



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:52 AM UTC

PDB ID : 1QAB / pdb_00001qab
Title : The structure of human retinol binding protein with its carrier protein transthyretin reveals interaction with the carboxy terminus of RBP
Authors : Naylor, H.M.; Newcomer, M.E.
Deposited on : 1999-02-03
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

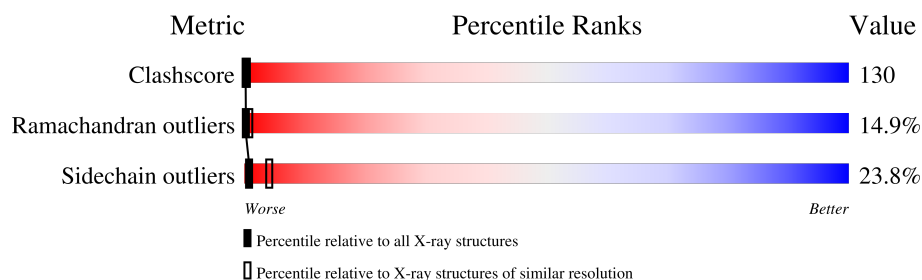
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	127	38% 46% 14% •
1	B	127	23% 48% 20% • 7%
1	C	127	30% 41% 16% • 10%
1	D	127	17% 44% 25% • 11%
2	E	180	7% 46% 35% 13%
2	F	180	• 43% 39% 9% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	RTL	E	1	-	-	X	-
3	RTL	F	2	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6454 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

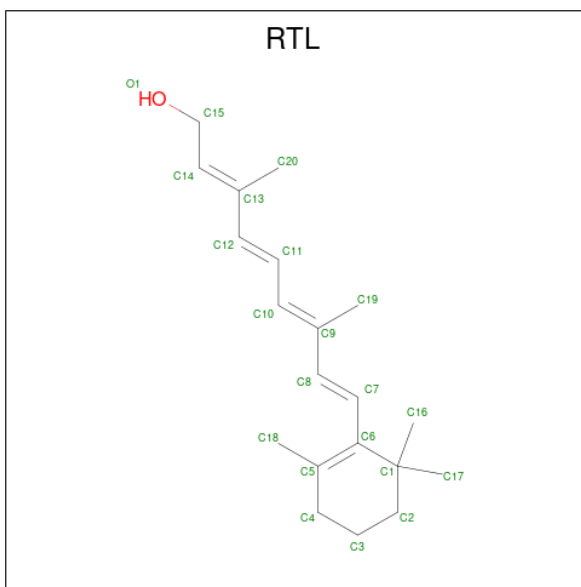
- Molecule 1 is a protein called PROTEIN (transthyretin).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	124	Total	C	N	O	S	0	0	0
			946	601	157	186	2			
1	B	118	Total	C	N	O	S	0	0	0
			915	584	151	178	2			
1	C	114	Total	C	N	O	S	0	0	0
			881	564	145	170	2			
1	D	113	Total	C	N	O	S	0	0	0
			874	560	144	168	2			

- Molecule 2 is a protein called PROTEIN (retinol binding protein).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	180	Total	C	N	O	S	0	0	0
			1435	902	245	278	10			
2	F	171	Total	C	N	O	S	0	0	0
			1361	860	229	262	10			

- Molecule 3 is RETINOL (CCD ID: RTL) (formula: C₂₀H₃₀O).



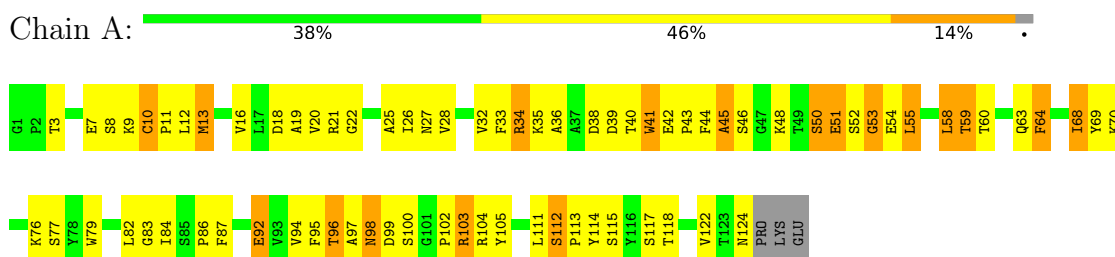
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			21	20	1		
3	F	1	Total	C	O	0	0
			21	20	1		

3 Residue-property plots

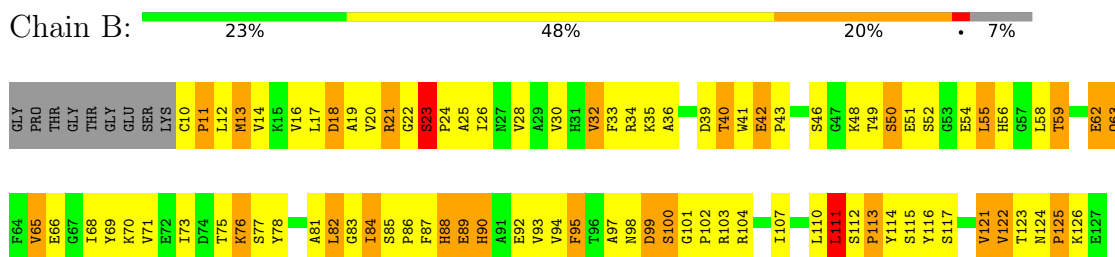
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

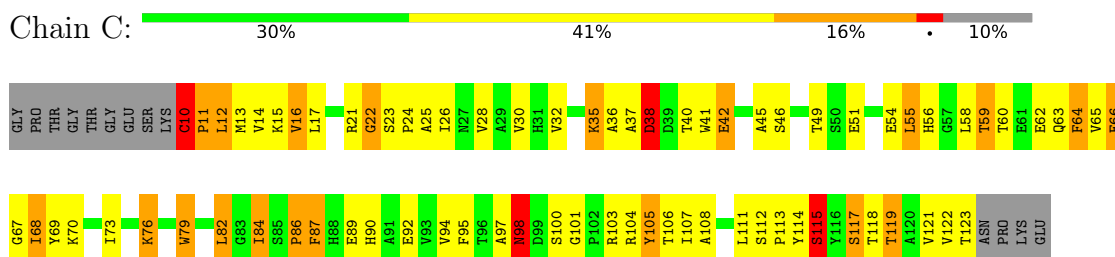
• Molecule 1: PROTEIN (transthyretin)



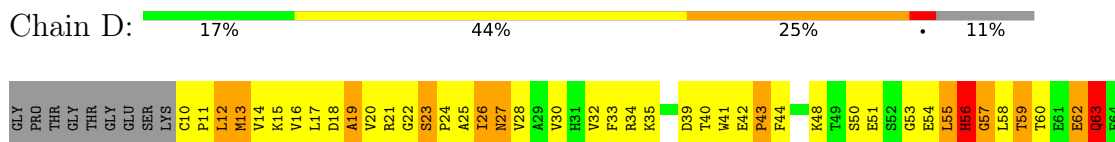
• Molecule 1: PROTEIN (transthyretin)

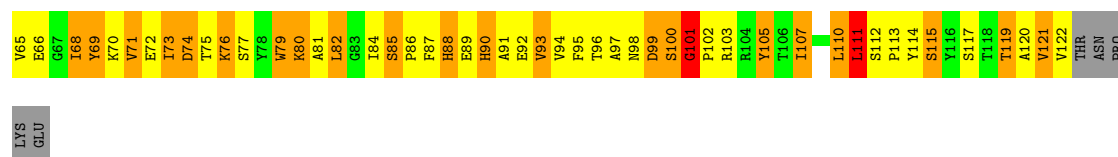


• Molecule 1: PROTEIN (transthyretin)



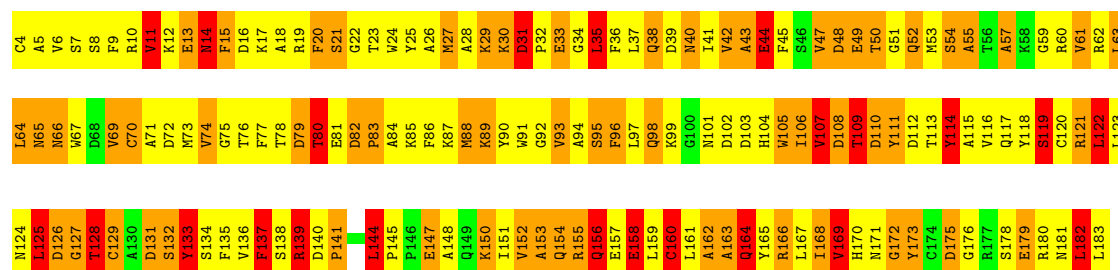
• Molecule 1: PROTEIN (transthyretin)





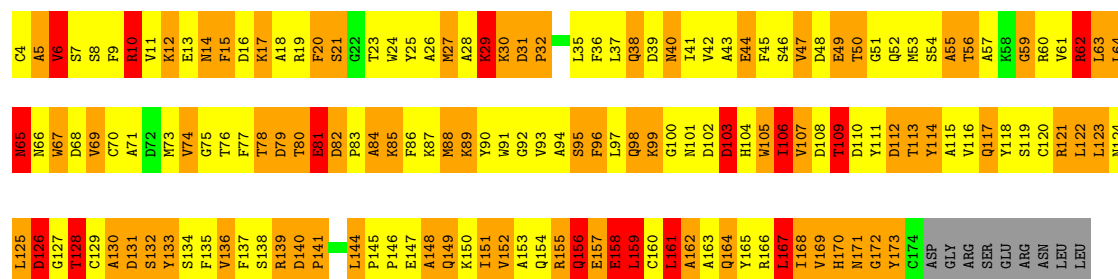
• Molecule 2: PROTEIN (retinol binding protein)

Chain E: 7% 46% 35% 13%



• Molecule 2: PROTEIN (retinol binding protein)

Chain F: 43% 39% 9% 5%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	140.23Å 140.23Å 124.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.20 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (6.20-3.20)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.278 , 0.403	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6454	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.68	0/970	1.17	7/1322 (0.5%)
1	B	0.67	0/939	1.19	11/1279 (0.9%)
1	C	0.75	0/904	1.32	13/1233 (1.1%)
1	D	0.72	1/897 (0.1%)	1.50	23/1223 (1.9%)
2	E	0.69	0/1467	1.34	29/1984 (1.5%)
2	F	0.69	0/1393	1.19	14/1887 (0.7%)
All	All	0.70	1/6570 (0.0%)	1.28	97/8928 (1.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	14	VAL	CA-CB	-5.28	1.47	1.54

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	85	SER	CA-C-N	12.86	134.51	120.11
1	D	85	SER	C-N-CA	12.86	134.51	120.11
1	D	63	GLN	N-CA-C	-10.94	99.77	113.55
1	D	23	SER	CA-C-N	10.55	130.63	119.76
1	D	23	SER	C-N-CA	10.55	130.63	119.76
1	D	19	ALA	N-CA-C	-9.49	101.82	113.97
1	C	122	VAL	N-CA-C	9.48	121.65	107.15
2	E	166	ARG	N-CA-C	-9.27	95.99	110.36
2	E	144	LEU	CA-C-N	8.79	129.43	120.38
2	E	144	LEU	C-N-CA	8.79	129.43	120.38
1	A	53	GLY	N-CA-C	-8.50	102.88	115.72
2	E	20	PHE	N-CA-C	-8.46	101.94	113.18
1	B	88	HIS	N-CA-C	8.20	120.36	110.19
1	A	51	GLU	N-CA-C	-8.12	102.00	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	103	ASP	N-CA-C	-7.82	100.19	110.43
1	D	26	ILE	N-CA-C	7.79	119.44	108.93
1	B	82	LEU	N-CA-C	-7.67	104.05	113.41
2	E	64	LEU	N-CA-C	7.59	121.86	111.39
2	E	57	ALA	N-CA-C	7.57	121.32	109.96
1	D	107	ILE	CB-CA-C	-7.46	102.25	111.88
2	E	154	GLN	N-CA-C	-7.46	103.80	113.12
2	E	158	GLU	N-CA-C	-7.30	104.62	113.97
1	D	111	LEU	N-CA-C	7.26	121.08	109.24
2	E	129	CYS	N-CA-C	7.23	120.57	108.13
2	E	173	TYR	N-CA-C	7.19	122.25	112.68
2	E	11	VAL	CB-CA-C	-7.07	105.09	111.74
2	F	140	ASP	CA-C-N	7.05	128.65	119.84
2	F	140	ASP	C-N-CA	7.05	128.65	119.84
1	D	101	GLY	CA-C-N	6.98	128.02	120.13
1	D	101	GLY	C-N-CA	6.98	128.02	120.13
2	E	163	ALA	N-CA-C	6.91	119.78	108.52
1	C	56	HIS	N-CA-C	6.90	119.64	110.53
1	C	76	LYS	N-CA-C	6.80	120.46	111.75
1	C	54	GLU	N-CA-C	6.70	120.44	110.52
1	C	23	SER	CA-C-N	-6.70	112.61	120.11
1	C	23	SER	C-N-CA	-6.70	112.61	120.11
1	C	111	LEU	N-CA-C	6.69	120.57	109.46
2	E	164	GLN	N-CA-C	-6.64	103.85	112.68
2	F	59	GLY	N-CA-C	6.60	120.75	110.91
1	B	89	GLU	N-CA-C	-6.58	105.83	114.31
1	D	88	HIS	N-CA-C	6.45	120.02	110.48
1	C	10	CYS	CA-C-N	6.43	127.88	119.84
1	C	10	CYS	C-N-CA	6.43	127.88	119.84
2	E	150	LYS	N-CA-C	-6.35	104.28	111.14
2	E	10	ARG	N-CA-C	6.33	119.67	109.86
1	D	79	TRP	N-CA-C	-6.33	104.61	112.90
1	A	58	LEU	N-CA-C	-6.11	105.78	113.72
2	F	128	THR	N-CA-C	6.11	123.81	110.80
1	C	38	ASP	N-CA-C	6.08	120.99	112.72
1	D	74	ASP	N-CA-C	-6.07	100.42	109.15
1	D	107	ILE	N-CA-C	5.92	116.20	107.15
2	F	112	ASP	N-CA-C	5.85	118.25	107.73
2	F	106	ILE	N-CA-C	-5.84	97.18	109.34
1	B	111	LEU	N-CA-C	5.83	118.45	109.07
1	C	115	SER	N-CA-C	5.82	117.53	107.93
2	E	63	LEU	N-CA-C	5.81	123.18	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	81	ALA	N-CA-C	-5.79	104.56	111.69
1	D	62	GLU	N-CA-C	5.75	119.92	113.02
2	F	32	PRO	N-CA-C	-5.73	103.20	111.22
2	E	156	GLN	N-CA-C	-5.72	105.89	112.92
2	E	61	VAL	N-CA-C	5.70	116.68	108.48
1	C	87	PHE	N-CA-C	-5.70	105.98	114.64
1	A	112	SER	CA-C-N	5.67	126.92	119.84
1	A	112	SER	C-N-CA	5.67	126.92	119.84
2	E	169	VAL	N-CA-C	5.64	116.22	107.99
1	A	92	GLU	N-CA-C	5.60	118.36	109.24
1	D	72	GLU	N-CA-C	5.55	117.78	108.96
2	E	137	PHE	N-CA-C	5.52	118.60	110.59
2	E	133	TYR	N-CA-C	-5.51	99.06	110.80
1	B	62	GLU	CB-CA-C	-5.50	104.30	111.40
2	E	40	ASN	N-CA-C	-5.47	103.69	111.24
1	B	65	VAL	N-CA-C	5.46	117.58	109.17
2	E	107	VAL	N-CA-C	5.41	120.59	109.34
2	F	155	ARG	N-CA-C	-5.39	99.31	110.80
1	D	59	THR	N-CA-C	5.39	115.50	108.07
1	D	105	TYR	N-CA-C	5.35	117.95	109.24
2	F	107	VAL	N-CA-C	5.33	116.11	110.72
2	E	10	ARG	CA-C-N	5.33	127.30	121.97
2	E	10	ARG	C-N-CA	5.33	127.30	121.97
1	B	99	ASP	N-CA-C	-5.30	106.65	113.01
1	D	73	ILE	N-CA-C	5.27	115.17	107.37
1	C	84	ILE	CB-CA-C	-5.23	102.45	110.50
2	E	153	ALA	N-CA-C	-5.23	106.69	114.64
2	E	139	ARG	N-CA-C	5.22	119.50	113.18
2	F	152	VAL	N-CA-C	-5.19	104.41	111.89
1	B	42	GLU	CA-C-N	5.17	126.31	119.84
1	B	42	GLU	C-N-CA	5.17	126.31	119.84
1	B	113	PRO	N-CA-C	5.17	121.45	113.75
1	D	99	ASP	N-CA-C	-5.16	106.08	112.38
1	A	45	ALA	N-CA-C	5.15	116.78	108.34
1	B	95	PHE	N-CA-C	5.14	116.89	108.55
2	F	40	ASN	N-CA-C	-5.13	104.34	111.52
2	E	127	GLY	N-CA-C	-5.12	101.05	113.18
2	E	42	VAL	N-CA-C	5.11	115.27	108.11
1	D	18	ASP	N-CA-C	-5.04	102.31	110.32
2	F	20	PHE	N-CA-C	-5.03	106.45	112.59
2	F	65	ASN	N-CA-C	5.01	121.47	110.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	946	0	921	146	0
1	B	915	0	890	208	0
1	C	881	0	856	109	0
1	D	874	0	851	207	0
2	E	1435	0	1356	524	15
2	F	1361	0	1285	534	16
3	E	21	0	29	12	0
3	F	21	0	29	15	0
All	All	6454	0	6217	1647	16

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 130.

All (1647) 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)
2:F:20:PHE:HE2	2:F:45:PHE:CE1	1.20	1.56
2:F:28:ALA:HB3	2:F:136:VAL:CG2	1.38	1.51
2:F:6:VAL:CG1	2:F:129:CYS:HB2	1.43	1.45
1:B:18:ASP:OD2	1:B:21:ARG:CG	1.64	1.43
2:F:20:PHE:CE2	2:F:45:PHE:CE1	2.07	1.40
2:F:103:ASP:OD1	2:F:105:TRP:CH2	1.75	1.39
1:B:18:ASP:CG	1:B:21:ARG:HG3	1.47	1.37
2:F:160:CYS:C	2:F:161:LEU:HD23	1.50	1.36
2:E:32:PRO:HG3	2:E:133:TYR:CB	1.54	1.35
2:F:30:LYS:HE3	2:F:31:ASP:N	1.41	1.34
2:F:122:LEU:HD23	2:F:123:LEU:N	1.39	1.34
1:B:104:ARG:O	1:B:122:VAL:CG2	1.74	1.34
2:F:160:CYS:C	2:F:161:LEU:CD2	2.02	1.32
2:E:38:GLN:CB	2:E:60:ARG:O	1.75	1.32
2:F:133:TYR:HD1	2:F:133:TYR:O	1.06	1.32
2:F:85:LYS:HD3	2:F:105:TRP:CD1	1.65	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:77:PHE:HE2	2:F:104:HIS:CD2	1.49	1.31
2:F:28:ALA:CB	2:F:136:VAL:HG21	1.58	1.30
2:E:123:LEU:HD12	2:E:128:THR:O	1.33	1.29
2:E:32:PRO:HB3	2:E:132:SER:O	1.31	1.28
2:F:133:TYR:O	2:F:133:TYR:CD1	1.87	1.28
1:B:104:ARG:O	1:B:122:VAL:HG21	1.19	1.26
2:F:28:ALA:O	2:F:29:LYS:HG2	1.24	1.26
2:F:90:TYR:HE1	2:F:102:ASP:OD2	1.10	1.26
1:B:102:PRO:CB	1:B:123:THR:O	1.84	1.25
2:F:5:ALA:HA	2:F:128:THR:OG1	1.34	1.25
1:B:102:PRO:CG	1:B:123:THR:O	1.84	1.24
2:E:164:GLN:O	2:E:165:TYR:CG	1.92	1.22
1:A:64:PHE:HE1	1:A:69:TYR:CE2	1.56	1.22
2:F:37:LEU:HA	2:F:61:VAL:CG2	1.68	1.22
1:D:87:PHE:HD2	1:D:88:HIS:CD2	1.55	1.22
2:F:38:GLN:HB2	2:F:60:ARG:O	1.31	1.21
1:B:102:PRO:HG3	1:B:123:THR:O	1.33	1.21
2:E:9:PHE:CE2	2:E:160:CYS:HB3	1.74	1.21
2:F:103:ASP:OD1	2:F:105:TRP:CZ2	1.93	1.21
2:E:153:ALA:N	2:E:156:GLN:HE22	1.40	1.20
2:E:38:GLN:HE21	2:E:60:ARG:NH2	1.37	1.19
2:E:152:VAL:C	2:E:156:GLN:HE22	1.51	1.18
1:A:13:MET:CE	1:A:104:ARG:HH12	1.57	1.18
2:E:6:VAL:H	2:E:128:THR:HB	1.08	1.18
1:A:26:ILE:HG13	1:A:50:SER:O	1.42	1.17
1:A:64:PHE:CE1	1:A:69:TYR:CE2	2.32	1.17
1:A:79:TRP:CH2	1:A:113:PRO:HD3	1.78	1.17
1:D:87:PHE:CD2	1:D:88:HIS:CD2	2.32	1.17
1:B:13:MET:HG3	1:B:56:HIS:CD2	1.78	1.17
2:F:66:ASN:CG	2:F:67:TRP:H	1.52	1.16
1:D:114:TYR:OH	2:E:95:SER:HB2	1.43	1.15
2:E:114:TYR:CG	2:E:114:TYR:O	1.98	1.15
1:A:18:ASP:OD2	1:A:21:ARG:CD	1.92	1.15
2:E:29:LYS:HB2	2:E:29:LYS:NZ	1.57	1.15
2:F:73:MET:HE1	2:F:97:LEU:HB3	1.18	1.15
1:B:102:PRO:HB2	1:B:122:VAL:HG12	1.29	1.14
1:A:18:ASP:OD2	1:A:21:ARG:HD3	1.46	1.14
1:A:79:TRP:CZ2	1:A:113:PRO:HD3	1.80	1.14
1:B:104:ARG:C	1:B:122:VAL:HG21	1.73	1.14
2:E:108:ASP:O	2:E:109:THR:HG22	1.45	1.14
2:F:37:LEU:HD23	2:F:61:VAL:CG2	1.78	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:88:MET:SD	2:F:104:HIS:HD2	1.70	1.13
2:F:90:TYR:CE1	2:F:102:ASP:OD2	2.02	1.13
1:B:12:LEU:HD11	1:B:107:ILE:CD1	1.79	1.12
2:E:9:PHE:HE2	2:E:160:CYS:HB3	1.02	1.12
2:F:85:LYS:HD3	2:F:105:TRP:NE1	1.64	1.12
1:B:20:VAL:HG11	2:F:64:LEU:HD21	1.16	1.12
1:B:75:THR:HG22	1:B:111:LEU:CD1	1.80	1.12
2:F:157:GLU:OE2	2:F:157:GLU:CA	1.97	1.12
2:E:153:ALA:CA	2:E:156:GLN:HE22	1.61	1.12
2:F:5:ALA:HA	2:F:128:THR:CB	1.79	1.12
1:C:115:SER:HB2	1:D:119:THR:OG1	1.47	1.12
2:E:19:ARG:O	2:E:111:TYR:CB	1.97	1.12
2:E:116:VAL:HG12	2:E:117:GLN:H	1.05	1.12
1:B:121:VAL:CG1	1:B:122:VAL:H	1.60	1.11
2:E:78:THR:OG1	2:E:87:LYS:HB2	1.48	1.11
1:A:18:ASP:OD2	1:A:21:ARG:NE	1.83	1.11
1:C:65:VAL:O	1:C:69:TYR:OH	1.67	1.11
2:F:122:LEU:HD23	2:F:122:LEU:C	1.72	1.11
1:B:102:PRO:HG3	1:B:123:THR:C	1.75	1.10
2:E:73:MET:HE1	2:E:97:LEU:HD13	1.31	1.10
2:F:27:MET:HE1	2:F:144:LEU:HD11	1.27	1.10
2:E:170:HIS:O	2:E:171:ASN:ND2	1.82	1.10
2:F:65:ASN:C	2:F:65:ASN:HD22	1.60	1.10
2:F:160:CYS:O	2:F:161:LEU:HD22	1.51	1.10
1:D:16:VAL:O	1:D:17:LEU:HD23	1.49	1.10
1:B:87:PHE:CD2	1:B:88:HIS:HD2	1.69	1.09
2:E:182:LEU:CD2	2:E:183:LEU:H	1.64	1.09
2:F:77:PHE:CE2	2:F:104:HIS:CD2	2.39	1.09
1:B:34:ARG:NH2	1:B:65:VAL:HG23	1.67	1.09
2:E:69:VAL:HA	2:E:182:LEU:HG	1.34	1.09
2:E:159:LEU:HD12	2:E:162:ALA:N	1.67	1.09
1:B:87:PHE:CD2	1:B:88:HIS:CD2	2.41	1.09
1:B:87:PHE:HD2	1:B:88:HIS:CD2	1.69	1.09
1:D:54:GLU:HB3	1:D:56:HIS:CE1	1.86	1.09
2:F:13:GLU:O	2:F:15:PHE:N	1.83	1.09
2:F:37:LEU:HA	2:F:61:VAL:HG22	1.34	1.09
2:E:181:ASN:O	2:E:182:LEU:HB2	1.50	1.09
2:F:6:VAL:HG12	2:F:129:CYS:HB2	1.35	1.09
2:E:6:VAL:HG13	2:E:129:CYS:HB2	1.14	1.08
2:F:6:VAL:CG1	2:F:129:CYS:CB	2.29	1.08
1:B:75:THR:CG2	1:B:111:LEU:HD13	1.83	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:ASP:O	1:D:101:GLY:N	1.86	1.08
2:E:152:VAL:C	2:E:156:GLN:NE2	2.11	1.08
1:D:66:GLU:OE2	1:D:99:ASP:N	1.85	1.08
1:B:102:PRO:HB3	1:B:123:THR:O	1.50	1.08
2:E:29:LYS:HG3	2:E:168:ILE:HD11	1.10	1.08
2:F:156:GLN:HG3	2:F:161:LEU:CD1	1.84	1.08
2:E:29:LYS:HB2	2:E:29:LYS:HZ2	1.02	1.08
2:F:5:ALA:C	2:F:128:THR:HB	1.79	1.08
1:A:117:SER:HB3	1:B:117:SER:HB3	1.34	1.07
1:C:10:CYS:O	1:C:104:ARG:HD2	1.52	1.07
2:E:29:LYS:HG3	2:E:168:ILE:CD1	1.84	1.07
2:E:159:LEU:O	2:E:161:LEU:N	1.87	1.07
1:C:64:PHE:HE1	1:C:69:TYR:CE2	1.71	1.07
2:E:116:VAL:CG1	2:E:117:GLN:H	1.68	1.07
2:F:66:ASN:O	2:F:67:TRP:O	1.73	1.07
2:F:95:SER:O	2:F:97:LEU:N	1.86	1.07
1:D:12:LEU:O	1:D:12:LEU:HG	1.39	1.06
1:C:112:SER:HB2	1:C:115:SER:O	1.55	1.06
1:D:54:GLU:HB3	1:D:56:HIS:HE1	1.15	1.06
2:F:28:ALA:O	2:F:29:LYS:CG	2.02	1.06
2:E:182:LEU:HD22	2:E:183:LEU:N	1.70	1.06
2:F:41:ILE:O	2:F:41:ILE:HG22	1.50	1.06
1:B:121:VAL:HG12	1:B:122:VAL:N	1.58	1.06
2:F:169:VAL:O	2:F:170:HIS:CG	2.08	1.05
2:E:38:GLN:HB2	2:E:60:ARG:O	0.88	1.05
2:F:38:GLN:HA	2:F:38:GLN:OE1	1.55	1.05
1:D:68:ILE:HD13	1:D:96:THR:OG1	1.54	1.05
2:F:17:LYS:NZ	2:F:51:GLY:O	1.89	1.04
2:F:6:VAL:HG11	2:F:129:CYS:HB2	1.38	1.04
2:E:19:ARG:O	2:E:111:TYR:HB3	1.52	1.04
2:E:39:ASP:OD1	2:E:60:ARG:NH1	1.88	1.04
2:E:114:TYR:H	2:E:138:SER:HA	1.18	1.03
2:E:116:VAL:HG12	2:E:117:GLN:N	1.59	1.03
1:A:98:ASN:OD1	1:A:102:PRO:HA	1.57	1.03
2:E:28:ALA:HB1	2:E:165:TYR:HB3	1.41	1.02
1:A:26:ILE:HD12	1:A:51:GLU:HA	1.04	1.02
1:C:64:PHE:CE1	1:C:69:TYR:CE2	2.47	1.02
1:C:115:SER:CB	1:D:119:THR:OG1	2.07	1.02
2:F:159:LEU:O	2:F:159:LEU:CD1	2.07	1.02
2:E:31:ASP:O	2:E:31:ASP:OD2	1.77	1.02
2:E:182:LEU:HD22	2:E:183:LEU:H	0.91	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ALA:HB3	1:A:40:THR:HG22	1.41	1.02
2:E:32:PRO:CG	2:E:133:TYR:HB2	1.88	1.01
1:B:85:SER:OG	2:F:96:PHE:HA	1.59	1.01
2:F:17:LYS:HD3	2:F:53:MET:HB2	1.42	1.01
1:B:20:VAL:CG1	2:F:64:LEU:HD21	1.89	1.01
1:D:13:MET:SD	1:D:54:GLU:HG2	2.01	1.01
2:E:40:ASN:ND2	2:E:173:TYR:HB2	1.74	1.01
1:A:26:ILE:CD1	1:A:51:GLU:HA	1.91	1.00
1:B:12:LEU:CD1	1:B:107:ILE:HD12	1.90	1.00
2:E:110:ASP:O	2:E:112:ASP:N	1.94	1.00
2:E:175:ASP:HB3	2:E:180:ARG:HD2	1.43	1.00
2:F:37:LEU:CD2	2:F:61:VAL:HG23	1.91	1.00
1:A:32:VAL:HG23	1:A:45:ALA:O	1.61	1.00
2:E:65:ASN:HB3	2:E:66:ASN:ND2	1.76	1.00
2:F:28:ALA:HB3	2:F:136:VAL:HG23	1.40	1.00
2:E:29:LYS:CG	2:E:168:ILE:HD11	1.91	1.00
2:F:161:LEU:HD23	2:F:161:LEU:N	1.71	1.00
2:F:159:LEU:O	2:F:159:LEU:HD13	1.60	1.00
2:E:123:LEU:N	2:E:123:LEU:HD22	1.76	1.00
1:B:41:TRP:CE2	1:B:70:LYS:HE2	1.97	1.00
1:D:70:LYS:HD2	1:D:92:GLU:OE1	1.60	0.99
2:F:123:LEU:N	2:F:123:LEU:CD2	2.23	0.99
2:F:20:PHE:CE2	2:F:45:PHE:CD1	2.49	0.99
1:B:66:GLU:HG3	1:B:99:ASP:OD1	1.61	0.99
1:C:38:ASP:OD1	1:C:40:THR:HG22	1.60	0.99
2:E:164:GLN:O	2:E:165:TYR:CD1	2.16	0.99
1:D:66:GLU:CD	1:D:99:ASP:H	1.71	0.99
2:F:11:VAL:CG2	2:F:84:ALA:CB	2.40	0.99
1:D:114:TYR:OH	2:E:95:SER:CB	2.11	0.98
2:E:29:LYS:NZ	2:E:29:LYS:CB	2.24	0.98
2:F:38:GLN:CB	2:F:60:ARG:O	2.11	0.98
2:F:14:ASN:O	2:F:15:PHE:O	1.81	0.98
2:F:40:ASN:OD1	2:F:170:HIS:HA	1.61	0.98
2:E:152:VAL:O	2:E:156:GLN:OE1	1.82	0.98
2:F:122:LEU:C	2:F:123:LEU:HD22	1.87	0.98
1:A:13:MET:CE	1:A:104:ARG:NH1	2.27	0.98
2:F:30:LYS:CE	2:F:31:ASP:N	2.27	0.98
1:A:118:THR:O	1:B:115:SER:OG	1.82	0.97
1:B:121:VAL:HG13	1:D:24:PRO:HD3	1.45	0.97
2:E:6:VAL:CG1	2:E:129:CYS:HB2	1.93	0.97
2:E:47:VAL:HG12	2:E:48:ASP:N	1.79	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:169:VAL:O	2:F:170:HIS:CD2	2.17	0.97
2:E:135:PHE:HB3	2:E:137:PHE:CE1	2.00	0.97
2:F:77:PHE:CE2	2:F:88:MET:SD	2.57	0.97
1:B:88:HIS:CE1	1:B:116:TYR:CD2	2.53	0.97
2:E:109:THR:HB	2:E:115:ALA:CB	1.94	0.96
2:F:11:VAL:HG23	2:F:84:ALA:CB	1.94	0.96
2:F:169:VAL:C	2:F:170:HIS:CD2	2.43	0.96
1:D:66:GLU:HA	1:D:97:ALA:O	1.66	0.96
2:E:120:CYS:C	2:E:121:ARG:NH1	2.23	0.96
2:E:131:ASP:OD2	2:E:131:ASP:C	2.06	0.96
2:E:156:GLN:HA	2:E:162:ALA:HB3	1.47	0.96
1:B:121:VAL:HG12	1:B:122:VAL:H	0.81	0.96
1:C:95:PHE:HA	1:D:89:GLU:HG2	1.47	0.96
1:D:16:VAL:CG1	1:D:111:LEU:HD11	1.95	0.95
1:D:55:LEU:HD22	1:D:55:LEU:C	1.91	0.95
2:E:108:ASP:OD1	2:E:155:ARG:NE	1.99	0.95
1:B:123:THR:HG23	1:B:125:PRO:HD3	1.48	0.95
2:E:182:LEU:HD22	2:E:183:LEU:HG	1.46	0.95
2:F:122:LEU:C	2:F:123:LEU:CD2	2.40	0.95
2:F:156:GLN:HG3	2:F:161:LEU:HG	1.47	0.95
2:E:38:GLN:HE21	2:E:60:ARG:HH22	1.14	0.95
2:F:156:GLN:HG3	2:F:161:LEU:CG	1.96	0.95
2:F:37:LEU:CA	2:F:61:VAL:HG22	1.96	0.94
1:D:68:ILE:CD1	1:D:96:THR:OG1	2.14	0.94
1:C:38:ASP:OD1	1:C:40:THR:CG2	2.14	0.94
2:F:26:ALA:HB2	2:F:41:ILE:HG22	1.49	0.94
2:E:159:LEU:CG	2:E:162:ALA:HB2	1.97	0.94
2:F:20:PHE:CE2	2:F:45:PHE:HE1	1.64	0.94
2:E:32:PRO:HG3	2:E:133:TYR:HB2	0.96	0.94
2:F:27:MET:N	2:F:168:ILE:HD11	1.83	0.94
2:F:37:LEU:HD23	2:F:61:VAL:HG21	1.50	0.94
1:C:36:ALA:HB2	1:C:42:GLU:HG3	1.47	0.94
2:E:138:SER:OG	2:E:144:LEU:HD22	1.68	0.94
2:F:122:LEU:C	2:F:122:LEU:CD2	2.39	0.94
2:F:123:LEU:N	2:F:123:LEU:HD23	1.82	0.94
2:F:160:CYS:C	2:F:161:LEU:HD22	1.88	0.94
2:E:64:LEU:O	2:E:65:ASN:HB2	1.66	0.94
2:E:153:ALA:CA	2:E:156:GLN:NE2	2.29	0.94
2:E:70:CYS:H	2:E:182:LEU:CD1	1.80	0.93
2:F:104:HIS:C	2:F:117:GLN:NE2	2.25	0.93
1:A:41:TRP:CD1	1:A:41:TRP:H	1.83	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:SER:HB2	2:F:91:TRP:CG	2.04	0.93
1:B:75:THR:HG22	1:B:111:LEU:HD13	0.94	0.93
1:B:12:LEU:HD11	1:B:107:ILE:HD12	0.96	0.93
1:A:36:ALA:CB	1:A:40:THR:HG22	1.98	0.93
1:B:20:VAL:HG11	2:F:64:LEU:CD2	1.99	0.93
2:E:38:GLN:NE2	2:E:60:ARG:NH2	2.15	0.93
2:F:173:TYR:HD1	2:F:173:TYR:O	1.48	0.93
2:E:155:ARG:HH21	2:E:155:ARG:CG	1.81	0.92
2:F:11:VAL:HG21	2:F:84:ALA:HB3	1.51	0.92
2:E:38:GLN:HB2	2:E:60:ARG:C	1.93	0.92
1:B:34:ARG:NH2	1:B:66:GLU:O	2.03	0.92
2:E:40:ASN:HD21	2:E:173:TYR:HB2	1.35	0.92
2:E:159:LEU:HB3	2:E:162:ALA:HB2	1.52	0.92
1:B:104:ARG:O	1:B:122:VAL:CB	2.18	0.92
2:E:156:GLN:HG2	2:E:163:ALA:HB3	1.48	0.92
2:E:6:VAL:N	2:E:128:THR:HB	1.84	0.92
1:A:95:PHE:HD2	1:A:96:THR:O	1.53	0.91
1:B:21:ARG:HD3	1:B:82:LEU:HD21	1.53	0.91
2:F:11:VAL:CG2	2:F:84:ALA:HB3	2.00	0.91
2:F:88:MET:SD	2:F:104:HIS:CD2	2.62	0.91
1:B:18:ASP:OD2	1:B:21:ARG:HG3	0.74	0.91
1:B:88:HIS:CE1	1:B:116:TYR:CE2	2.58	0.91
1:D:16:VAL:HG11	1:D:111:LEU:HD11	1.53	0.91
2:E:178:SER:O	2:E:180:ARG:N	2.04	0.91
2:F:28:ALA:CB	2:F:136:VAL:CG2	2.30	0.91
2:E:165:TYR:HD1	2:E:165:TYR:O	1.54	0.91
1:A:13:MET:HE3	1:A:104:ARG:NH1	1.86	0.91
2:E:153:ALA:N	2:E:156:GLN:NE2	2.18	0.90
2:E:40:ASN:ND2	2:E:173:TYR:CB	2.34	0.90
2:E:47:VAL:O	2:E:48:ASP:HB2	1.70	0.90
2:E:120:CYS:O	2:E:121:ARG:CZ	2.20	0.90
1:A:32:VAL:HG13	1:A:70:LYS:O	1.72	0.90
2:E:113:THR:O	2:E:114:TYR:HB3	1.71	0.90
2:F:77:PHE:CZ	2:F:88:MET:SD	2.64	0.90
2:E:159:LEU:HD12	2:E:162:ALA:CA	2.00	0.90
2:E:108:ASP:O	2:E:109:THR:CG2	2.19	0.90
2:E:24:TRP:CH2	2:E:139:ARG:HD2	2.07	0.90
2:E:103:ASP:O	2:E:119:SER:HB2	1.70	0.90
2:F:80:THR:O	2:F:81:GLU:O	1.89	0.89
2:F:20:PHE:CD2	2:F:45:PHE:CD1	2.60	0.89
2:E:127:GLY:O	2:E:128:THR:OG1	1.91	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:118:TYR:CD2	2:F:159:LEU:HD21	2.08	0.89
2:E:159:LEU:CB	2:E:162:ALA:HB2	2.02	0.89
2:E:77:PHE:CE1	2:E:88:MET:HG3	2.08	0.89
1:B:85:SER:OG	2:F:96:PHE:CA	2.20	0.89
2:F:27:MET:HE1	2:F:144:LEU:CD1	2.03	0.89
2:E:123:LEU:CD1	2:E:128:THR:O	2.20	0.89
2:F:41:ILE:O	2:F:41:ILE:CG2	2.19	0.89
2:F:28:ALA:HB3	2:F:136:VAL:HG21	0.90	0.88
2:E:43:ALA:O	2:E:44:GLU:HB2	1.71	0.88
2:E:52:GLN:NE2	2:E:77:PHE:O	2.05	0.88
2:F:65:ASN:C	2:F:65:ASN:ND2	2.30	0.88
2:F:157:GLU:OE2	2:F:157:GLU:HA	1.09	0.88
2:E:32:PRO:HG3	2:E:133:TYR:HB3	1.52	0.88
2:E:32:PRO:CG	2:E:133:TYR:CB	2.46	0.88
2:F:114:TYR:HD1	2:F:114:TYR:C	1.81	0.88
2:F:129:CYS:SG	2:F:130:ALA:N	2.45	0.88
2:F:48:ASP:O	2:F:50:THR:N	2.06	0.88
2:E:152:VAL:O	2:E:156:GLN:CD	2.17	0.88
1:B:23:SER:HB2	1:B:24:PRO:CD	2.04	0.88
1:D:73:ILE:HB	1:D:91:ALA:HB3	1.56	0.88
2:F:37:LEU:CD2	2:F:61:VAL:CG2	2.50	0.88
2:E:11:VAL:HB	2:E:84:ALA:CB	2.04	0.88
2:F:74:VAL:HG12	2:F:91:TRP:O	1.74	0.88
2:F:138:SER:HB2	2:F:144:LEU:HD21	1.56	0.88
1:A:41:TRP:H	1:A:41:TRP:HD1	1.20	0.87
2:E:24:TRP:CZ2	2:E:139:ARG:HD2	2.10	0.87
2:E:38:GLN:NE2	2:E:60:ARG:HH22	1.69	0.87
1:D:16:VAL:CG1	1:D:111:LEU:CD1	2.52	0.87
1:D:54:GLU:CB	1:D:56:HIS:HE1	1.86	0.87
2:F:66:ASN:CG	2:F:67:TRP:N	2.26	0.87
1:A:13:MET:HE1	1:A:104:ARG:HH12	1.37	0.87
1:A:16:VAL:HG11	1:A:111:LEU:HD11	1.56	0.87
2:E:108:ASP:OD2	2:E:109:THR:N	2.06	0.87
2:F:30:LYS:HE3	2:F:30:LYS:C	2.00	0.87
1:D:70:LYS:HA	1:D:93:VAL:O	1.75	0.87
2:E:66:ASN:ND2	2:E:66:ASN:N	2.19	0.87
2:E:132:SER:O	2:E:133:TYR:HB3	1.72	0.87
2:F:26:ALA:HB2	2:F:41:ILE:CG2	2.02	0.87
2:F:40:ASN:OD1	2:F:170:HIS:CA	2.21	0.87
1:C:10:CYS:O	1:C:104:ARG:CD	2.23	0.87
2:E:16:ASP:OD2	2:E:18:ALA:N	2.08	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:17:LYS:HB3	2:E:53:MET:SD	2.15	0.87
1:B:41:TRP:NE1	1:B:70:LYS:HE2	1.90	0.86
2:F:104:HIS:CA	2:F:117:GLN:HE22	1.86	0.86
2:F:160:CYS:O	2:F:161:LEU:CD2	2.12	0.86
2:E:153:ALA:HA	2:E:156:GLN:NE2	1.90	0.86
2:F:112:ASP:O	2:F:113:THR:OG1	1.92	0.86
1:D:65:VAL:O	1:D:69:TYR:OH	1.91	0.86
1:A:13:MET:HE3	1:A:104:ARG:HH12	1.39	0.86
1:D:114:TYR:HH	2:E:95:SER:HB2	1.40	0.86
2:E:4:CYS:SG	2:E:5:ALA:N	2.48	0.86
2:E:79:ASP:O	2:E:80:THR:HG22	1.74	0.86
2:F:5:ALA:CA	2:F:128:THR:CB	2.53	0.86
1:D:12:LEU:HD23	1:D:58:LEU:HB2	1.56	0.86
2:F:30:LYS:HD3	2:F:164:GLN:HE21	1.41	0.86
2:E:165:TYR:CD1	2:E:165:TYR:O	2.28	0.85
1:D:87:PHE:CD2	1:D:88:HIS:HD2	1.91	0.85
2:F:67:TRP:HD1	2:F:68:ASP:N	1.74	0.85
2:E:113:THR:H	2:E:139:ARG:HD3	1.41	0.85
2:F:5:ALA:CA	2:F:128:THR:HB	2.05	0.85
1:D:26:ILE:O	1:D:27:ASN:HB2	1.73	0.85
2:E:13:GLU:O	2:E:15:PHE:N	2.10	0.85
2:E:122:LEU:C	2:E:123:LEU:HD22	2.02	0.85
2:F:111:TYR:O	2:F:139:ARG:NE	2.09	0.85
2:E:9:PHE:HE2	2:E:160:CYS:CB	1.87	0.85
2:E:114:TYR:O	2:E:114:TYR:CD2	2.29	0.85
2:E:124:ASN:O	2:E:126:ASP:N	2.09	0.85
2:E:153:ALA:HA	2:E:156:GLN:HE22	1.42	0.85
2:E:36:PHE:HE2	3:E:1:RTL:C19	1.90	0.84
2:E:152:VAL:O	2:E:152:VAL:HG12	1.76	0.84
2:E:26:ALA:HB1	2:E:168:ILE:HD13	1.57	0.84
2:F:113:THR:H	2:F:139:ARG:HD3	1.41	0.84
2:F:158:GLU:OE2	2:F:158:GLU:N	2.10	0.84
1:C:97:ALA:HB1	1:C:98:ASN:ND2	1.90	0.84
2:F:53:MET:HE1	2:F:86:PHE:CE2	2.13	0.84
1:B:66:GLU:HG3	1:B:99:ASP:CG	2.03	0.84
2:E:159:LEU:O	2:E:159:LEU:CD1	2.24	0.84
2:F:30:LYS:NZ	2:F:31:ASP:O	2.09	0.84
2:F:94:ALA:O	2:F:97:LEU:HD12	1.77	0.84
2:E:108:ASP:C	2:E:109:THR:HG22	2.02	0.84
2:E:114:TYR:O	2:E:114:TYR:CD1	2.31	0.84
2:E:120:CYS:O	2:E:121:ARG:NH2	2.10	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:9:PHE:O	2:F:10:ARG:O	1.96	0.84
2:E:30:LYS:HB2	2:E:134:SER:H	1.43	0.84
2:E:135:PHE:CB	2:E:137:PHE:CE1	2.59	0.84
2:E:109:THR:HB	2:E:115:ALA:HB1	1.59	0.83
2:F:133:TYR:CD1	2:F:133:TYR:C	2.56	0.83
2:E:65:ASN:HB3	2:E:66:ASN:HD21	1.39	0.83
2:F:156:GLN:CD	2:F:165:TYR:HE2	1.86	0.83
2:F:11:VAL:HG21	2:F:84:ALA:CB	2.07	0.83
1:B:66:GLU:CG	1:B:99:ASP:OD1	2.25	0.83
2:E:5:ALA:HA	2:E:129:CYS:N	1.92	0.83
2:E:114:TYR:N	2:E:138:SER:HA	1.92	0.83
2:E:159:LEU:O	2:E:159:LEU:HD13	1.77	0.83
1:D:12:LEU:HD21	1:D:58:LEU:CD1	2.08	0.83
2:F:6:VAL:HG13	2:F:129:CYS:CB	2.09	0.83
2:E:118:TYR:CD1	2:E:119:SER:N	2.46	0.83
2:E:164:GLN:O	2:E:165:TYR:CD2	2.32	0.83
2:F:84:ALA:O	2:F:85:LYS:O	1.97	0.83
2:F:104:HIS:O	2:F:117:GLN:NE2	2.11	0.83
1:B:104:ARG:CB	1:B:122:VAL:HG21	2.09	0.82
2:E:70:CYS:HB2	2:E:182:LEU:HD12	1.58	0.82
1:A:26:ILE:CG1	1:A:50:SER:O	2.27	0.82
1:B:21:ARG:C	1:C:114:TYR:CD1	2.57	0.82
2:E:107:VAL:HG11	2:E:159:LEU:HD23	1.61	0.82
2:F:133:TYR:HD1	2:F:133:TYR:C	1.85	0.82
2:E:155:ARG:HH21	2:E:155:ARG:HG3	1.39	0.82
1:B:102:PRO:HB2	1:B:122:VAL:CG1	2.08	0.82
2:E:107:VAL:HG12	2:E:107:VAL:O	1.79	0.82
2:E:114:TYR:HA	2:E:137:PHE:O	1.79	0.82
1:B:18:ASP:CG	1:B:21:ARG:CG	2.34	0.82
2:E:152:VAL:O	2:E:156:GLN:NE2	2.13	0.82
1:D:55:LEU:C	1:D:55:LEU:CD2	2.53	0.82
1:B:54:GLU:HB3	1:B:56:HIS:CE1	2.14	0.81
1:C:84:ILE:HD11	2:F:67:TRP:CE3	2.14	0.81
2:E:5:ALA:HB1	2:E:128:THR:OG1	1.80	0.81
2:E:105:TRP:O	2:E:106:ILE:HG13	1.80	0.81
1:A:16:VAL:CG1	1:A:111:LEU:HD11	2.10	0.81
1:A:100:SER:HB2	2:F:91:TRP:CD2	2.15	0.81
2:E:32:PRO:CB	2:E:132:SER:O	2.24	0.81
2:E:107:VAL:HG21	2:E:159:LEU:CD2	2.10	0.81
1:A:84:ILE:O	1:A:86:PRO:HD3	1.80	0.81
2:E:16:ASP:OD2	2:E:16:ASP:C	2.20	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:107:VAL:HG21	2:E:159:LEU:HD21	1.63	0.81
2:F:6:VAL:HG13	2:F:129:CYS:HB2	1.58	0.81
2:F:171:ASN:O	2:F:172:GLY:C	2.22	0.81
2:F:11:VAL:O	2:F:12:LYS:O	1.99	0.81
1:A:122:VAL:HG11	1:B:114:TYR:HE2	1.46	0.81
2:F:114:TYR:C	2:F:114:TYR:CD1	2.52	0.81
2:E:72:ASP:O	2:E:93:VAL:HG22	1.80	0.81
2:E:120:CYS:O	2:E:121:ARG:NH1	2.13	0.81
2:F:104:HIS:O	2:F:104:HIS:ND1	2.14	0.81
2:F:73:MET:HE3	3:F:2:RTL:H12	1.62	0.81
1:A:122:VAL:CG1	1:B:114:TYR:HE2	1.93	0.81
1:D:33:PHE:O	1:D:69:TYR:HA	1.80	0.81
2:F:109:THR:OG1	2:F:115:ALA:HB2	1.81	0.81
1:A:79:TRP:CZ2	1:A:113:PRO:CD	2.63	0.80
2:E:113:THR:HG23	2:E:138:SER:OG	1.81	0.80
2:E:173:TYR:HD2	2:E:173:TYR:O	1.64	0.80
2:E:159:LEU:HG	2:E:162:ALA:HB2	1.63	0.80
2:E:120:CYS:C	2:E:121:ARG:HH12	1.88	0.80
2:E:173:TYR:HE2	2:E:181:ASN:HB2	1.44	0.80
2:F:37:LEU:HD22	2:F:61:VAL:HG23	1.62	0.80
1:D:56:HIS:O	1:D:58:LEU:N	2.15	0.80
2:F:67:TRP:CD1	2:F:68:ASP:N	2.50	0.80
1:B:16:VAL:HB	1:B:25:ALA:HB3	1.63	0.80
2:F:154:GLN:O	2:F:155:ARG:NH2	2.15	0.80
2:F:79:ASP:O	2:F:80:THR:HG22	1.82	0.79
2:F:23:THR:O	2:F:139:ARG:NH1	2.15	0.79
2:F:53:MET:HE1	2:F:86:PHE:CD2	2.17	0.79
1:A:7:GLU:HG2	1:A:8:SER:H	1.47	0.79
1:A:26:ILE:HD12	1:A:51:GLU:CA	2.01	0.79
2:F:5:ALA:HA	2:F:128:THR:HB	1.62	0.79
2:F:63:LEU:HD23	2:F:69:VAL:HG11	1.65	0.79
2:E:80:THR:OG1	2:E:81:GLU:N	2.08	0.79
1:C:76:LYS:HB2	1:C:89:GLU:O	1.82	0.79
2:E:38:GLN:HG2	2:E:61:VAL:HA	1.63	0.79
2:F:156:GLN:O	2:F:161:LEU:HD23	1.82	0.79
1:D:66:GLU:HG2	1:D:103:ARG:HH12	1.48	0.78
2:F:88:MET:O	2:F:101:ASN:HA	1.82	0.78
2:E:157:GLU:O	2:E:157:GLU:HG3	1.81	0.78
2:F:85:LYS:CD	2:F:105:TRP:NE1	2.46	0.78
2:F:124:ASN:HB2	2:F:130:ALA:HB2	1.63	0.78
2:F:169:VAL:C	2:F:170:HIS:CG	2.57	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:TRP:CH2	1:A:113:PRO:CD	2.66	0.78
1:B:13:MET:CG	1:B:56:HIS:CD2	2.63	0.78
2:F:48:ASP:O	2:F:50:THR:HG23	1.84	0.78
1:B:88:HIS:HE1	1:B:116:TYR:CD2	1.98	0.78
2:E:29:LYS:CB	2:E:29:LYS:HZ3	1.96	0.78
2:E:69:VAL:HG23	2:E:182:LEU:HD21	1.64	0.78
2:F:81:GLU:O	2:F:82:ASP:O	2.01	0.78
1:A:64:PHE:HE1	1:A:69:TYR:CD2	2.02	0.78
2:E:66:ASN:N	2:E:66:ASN:HD22	1.77	0.78
2:E:104:HIS:CE1	2:E:117:GLN:HE21	2.02	0.78
2:E:106:ILE:HG22	2:E:106:ILE:O	1.83	0.78
2:F:156:GLN:HG3	2:F:161:LEU:HD12	1.65	0.78
2:E:5:ALA:HA	2:E:129:CYS:H	1.49	0.78
2:E:175:ASP:HB3	2:E:180:ARG:CD	2.13	0.78
2:F:107:VAL:HG21	2:F:159:LEU:HD23	1.65	0.77
2:F:122:LEU:HD23	2:F:123:LEU:CA	2.13	0.77
2:E:24:TRP:NE1	2:E:139:ARG:NH1	2.33	0.77
1:B:90:HIS:NE2	1:B:92:GLU:OE2	2.17	0.77
1:B:98:ASN:C	1:B:103:ARG:NH1	2.43	0.77
2:F:118:TYR:CD1	2:F:119:SER:N	2.52	0.77
2:F:38:GLN:NE2	2:F:62:ARG:NH1	2.32	0.77
2:F:109:THR:CG2	2:F:109:THR:O	2.32	0.77
2:F:159:LEU:O	2:F:159:LEU:HD12	1.85	0.77
2:F:29:LYS:H	2:F:165:TYR:HD1	1.30	0.77
2:F:29:LYS:HG3	2:F:168:ILE:CG2	2.13	0.77
2:F:89:LYS:CG	2:F:89:LYS:O	2.32	0.77
1:A:7:GLU:HG2	1:A:8:SER:N	1.99	0.77
2:E:66:ASN:HD22	2:E:66:ASN:H	1.33	0.77
2:F:104:HIS:O	2:F:105:TRP:O	2.03	0.77
2:E:82:ASP:O	2:E:84:ALA:N	2.18	0.77
2:F:124:ASN:ND2	2:F:125:LEU:HG	2.00	0.77
2:F:109:THR:O	2:F:109:THR:HG23	1.85	0.76
2:E:19:ARG:O	2:E:111:TYR:CG	2.38	0.76
1:B:54:GLU:HB3	1:B:56:HIS:HE1	1.49	0.76
2:F:103:ASP:H	2:F:121:ARG:HD3	1.50	0.76
1:D:76:LYS:HA	1:D:86:PRO:HG3	1.66	0.76
2:E:39:ASP:CB	2:E:169:VAL:HG13	2.16	0.76
1:C:98:ASN:ND2	1:C:98:ASN:N	2.33	0.76
2:E:47:VAL:HG12	2:E:48:ASP:H	1.49	0.76
2:F:73:MET:HE3	3:F:2:RTL:H14	1.67	0.76
2:F:168:ILE:O	2:F:170:HIS:NE2	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:SER:HB3	1:B:117:SER:CB	2.15	0.76
2:E:15:PHE:CE1	2:E:17:LYS:HA	2.19	0.76
1:D:69:TYR:N	1:D:69:TYR:CD1	2.53	0.76
2:F:104:HIS:HA	2:F:117:GLN:HE22	1.51	0.76
2:F:29:LYS:C	2:F:165:TYR:HD1	1.93	0.76
2:F:94:ALA:O	2:F:95:SER:O	2.04	0.76
1:B:18:ASP:OD1	1:B:21:ARG:CB	2.34	0.75
2:E:28:ALA:HB1	2:E:165:TYR:CB	2.17	0.75
2:E:63:LEU:HD12	2:E:64:LEU:N	2.01	0.75
2:E:65:ASN:CB	2:E:66:ASN:ND2	2.48	0.75
2:E:75:GLY:HA3	2:E:88:MET:SD	2.26	0.75
2:E:76:THR:O	2:E:88:MET:HG2	1.87	0.75
2:F:168:ILE:HD13	2:F:168:ILE:H	1.51	0.75
2:E:15:PHE:CD1	2:E:15:PHE:C	2.64	0.75
2:E:123:LEU:N	2:E:123:LEU:CD2	2.46	0.75
1:B:18:ASP:OD2	1:B:21:ARG:CD	2.35	0.75
1:B:23:SER:HB2	1:B:24:PRO:HD2	1.67	0.75
2:E:15:PHE:CE2	2:E:106:ILE:HD12	2.20	0.75
2:E:133:TYR:CD1	2:E:133:TYR:C	2.63	0.75
2:E:113:THR:HA	2:E:139:ARG:H	1.52	0.75
2:F:11:VAL:HG23	2:F:84:ALA:HB2	1.68	0.75
2:F:28:ALA:HB2	2:F:136:VAL:HG21	1.68	0.75
1:D:25:ALA:HB1	1:D:28:VAL:HG21	1.67	0.75
1:C:84:ILE:HD11	2:F:67:TRP:CZ3	2.22	0.75
2:E:92:GLY:C	2:E:94:ALA:N	2.38	0.75
2:F:66:ASN:ND2	2:F:67:TRP:H	1.85	0.75
2:F:77:PHE:CE2	2:F:104:HIS:HD2	2.03	0.75
2:F:20:PHE:CD2	2:F:45:PHE:HD1	2.04	0.75
1:D:16:VAL:HG11	1:D:111:LEU:CD1	2.15	0.74
2:E:92:GLY:C	2:E:94:ALA:H	1.94	0.74
2:F:30:LYS:HE3	2:F:31:ASP:CA	2.17	0.74
1:B:22:GLY:O	1:D:121:VAL:HA	1.87	0.74
2:F:30:LYS:HE3	2:F:31:ASP:H	1.49	0.74
2:F:156:GLN:CG	2:F:161:LEU:HG	2.16	0.74
2:E:118:TYR:CE1	2:E:132:SER:HB2	2.22	0.74
2:E:137:PHE:CD1	2:E:137:PHE:N	2.54	0.74
2:F:85:LYS:CD	2:F:105:TRP:CD1	2.60	0.74
2:F:5:ALA:C	2:F:128:THR:CB	2.60	0.74
1:A:41:TRP:CD1	1:A:41:TRP:N	2.53	0.74
2:E:127:GLY:C	2:E:128:THR:OG1	2.29	0.74
2:F:85:LYS:CD	2:F:105:TRP:HE1	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:122:LEU:HD22	2:F:130:ALA:HB3	1.70	0.74
2:E:107:VAL:O	2:E:108:ASP:HB2	1.88	0.73
2:F:156:GLN:HA	2:F:161:LEU:HD21	1.69	0.73
2:F:160:CYS:CA	2:F:161:LEU:HD23	2.18	0.73
1:D:25:ALA:O	1:D:28:VAL:HG23	1.88	0.73
2:E:36:PHE:HE2	3:E:1:RTL:H193	1.53	0.73
2:E:138:SER:CB	2:E:144:LEU:HD22	2.19	0.73
2:E:164:GLN:C	2:E:165:TYR:CG	2.66	0.73
1:A:64:PHE:CE1	1:A:69:TYR:CZ	2.75	0.73
2:F:29:LYS:N	2:F:165:TYR:HD1	1.86	0.73
2:F:48:ASP:O	2:F:50:THR:CG2	2.36	0.73
1:A:16:VAL:HG12	1:A:25:ALA:HB2	1.71	0.73
2:E:38:GLN:HE21	2:E:60:ARG:HH21	1.31	0.73
2:E:82:ASP:N	2:E:82:ASP:OD1	2.21	0.73
2:F:74:VAL:CG1	2:F:91:TRP:O	2.35	0.73
2:E:125:LEU:C	2:E:127:GLY:H	1.97	0.73
2:E:156:GLN:HG2	2:E:163:ALA:CB	2.18	0.73
2:F:20:PHE:CD2	2:F:45:PHE:CE1	2.76	0.73
2:F:29:LYS:N	2:F:165:TYR:CD1	2.55	0.73
1:A:16:VAL:HG12	1:A:25:ALA:CB	2.19	0.73
2:E:28:ALA:CB	2:E:165:TYR:HB3	2.17	0.73
2:F:5:ALA:CA	2:F:128:THR:OG1	2.27	0.72
1:A:18:ASP:CG	1:A:21:ARG:HD3	2.14	0.72
2:E:110:ASP:C	2:E:112:ASP:H	1.97	0.72
2:E:134:SER:HB3	2:E:162:ALA:O	1.88	0.72
2:F:57:ALA:HB2	3:F:2:RTL:H173	1.70	0.72
2:E:135:PHE:CB	2:E:137:PHE:HE1	2.01	0.72
2:F:38:GLN:HE22	2:F:62:ARG:NH1	1.88	0.72
1:B:22:GLY:HA3	1:C:114:TYR:CG	2.24	0.72
2:E:25:TYR:CE2	2:E:141:PRO:HD3	2.24	0.72
2:E:85:LYS:HG2	2:E:105:TRP:CD1	2.24	0.72
2:F:80:THR:O	2:F:81:GLU:C	2.29	0.72
2:F:123:LEU:HD13	2:F:129:CYS:H	1.54	0.72
2:F:156:GLN:O	2:F:161:LEU:CD2	2.38	0.72
2:E:70:CYS:H	2:E:182:LEU:HD12	1.54	0.72
1:B:13:MET:SD	1:B:56:HIS:NE2	2.62	0.72
1:C:64:PHE:HE1	1:C:69:TYR:CD2	2.06	0.72
1:D:66:GLU:CA	1:D:97:ALA:O	2.38	0.72
2:E:4:CYS:N	2:E:129:CYS:O	2.22	0.72
2:F:85:LYS:HD3	2:F:105:TRP:HE1	1.48	0.72
2:F:171:ASN:O	2:F:172:GLY:O	2.08	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:VAL:HB	1:A:25:ALA:HB3	1.71	0.72
1:B:98:ASN:C	1:B:103:ARG:HH11	1.97	0.72
1:B:121:VAL:CG1	1:B:122:VAL:N	2.33	0.72
2:F:66:ASN:O	2:F:67:TRP:C	2.32	0.72
2:E:151:ILE:C	2:E:153:ALA:H	1.97	0.72
2:E:171:ASN:O	2:E:172:GLY:C	2.33	0.72
2:F:26:ALA:C	2:F:168:ILE:HD11	2.13	0.72
1:D:102:PRO:HG2	1:D:122:VAL:HG12	1.71	0.72
1:C:11:PRO:HA	1:C:104:ARG:HG2	1.71	0.72
2:F:27:MET:N	2:F:168:ILE:CD1	2.53	0.72
1:A:97:ALA:O	1:A:99:ASP:N	2.22	0.71
2:F:36:PHE:O	2:F:61:VAL:CG2	2.38	0.71
1:B:16:VAL:O	1:B:17:LEU:HD23	1.90	0.71
1:A:7:GLU:OE2	1:A:9:LYS:HB2	1.90	0.71
2:E:11:VAL:HB	2:E:84:ALA:HB1	1.71	0.71
2:F:38:GLN:NE2	2:F:62:ARG:CZ	2.53	0.71
2:E:155:ARG:HG3	2:E:155:ARG:NH2	2.00	0.71
2:F:11:VAL:O	2:F:12:LYS:C	2.31	0.71
2:F:53:MET:CE	2:F:86:PHE:CE2	2.73	0.71
1:B:41:TRP:CE2	1:B:70:LYS:CE	2.74	0.71
1:D:73:ILE:HD12	1:D:91:ALA:O	1.91	0.71
2:F:122:LEU:O	2:F:123:LEU:HD22	1.89	0.71
1:B:88:HIS:CE1	1:B:116:TYR:HD2	2.06	0.71
1:C:70:LYS:HD2	1:C:92:GLU:OE1	1.91	0.71
1:D:66:GLU:OE2	1:D:99:ASP:CB	2.39	0.71
1:D:12:LEU:HD21	1:D:58:LEU:HD12	1.73	0.70
1:D:16:VAL:C	1:D:17:LEU:HD23	2.16	0.70
2:F:12:LYS:HE2	2:F:109:THR:O	1.90	0.70
2:F:95:SER:C	2:F:97:LEU:H	1.95	0.70
1:D:84:ILE:O	1:D:86:PRO:HD3	1.90	0.70
2:E:103:ASP:HB2	2:E:121:ARG:NH2	2.06	0.70
1:D:13:MET:SD	1:D:54:GLU:CG	2.79	0.70
1:D:121:VAL:HG23	1:D:121:VAL:O	1.91	0.70
2:E:6:VAL:H	2:E:128:THR:CB	1.96	0.70
2:F:52:GLN:OE1	2:F:77:PHE:O	2.09	0.70
2:F:122:LEU:C	2:F:123:LEU:HD23	2.14	0.70
2:E:72:ASP:C	2:E:73:MET:HE2	2.16	0.70
2:E:107:VAL:CG1	2:E:159:LEU:HD23	2.21	0.70
2:E:125:LEU:O	2:E:127:GLY:N	2.25	0.70
2:F:155:ARG:C	2:F:157:GLU:H	1.99	0.70
1:A:19:ALA:CB	1:A:111:LEU:O	2.40	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:15:PHE:HE1	2:E:17:LYS:HA	1.57	0.70
2:E:131:ASP:OD2	2:E:132:SER:N	2.25	0.70
1:B:25:ALA:O	1:B:28:VAL:HG23	1.91	0.70
1:D:12:LEU:O	1:D:12:LEU:CG	2.25	0.70
2:F:105:TRP:O	2:F:117:GLN:NE2	2.24	0.70
2:E:13:GLU:O	2:E:14:ASN:C	2.35	0.69
2:E:77:PHE:CD1	2:E:88:MET:HG3	2.27	0.69
2:F:104:HIS:C	2:F:117:GLN:HE22	1.93	0.69
1:B:17:LEU:HB2	1:B:110:LEU:HD13	1.74	0.69
1:D:76:LYS:CG	1:D:80:LYS:HE2	2.22	0.69
2:E:139:ARG:HH11	2:E:139:ARG:CG	2.05	0.69
2:E:22:GLY:O	2:E:24:TRP:CD1	2.45	0.69
2:E:69:VAL:CA	2:E:182:LEU:HG	2.18	0.69
1:B:84:ILE:HG23	2:F:96:PHE:HB2	1.74	0.69
1:D:12:LEU:HD21	1:D:58:LEU:HD13	1.73	0.69
2:F:14:ASN:O	2:F:15:PHE:C	2.36	0.69
1:B:18:ASP:OD1	1:B:21:ARG:N	2.26	0.69
2:E:45:PHE:CE2	2:E:55:ALA:HB1	2.28	0.69
2:F:38:GLN:OE1	2:F:38:GLN:CA	2.38	0.69
1:A:115:SER:HB3	1:D:19:ALA:HB1	1.72	0.69
2:F:5:ALA:HA	2:F:128:THR:HG1	1.53	0.69
1:A:41:TRP:HD1	1:A:41:TRP:N	1.91	0.69
1:D:71:VAL:O	1:D:93:VAL:HG23	1.91	0.69
1:D:76:LYS:HG3	1:D:80:LYS:HE2	1.74	0.69
2:E:24:TRP:CZ2	2:E:139:ARG:CD	2.76	0.69
2:E:39:ASP:HB2	2:E:169:VAL:HG13	1.74	0.69
2:E:182:LEU:CD2	2:E:183:LEU:N	2.44	0.69
2:F:36:PHE:O	2:F:61:VAL:HG22	1.93	0.69
2:F:85:LYS:HD3	2:F:105:TRP:HD1	1.49	0.69
1:C:115:SER:HB3	1:D:119:THR:OG1	1.91	0.69
1:D:66:GLU:OE2	1:D:99:ASP:HB2	1.93	0.69
2:E:138:SER:CB	2:E:144:LEU:CD2	2.71	0.69
2:F:14:ASN:C	2:F:15:PHE:O	2.33	0.69
1:B:90:HIS:CD2	1:B:92:GLU:HG3	2.28	0.68
1:B:10:CYS:N	1:B:11:PRO:CD	2.56	0.68
1:C:21:ARG:O	1:C:22:GLY:O	2.11	0.68
2:F:148:ALA:O	2:F:151:ILE:N	2.25	0.68
2:F:24:TRP:CZ2	2:F:111:TYR:O	2.47	0.68
2:F:140:ASP:OD2	2:F:141:PRO:HD2	1.93	0.68
2:F:156:GLN:CD	2:F:165:TYR:CE2	2.71	0.68
2:F:81:GLU:O	2:F:82:ASP:C	2.36	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:173:TYR:O	2:F:173:TYR:CD1	2.39	0.68
1:B:34:ARG:HH21	1:B:65:VAL:HG23	1.56	0.68
2:E:89:LYS:HB3	2:E:101:ASN:OD1	1.93	0.68
1:A:16:VAL:CG1	1:A:111:LEU:CD1	2.71	0.68
1:A:95:PHE:CD2	1:A:96:THR:O	2.42	0.68
1:B:19:ALA:O	1:C:114:TYR:HB2	1.93	0.68
2:F:70:CYS:SG	2:F:173:TYR:O	2.52	0.68
2:F:89:LYS:O	2:F:89:LYS:HG3	1.93	0.68
1:B:104:ARG:H	1:B:122:VAL:HG11	1.56	0.68
1:C:21:ARG:O	1:C:22:GLY:C	2.37	0.68
2:E:118:TYR:CG	2:E:119:SER:N	2.62	0.68
1:A:114:TYR:CD2	1:D:22:GLY:HA3	2.29	0.68
1:C:30:VAL:HG21	1:C:55:LEU:HD12	1.76	0.68
1:D:34:ARG:HH11	1:D:34:ARG:HG2	1.58	0.68
2:F:29:LYS:C	2:F:165:TYR:CD1	2.71	0.68
2:F:38:GLN:N	2:F:60:ARG:O	2.27	0.68
2:E:30:LYS:HB2	2:E:134:SER:N	2.09	0.67
2:F:167:LEU:O	2:F:167:LEU:HD22	1.94	0.67
1:B:104:ARG:CA	1:B:122:VAL:HG21	2.24	0.67
1:D:66:GLU:CG	1:D:99:ASP:H	2.07	0.67
2:E:124:ASN:O	2:E:125:LEU:C	2.37	0.67
2:F:6:VAL:N	2:F:128:THR:HB	2.09	0.67
2:F:65:ASN:HD22	2:F:66:ASN:N	1.92	0.67
2:F:85:LYS:O	2:F:86:PHE:CG	2.48	0.67
2:E:118:TYR:HE1	2:E:132:SER:HB2	1.60	0.67
2:E:179:GLU:HG3	2:E:182:LEU:O	1.93	0.67
2:F:9:PHE:O	2:F:10:ARG:C	2.36	0.67
2:F:150:LYS:O	2:F:150:LYS:HG3	1.95	0.67
2:F:155:ARG:O	2:F:157:GLU:N	2.27	0.67
1:D:13:MET:HG3	1:D:56:HIS:CG	2.30	0.67
2:E:137:PHE:N	2:E:137:PHE:HD1	1.93	0.67
2:F:78:THR:O	2:F:87:LYS:HE3	1.95	0.67
1:D:90:HIS:O	1:D:90:HIS:CD2	2.48	0.67
2:E:15:PHE:CE2	2:E:106:ILE:CD1	2.78	0.67
2:E:36:PHE:CE2	3:E:1:RTL:C19	2.78	0.67
1:A:16:VAL:CG1	1:A:25:ALA:CB	2.73	0.67
2:F:29:LYS:HG3	2:F:168:ILE:HG23	1.75	0.67
2:F:67:TRP:HD1	2:F:68:ASP:H	1.41	0.67
2:F:147:GLU:O	2:F:148:ALA:O	2.13	0.67
1:A:87:PHE:CZ	1:B:95:PHE:CG	2.82	0.67
2:E:182:LEU:CD2	2:E:183:LEU:HG	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:25:TYR:O	2:F:137:PHE:HA	1.95	0.67
2:F:53:MET:CE	2:F:86:PHE:CD2	2.77	0.67
2:F:113:THR:O	2:F:138:SER:HA	1.94	0.66
2:F:148:ALA:O	2:F:150:LYS:N	2.28	0.66
2:E:108:ASP:O	2:E:109:THR:CB	2.44	0.66
1:A:102:PRO:C	1:A:103:ARG:HG2	2.21	0.66
2:E:39:ASP:CG	2:E:60:ARG:NH1	2.52	0.66
2:F:98:GLN:HG2	2:F:98:GLN:O	1.93	0.66
2:F:168:ILE:HG12	2:F:170:HIS:CE1	2.31	0.66
1:B:40:THR:CG2	1:B:41:TRP:N	2.58	0.66
2:E:22:GLY:O	2:E:139:ARG:NH1	2.27	0.66
1:B:18:ASP:OD1	1:B:21:ARG:CA	2.43	0.66
2:E:36:PHE:CE2	3:E:1:RTL:H193	2.30	0.66
2:F:20:PHE:HD2	2:F:45:PHE:HD1	1.41	0.66
2:E:76:THR:O	2:E:88:MET:CG	2.44	0.66
1:C:100:SER:HB2	2:E:91:TRP:CG	2.31	0.66
2:F:30:LYS:O	2:F:32:PRO:HD3	1.96	0.65
1:C:14:VAL:HG12	1:C:14:VAL:O	1.96	0.65
1:C:79:TRP:HZ2	1:C:112:SER:C	2.04	0.65
2:E:38:GLN:CG	2:E:60:ARG:O	2.43	0.65
2:E:33:GLU:HG3	2:E:33:GLU:O	1.95	0.65
1:A:32:VAL:CG1	1:A:70:LYS:O	2.42	0.65
1:A:52:SER:OG	1:A:54:GLU:HB2	1.95	0.65
2:E:4:CYS:C	2:E:129:CYS:O	2.40	0.65
2:F:73:MET:HG3	3:F:2:RTL:H10	1.78	0.65
1:D:98:ASN:C	1:D:103:ARG:HH11	2.03	0.65
2:E:4:CYS:O	2:E:129:CYS:O	2.15	0.65
2:E:168:ILE:O	2:E:168:ILE:HG22	1.96	0.65
2:E:114:TYR:CD1	2:E:152:VAL:CG2	2.80	0.65
2:F:19:ARG:HD2	2:F:111:TYR:CE2	2.32	0.65
1:C:97:ALA:HB1	1:C:98:ASN:HD21	1.61	0.65
2:F:122:LEU:CD2	2:F:123:LEU:N	2.35	0.65
2:E:47:VAL:O	2:E:48:ASP:CB	2.45	0.65
2:F:6:VAL:HG23	2:F:7:SER:N	2.10	0.65
2:E:108:ASP:CG	2:E:109:THR:H	2.05	0.65
1:D:12:LEU:CD2	1:D:58:LEU:HD12	2.27	0.64
2:F:19:ARG:HD2	2:F:111:TYR:CD2	2.32	0.64
1:A:32:VAL:O	1:A:44:PHE:N	2.28	0.64
2:F:30:LYS:CE	2:F:31:ASP:H	2.04	0.64
2:F:167:LEU:HD22	2:F:167:LEU:C	2.21	0.64
1:B:25:ALA:HB1	1:B:28:VAL:HG21	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:114:TYR:HD2	2:F:148:ALA:CB	2.10	0.64
1:D:26:ILE:HG23	1:D:50:SER:O	1.97	0.64
2:E:70:CYS:H	2:E:182:LEU:CG	2.10	0.64
2:F:6:VAL:HG13	2:F:128:THR:C	2.22	0.64
2:F:155:ARG:C	2:F:157:GLU:N	2.52	0.64
1:B:58:LEU:O	1:B:59:THR:HB	1.97	0.64
1:B:104:ARG:O	1:B:122:VAL:HB	1.96	0.64
1:C:38:ASP:OD1	1:C:40:THR:HG21	1.97	0.64
2:E:175:ASP:CG	2:E:176:GLY:N	2.55	0.64
1:D:10:CYS:HB3	1:D:56:HIS:HB3	1.79	0.64
1:D:12:LEU:HD23	1:D:58:LEU:CB	2.26	0.64
1:D:87:PHE:CE2	1:D:88:HIS:CD2	2.84	0.64
2:F:79:ASP:C	2:F:80:THR:CG2	2.70	0.64
2:F:107:VAL:HG21	2:F:159:LEU:CD2	2.28	0.64
1:B:34:ARG:HB2	1:B:69:TYR:CE2	2.32	0.64
2:E:57:ALA:HB3	3:E:1:RTL:H41	1.80	0.64
2:F:45:PHE:CE2	2:F:55:ALA:HB1	2.32	0.64
1:D:13:MET:HG3	1:D:56:HIS:CE1	2.33	0.64
2:E:70:CYS:N	2:E:182:LEU:CD1	2.57	0.64
2:F:27:MET:CE	2:F:144:LEU:HD11	2.16	0.64
2:F:155:ARG:O	2:F:158:GLU:N	2.31	0.64
1:A:64:PHE:CD1	1:A:69:TYR:CE2	2.84	0.64
2:E:125:LEU:C	2:E:127:GLY:N	2.52	0.64
2:F:118:TYR:HD2	2:F:159:LEU:HD21	1.62	0.64
1:A:117:SER:CB	1:B:117:SER:HB3	2.20	0.63
1:D:54:GLU:OE1	1:D:56:HIS:CE1	2.51	0.63
2:E:22:GLY:C	2:E:139:ARG:HH12	2.05	0.63
2:E:79:ASP:C	2:E:80:THR:CG2	2.72	0.63
2:F:20:PHE:CD2	2:F:20:PHE:O	2.52	0.63
2:F:161:LEU:O	2:F:164:GLN:CB	2.46	0.63
1:D:13:MET:HG3	1:D:56:HIS:CD2	2.33	0.63
1:D:79:TRP:HD1	1:D:86:PRO:HB3	1.64	0.63
2:E:6:VAL:HG13	2:E:129:CYS:CB	2.09	0.63
2:F:36:PHE:CE1	2:F:135:PHE:CZ	2.86	0.63
1:C:36:ALA:HB2	1:C:42:GLU:CG	2.25	0.63
1:D:16:VAL:HB	1:D:25:ALA:HB3	1.80	0.63
1:A:124:ASN:HD22	1:A:124:ASN:C	2.05	0.63
1:A:19:ALA:HB3	1:A:111:LEU:O	1.97	0.63
1:B:121:VAL:HA	1:D:22:GLY:O	1.98	0.63
1:D:87:PHE:CD2	1:D:88:HIS:NE2	2.65	0.63
2:E:113:THR:N	2:E:139:ARG:HD3	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:166:ARG:HG3	2:E:167:LEU:N	2.14	0.63
1:A:100:SER:O	1:A:103:ARG:NH2	2.32	0.63
2:E:24:TRP:CZ2	2:E:139:ARG:NE	2.66	0.63
2:F:118:TYR:HD1	2:F:119:SER:H	1.44	0.63
1:A:19:ALA:CB	1:A:112:SER:OG	2.47	0.63
2:F:70:CYS:SG	2:F:173:TYR:CD1	2.92	0.63
1:B:102:PRO:HD3	1:B:124:ASN:HA	1.79	0.63
2:E:97:LEU:O	2:E:98:GLN:C	2.42	0.63
2:E:9:PHE:CZ	2:E:160:CYS:HB3	2.32	0.62
2:E:135:PHE:HB2	2:E:137:PHE:HE1	1.64	0.62
2:F:119:SER:C	2:F:132:SER:HB2	2.24	0.62
2:F:161:LEU:HD12	2:F:165:TYR:CE2	2.33	0.62
1:D:16:VAL:HG13	1:D:111:LEU:HD11	1.80	0.62
2:F:29:LYS:HD3	2:F:41:ILE:CD1	2.29	0.62
1:A:12:LEU:HD12	1:A:13:MET:H	1.64	0.62
1:D:13:MET:SD	1:D:56:HIS:NE2	2.73	0.62
2:E:138:SER:OG	2:E:144:LEU:CD2	2.44	0.62
2:F:13:GLU:C	2:F:15:PHE:N	2.57	0.62
1:A:97:ALA:C	1:A:99:ASP:N	2.57	0.62
1:C:115:SER:HB2	1:D:119:THR:CB	2.28	0.62
2:E:72:ASP:HB3	2:E:93:VAL:HG21	1.80	0.62
1:C:97:ALA:O	1:C:98:ASN:C	2.42	0.62
1:D:102:PRO:HG2	1:D:122:VAL:CG1	2.29	0.62
2:E:92:GLY:O	2:E:94:ALA:N	2.31	0.62
2:F:109:THR:OG1	2:F:115:ALA:CB	2.48	0.62
2:F:113:THR:N	2:F:139:ARG:HD3	2.11	0.62
1:A:70:LYS:HD2	1:A:92:GLU:CD	2.25	0.62
2:E:109:THR:OG1	2:E:110:ASP:N	2.32	0.62
2:F:40:ASN:OD1	2:F:170:HIS:C	2.43	0.62
1:B:84:ILE:CG2	2:F:96:PHE:HB2	2.29	0.62
2:E:135:PHE:HB2	2:E:137:PHE:CE1	2.34	0.62
2:F:17:LYS:HZ3	2:F:53:MET:H	1.46	0.62
2:F:114:TYR:HD2	2:F:148:ALA:HB1	1.64	0.62
1:B:71:VAL:HB	1:B:93:VAL:HB	1.81	0.62
2:E:182:LEU:O	2:E:183:LEU:C	2.42	0.62
1:A:33:PHE:HD2	1:A:43:PRO:HA	1.65	0.61
1:C:76:LYS:HG2	1:C:76:LYS:O	1.99	0.61
2:F:98:GLN:HB3	3:F:2:RTL:H151	1.82	0.61
2:E:137:PHE:HD1	2:E:137:PHE:H	1.48	0.61
1:B:88:HIS:CE1	1:B:116:TYR:HE2	2.19	0.61
1:D:70:LYS:CD	1:D:92:GLU:OE1	2.43	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:VAL:HB	1:C:25:ALA:HB3	1.82	0.61
1:C:79:TRP:CZ2	1:C:112:SER:C	2.79	0.61
1:C:97:ALA:CB	1:C:98:ASN:ND2	2.62	0.61
1:D:33:PHE:O	1:D:69:TYR:CA	2.49	0.61
2:E:12:LYS:CG	2:E:15:PHE:HB2	2.29	0.61
2:E:25:TYR:CD2	2:E:141:PRO:HD3	2.35	0.61
2:E:39:ASP:HB2	2:E:169:VAL:O	2.00	0.61
2:E:73:MET:HE2	2:E:73:MET:HA	1.81	0.61
2:F:37:LEU:CA	2:F:61:VAL:CG2	2.56	0.61
2:E:4:CYS:SG	2:E:129:CYS:HB3	2.41	0.61
1:A:16:VAL:CG1	1:A:25:ALA:HB3	2.31	0.61
1:B:20:VAL:HA	1:C:113:PRO:HD2	1.81	0.61
1:D:21:ARG:HD2	2:E:65:ASN:HD21	1.64	0.61
2:E:29:LYS:HZ3	2:E:29:LYS:HB3	1.64	0.61
2:E:67:TRP:CG	2:E:67:TRP:O	2.51	0.61
1:A:55:LEU:HD13	1:A:58:LEU:HD11	1.82	0.61
1:C:30:VAL:CG2	1:C:55:LEU:HD12	2.31	0.61
2:E:155:ARG:HH21	2:E:155:ARG:HG2	1.66	0.61
2:E:170:HIS:O	2:E:171:ASN:CG	2.43	0.61
2:F:162:ALA:O	2:F:163:ALA:HB3	2.01	0.61
2:E:133:TYR:C	2:E:133:TYR:HD1	2.07	0.61
1:A:55:LEU:HD22	1:A:58:LEU:HD21	1.81	0.61
1:A:70:LYS:HD3	1:A:94:VAL:HG22	1.82	0.61
2:E:17:LYS:NZ	2:E:51:GLY:O	2.33	0.61
2:E:32:PRO:CG	2:E:133:TYR:HB3	2.24	0.61
2:E:138:SER:HB2	2:E:144:LEU:CD2	2.31	0.61
1:B:23:SER:CB	1:B:24:PRO:CD	2.76	0.60
2:F:92:GLY:C	2:F:94:ALA:N	2.55	0.60
2:F:123:LEU:HD13	2:F:129:CYS:N	2.15	0.60
1:C:100:SER:HB2	2:E:91:TRP:CD2	2.37	0.60
2:F:37:LEU:C	2:F:61:VAL:HG22	2.25	0.60
1:B:88:HIS:ND1	1:B:116:TYR:CD2	2.69	0.60
1:D:98:ASN:C	1:D:103:ARG:NH1	2.59	0.60
2:E:114:TYR:HD1	2:E:152:VAL:CG2	2.13	0.60
1:B:18:ASP:OD1	1:B:21:ARG:CG	2.49	0.60
2:E:79:ASP:O	2:E:80:THR:CG2	2.48	0.60
2:F:42:VAL:HG12	2:F:43:ALA:N	2.16	0.60
1:B:63:GLN:OE1	1:B:63:GLN:HA	1.91	0.60
2:E:30:LYS:HD2	2:E:164:GLN:HB3	1.84	0.60
2:E:36:PHE:HE2	3:E:1:RTL:H191	1.65	0.60
2:F:161:LEU:O	2:F:162:ALA:C	2.44	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:110:ASP:O	2:F:111:TYR:HB2	2.02	0.60
2:F:114:TYR:HD1	2:F:114:TYR:O	1.85	0.60
2:F:138:SER:HB2	2:F:144:LEU:CD2	2.29	0.60
1:D:69:TYR:N	1:D:69:TYR:HD1	2.00	0.60
1:A:16:VAL:CB	1:A:25:ALA:HB3	2.31	0.60
1:A:33:PHE:CD2	1:A:43:PRO:HA	2.37	0.60
1:A:122:VAL:CG1	1:B:114:TYR:CE2	2.80	0.60
1:B:41:TRP:CH2	1:B:70:LYS:HB2	2.37	0.60
2:E:77:PHE:CZ	2:E:88:MET:HE2	2.37	0.60
2:E:157:GLU:O	2:E:157:GLU:CG	2.49	0.60
1:D:16:VAL:CG1	1:D:111:LEU:HD12	2.31	0.59
2:F:36:PHE:O	2:F:61:VAL:CG1	2.50	0.59
2:F:150:LYS:O	2:F:150:LYS:CG	2.49	0.59
1:A:26:ILE:HG13	1:A:50:SER:C	2.24	0.59
2:F:4:CYS:O	2:F:5:ALA:CB	2.49	0.59
1:B:55:LEU:HD13	1:B:58:LEU:HD11	1.82	0.59
2:E:73:MET:CE	2:E:97:LEU:HD13	2.20	0.59
2:E:113:THR:CG2	2:E:138:SER:OG	2.50	0.59
2:F:5:ALA:O	2:F:7:SER:N	2.36	0.59
2:F:73:MET:HE3	3:F:2:RTL:C12	2.32	0.59
2:F:156:GLN:HA	2:F:161:LEU:CD2	2.32	0.59
1:B:88:HIS:ND1	1:B:116:TYR:CE2	2.70	0.59
2:E:95:SER:O	2:E:97:LEU:N	2.35	0.59
2:E:173:TYR:CE2	2:E:181:ASN:HB2	2.33	0.59
2:F:64:LEU:O	2:F:66:ASN:N	2.35	0.59
2:F:118:TYR:CG	2:F:159:LEU:HD11	2.37	0.59
2:F:99:LYS:CD	2:F:99:LYS:O	2.50	0.59
2:E:95:SER:O	2:E:96:PHE:CD1	2.56	0.59
1:B:104:ARG:CB	1:B:122:VAL:CG2	2.79	0.59
1:D:107:ILE:HG22	1:D:107:ILE:O	2.03	0.59
2:E:73:MET:O	2:E:74:VAL:HB	2.02	0.59
2:E:113:THR:O	2:E:114:TYR:CB	2.47	0.59
2:F:99:LYS:O	2:F:99:LYS:HD2	2.02	0.59
2:F:124:ASN:C	2:F:124:ASN:HD22	2.10	0.59
1:A:114:TYR:CG	1:D:22:GLY:HA3	2.37	0.59
2:F:18:ALA:O	2:F:21:SER:HB3	2.02	0.59
2:F:122:LEU:HD23	2:F:123:LEU:C	2.28	0.59
2:F:160:CYS:O	2:F:161:LEU:CB	2.50	0.59
2:E:38:GLN:CG	2:E:61:VAL:HA	2.32	0.59
2:E:109:THR:HB	2:E:115:ALA:HB2	1.81	0.59
2:E:159:LEU:HD13	2:E:159:LEU:C	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ALA:CB	1:A:40:THR:CG2	2.79	0.59
1:D:99:ASP:O	1:D:100:SER:C	2.45	0.59
2:F:4:CYS:O	2:F:5:ALA:HB2	2.03	0.59
1:D:12:LEU:HA	1:D:105:TYR:O	2.03	0.58
1:D:35:LYS:HB2	1:D:41:TRP:CZ3	2.37	0.58
2:E:134:SER:CB	2:E:162:ALA:O	2.50	0.58
2:F:99:LYS:HD2	2:F:99:LYS:H	1.67	0.58
2:F:147:GLU:O	2:F:148:ALA:C	2.45	0.58
2:F:156:GLN:OE1	2:F:165:TYR:CE2	2.56	0.58
1:D:34:ARG:HH21	1:D:65:VAL:HG23	1.67	0.58
2:E:69:VAL:HA	2:E:182:LEU:CG	2.22	0.58
1:B:114:TYR:O	1:B:115:SER:HB2	2.02	0.58
1:D:68:ILE:HD11	1:D:96:THR:OG1	2.02	0.58
2:E:4:CYS:SG	2:E:5:ALA:O	2.62	0.58
2:E:48:ASP:O	2:E:50:THR:N	2.36	0.58
2:F:160:CYS:O	2:F:161:LEU:HB3	2.02	0.58
1:A:20:VAL:HG23	1:A:79:TRP:HH2	1.68	0.58
1:B:89:GLU:O	1:B:90:HIS:HB3	2.03	0.58
1:B:18:ASP:CG	1:B:21:ARG:CB	2.77	0.58
1:D:99:ASP:C	1:D:101:GLY:N	2.60	0.58
2:E:19:ARG:O	2:E:111:TYR:HB2	1.99	0.58
2:E:61:VAL:HG12	2:E:63:LEU:H	1.68	0.58
2:E:155:ARG:O	2:E:159:LEU:HB2	2.04	0.58
2:F:73:MET:CE	3:F:2:RTL:H14	2.33	0.58
2:F:160:CYS:CA	2:F:161:LEU:CD2	2.80	0.58
2:F:77:PHE:CD2	2:F:88:MET:HG3	2.39	0.58
1:A:55:LEU:CD2	1:A:58:LEU:HD21	2.33	0.57
1:A:100:SER:CB	2:F:91:TRP:CG	2.84	0.57
2:E:76:THR:O	2:E:88:MET:HA	2.04	0.57
2:E:84:ALA:O	2:E:86:PHE:CE2	2.57	0.57
2:E:102:ASP:OD1	2:E:121:ARG:HD2	2.03	0.57
1:D:59:THR:OG1	1:D:60:THR:N	2.37	0.57
2:E:70:CYS:H	2:E:182:LEU:HG	1.70	0.57
2:E:181:ASN:O	2:E:182:LEU:CB	2.35	0.57
2:F:30:LYS:HE3	2:F:31:ASP:C	2.28	0.57
2:F:99:LYS:CD	2:F:99:LYS:C	2.77	0.57
1:A:70:LYS:HD2	1:A:92:GLU:OE1	2.04	0.57
1:B:22:GLY:N	1:C:114:TYR:CD1	2.71	0.57
1:D:21:ARG:NH1	1:D:82:LEU:HD11	2.19	0.57
2:E:78:THR:HG1	2:E:87:LYS:HB2	1.65	0.57
2:E:112:ASP:O	2:E:113:THR:HB	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:160:CYS:N	2:F:161:LEU:CD2	2.68	0.57
2:E:15:PHE:HA	2:E:111:TYR:OH	2.04	0.57
2:F:67:TRP:CD1	2:F:67:TRP:C	2.83	0.57
1:D:26:ILE:HG23	1:D:50:SER:C	2.30	0.57
2:E:24:TRP:CE2	2:E:139:ARG:NH1	2.72	0.57
2:E:64:LEU:O	2:E:65:ASN:CB	2.44	0.57
2:E:159:LEU:HD12	2:E:162:ALA:HA	1.86	0.57
2:F:79:ASP:C	2:F:80:THR:HG22	2.30	0.57
2:E:29:LYS:HG3	2:E:168:ILE:CG1	2.35	0.57
1:B:83:GLY:HA3	2:F:35:LEU:HD12	1.86	0.56
1:B:97:ALA:C	1:B:103:ARG:HH12	2.13	0.56
1:C:26:ILE:HD11	1:C:51:GLU:CD	2.30	0.56
1:D:56:HIS:ND1	1:D:56:HIS:N	2.52	0.56
1:D:66:GLU:OE2	1:D:99:ASP:CA	2.53	0.56
2:E:159:LEU:HD12	2:E:159:LEU:O	2.04	0.56
2:F:85:LYS:O	2:F:86:PHE:CD2	2.58	0.56
1:A:100:SER:HB2	2:F:91:TRP:CD1	2.40	0.56
2:E:73:MET:HE2	2:E:73:MET:N	2.20	0.56
2:E:121:ARG:NH1	2:E:121:ARG:N	2.53	0.56
1:C:94:VAL:HG12	1:D:89:GLU:HG3	1.86	0.56
1:D:39:ASP:CG	1:D:39:ASP:O	2.48	0.56
1:D:90:HIS:O	1:D:90:HIS:HD2	1.87	0.56
2:E:109:THR:CB	2:E:115:ALA:CB	2.77	0.56
2:E:107:VAL:CG2	2:E:159:LEU:CD2	2.84	0.56
2:E:127:GLY:O	2:E:128:THR:CB	2.53	0.56
2:F:73:MET:HE1	2:F:97:LEU:CB	2.12	0.56
1:B:16:VAL:CB	1:B:25:ALA:HB3	2.34	0.56
1:B:121:VAL:CG1	1:D:24:PRO:HD3	2.27	0.56
2:E:9:PHE:HB3	2:E:158:GLU:O	2.06	0.56
2:E:40:ASN:ND2	2:E:173:TYR:HB3	2.19	0.56
2:E:71:ALA:HB1	2:E:73:MET:HE3	1.87	0.56
2:E:110:ASP:C	2:E:112:ASP:N	2.60	0.56
2:F:20:PHE:HD2	2:F:45:PHE:CD1	2.18	0.56
1:A:25:ALA:O	1:A:53:GLY:HA2	2.05	0.56
1:B:13:MET:CG	1:B:56:HIS:NE2	2.69	0.56
1:B:104:ARG:HB2	1:B:122:VAL:CG2	2.35	0.56
1:C:97:ALA:C	1:C:98:ASN:HD22	2.14	0.56
2:F:38:GLN:HB2	2:F:60:ARG:C	2.22	0.56
2:F:156:GLN:HA	2:F:161:LEU:CG	2.36	0.56
2:E:109:THR:CB	2:E:115:ALA:HB2	2.36	0.56
2:F:124:ASN:HD22	2:F:125:LEU:HG	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:TYR:N	1:C:105:TYR:CD2	2.73	0.56
2:E:159:LEU:O	2:E:160:CYS:C	2.49	0.56
1:D:20:VAL:CG1	2:E:64:LEU:HD21	2.36	0.56
2:F:52:GLN:HE22	2:F:76:THR:HG22	1.71	0.56
2:F:128:THR:O	2:F:129:CYS:HB3	2.06	0.56
1:A:9:LYS:O	1:A:10:CYS:C	2.49	0.56
1:B:21:ARG:O	1:C:114:TYR:CE1	2.59	0.56
2:E:77:PHE:CZ	2:E:88:MET:HG3	2.41	0.56
1:B:104:ARG:HB2	1:B:122:VAL:HG21	1.88	0.55
1:D:16:VAL:O	1:D:17:LEU:CD2	2.40	0.55
1:D:66:GLU:HG2	1:D:99:ASP:N	2.21	0.55
1:D:76:LYS:O	1:D:80:LYS:HB2	2.05	0.55
2:E:52:GLN:CD	2:E:77:PHE:O	2.49	0.55
2:E:136:VAL:CG2	2:E:163:ALA:HB2	2.36	0.55
1:A:83:GLY:O	2:E:67:TRP:HA	2.06	0.55
1:D:21:ARG:CZ	1:D:82:LEU:HD21	2.36	0.55
2:E:20:PHE:HD1	2:E:111:TYR:CD1	2.23	0.55
1:A:7:GLU:CG	1:A:8:SER:H	2.17	0.55
2:E:139:ARG:NH1	2:E:139:ARG:CG	2.67	0.55
2:F:57:ALA:HB2	3:F:2:RTL:H41	1.88	0.55
2:F:122:LEU:CD2	2:F:123:LEU:C	2.79	0.55
2:E:182:LEU:O	2:E:183:LEU:OXT	2.25	0.55
2:F:38:GLN:CA	2:F:60:ARG:O	2.55	0.55
1:B:21:ARG:HD3	1:B:82:LEU:CD2	2.32	0.55
2:F:6:VAL:CG2	2:F:7:SER:N	2.68	0.55
2:F:11:VAL:C	2:F:12:LYS:O	2.47	0.55
2:F:45:PHE:CE2	2:F:55:ALA:CB	2.90	0.55
2:F:48:ASP:O	2:F:49:GLU:C	2.49	0.55
2:E:6:VAL:CG2	2:E:128:THR:HG22	2.36	0.55
1:A:68:ILE:HD13	1:B:89:GLU:HG3	1.88	0.55
2:E:173:TYR:C	2:E:173:TYR:CD2	2.83	0.55
2:F:114:TYR:HB3	2:F:144:LEU:HD22	1.88	0.55
1:A:34:ARG:O	1:A:34:ARG:CG	2.55	0.55
1:C:95:PHE:CA	1:D:89:GLU:HG2	2.29	0.55
2:E:39:ASP:O	2:E:40:ASN:C	2.50	0.55
2:E:108:ASP:OD1	2:E:155:ARG:CZ	2.55	0.55
2:E:169:VAL:CG2	2:E:171:ASN:OD1	2.55	0.55
1:B:10:CYS:SG	1:B:104:ARG:NH1	2.80	0.55
2:F:28:ALA:C	2:F:29:LYS:CG	2.78	0.55
2:F:161:LEU:O	2:F:164:GLN:HB3	2.05	0.55
1:A:19:ALA:HB3	1:A:112:SER:OG	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:THR:OG1	1:A:63:GLN:HB3	2.07	0.54
1:B:85:SER:OG	2:F:96:PHE:C	2.49	0.54
1:B:98:ASN:O	1:B:103:ARG:NH1	2.29	0.54
2:E:35:LEU:HD22	2:E:62:ARG:CZ	2.37	0.54
2:F:11:VAL:CG2	2:F:84:ALA:HB1	2.36	0.54
2:F:158:GLU:O	2:F:160:CYS:N	2.40	0.54
1:B:32:VAL:HG13	1:B:71:VAL:HG22	1.88	0.54
1:D:76:LYS:HD3	1:D:80:LYS:HE2	1.88	0.54
2:F:126:ASP:OD1	2:F:126:ASP:N	2.40	0.54
2:F:130:ALA:O	2:F:131:ASP:HB3	2.07	0.54
1:A:32:VAL:O	1:A:33:PHE:CD2	2.60	0.54
1:B:13:MET:HG3	1:B:56:HIS:NE2	2.19	0.54
1:B:26:ILE:HG23	1:B:50:SER:O	2.07	0.54
1:A:113:PRO:HG2	1:D:20:VAL:HG13	1.89	0.54
1:D:79:TRP:HA	1:D:79:TRP:CE3	2.43	0.54
2:E:15:PHE:HE2	2:E:106:ILE:HD12	1.69	0.54
2:E:73:MET:HE2	2:E:73:MET:CA	2.36	0.54
2:F:19:ARG:CD	2:F:111:TYR:CD2	2.91	0.54
2:F:29:LYS:CA	2:F:165:TYR:HD1	2.20	0.54
2:F:99:LYS:HD2	2:F:99:LYS:N	2.23	0.54
2:F:156:GLN:CA	2:F:161:LEU:HD21	2.36	0.54
2:E:113:THR:H	2:E:139:ARG:CD	2.17	0.54
2:E:159:LEU:HB3	2:E:162:ALA:CB	2.31	0.54
3:E:1:RTL:C18	3:E:1:RTL:H8	2.37	0.54
1:A:22:GLY:HA3	1:D:114:TYR:CD2	2.43	0.54
2:E:166:ARG:HG3	2:E:167:LEU:H	1.71	0.54
2:F:39:ASP:OD2	2:F:60:ARG:HB3	2.08	0.54
2:F:118:TYR:HE1	2:F:132:SER:CB	2.21	0.54
1:C:98:ASN:N	1:C:98:ASN:HD22	2.06	0.54
1:D:19:ALA:HB2	1:D:110:LEU:HD11	1.88	0.54
1:D:39:ASP:O	1:D:39:ASP:OD1	2.25	0.54
2:E:107:VAL:CG2	2:E:159:LEU:HD21	2.37	0.54
2:E:155:ARG:O	2:E:159:LEU:CB	2.56	0.54
1:B:20:VAL:O	1:C:114:TYR:HD1	1.89	0.54
1:D:66:GLU:HG2	1:D:98:ASN:HA	1.88	0.54
1:D:74:ASP:OD2	1:D:77:SER:HB2	2.07	0.54
2:E:36:PHE:CE2	3:E:1:RTL:H191	2.42	0.54
2:E:86:PHE:C	2:E:87:LYS:HG2	2.33	0.54
2:F:32:PRO:HB3	2:F:133:TYR:HB3	1.89	0.54
2:F:48:ASP:OD1	2:F:50:THR:HG22	2.08	0.54
2:F:112:ASP:O	2:F:113:THR:CB	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:CYS:CB	1:D:56:HIS:HD2	2.21	0.54
1:A:35:LYS:HE3	1:A:39:ASP:OD1	2.08	0.53
1:B:34:ARG:NH2	1:B:65:VAL:CG2	2.59	0.53
2:F:5:ALA:O	2:F:7:SER:O	2.27	0.53
2:F:114:TYR:CD1	2:F:114:TYR:O	2.59	0.53
1:B:121:VAL:O	1:B:122:VAL:O	2.25	0.53
1:D:32:VAL:C	1:D:33:PHE:CD1	2.86	0.53
2:F:90:TYR:HE2	2:F:98:GLN:O	1.91	0.53
2:F:103:ASP:N	2:F:121:ARG:HD3	2.20	0.53
1:B:16:VAL:HG12	1:B:17:LEU:H	1.73	0.53
1:D:13:MET:SD	1:D:56:HIS:CE1	3.02	0.53
1:D:21:ARG:HD3	2:E:64:LEU:CD1	2.38	0.53
2:E:24:TRP:CZ3	2:E:139:ARG:HD2	2.43	0.53
1:C:35:LYS:N	1:C:41:TRP:CZ3	2.77	0.53
2:E:13:GLU:C	2:E:15:PHE:N	2.66	0.53
1:A:34:ARG:O	1:A:34:ARG:HG2	2.08	0.53
1:D:90:HIS:CD2	1:D:90:HIS:C	2.86	0.53
2:F:17:LYS:CD	2:F:53:MET:HB2	2.28	0.53
1:A:50:SER:OG	1:A:52:SER:N	2.37	0.53
1:B:124:ASN:O	1:B:126:LYS:N	2.41	0.53
1:D:66:GLU:CG	1:D:103:ARG:HH12	2.18	0.53
1:D:69:TYR:HD1	1:D:69:TYR:H	1.55	0.53
2:E:39:ASP:HB3	2:E:169:VAL:CG1	2.39	0.53
2:E:107:VAL:O	2:E:107:VAL:CG1	2.52	0.53
2:E:159:LEU:HD12	2:E:161:LEU:C	2.31	0.53
2:F:53:MET:O	2:F:77:PHE:CD1	2.62	0.53
2:F:60:ARG:HD3	2:F:173:TYR:CD2	2.42	0.53
2:F:104:HIS:C	2:F:105:TRP:O	2.52	0.53
1:A:18:ASP:OD1	1:A:20:VAL:N	2.41	0.53
1:D:119:THR:HG23	1:D:120:ALA:N	2.24	0.53
2:E:15:PHE:HD1	2:E:16:ASP:N	2.07	0.53
2:E:81:GLU:OE1	2:E:81:GLU:HA	2.09	0.53
2:E:95:SER:C	2:E:97:LEU:H	2.17	0.53
2:F:164:GLN:O	2:F:164:GLN:CG	2.56	0.53
2:E:49:GLU:O	2:E:50:THR:C	2.51	0.53
1:D:20:VAL:HG12	2:E:64:LEU:HD21	1.91	0.53
2:E:82:ASP:C	2:E:84:ALA:H	2.17	0.53
2:E:139:ARG:HH11	2:E:139:ARG:HG3	1.74	0.53
2:E:173:TYR:HD2	2:E:173:TYR:C	2.14	0.53
2:F:73:MET:HE3	3:F:2:RTL:C14	2.37	0.53
2:F:6:VAL:HA	2:F:9:PHE:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:124:ASN:HD22	2:F:125:LEU:N	2.07	0.52
2:E:52:GLN:OE1	2:E:52:GLN:HA	2.09	0.52
2:F:77:PHE:CD1	2:F:77:PHE:N	2.76	0.52
2:F:108:ASP:O	2:F:109:THR:HB	2.08	0.52
1:B:17:LEU:HB2	1:B:110:LEU:CD1	2.38	0.52
1:B:39:ASP:CG	1:B:39:ASP:O	2.53	0.52
1:C:79:TRP:CE3	1:C:79:TRP:HA	2.44	0.52
1:D:70:LYS:CA	1:D:93:VAL:O	2.54	0.52
2:E:20:PHE:HB2	2:E:111:TYR:CD1	2.44	0.52
2:E:63:LEU:HG	2:E:67:TRP:CE3	2.45	0.52
2:E:159:LEU:CD1	2:E:162:ALA:CA	2.81	0.52
2:E:26:ALA:O	2:E:27:MET:HE3	2.10	0.52
2:F:52:GLN:NE2	2:F:76:THR:HG22	2.24	0.52
2:F:124:ASN:CB	2:F:130:ALA:HB2	2.36	0.52
1:A:87:PHE:CE2	1:B:95:PHE:CB	2.93	0.52
1:A:112:SER:O	1:A:115:SER:O	2.27	0.52
1:D:41:TRP:HZ3	1:D:68:ILE:O	1.92	0.52
2:F:124:ASN:HB2	2:F:130:ALA:CB	2.38	0.52
2:F:159:LEU:CD1	2:F:159:LEU:C	2.81	0.52
2:E:124:ASN:O	2:E:127:GLY:N	2.42	0.52
1:A:28:VAL:O	1:A:48:LYS:HA	2.10	0.52
1:B:87:PHE:HD2	1:B:88:HIS:NE2	2.03	0.52
1:D:99:ASP:N	1:D:103:ARG:NH1	2.57	0.52
2:F:118:TYR:CG	2:F:159:LEU:HD21	2.44	0.52
1:D:15:LYS:HA	1:D:53:GLY:O	2.10	0.52
1:D:21:ARG:O	1:D:22:GLY:C	2.53	0.52
2:E:20:PHE:CD1	2:E:111:TYR:HD1	2.28	0.52
2:E:63:LEU:HD23	2:E:69:VAL:HG11	1.92	0.52
2:E:90:TYR:OH	2:E:98:GLN:NE2	2.40	0.52
2:E:113:THR:HG23	2:E:138:SER:HG	1.73	0.52
2:F:163:ALA:C	2:F:165:TYR:H	2.18	0.52
1:A:97:ALA:C	1:A:99:ASP:H	2.18	0.52
2:F:25:TYR:O	2:F:137:PHE:HD1	1.93	0.52
1:D:34:ARG:HH11	1:D:34:ARG:CG	2.21	0.52
1:B:114:TYR:CD2	1:C:22:GLY:HA3	2.45	0.51
1:C:87:PHE:HB2	1:C:114:TYR:CD2	2.45	0.51
1:D:12:LEU:CD2	1:D:58:LEU:CD1	2.82	0.51
1:D:73:ILE:HG22	1:D:75:THR:CG2	2.40	0.51
2:E:32:PRO:CB	2:E:133:TYR:HB3	2.40	0.51
2:F:124:ASN:ND2	2:F:124:ASN:C	2.65	0.51
1:B:116:TYR:O	1:B:116:TYR:CD1	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:57:ALA:HB3	3:E:1:RTL:H173	1.92	0.51
2:E:74:VAL:HG12	2:E:91:TRP:O	2.09	0.51
2:F:29:LYS:O	2:F:165:TYR:HD1	1.93	0.51
2:F:82:ASP:HB2	2:F:85:LYS:HG3	1.92	0.51
1:B:30:VAL:O	1:B:46:SER:HA	2.10	0.51
2:E:24:TRP:CE2	2:E:139:ARG:CZ	2.93	0.51
2:F:78:THR:O	2:F:79:ASP:O	2.28	0.51
1:C:28:VAL:HB	1:C:49:THR:CG2	2.40	0.51
1:D:25:ALA:HB1	1:D:28:VAL:CG2	2.37	0.51
2:E:103:ASP:HB2	2:E:121:ARG:CZ	2.41	0.51
1:B:40:THR:HG22	1:B:41:TRP:N	2.25	0.51
1:B:123:THR:C	1:B:125:PRO:HD3	2.35	0.51
1:C:103:ARG:HB2	1:C:105:TYR:CE2	2.46	0.51
2:E:24:TRP:HZ3	2:E:114:TYR:H	1.58	0.51
2:E:82:ASP:C	2:E:84:ALA:N	2.69	0.51
2:E:106:ILE:O	2:E:106:ILE:CG2	2.56	0.51
2:F:118:TYR:CD2	2:F:159:LEU:HD11	2.45	0.51
1:A:95:PHE:HA	1:B:89:GLU:HG2	1.93	0.51
1:A:102:PRO:O	1:A:103:ARG:HG2	2.11	0.51
2:E:20:PHE:HD1	2:E:111:TYR:HD1	1.57	0.51
2:E:94:ALA:O	2:E:95:SER:O	2.28	0.51
2:E:114:TYR:CD1	2:E:152:VAL:HG22	2.46	0.51
2:E:145:PRO:HB2	2:E:147:GLU:OE1	2.10	0.51
2:F:36:PHE:O	2:F:61:VAL:HG13	2.10	0.51
2:F:118:TYR:CD2	2:F:159:LEU:CD2	2.87	0.51
1:A:64:PHE:CD1	1:A:69:TYR:CZ	2.98	0.51
1:A:98:ASN:OD1	1:A:102:PRO:CA	2.45	0.51
1:B:21:ARG:C	1:C:114:TYR:CE1	2.89	0.51
2:E:47:VAL:CG1	2:E:48:ASP:H	2.10	0.51
2:E:52:GLN:NE2	2:E:76:THR:HG22	2.25	0.51
2:E:39:ASP:CB	2:E:169:VAL:CG1	2.88	0.51
2:E:84:ALA:O	2:E:86:PHE:CD2	2.64	0.51
2:F:110:ASP:O	2:F:111:TYR:CB	2.59	0.51
2:F:173:TYR:CD1	2:F:173:TYR:C	2.88	0.51
1:A:32:VAL:C	1:A:33:PHE:CD2	2.88	0.51
1:B:16:VAL:HG12	1:B:17:LEU:N	2.26	0.51
1:B:16:VAL:CG2	1:B:49:THR:HG21	2.41	0.51
1:C:64:PHE:CD1	1:C:69:TYR:CE2	2.99	0.51
1:A:98:ASN:OD1	1:A:103:ARG:N	2.44	0.51
1:B:78:TYR:O	1:B:81:ALA:HB3	2.10	0.51
1:D:55:LEU:HD11	1:D:58:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:GLU:CG	1:D:99:ASP:N	2.71	0.51
1:A:79:TRP:HE3	1:A:84:ILE:HD12	1.77	0.50
1:A:97:ALA:O	1:A:98:ASN:C	2.52	0.50
1:D:55:LEU:HD22	1:D:55:LEU:O	2.10	0.50
2:E:159:LEU:HG	2:E:162:ALA:CB	2.37	0.50
2:F:27:MET:HE1	2:F:144:LEU:CG	2.41	0.50
2:F:156:GLN:C	2:F:161:LEU:CD2	2.85	0.50
1:A:16:VAL:HG11	1:A:111:LEU:CD1	2.30	0.50
2:E:92:GLY:O	2:E:93:VAL:C	2.55	0.50
2:E:64:LEU:O	2:E:64:LEU:HG	2.11	0.50
1:A:87:PHE:C	1:A:87:PHE:CD2	2.89	0.50
1:C:79:TRP:CD1	1:C:86:PRO:HB3	2.46	0.50
2:E:30:LYS:HE2	2:E:161:LEU:HG	1.94	0.50
2:E:85:LYS:HG2	2:E:105:TRP:CG	2.45	0.50
2:E:95:SER:C	2:E:97:LEU:N	2.69	0.50
2:F:173:TYR:HD1	2:F:173:TYR:C	2.19	0.50
1:B:10:CYS:N	1:B:11:PRO:HD3	2.27	0.50
1:A:33:PHE:O	1:A:69:TYR:HA	2.11	0.50
2:E:41:ILE:HD13	2:E:135:PHE:HE2	1.77	0.50
2:E:54:SER:O	2:E:55:ALA:HB2	2.10	0.50
1:C:79:TRP:CZ2	1:C:113:PRO:N	2.80	0.50
1:D:54:GLU:OE1	1:D:56:HIS:NE2	2.44	0.50
2:E:24:TRP:CE2	2:E:139:ARG:HD2	2.45	0.50
2:F:74:VAL:HG22	2:F:75:GLY:N	2.27	0.50
2:F:81:GLU:C	2:F:81:GLU:CD	2.79	0.50
1:B:69:TYR:O	1:B:94:VAL:HA	2.12	0.50
1:D:56:HIS:O	1:D:57:GLY:C	2.54	0.50
1:D:76:LYS:CD	1:D:80:LYS:HE2	2.42	0.50
1:D:89:GLU:O	1:D:90:HIS:HB3	2.12	0.50
1:D:99:ASP:N	1:D:103:ARG:HH11	2.09	0.50
2:E:77:PHE:CE2	2:E:88:MET:HB2	2.47	0.50
1:B:98:ASN:HB3	1:B:100:SER:OG	2.12	0.50
1:D:74:ASP:OD2	1:D:77:SER:CB	2.60	0.50
2:E:15:PHE:CE1	2:E:17:LYS:CA	2.93	0.50
2:F:63:LEU:CD2	2:F:96:PHE:HE1	2.25	0.50
2:F:147:GLU:OE1	2:F:147:GLU:N	2.36	0.50
1:D:10:CYS:HB3	1:D:56:HIS:CD2	2.47	0.49
2:F:140:ASP:OD2	2:F:141:PRO:CD	2.59	0.49
2:E:35:LEU:HD22	2:E:62:ARG:NE	2.27	0.49
2:E:72:ASP:HB3	2:E:93:VAL:CG2	2.43	0.49
2:F:151:ILE:C	2:F:153:ALA:N	2.67	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:VAL:HB	1:C:49:THR:HG21	1.93	0.49
1:D:28:VAL:O	1:D:30:VAL:HG23	2.12	0.49
2:E:156:GLN:CG	2:E:163:ALA:HB3	2.33	0.49
2:F:30:LYS:CE	2:F:31:ASP:C	2.86	0.49
1:C:94:VAL:HG12	1:D:89:GLU:HB2	1.93	0.49
1:C:97:ALA:CB	1:C:98:ASN:HD22	2.25	0.49
2:F:38:GLN:CG	2:F:62:ARG:HD2	2.42	0.49
1:B:66:GLU:HG2	1:B:99:ASP:OD1	2.12	0.49
2:E:45:PHE:CD2	2:E:55:ALA:HB1	2.47	0.49
2:E:73:MET:HG3	3:E:1:RTL:H10	1.95	0.49
2:F:89:LYS:HA	2:F:100:GLY:O	2.12	0.49
1:B:34:ARG:CZ	1:B:65:VAL:HG23	2.40	0.49
1:B:123:THR:HG23	1:B:125:PRO:CD	2.32	0.49
2:E:44:GLU:O	2:E:55:ALA:HA	2.12	0.49
1:B:83:GLY:O	2:F:63:LEU:HD11	2.12	0.49
1:C:87:PHE:HB2	1:C:114:TYR:CE2	2.47	0.49
1:A:8:SER:O	1:A:8:SER:OG	2.29	0.49
1:A:103:ARG:O	1:A:105:TYR:CE2	2.65	0.49
1:C:123:THR:O	1:C:123:THR:OG1	2.30	0.49
1:D:21:ARG:HD3	1:D:82:LEU:HD21	1.93	0.49
2:E:9:PHE:CE2	2:E:160:CYS:CB	2.68	0.49
2:F:27:MET:O	2:F:27:MET:HG2	2.11	0.49
2:F:81:GLU:C	2:F:82:ASP:O	2.55	0.49
1:D:102:PRO:CG	1:D:122:VAL:HG12	2.41	0.49
2:E:45:PHE:CD2	2:E:55:ALA:CB	2.96	0.49
2:F:44:GLU:HB3	2:F:56:THR:HG23	1.95	0.49
2:F:77:PHE:CE2	2:F:88:MET:CG	2.96	0.49
2:F:78:THR:O	2:F:87:LYS:HG3	2.13	0.49
1:A:79:TRP:CE3	1:A:84:ILE:HD12	2.48	0.49
1:B:102:PRO:HD2	1:B:124:ASN:ND2	2.28	0.49
1:C:69:TYR:N	1:C:69:TYR:CD1	2.81	0.49
1:C:79:TRP:HZ2	1:C:112:SER:CA	2.26	0.49
2:E:151:ILE:C	2:E:153:ALA:N	2.66	0.49
2:F:107:VAL:CG2	2:F:159:LEU:HD23	2.40	0.49
1:A:124:ASN:C	1:A:124:ASN:ND2	2.71	0.48
1:C:26:ILE:HD11	1:C:51:GLU:OE2	2.13	0.48
2:F:138:SER:OG	2:F:144:LEU:HD23	2.13	0.48
2:E:6:VAL:HG22	2:E:128:THR:HG22	1.95	0.48
2:F:118:TYR:CB	2:F:159:LEU:HD21	2.42	0.48
1:A:26:ILE:O	1:A:27:ASN:HB2	2.12	0.48
1:A:34:ARG:O	1:A:35:LYS:C	2.55	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:TYR:N	1:A:105:TYR:CD2	2.81	0.48
1:C:87:PHE:O	1:D:95:PHE:HB2	2.14	0.48
2:E:35:LEU:HD23	2:E:35:LEU:H	1.79	0.48
2:F:134:SER:O	2:F:165:TYR:HE1	1.96	0.48
1:A:18:ASP:CG	1:A:21:ARG:H	2.21	0.48
1:D:11:PRO:O	1:D:12:LEU:C	2.56	0.48
2:E:30:LYS:HG2	2:E:134:SER:HB3	1.95	0.48
2:F:54:SER:O	2:F:55:ALA:HB2	2.14	0.48
1:A:7:GLU:CG	1:A:8:SER:N	2.70	0.48
1:C:17:LEU:HD23	1:C:24:PRO:HA	1.95	0.48
2:E:118:TYR:HE1	2:E:132:SER:CB	2.25	0.48
1:B:34:ARG:HB2	1:B:69:TYR:CD2	2.49	0.48
1:B:41:TRP:CD1	1:B:70:LYS:HE2	2.49	0.48
1:B:70:LYS:HA	1:B:93:VAL:O	2.14	0.48
2:E:48:ASP:O	2:E:49:GLU:C	2.57	0.48
1:A:87:PHE:CE2	1:B:95:PHE:HB3	2.48	0.48
2:E:15:PHE:CD1	2:E:16:ASP:N	2.81	0.48
2:F:37:LEU:HD13	2:F:59:GLY:HA3	1.95	0.48
1:A:59:THR:HG23	1:A:60:THR:N	2.28	0.48
1:D:85:SER:HA	1:D:86:PRO:HD2	1.51	0.48
3:E:1:RTL:C18	3:E:1:RTL:C8	2.89	0.48
2:F:8:SER:C	2:F:10:ARG:H	2.22	0.48
2:F:70:CYS:SG	2:F:173:TYR:C	2.97	0.48
2:F:85:LYS:HD2	2:F:105:TRP:HE1	1.78	0.48
1:C:36:ALA:O	1:C:37:ALA:C	2.56	0.48
1:C:70:LYS:HD2	1:C:92:GLU:CD	2.38	0.48
2:E:23:THR:O	2:E:139:ARG:HG3	2.13	0.48
2:F:144:LEU:HD12	2:F:149:GLN:OE1	2.14	0.48
2:E:19:ARG:O	2:E:19:ARG:HG2	2.14	0.47
2:E:95:SER:O	2:E:96:PHE:CG	2.67	0.47
2:F:26:ALA:HB1	2:F:168:ILE:CD1	2.44	0.47
1:B:21:ARG:HB2	1:B:23:SER:OG	2.13	0.47
1:B:102:PRO:CD	1:B:124:ASN:ND2	2.77	0.47
1:D:21:ARG:HD3	2:E:64:LEU:HD11	1.96	0.47
2:E:107:VAL:HG21	2:E:159:LEU:HD23	1.94	0.47
3:E:1:RTL:C8	3:E:1:RTL:H181	2.44	0.47
2:F:104:HIS:O	2:F:104:HIS:CG	2.66	0.47
2:F:118:TYR:HE1	2:F:132:SER:OG	1.97	0.47
2:F:124:ASN:O	2:F:125:LEU:C	2.57	0.47
2:E:159:LEU:CD1	2:E:162:ALA:HB2	2.43	0.47
2:F:21:SER:O	2:F:21:SER:OG	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:29:LYS:HD3	2:F:41:ILE:HD13	1.96	0.47
1:B:85:SER:H	2:F:96:PHE:C	2.21	0.47
1:D:66:GLU:HG3	1:D:99:ASP:CG	2.40	0.47
2:E:20:PHE:CD1	2:E:111:TYR:CD1	3.02	0.47
2:E:32:PRO:HB3	2:E:133:TYR:HB3	1.96	0.47
2:F:92:GLY:HA3	2:F:97:LEU:HD12	1.97	0.47
2:F:99:LYS:O	2:F:99:LYS:HD3	2.15	0.47
1:C:118:THR:O	1:D:115:SER:HA	2.15	0.47
2:E:147:GLU:O	2:E:150:LYS:CB	2.62	0.47
2:F:36:PHE:HE2	3:F:2:RTL:H191	1.78	0.47
2:F:66:ASN:C	2:F:67:TRP:O	2.48	0.47
1:B:18:ASP:OD1	1:B:21:ARG:HB2	2.11	0.47
1:B:36:ALA:HB2	1:B:42:GLU:CD	2.39	0.47
2:E:24:TRP:HZ3	2:E:114:TYR:N	2.13	0.47
2:E:29:LYS:H	2:E:165:TYR:HA	1.80	0.47
2:E:138:SER:HB2	2:E:144:LEU:HD21	1.96	0.47
2:F:63:LEU:HD23	2:F:69:VAL:CG1	2.38	0.47
2:E:12:LYS:HG2	2:E:15:PHE:HB2	1.95	0.47
2:E:35:LEU:HD13	2:E:62:ARG:HG3	1.96	0.47
2:E:182:LEU:HD22	2:E:183:LEU:CG	2.32	0.47
2:F:36:PHE:HE2	3:F:2:RTL:C19	2.27	0.47
2:F:105:TRP:O	2:F:117:GLN:HG2	2.14	0.47
2:F:115:ALA:C	2:F:116:VAL:HG23	2.40	0.47
2:F:156:GLN:C	2:F:161:LEU:HD21	2.40	0.47
2:F:157:GLU:HB3	2:F:158:GLU:OE2	2.14	0.47
1:D:13:MET:HG3	1:D:56:HIS:ND1	2.29	0.47
2:E:30:LYS:O	2:E:32:PRO:HD2	2.15	0.47
2:E:164:GLN:HG2	2:E:165:TYR:N	2.20	0.47
2:F:6:VAL:HG12	2:F:129:CYS:CB	2.20	0.47
2:F:77:PHE:HE2	2:F:104:HIS:NE2	2.03	0.47
1:B:35:LYS:HB2	1:B:35:LYS:HE3	1.58	0.47
1:D:66:GLU:CB	1:D:97:ALA:O	2.63	0.47
2:E:24:TRP:NE1	2:E:139:ARG:CZ	2.78	0.47
1:B:104:ARG:HB3	1:B:122:VAL:HG21	1.96	0.47
1:D:44:PHE:HE2	1:D:59:THR:HB	1.80	0.47
1:D:84:ILE:HG23	2:E:96:PHE:HB2	1.97	0.47
2:E:78:THR:O	2:E:79:ASP:O	2.33	0.47
2:E:107:VAL:O	2:E:108:ASP:CB	2.60	0.47
2:F:28:ALA:HB1	2:F:165:TYR:CG	2.50	0.47
1:B:116:TYR:CD1	1:B:116:TYR:C	2.91	0.46
1:C:79:TRP:HA	1:C:79:TRP:HE3	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:38:GLN:HB2	2:F:61:VAL:HA	1.96	0.46
1:A:50:SER:OG	1:A:51:GLU:N	2.45	0.46
1:A:36:ALA:HB3	1:A:40:THR:CG2	2.30	0.46
1:B:16:VAL:HG23	1:B:49:THR:HG21	1.98	0.46
1:B:123:THR:OG1	1:B:124:ASN:N	2.46	0.46
1:C:35:LYS:HD2	1:C:41:TRP:CZ2	2.51	0.46
1:C:58:LEU:HA	1:C:58:LEU:HD23	1.62	0.46
1:D:44:PHE:C	1:D:44:PHE:CD2	2.93	0.46
2:F:6:VAL:HG11	2:F:129:CYS:CB	2.22	0.46
1:C:106:THR:HB	1:C:121:VAL:HB	1.96	0.46
2:F:77:PHE:CE2	2:F:88:MET:HG3	2.49	0.46
2:F:146:PRO:HD2	2:F:147:GLU:OE1	2.15	0.46
1:B:66:GLU:HA	1:B:97:ALA:O	2.15	0.46
1:C:66:GLU:HB3	1:C:98:ASN:O	2.16	0.46
2:E:5:ALA:C	2:E:129:CYS:HB3	2.41	0.46
2:E:108:ASP:OD1	2:E:155:ARG:NH1	2.48	0.46
2:F:38:GLN:NE2	2:F:62:ARG:HD2	2.31	0.46
2:F:71:ALA:HB1	2:F:97:LEU:HD22	1.97	0.46
2:F:156:GLN:CB	2:F:161:LEU:HG	2.45	0.46
2:E:52:GLN:HE21	2:E:76:THR:HG22	1.81	0.46
2:E:138:SER:HB2	2:E:144:LEU:HD22	1.92	0.46
2:F:5:ALA:O	2:F:6:VAL:C	2.59	0.46
2:F:113:THR:O	2:F:138:SER:CA	2.60	0.46
2:F:148:ALA:O	2:F:149:GLN:C	2.58	0.46
1:B:82:LEU:HB3	1:B:84:ILE:HD12	1.97	0.46
1:C:67:GLY:O	1:C:69:TYR:CE1	2.68	0.46
2:E:114:TYR:CD1	2:E:114:TYR:C	2.89	0.46
2:F:17:LYS:HD3	2:F:53:MET:CB	2.29	0.46
2:F:29:LYS:O	2:F:165:TYR:CD1	2.68	0.46
2:F:29:LYS:O	2:F:165:TYR:HA	2.16	0.46
2:F:44:GLU:O	2:F:44:GLU:HG3	2.15	0.46
2:F:92:GLY:C	2:F:94:ALA:H	2.23	0.46
2:F:106:ILE:O	2:F:106:ILE:HG22	2.15	0.46
1:A:32:VAL:HB	1:A:45:ALA:H	1.80	0.46
1:C:67:GLY:O	1:C:69:TYR:CD1	2.69	0.46
1:C:94:VAL:O	1:D:89:GLU:HB2	2.16	0.46
1:D:16:VAL:C	1:D:17:LEU:CD2	2.88	0.46
2:E:40:ASN:O	2:E:59:GLY:HA2	2.16	0.46
2:E:132:SER:OG	2:E:133:TYR:N	2.49	0.46
2:E:159:LEU:CD1	2:E:162:ALA:HA	2.45	0.46
2:F:74:VAL:CG2	2:F:75:GLY:N	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:LEU:CB	1:B:110:LEU:HD13	2.43	0.46
1:D:21:ARG:HG2	2:E:64:LEU:HD11	1.98	0.46
2:E:120:CYS:SG	2:E:131:ASP:O	2.74	0.46
1:C:59:THR:OG1	1:C:60:THR:N	2.48	0.45
1:D:42:GLU:O	1:D:43:PRO:C	2.57	0.45
2:F:81:GLU:CD	2:F:82:ASP:N	2.74	0.45
1:B:76:LYS:O	1:B:77:SER:C	2.59	0.45
1:C:60:THR:OG1	1:C:63:GLN:HB2	2.15	0.45
2:E:70:CYS:N	2:E:182:LEU:HD12	2.26	0.45
2:F:27:MET:CA	2:F:168:ILE:CD1	2.95	0.45
1:C:26:ILE:HD11	1:C:51:GLU:OE1	2.16	0.45
1:D:13:MET:CG	1:D:56:HIS:CE1	3.00	0.45
1:B:24:PRO:CB	1:B:52:SER:O	2.65	0.45
2:E:9:PHE:CB	2:E:158:GLU:O	2.65	0.45
2:E:70:CYS:N	2:E:182:LEU:HG	2.31	0.45
2:E:107:VAL:CG2	2:E:159:LEU:HD23	2.46	0.45
2:F:92:GLY:O	2:F:93:VAL:C	2.57	0.45
1:C:10:CYS:HA	1:C:11:PRO:HD3	1.75	0.45
1:D:25:ALA:O	1:D:28:VAL:CG2	2.62	0.45
1:D:28:VAL:O	1:D:28:VAL:HG12	2.17	0.45
1:D:60:THR:OG1	1:D:63:GLN:HB2	2.16	0.45
2:E:11:VAL:CB	2:E:84:ALA:HB1	2.43	0.45
1:D:66:GLU:HG2	1:D:103:ARG:NH1	2.26	0.45
2:E:159:LEU:HD12	2:E:162:ALA:CB	2.44	0.45
2:F:99:LYS:C	2:F:99:LYS:HD3	2.40	0.45
2:F:156:GLN:CA	2:F:161:LEU:HG	2.46	0.45
1:B:10:CYS:SG	1:B:104:ARG:CZ	3.05	0.45
2:E:20:PHE:CB	2:E:111:TYR:HD1	2.30	0.45
2:E:35:LEU:HD23	2:E:35:LEU:N	2.32	0.45
2:E:136:VAL:CG1	2:E:152:VAL:HG11	2.46	0.45
2:F:37:LEU:HA	2:F:61:VAL:HG21	1.84	0.45
1:A:12:LEU:O	1:A:13:MET:HG2	2.17	0.45
2:E:89:LYS:HE2	2:E:89:LYS:HB2	1.39	0.45
2:F:40:ASN:CG	2:F:170:HIS:HA	2.39	0.45
1:B:97:ALA:C	1:B:103:ARG:NH1	2.75	0.45
2:F:32:PRO:HG3	2:F:133:TYR:HB3	1.99	0.45
1:A:55:LEU:HD22	1:A:58:LEU:CD2	2.47	0.45
2:F:18:ALA:O	2:F:21:SER:N	2.48	0.45
1:D:21:ARG:NE	1:D:82:LEU:HD21	2.33	0.44
1:D:76:LYS:HD3	1:D:80:LYS:CE	2.47	0.44
2:E:111:TYR:O	2:E:139:ARG:NE	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:26:ALA:CB	2:F:168:ILE:HD11	2.47	0.44
2:F:71:ALA:HB1	2:F:73:MET:HE2	1.99	0.44
2:F:102:ASP:HA	2:F:121:ARG:HH11	1.83	0.44
1:B:77:SER:O	1:B:78:TYR:C	2.60	0.44
1:C:26:ILE:CD1	1:C:51:GLU:OE1	2.65	0.44
1:C:92:GLU:OE2	1:D:92:GLU:OE2	2.35	0.44
2:E:24:TRP:CD1	2:E:139:ARG:NH1	2.84	0.44
2:E:64:LEU:HB3	2:E:67:TRP:HE3	1.81	0.44
1:A:12:LEU:C	1:A:13:MET:CG	2.90	0.44
1:A:36:ALA:CB	1:A:40:THR:O	2.66	0.44
2:E:90:TYR:HE2	2:E:98:GLN:O	2.00	0.44
2:F:120:CYS:HA	2:F:132:SER:HB2	1.99	0.44
1:B:88:HIS:ND1	1:B:116:TYR:HD2	2.11	0.44
1:B:90:HIS:HD2	1:B:92:GLU:HG3	1.76	0.44
1:B:102:PRO:CB	1:B:122:VAL:HG12	2.21	0.44
1:D:113:PRO:C	1:D:114:TYR:CD1	2.96	0.44
2:E:65:ASN:CB	2:E:66:ASN:HD21	2.17	0.44
2:F:84:ALA:O	2:F:86:PHE:CE2	2.71	0.44
2:F:121:ARG:HA	2:F:121:ARG:HD2	1.37	0.44
1:C:79:TRP:O	1:C:82:LEU:HB2	2.17	0.44
1:C:100:SER:CB	2:E:91:TRP:CG	3.01	0.44
2:E:140:ASP:OD2	2:E:141:PRO:HD2	2.18	0.44
1:D:20:VAL:HG12	1:D:20:VAL:O	2.17	0.44
2:E:85:LYS:HA	2:E:105:TRP:HA	2.00	0.44
2:F:24:TRP:CZ2	2:F:139:ARG:NE	2.86	0.44
2:F:158:GLU:C	2:F:160:CYS:H	2.25	0.44
1:A:16:VAL:HG13	1:A:111:LEU:HD11	1.99	0.44
1:D:71:VAL:HG23	1:D:93:VAL:HB	1.98	0.44
1:D:79:TRP:HA	1:D:79:TRP:HE3	1.83	0.44
2:E:11:VAL:HB	2:E:84:ALA:HB2	1.95	0.44
2:E:70:CYS:CB	2:E:182:LEU:HD12	2.38	0.44
2:E:154:GLN:C	2:E:154:GLN:OE1	2.61	0.44
2:F:63:LEU:HD21	2:F:96:PHE:CE1	2.52	0.44
2:F:115:ALA:O	2:F:116:VAL:CG2	2.65	0.44
1:B:85:SER:OG	2:F:96:PHE:N	2.50	0.44
1:C:90:HIS:NE2	1:D:94:VAL:HG21	2.33	0.44
2:E:77:PHE:CE1	2:E:88:MET:CG	2.92	0.44
2:F:65:ASN:ND2	2:F:65:ASN:O	2.51	0.44
2:F:90:TYR:HB3	3:F:2:RTL:H181	1.98	0.44
2:F:105:TRP:O	2:F:106:ILE:HG13	2.18	0.44
2:F:120:CYS:N	2:F:132:SER:HB2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:TRP:CE3	1:A:70:LYS:NZ	2.72	0.43
1:B:88:HIS:ND1	1:B:116:TYR:HE2	2.16	0.43
1:D:76:LYS:O	1:D:80:LYS:CB	2.66	0.43
2:E:24:TRP:CZ2	2:E:139:ARG:CZ	3.01	0.43
2:E:77:PHE:CZ	2:E:88:MET:CG	3.01	0.43
2:E:95:SER:C	2:E:96:PHE:CG	2.96	0.43
2:F:84:ALA:O	2:F:85:LYS:C	2.61	0.43
2:F:98:GLN:HB3	3:F:2:RTL:C13	2.48	0.43
1:B:66:GLU:OE2	1:B:98:ASN:OD1	2.37	0.43
1:C:55:LEU:C	1:C:55:LEU:CD2	2.91	0.43
1:D:13:MET:HE2	1:D:13:MET:HB3	1.88	0.43
1:D:21:ARG:O	1:D:23:SER:HB3	2.18	0.43
2:E:30:LYS:HD2	2:E:30:LYS:HA	1.57	0.43
2:F:97:LEU:O	2:F:98:GLN:C	2.60	0.43
1:B:11:PRO:HB2	1:B:59:THR:CG2	2.49	0.43
1:D:73:ILE:HG22	1:D:75:THR:HG23	1.99	0.43
2:E:21:SER:O	2:E:45:PHE:O	2.36	0.43
1:B:40:THR:HG23	1:B:41:TRP:N	2.32	0.43
1:D:87:PHE:CE2	1:D:88:HIS:NE2	2.86	0.43
2:E:126:ASP:N	2:E:126:ASP:OD1	2.51	0.43
2:F:120:CYS:CA	2:F:132:SER:HB2	2.48	0.43
2:F:154:GLN:O	2:F:155:ARG:HG2	2.18	0.43
1:A:79:TRP:CZ3	1:A:113:PRO:HG3	2.52	0.43
1:B:33:PHE:N	1:B:33:PHE:CD1	2.86	0.43
1:B:54:GLU:CB	1:B:56:HIS:HE1	2.25	0.43
1:B:102:PRO:CD	1:B:124:ASN:CG	2.91	0.43
2:E:30:LYS:NZ	2:E:161:LEU:HD11	2.34	0.43
2:E:156:GLN:HG2	2:E:163:ALA:H	1.83	0.43
2:F:29:LYS:NZ	2:F:29:LYS:HB3	2.34	0.43
2:F:38:GLN:NE2	2:F:62:ARG:CD	2.81	0.43
1:A:87:PHE:CZ	1:B:95:PHE:CD2	3.06	0.43
1:B:28:VAL:O	1:B:48:LYS:HA	2.18	0.43
1:D:66:GLU:HG2	1:D:98:ASN:CA	2.49	0.43
2:E:34:GLY:O	2:E:35:LEU:C	2.61	0.43
2:F:112:ASP:HA	2:F:139:ARG:HE	1.83	0.43
1:B:66:GLU:CG	1:B:99:ASP:CG	2.80	0.43
1:C:68:ILE:C	1:C:69:TYR:HD1	2.27	0.43
2:E:104:HIS:CE1	2:E:117:GLN:NE2	2.80	0.43
2:F:92:GLY:HA3	2:F:97:LEU:CD1	2.49	0.43
2:F:131:ASP:O	2:F:131:ASP:OD2	2.36	0.43
2:E:24:TRP:CH2	2:E:139:ARG:CD	2.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:15:PHE:HB3	2:F:83:PRO:HB2	2.01	0.43
1:B:82:LEU:O	2:F:35:LEU:HD12	2.18	0.43
2:E:136:VAL:HG11	2:E:152:VAL:HG11	2.01	0.43
2:F:6:VAL:HG12	2:F:118:TYR:OH	2.19	0.43
2:F:24:TRP:CH2	2:F:111:TYR:O	2.72	0.43
2:F:42:VAL:CG1	2:F:43:ALA:N	2.80	0.43
1:D:13:MET:HG3	1:D:56:HIS:NE2	2.34	0.43
2:F:119:SER:HB3	2:F:133:TYR:CE1	2.54	0.43
2:F:151:ILE:HG22	2:F:152:VAL:N	2.33	0.43
2:F:158:GLU:C	2:F:160:CYS:N	2.77	0.43
1:B:16:VAL:O	1:B:17:LEU:CD2	2.66	0.42
1:B:76:LYS:HG3	1:B:86:PRO:HG2	2.00	0.42
1:B:102:PRO:HD3	1:B:124:ASN:CG	2.43	0.42
1:D:34:ARG:CG	1:D:34:ARG:NH1	2.79	0.42
2:E:63:LEU:HD12	2:E:63:LEU:C	2.44	0.42
2:E:63:LEU:HD21	2:E:67:TRP:CH2	2.54	0.42
2:F:123:LEU:CD1	2:F:129:CYS:H	2.28	0.42
2:F:168:ILE:O	2:F:168:ILE:HG12	2.18	0.42
1:C:69:TYR:N	1:C:69:TYR:HD1	2.16	0.42
1:C:94:VAL:HG12	1:D:89:GLU:CG	2.49	0.42
2:E:117:GLN:HE22	2:E:133:TYR:HE1	1.65	0.42
2:F:29:LYS:CA	2:F:165:TYR:CD1	3.01	0.42
2:F:79:ASP:O	2:F:87:LYS:HE3	2.19	0.42
2:F:90:TYR:CE2	2:F:98:GLN:O	2.71	0.42
1:A:11:PRO:HG2	1:A:12:LEU:H	1.84	0.42
2:F:19:ARG:HG2	2:F:111:TYR:CG	2.54	0.42
2:F:30:LYS:CE	2:F:31:ASP:O	2.67	0.42
2:E:9:PHE:CE2	2:E:160:CYS:N	2.88	0.42
2:F:6:VAL:HA	2:F:9:PHE:CD1	2.54	0.42
2:F:48:ASP:O	2:F:50:THR:HG22	2.16	0.42
2:F:90:TYR:HE2	2:F:98:GLN:HG2	1.84	0.42
2:F:156:GLN:HA	2:F:161:LEU:HD11	2.00	0.42
1:B:98:ASN:O	1:B:103:ARG:HD3	2.18	0.42
2:E:173:TYR:O	2:E:173:TYR:CD2	2.55	0.42
2:F:60:ARG:HD3	2:F:173:TYR:CE2	2.54	0.42
2:F:89:LYS:O	2:F:89:LYS:HG2	2.17	0.42
2:F:104:HIS:O	2:F:105:TRP:C	2.61	0.42
2:F:124:ASN:HD21	2:F:125:LEU:HG	1.80	0.42
1:C:94:VAL:HG12	1:D:89:GLU:CB	2.49	0.42
1:C:117:SER:HB2	1:D:117:SER:CB	2.49	0.42
1:D:66:GLU:CD	1:D:99:ASP:OD2	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:LYS:O	1:D:80:LYS:HG3	2.19	0.42
2:E:5:ALA:CB	2:E:128:THR:OG1	2.59	0.42
2:E:148:ALA:O	2:E:152:VAL:HG23	2.20	0.42
1:B:24:PRO:HB3	1:B:52:SER:O	2.20	0.42
1:B:25:ALA:HB1	1:B:28:VAL:CG2	2.48	0.42
1:C:32:VAL:HB	1:C:45:ALA:HB3	2.02	0.42
1:C:100:SER:HB2	2:E:91:TRP:CD1	2.54	0.42
1:C:108:ALA:HB3	1:C:119:THR:HG22	2.02	0.42
1:D:16:VAL:HG12	1:D:111:LEU:HD12	2.00	0.42
1:D:82:LEU:HD12	1:D:82:LEU:HA	1.73	0.42
2:E:39:ASP:OD2	2:E:60:ARG:NH1	2.52	0.42
2:E:108:ASP:C	2:E:109:THR:CG2	2.73	0.42
2:F:158:GLU:OE2	2:F:158:GLU:CA	2.67	0.42
3:F:2:RTL:H201	3:F:2:RTL:H152	1.73	0.42
1:D:26:ILE:O	1:D:27:ASN:CB	2.53	0.42
1:D:66:GLU:CD	1:D:99:ASP:CG	2.88	0.42
2:E:5:ALA:HB1	2:E:128:THR:CB	2.48	0.42
2:E:6:VAL:HG23	2:E:128:THR:HG22	2.01	0.42
2:E:69:VAL:CG2	2:E:182:LEU:HD21	2.43	0.42
2:F:52:GLN:NE2	2:F:76:THR:CG2	2.83	0.42
1:A:112:SER:HB2	1:A:115:SER:O	2.19	0.42
1:D:21:ARG:CG	2:E:64:LEU:HD11	2.50	0.42
2:E:24:TRP:HB3	2:E:137:PHE:HD2	1.85	0.42
2:E:37:LEU:HA	2:E:37:LEU:HD23	1.60	0.42
2:E:82:ASP:O	2:E:83:PRO:C	2.63	0.42
2:F:28:ALA:CB	2:F:136:VAL:HG23	2.27	0.42
2:F:138:SER:CB	2:F:144:LEU:CD2	2.96	0.42
2:F:169:VAL:O	2:F:170:HIS:ND1	2.46	0.42
1:C:68:ILE:C	1:C:69:TYR:CD1	2.98	0.42
2:E:11:VAL:CG1	2:E:84:ALA:HB1	2.50	0.42
2:E:19:ARG:O	2:E:19:ARG:CG	2.66	0.42
2:E:28:ALA:HB1	2:E:165:TYR:CA	2.50	0.42
2:E:69:VAL:HG23	2:E:182:LEU:HD11	2.01	0.42
2:E:151:ILE:O	2:E:153:ALA:N	2.51	0.42
1:A:18:ASP:OD1	1:A:18:ASP:C	2.62	0.41
1:A:19:ALA:HB2	1:A:111:LEU:O	2.15	0.41
1:B:55:LEU:HA	1:B:55:LEU:HD23	1.80	0.41
2:F:24:TRP:HE3	2:F:137:PHE:HB3	1.85	0.41
2:F:46:SER:O	2:F:47:VAL:HB	2.19	0.41
2:F:167:LEU:C	2:F:167:LEU:CD2	2.91	0.41
2:F:169:VAL:O	2:F:170:HIS:CE1	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2:RTL:C18	3:F:2:RTL:C8	2.98	0.41
1:B:20:VAL:O	1:C:114:TYR:CD1	2.72	0.41
1:D:92:GLU:C	1:D:93:VAL:CG2	2.92	0.41
2:E:135:PHE:CB	2:E:137:PHE:CZ	3.03	0.41
2:F:23:THR:H	2:F:139:ARG:HH12	1.67	0.41
1:B:14:VAL:HA	1:B:107:ILE:O	2.20	0.41
1:B:18:ASP:HB2	1:B:78:TYR:OH	2.20	0.41
1:B:36:ALA:HB2	1:B:42:GLU:OE1	2.20	0.41
1:C:105:TYR:H	1:C:105:TYR:HD2	1.67	0.41
1:D:34:ARG:HG2	1:D:34:ARG:NH1	2.33	0.41
1:D:73:ILE:HG22	1:D:75:THR:HG22	2.02	0.41
2:E:52:GLN:OE1	2:E:77:PHE:O	2.38	0.41
2:E:67:TRP:CD1	2:E:67:TRP:C	2.98	0.41
2:F:19:ARG:HG2	2:F:111:TYR:HB3	2.03	0.41
2:F:66:ASN:N	2:F:66:ASN:OD1	2.52	0.41
1:B:75:THR:O	1:B:78:TYR:HB3	2.20	0.41
2:E:79:ASP:C	2:E:80:THR:HG23	2.43	0.41
2:F:95:SER:HB2	2:F:96:PHE:H	1.50	0.41
2:F:120:CYS:HA	2:F:132:SER:CB	2.50	0.41
1:A:70:LYS:HD3	1:A:94:VAL:CG2	2.46	0.41
1:C:79:TRP:NE1	1:C:113:PRO:HA	2.36	0.41
2:E:108:ASP:HB2	2:E:155:ARG:HD3	2.02	0.41
2:F:45:PHE:CD2	2:F:55:ALA:CB	3.03	0.41
1:A:114:TYR:CB	1:D:22:GLY:HA3	2.51	0.41
1:C:12:LEU:HD12	1:C:105:TYR:HB2	2.01	0.41
2:E:15:PHE:HA	2:E:111:TYR:HH	1.85	0.41
1:B:21:ARG:O	1:B:22:GLY:C	2.63	0.41
2:E:29:LYS:NZ	2:E:166:ARG:HB3	2.35	0.41
2:E:45:PHE:CE2	2:E:55:ALA:CB	3.01	0.41
2:E:120:CYS:SG	2:E:122:LEU:O	2.79	0.41
2:F:88:MET:HE2	2:F:88:MET:HB3	1.71	0.41
1:B:82:LEU:O	2:F:35:LEU:CD1	2.69	0.41
1:D:21:ARG:CD	1:D:82:LEU:HD21	2.51	0.41
2:E:24:TRP:HZ2	2:E:111:TYR:HA	1.86	0.41
2:E:144:LEU:N	2:E:144:LEU:HD23	2.36	0.41
2:F:13:GLU:HB3	2:F:14:ASN:H	1.47	0.41
2:F:60:ARG:HD2	2:F:68:ASP:OD1	2.21	0.41
2:F:151:ILE:C	2:F:153:ALA:H	2.28	0.41
1:A:20:VAL:CG2	1:A:79:TRP:HH2	2.32	0.41
1:B:16:VAL:CG1	1:B:25:ALA:HB3	2.51	0.41
1:B:22:GLY:CA	1:C:114:TYR:CG	3.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ALA:CB	1:B:28:VAL:HG21	2.50	0.41
1:D:70:LYS:HD2	1:D:92:GLU:CD	2.40	0.41
1:D:74:ASP:OD2	1:D:77:SER:OG	2.37	0.41
1:D:79:TRP:CD1	1:D:86:PRO:HB3	2.50	0.41
2:E:22:GLY:O	2:E:23:THR:C	2.63	0.41
2:E:31:ASP:OD2	2:E:31:ASP:C	2.59	0.41
2:E:133:TYR:HD1	2:E:134:SER:N	2.19	0.41
2:F:15:PHE:CG	2:F:16:ASP:N	2.88	0.41
2:F:124:ASN:N	2:F:130:ALA:HB2	2.36	0.41
1:B:20:VAL:CG2	1:B:113:PRO:HD3	2.51	0.41
2:E:11:VAL:CB	2:E:84:ALA:CB	2.89	0.41
2:E:112:ASP:O	2:E:113:THR:CB	2.69	0.41
2:F:29:LYS:HD2	2:F:135:PHE:CE1	2.56	0.41
2:F:109:THR:HA	2:F:114:TYR:CE1	2.56	0.41
2:F:115:ALA:C	2:F:116:VAL:CG2	2.94	0.41
1:B:18:ASP:CG	1:B:21:ARG:HB2	2.46	0.40
2:E:20:PHE:HB2	2:E:111:TYR:HD1	1.87	0.40
1:A:32:VAL:HB	1:A:44:PHE:HB3	2.03	0.40
1:B:102:PRO:HD3	1:B:124:ASN:CA	2.49	0.40
1:C:101:GLY:O	1:C:103:ARG:HG2	2.22	0.40
1:C:105:TYR:N	1:C:105:TYR:HD2	2.19	0.40
1:D:10:CYS:CB	1:D:56:HIS:CD2	3.02	0.40
2:E:26:ALA:O	2:E:27:MET:CE	2.70	0.40
2:E:139:ARG:NH1	2:E:139:ARG:HG2	2.35	0.40
1:A:33:PHE:O	1:A:70:LYS:N	2.54	0.40
2:E:32:PRO:HD3	2:E:133:TYR:HA	2.03	0.40
2:F:53:MET:O	2:F:77:PHE:HB2	2.22	0.40
2:F:92:GLY:HA3	2:F:97:LEU:HB2	2.04	0.40
1:C:28:VAL:O	1:C:49:THR:HG23	2.22	0.40
1:D:12:LEU:CD2	1:D:58:LEU:CB	2.95	0.40
2:E:23:THR:O	2:E:139:ARG:NH1	2.54	0.40
2:E:38:GLN:HG3	2:E:60:ARG:NH2	2.37	0.40

All (16) 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:E:154:GLN:O	2:F:164:GLN:OE1[8_455]	1.44	0.76
2:E:8:SER:OG	2:F:128:THR:O[8_455]	1.57	0.63
2:F:27:MET:SD	2:F:126:ASP:OD1[4_444]	1.58	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:160:CYS:N	2:F:4:CYS:N[8_455]	1.74	0.46
2:E:163:ALA:N	2:F:157:GLU:OE1[8_455]	1.78	0.42
2:E:9:PHE:CE2	2:F:4:CYS:N[8_455]	1.82	0.38
2:E:157:GLU:OE2	2:F:160:CYS:O[8_455]	1.85	0.35
2:E:4:CYS:O	2:F:8:SER:OG[8_455]	1.87	0.33
2:E:158:GLU:O	2:F:4:CYS:SG[8_455]	1.87	0.33
2:E:157:GLU:CB	2:F:161:LEU:CA[8_455]	1.88	0.32
2:E:160:CYS:O	2:F:158:GLU:O[8_455]	1.89	0.31
2:E:9:PHE:CD2	2:F:4:CYS:N[8_455]	1.95	0.25
2:E:156:GLN:O	2:F:161:LEU:N[8_455]	1.96	0.24
2:E:157:GLU:CA	2:F:161:LEU:N[8_455]	2.02	0.18
2:E:153:ALA:O	2:F:164:GLN:N[8_455]	2.09	0.11
2:E:5:ALA:CB	2:F:5:ALA:CB[8_455]	2.12	0.08

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	122/127 (96%)	102 (84%)	17 (14%)	3 (2%)	4	27
1	B	116/127 (91%)	84 (72%)	21 (18%)	11 (10%)	0	3
1	C	112/127 (88%)	94 (84%)	13 (12%)	5 (4%)	2	15
1	D	111/127 (87%)	94 (85%)	9 (8%)	8 (7%)	1	6
2	E	178/180 (99%)	96 (54%)	39 (22%)	43 (24%)	0	0
2	F	169/180 (94%)	90 (53%)	29 (17%)	50 (30%)	0	0
All	All	808/868 (93%)	560 (69%)	128 (16%)	120 (15%)	0	1

All (120) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	B	50	SER

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Mol	Chain	Res	Type
1	B	100	SER
1	C	11	PRO
1	D	57	GLY
1	D	100	SER
2	E	14	ASN
2	E	38	GLN
2	E	44	GLU
2	E	48	ASP
2	E	49	GLU
2	E	74	VAL
2	E	79	ASP
2	E	83	PRO
2	E	95	SER
2	E	96	PHE
2	E	105	TRP
2	E	106	ILE
2	E	108	ASP
2	E	109	THR
2	E	111	TYR
2	E	114	TYR
2	E	125	LEU
2	E	126	ASP
2	E	128	THR
2	E	133	TYR
2	E	160	CYS
2	E	179	GLU
2	E	182	LEU
2	F	5	ALA
2	F	6	VAL
2	F	10	ARG
2	F	12	LYS
2	F	14	ASN
2	F	15	PHE
2	F	49	GLU
2	F	64	LEU
2	F	65	ASN
2	F	67	TRP
2	F	79	ASP
2	F	81	GLU
2	F	85	LYS
2	F	95	SER
2	F	96	PHE

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Mol	Chain	Res	Type
2	F	105	TRP
2	F	113	THR
2	F	125	LEU
2	F	126	ASP
2	F	128	THR
2	F	145	PRO
2	F	148	ALA
2	F	149	GLN
2	F	161	LEU
1	B	90	HIS
1	B	122	VAL
1	C	22	GLY
1	C	64	PHE
2	E	7	SER
2	E	21	SER
2	E	43	ALA
2	E	98	GLN
2	E	122	LEU
2	E	152	VAL
2	E	172	GLY
2	F	82	ASP
2	F	84	ALA
2	F	109	THR
2	F	131	ASP
2	F	156	GLN
2	F	159	LEU
2	F	162	ALA
2	F	169	VAL
2	F	170	HIS
2	F	172	GLY
1	A	50	SER
1	B	59	THR
1	B	125	PRO
2	E	55	ALA
2	E	65	ASN
2	E	80	THR
2	E	110	ASP
2	E	119	SER
2	E	162	ALA
2	F	27	MET
2	F	55	ALA
2	F	98	GLN

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Mol	Chain	Res	Type
2	F	164	GLN
2	F	167	LEU
1	B	11	PRO
1	C	98	ASN
1	D	27	ASN
1	D	43	PRO
1	D	56	HIS
1	D	90	HIS
2	E	107	VAL
2	F	17	LYS
2	F	130	ALA
2	F	158	GLU
2	E	31	ASP
2	E	35	LEU
2	E	132	SER
2	F	47	VAL
2	F	62	ARG
2	F	166	ARG
2	F	173	TYR
1	B	23	SER
1	C	86	PRO
2	E	47	VAL
2	F	29	LYS
1	B	43	PRO
1	A	10	CYS
1	B	121	VAL
2	F	127	GLY
1	D	101	GLY
1	D	121	VAL
2	E	93	VAL
2	E	141	PRO
2	F	106	ILE
1	B	101	GLY
2	F	141	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	102/105 (97%)	86 (84%)	16 (16%)	2	13
1	B	99/105 (94%)	83 (84%)	16 (16%)	2	12
1	C	95/105 (90%)	72 (76%)	23 (24%)	1	4
1	D	94/105 (90%)	73 (78%)	21 (22%)	1	5
2	E	153/153 (100%)	108 (71%)	45 (29%)	0	1
2	F	145/153 (95%)	102 (70%)	43 (30%)	0	1
All	All	688/726 (95%)	524 (76%)	164 (24%)	1	4

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	13	MET
1	A	34	ARG
1	A	38	ASP
1	A	41	TRP
1	A	42	GLU
1	A	46	SER
1	A	55	LEU
1	A	59	THR
1	A	64	PHE
1	A	68	ILE
1	A	76	LYS
1	A	77	SER
1	A	82	LEU
1	A	96	THR
1	A	103	ARG
1	B	13	MET
1	B	18	ASP
1	B	21	ARG
1	B	23	SER
1	B	32	VAL
1	B	40	THR
1	B	51	GLU
1	B	55	LEU
1	B	62	GLU
1	B	63	GLN
1	B	68	ILE
1	B	73	ILE
1	B	76	LYS
1	B	84	ILE

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Mol	Chain	Res	Type
1	B	111	LEU
1	B	112	SER
1	C	10	CYS
1	C	12	LEU
1	C	13	MET
1	C	15	LYS
1	C	16	VAL
1	C	35	LYS
1	C	38	ASP
1	C	42	GLU
1	C	46	SER
1	C	55	LEU
1	C	59	THR
1	C	62	GLU
1	C	66	GLU
1	C	68	ILE
1	C	73	ILE
1	C	79	TRP
1	C	82	LEU
1	C	98	ASN
1	C	105	TYR
1	C	107	ILE
1	C	115	SER
1	C	117	SER
1	C	119	THR
1	D	12	LEU
1	D	13	MET
1	D	40	THR
1	D	48	LYS
1	D	51	GLU
1	D	55	LEU
1	D	56	HIS
1	D	62	GLU
1	D	63	GLN
1	D	68	ILE
1	D	69	TYR
1	D	71	VAL
1	D	76	LYS
1	D	80	LYS
1	D	82	LEU
1	D	93	VAL
1	D	110	LEU

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Mol	Chain	Res	Type
1	D	111	LEU
1	D	112	SER
1	D	115	SER
1	D	119	THR
2	E	11	VAL
2	E	13	GLU
2	E	14	ASN
2	E	15	PHE
2	E	27	MET
2	E	29	LYS
2	E	30	LYS
2	E	31	ASP
2	E	33	GLU
2	E	35	LEU
2	E	42	VAL
2	E	44	GLU
2	E	50	THR
2	E	52	GLN
2	E	54	SER
2	E	66	ASN
2	E	69	VAL
2	E	70	CYS
2	E	80	THR
2	E	82	ASP
2	E	88	MET
2	E	89	LYS
2	E	99	LYS
2	E	109	THR
2	E	114	TYR
2	E	119	SER
2	E	121	ARG
2	E	122	LEU
2	E	125	LEU
2	E	128	THR
2	E	131	ASP
2	E	133	TYR
2	E	137	PHE
2	E	139	ARG
2	E	144	LEU
2	E	147	GLU
2	E	155	ARG
2	E	156	GLN

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Mol	Chain	Res	Type
2	E	158	GLU
2	E	160	CYS
2	E	164	GLN
2	E	168	ILE
2	E	169	VAL
2	E	175	ASP
2	E	182	LEU
2	F	6	VAL
2	F	10	ARG
2	F	21	SER
2	F	29	LYS
2	F	30	LYS
2	F	31	ASP
2	F	38	GLN
2	F	44	GLU
2	F	50	THR
2	F	56	THR
2	F	62	ARG
2	F	63	LEU
2	F	65	ASN
2	F	69	VAL
2	F	74	VAL
2	F	78	THR
2	F	80	THR
2	F	81	GLU
2	F	88	MET
2	F	89	LYS
2	F	99	LYS
2	F	103	ASP
2	F	109	THR
2	F	114	TYR
2	F	117	GLN
2	F	121	ARG
2	F	122	LEU
2	F	123	LEU
2	F	126	ASP
2	F	132	SER
2	F	133	TYR
2	F	136	VAL
2	F	139	ARG
2	F	144	LEU
2	F	151	ILE

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Mol	Chain	Res	Type
2	F	156	GLN
2	F	157	GLU
2	F	158	GLU
2	F	159	LEU
2	F	161	LEU
2	F	167	LEU
2	F	168	ILE
2	F	171	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	HIS
1	A	124	ASN
1	B	88	HIS
1	C	31	HIS
1	C	56	HIS
1	C	88	HIS
1	C	98	ASN
1	D	27	ASN
1	D	88	HIS
2	E	14	ASN
2	E	38	GLN
2	E	65	ASN
2	E	66	ASN
2	E	98	GLN
2	E	104	HIS
2	E	117	GLN
2	E	156	GLN
2	E	170	HIS
2	F	14	ASN
2	F	38	GLN
2	F	52	GLN
2	F	65	ASN
2	F	124	ASN
2	F	164	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	RTL	F	2	-	21,21,21	1.33	2 (9%)	28,28,28	5.89	19 (67%)
3	RTL	E	1	-	21,21,21	1.20	2 (9%)	28,28,28	5.97	19 (67%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	RTL	F	2	-	-	3/14/31/31	0/1/1/1
3	RTL	E	1	-	-	3/14/31/31	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	RTL	C15-C14	-2.47	1.45	1.50
3	F	2	RTL	C5-C6	2.37	1.38	1.34
3	E	1	RTL	C16-C1	-2.35	1.49	1.53
3	F	2	RTL	C15-C14	-2.09	1.45	1.50

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	RTL	C11-C10-C9	-13.13	108.86	127.28
3	E	1	RTL	C11-C10-C9	-12.87	109.23	127.28
3	E	1	RTL	C1-C6-C5	-12.44	105.64	122.64
3	F	2	RTL	C1-C6-C5	-11.80	106.51	122.64
3	E	1	RTL	C19-C9-C10	11.54	141.50	122.82
3	F	2	RTL	C19-C9-C10	11.24	141.03	122.82
3	E	1	RTL	C15-C14-C13	-10.63	109.36	126.61
3	F	2	RTL	C15-C14-C13	-10.15	110.13	126.61
3	E	1	RTL	C20-C13-C14	-9.25	107.70	123.73
3	F	2	RTL	C20-C13-C14	-9.07	108.02	123.73
3	F	2	RTL	C7-C8-C9	-8.63	113.47	126.23
3	E	1	RTL	C12-C13-C14	-8.24	107.02	118.49
3	E	1	RTL	C8-C9-C10	-8.00	106.43	119.01
3	F	2	RTL	C12-C13-C14	-7.84	107.58	118.49
3	E	1	RTL	C7-C8-C9	-7.46	115.20	126.23
3	F	2	RTL	C8-C9-C10	-7.15	107.76	119.01
3	F	2	RTL	C17-C1-C6	5.33	118.60	110.24
3	E	1	RTL	C10-C11-C12	-5.18	108.20	123.20
3	E	1	RTL	C17-C1-C6	5.06	118.17	110.24
3	F	2	RTL	C11-C12-C13	-4.92	112.89	126.36
3	E	1	RTL	C11-C12-C13	-4.77	113.29	126.36
3	F	2	RTL	C10-C11-C12	-4.51	110.12	123.20
3	F	2	RTL	C19-C9-C8	-4.50	111.21	118.09
3	E	1	RTL	C16-C1-C6	-4.03	103.93	110.24
3	E	1	RTL	C19-C9-C8	-3.94	112.07	118.09
3	F	2	RTL	C16-C1-C6	-3.69	104.45	110.24
3	F	2	RTL	C7-C6-C5	-3.31	113.94	121.56
3	E	1	RTL	C2-C1-C6	3.03	114.84	110.44
3	E	1	RTL	C7-C6-C5	-3.00	114.64	121.56
3	F	2	RTL	C2-C1-C6	2.92	114.69	110.44
3	F	2	RTL	C16-C1-C2	-2.68	98.67	108.95
3	F	2	RTL	C20-C13-C12	-2.61	114.10	118.09
3	F	2	RTL	C18-C5-C4	-2.60	108.05	113.60
3	E	1	RTL	C16-C1-C2	-2.55	99.18	108.95
3	E	1	RTL	C18-C5-C4	-2.54	108.19	113.60
3	F	2	RTL	C4-C5-C6	2.48	126.06	122.70
3	E	1	RTL	C20-C13-C12	-2.45	114.34	118.09
3	E	1	RTL	C4-C5-C6	2.43	125.99	122.70

There are no chirality outliers.

All (6) torsion outliers are listed below:

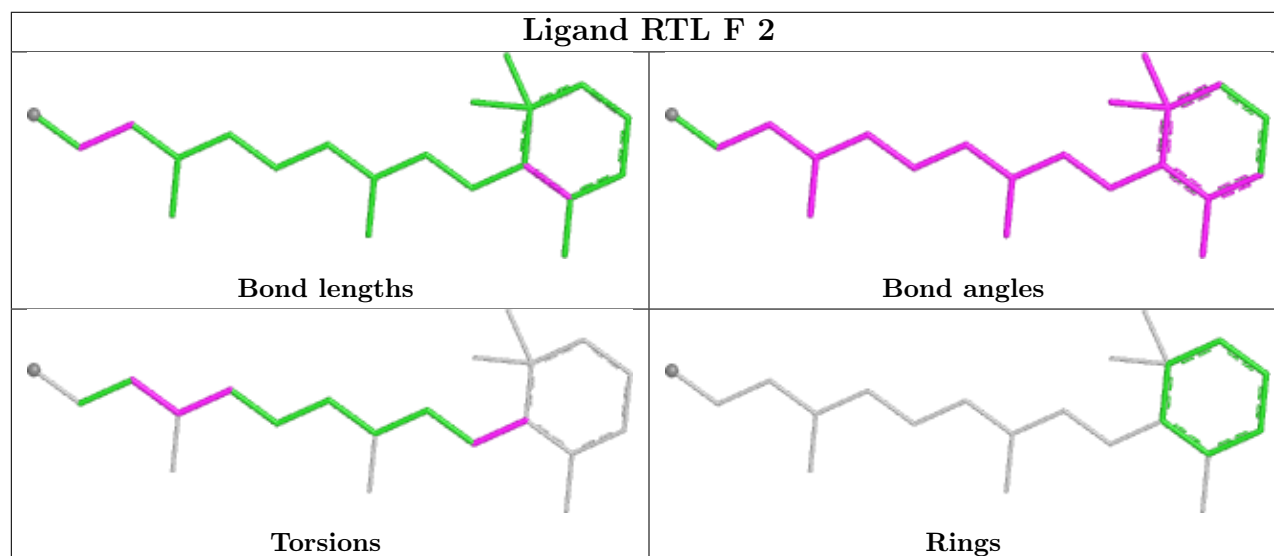
Mol	Chain	Res	Type	Atoms
3	E	1	RTL	C5-C6-C7-C8
3	E	1	RTL	C20-C13-C14-C15
3	F	2	RTL	C20-C13-C14-C15
3	E	1	RTL	C11-C12-C13-C20
3	F	2	RTL	C11-C12-C13-C20
3	F	2	RTL	C5-C6-C7-C8

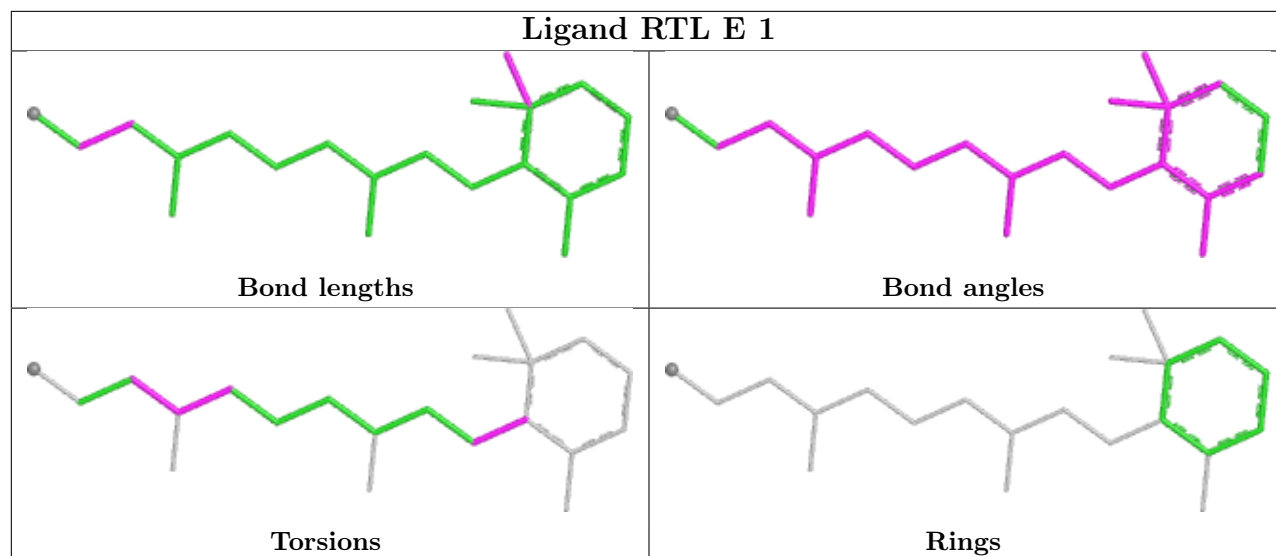
There are no ring outliers.

2 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	RTL	15	0
3	E	1	RTL	12	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.