY:N	2.75	0.40
2:B:3:GLN:CG	3:B:219:HOH:O	2.49	0.40
1:C:29:ILE:O	1:C:30:ASN:C	2.60	0.40
2:D:20:LEU:CD2	2:D:102:PHE:HE2	2.17	0.40
2:D:103:TRP:HE1	2:D:168:TYR:HH	1.58	0.40
2:B:114:VAL:HG11	2:B:201:LYS:HB2	2.04	0.40
2:B:80:LEU:HA	2:B:80:LEU:HD23	1.95	0.40
1:C:120:GLU:N	1:C:120:GLU:OE2	2.54	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 (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	192/211 (91%)	120 (62%)	35 (18%)	37 (19%)	0	0
1	C	209/211 (99%)	151 (72%)	31 (15%)	27 (13%)	0	1
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	1
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	128 (68%)	60 (32%)	0 0
1	C	188/188 (100%)	111 (59%)	77 (41%)	0 0
2	B	189/189 (100%)	136 (72%)	53 (28%)	0 1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	189/189 (100%)	120 (64%)	69 (36%)	0 0
All	All	754/754 (100%)	495 (66%)	259 (34%)	0 0

All (259) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	10	LEU
1	A	11	LEU
1	A	12	SER
1	A	14	SER
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
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	107	ARG
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

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Mol	Chain	Res	Type
1	A	140	ASP
1	A	141	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	191	CYS
1	A	192	GLU
1	A	194	VAL
1	A	196	LYS
1	A	202	VAL
1	A	205	SER
1	A	210	GLU
2	B	1	GLN
2	B	6	GLU
2	B	7	SER
2	B	18	LEU
2	B	19	SER
2	B	23	THR
2	B	28	SER
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	71	ARG

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Mol	Chain	Res	Type
2	B	75	LYS
2	B	77	GLN
2	B	80	LEU
2	B	82(A)	ASN
2	B	82(B)	SER
2	B	84	THR
2	B	89	THR
2	B	100	TYR
2	B	100(E)	TRP
2	B	100(F)	TYR
2	B	103	TRP
2	B	107	THR
2	B	111	VAL
2	B	112	SER
2	B	113	SER
2	B	125	THR
2	B	127	SER
2	B	131	LEU
2	B	141	GLU
2	B	148	ASN
2	B	152	LEU
2	B	157	HIS
2	B	159	PHE
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	187	THR
2	B	189	ASN
2	B	195	SER
2	B	198	LYS
2	B	204	VAL
2	B	207	ASP
1	C	3	LYS
1	C	6	GLN
1	C	10	LEU
1	C	11	LEU
1	C	12	SER
1	C	14	SER
1	C	17	ASP

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Mol	Chain	Res	Type
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	45	LYS
1	C	48	ILE
1	C	50	ASN
1	C	51	THR
1	C	53	SER
1	C	54	LEU
1	C	55	GLN
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	106(A)	LYS
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	133	MET
1	C	139	ARG
1	C	141	ILE
1	C	142	SER

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Mol	Chain	Res	Type
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	164	ASP
1	C	166	LYS
1	C	172	MET
1	C	173	SER
1	C	174	SER
1	C	175	THR
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	196	LYS
1	C	202	VAL
1	C	205	SER
1	C	206	PHE
1	C	210	GLU
2	D	1	GLN
2	D	3	GLN
2	D	6	GLU
2	D	7	SER
2	D	15	SER
2	D	18	LEU
2	D	19	SER
2	D	23	THR
2	D	25	SER
2	D	35	SER
2	D	38	ARG
2	D	39	HIS
2	D	41	SER
2	D	43	LYS

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Mol	Chain	Res	Type
2	D	57	THR
2	D	61	SER
2	D	65	SER
2	D	66	ARG
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	82(A)	ASN
2	D	82(B)	SER
2	D	82(C)	LEU
2	D	85	ASP
2	D	89	THR
2	D	94	ARG
2	D	100	TYR
2	D	100(B)	LEU
2	D	100(E)	TRP
2	D	101	ASP
2	D	102	PHE
2	D	103	TRP
2	D	105	PRO
2	D	107	THR
2	D	112	SER
2	D	113	SER
2	D	125	THR
2	D	127	SER
2	D	128	MET
2	D	131	LEU
2	D	136	LYS
2	D	139	PHE
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

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Mol	Chain	Res	Type
2	D	172	SER
2	D	176	VAL
2	D	181	TRP
2	D	183	SER
2	D	184	GLN
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
2	D	207	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	37	GLN
1	A	55	GLN
1	A	90	GLN
1	A	93	ASN
1	A	135	ASN
1	A	187	ASN
2	B	39	HIS
2	B	77	GLN
2	B	148	ASN
2	B	157	HIS
2	B	164	GLN
1	C	28	ASN
1	C	30	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	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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
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
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.