



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Aug 17, 2017 – 12:37 PM EDT

PDB ID : 4UX8
EMDB ID: : EMD-2712
Title : RET recognition of GDNF-GFRalpha1 ligand by a composite binding site promotes membrane-proximal self-association
Authors : Goodman, K.; Kjaer, S.; Beuron, F.; Knowles, P.; Nawrotek, A.; Burns, E.; Purkiss, A.; George, R.; Santoro, M.; Morris, E.P.; McDonald, N.Q.
Deposited on : unknown
Resolution : 24.00 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

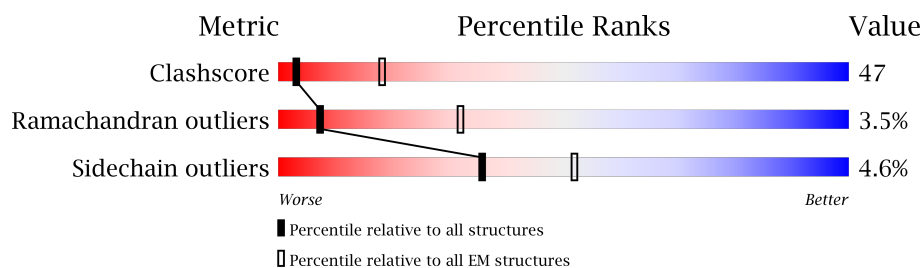
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 24.00 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	607	
1	B	607	
2	C	463	
2	E	463	
3	D	134	
3	F	134	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13046 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 PROTO-ONCOGENE TYROSINE-PROTEIN KINASE RECEPTOR RET.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	448	Total	C	N	O	S	0	0
			3569	2264	632	660	13		
1	B	448	Total	C	N	O	S	0	0
			3569	2264	632	660	13		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	87	ARG	CYS	engineered mutation	UNP P07949
A	98	GLN	ASN	conflict	UNP P07949
A	199	GLN	ASN	conflict	UNP P07949
A	216	SER	CYS	engineered mutation	UNP P07949
B	87	ARG	CYS	engineered mutation	UNP P07949
B	98	GLN	ASN	conflict	UNP P07949
B	199	GLN	ASN	conflict	UNP P07949
B	216	SER	CYS	engineered mutation	UNP P07949

- Molecule 2 is a protein called GDNF FAMILY RECEPTOR ALPHA-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	284	Total	C	N	O	S	0	0
			2203	1349	398	422	34		
2	E	284	Total	C	N	O	S	0	0
			2203	1349	398	422	34		

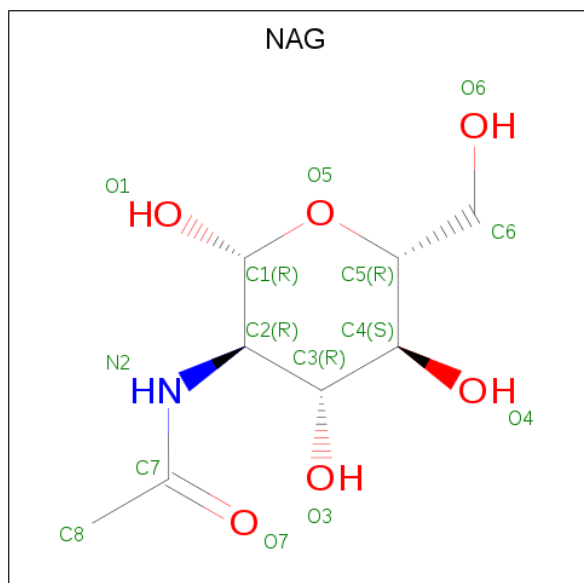
- Molecule 3 is a protein called GLIAL CELL LINE-DERIVED NEUROTROPHIC FACTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	93	Total	C	N	O	S	0	0
			720	450	126	138	6		
3	F	93	Total	C	N	O	S	0	0
			720	450	126	138	6		

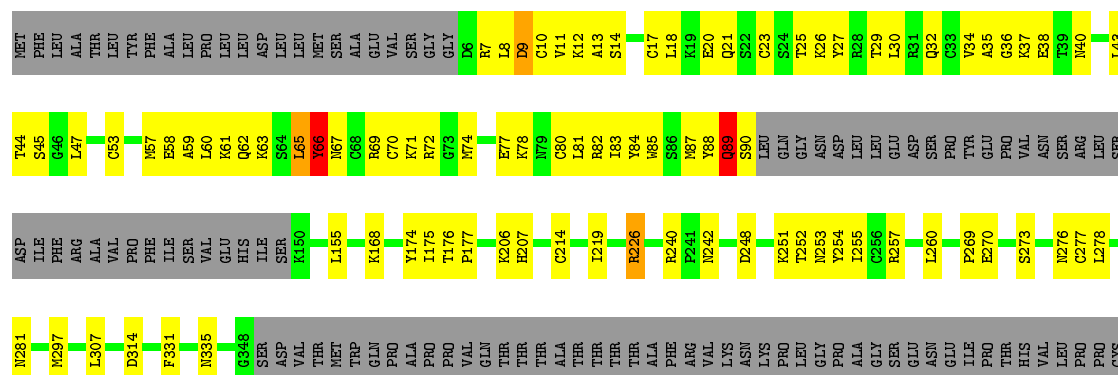
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

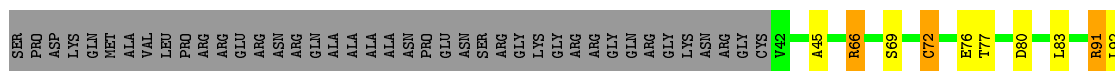
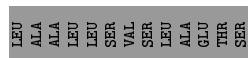
Mol	Chain	Residues	Atoms		AltConf
4	B	3	Total	Ca	0
			3	3	
4	A	3	Total	Ca	0
			3	3	

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).

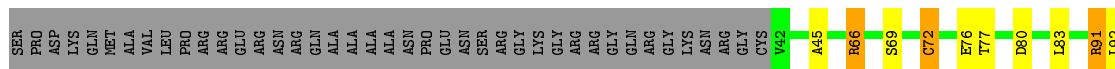


Mol	Chain	Residues	Atoms				AltConf
5	D	1	Total	C	N	O	0
			28	16	2	10	
5	D	1	Total	C	N	O	0
			28	16	2	10	
5	F	1	Total	C	N	O	0
			28	16	2	10	
5	F	1	Total	C	N	O	0
			28	16	2	10	





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4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	8519	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	100	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	80000	Depositor
Image detector	TVIPS TEMCAM-F415 (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	1.59	43/3655 (1.2%)	1.94	130/4977 (2.6%)
1	B	1.59	45/3655 (1.2%)	1.94	128/4977 (2.6%)
2	C	0.62	0/2236	0.80	3/3005 (0.1%)
2	E	0.62	0/2236	0.80	3/3005 (0.1%)
3	D	0.37	0/730	0.56	0/985
3	F	0.36	0/730	0.56	0/985
All	All	1.24	88/13242 (0.7%)	1.53	264/17934 (1.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	4	2
1	B	4	2
All	All	8	4

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	269	ALA	C-N	16.06	1.64	1.34
1	B	269	ALA	C-N	16.06	1.64	1.34
1	B	405	PRO	N-CD	15.82	1.70	1.47
1	A	405	PRO	N-CD	15.81	1.70	1.47
1	A	410	LEU	N-CA	15.03	1.76	1.46
1	B	451	THR	CA-C	15.02	1.92	1.52
1	B	410	LEU	N-CA	15.01	1.76	1.46
1	A	451	THR	CA-C	14.99	1.92	1.52
1	B	452	LEU	N-CA	-12.30	1.21	1.46
1	A	452	LEU	N-CA	-12.24	1.21	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	456	THR	N-CA	10.11	1.66	1.46
1	A	456	THR	N-CA	10.07	1.66	1.46
1	A	415	ARG	N-CA	9.73	1.65	1.46
1	B	415	ARG	N-CA	9.72	1.65	1.46
1	A	476	PRO	N-CD	9.45	1.61	1.47
1	B	476	PRO	N-CD	9.45	1.61	1.47
1	A	488	THR	N-CA	8.52	1.63	1.46
1	B	488	THR	N-CA	8.48	1.63	1.46
1	A	490	GLN	N-CA	8.41	1.63	1.46
1	B	490	GLN	N-CA	8.40	1.63	1.46
1	A	474	ARG	CA-C	-8.11	1.31	1.52
1	B	474	ARG	CA-C	-8.10	1.31	1.52
1	A	251	GLU	CB-CG	-7.79	1.37	1.52
1	B	251	GLU	CB-CG	-7.76	1.37	1.52
1	A	423	GLY	CA-C	7.47	1.63	1.51
1	B	423	GLY	CA-C	7.44	1.63	1.51
1	A	477	LYS	CA-C	7.37	1.72	1.52
1	B	477	LYS	CA-C	7.37	1.72	1.52
1	B	453	GLY	N-CA	7.28	1.56	1.46
1	A	453	GLY	N-CA	7.22	1.56	1.46
1	B	483	TYR	CA-C	7.21	1.71	1.52
1	A	483	TYR	CA-C	7.20	1.71	1.52
1	B	466	PHE	N-CA	-6.78	1.32	1.46
1	A	458	ALA	CA-C	-6.78	1.35	1.52
1	B	458	ALA	CA-C	-6.78	1.35	1.52
1	A	466	PHE	N-CA	-6.76	1.32	1.46
1	A	263	TYR	C-N	6.69	1.49	1.34
1	A	508	TYR	N-CA	6.68	1.59	1.46
1	B	508	TYR	N-CA	6.68	1.59	1.46
1	B	263	TYR	C-N	6.67	1.49	1.34
1	B	508	TYR	CA-C	6.66	1.70	1.52
1	A	508	TYR	CA-C	6.62	1.70	1.52
1	A	446	GLY	N-CA	6.57	1.55	1.46
1	B	446	GLY	N-CA	6.55	1.55	1.46
1	A	174	PHE	CE1-CZ	6.53	1.49	1.37
1	B	174	PHE	CE1-CZ	6.53	1.49	1.37
1	B	164	GLU	CG-CD	6.50	1.61	1.51
1	A	164	GLU	CG-CD	6.48	1.61	1.51
1	A	147	PHE	CD1-CE1	6.40	1.52	1.39
1	B	147	PHE	CD1-CE1	6.39	1.52	1.39
1	A	489	ASP	CA-C	6.28	1.69	1.52
1	B	489	ASP	CA-C	6.25	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	ARG	CG-CD	6.20	1.67	1.51
1	A	416	ALA	N-CA	6.18	1.58	1.46
1	B	205	ARG	CG-CD	6.17	1.67	1.51
1	B	506	GLY	CA-C	6.17	1.61	1.51
1	B	416	ALA	N-CA	6.15	1.58	1.46
1	A	506	GLY	CA-C	6.13	1.61	1.51
1	B	122	TYR	CD2-CE2	6.02	1.48	1.39
1	B	463	GLY	N-CA	6.01	1.55	1.46
1	A	122	TYR	CD2-CE2	5.97	1.48	1.39
1	A	463	GLY	N-CA	5.96	1.54	1.46
1	A	455	VAL	CA-C	-5.79	1.38	1.52
1	B	455	VAL	CA-C	-5.79	1.38	1.52
1	A	487	ALA	CA-C	-5.71	1.38	1.52
1	B	487	ALA	CA-C	-5.71	1.38	1.52
1	B	205	ARG	CZ-NH1	5.66	1.40	1.33
1	A	205	ARG	CZ-NH1	5.63	1.40	1.33
1	A	187	GLN	CB-CG	-5.62	1.37	1.52
1	B	187	GLN	CB-CG	-5.59	1.37	1.52
1	A	31	PHE	CB-CG	-5.43	1.42	1.51
1	B	31	PHE	CB-CG	-5.43	1.42	1.51
1	B	207	LEU	C-O	5.43	1.33	1.23
1	A	207	LEU	C-O	5.39	1.33	1.23
1	A	36	TYR	CD1-CE1	5.37	1.47	1.39
1	B	36	TYR	CD1-CE1	5.31	1.47	1.39
1	A	473	LEU	CA-C	5.19	1.66	1.52
1	B	473	LEU	CA-C	5.19	1.66	1.52
1	A	188	PHE	CE2-CZ	5.18	1.47	1.37
1	B	188	PHE	CE2-CZ	5.13	1.47	1.37
1	A	475	ARG	N-CA	5.08	1.56	1.46
1	A	431	GLN	N-CA	5.07	1.56	1.46
1	B	431	GLN	N-CA	5.07	1.56	1.46
1	B	475	ARG	N-CA	5.06	1.56	1.46
1	B	112	ARG	CG-CD	5.04	1.64	1.51
1	B	112	ARG	CD-NE	-5.03	1.37	1.46
1	B	444	SER	N-CA	5.01	1.56	1.46
1	A	112	ARG	CD-NE	-5.01	1.38	1.46

All (264) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	TYR	O-C-N	-27.83	78.17	122.70
1	B	263	TYR	O-C-N	-27.79	78.23	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	ARG	NE-CZ-NH1	-27.21	106.70	120.30
1	B	112	ARG	NE-CZ-NH1	-27.05	106.78	120.30
1	A	450	SER	CB-CA-C	-22.51	67.33	110.10
1	B	450	SER	CB-CA-C	-22.49	67.36	110.10
1	A	447	ALA	CB-CA-C	-22.30	76.65	110.10
1	B	447	ALA	CB-CA-C	-22.29	76.66	110.10
1	B	263	TYR	CA-C-N	19.02	159.05	117.20
1	A	263	TYR	CA-C-N	19.02	159.05	117.20
1	A	112	ARG	NE-CZ-NH2	18.94	129.77	120.30
1	B	112	ARG	NE-CZ-NH2	18.77	129.69	120.30
1	A	434	SER	N-CA-CB	16.39	135.09	110.50
1	B	434	SER	N-CA-CB	16.39	135.09	110.50
1	B	477	LYS	N-CA-CB	13.93	135.67	110.60
1	A	477	LYS	N-CA-CB	13.92	135.66	110.60
1	A	458	ALA	N-CA-CB	12.91	128.17	110.10
1	B	458	ALA	N-CA-CB	12.88	128.14	110.10
1	B	435	GLY	CA-C-O	-12.45	98.19	120.60
1	A	435	GLY	CA-C-O	-12.44	98.21	120.60
1	B	269	ALA	C-N-CD	-12.25	93.65	120.60
1	A	269	ALA	C-N-CD	-12.23	93.70	120.60
1	B	508	TYR	N-CA-CB	11.47	131.25	110.60
1	A	508	TYR	N-CA-CB	11.44	131.19	110.60
1	B	451	THR	N-CA-C	-11.33	80.41	111.00
1	A	451	THR	N-CA-C	-11.31	80.45	111.00
1	B	462	SER	CB-CA-C	-10.94	89.31	110.10
1	A	462	SER	CB-CA-C	-10.94	89.31	110.10
1	A	205	ARG	NE-CZ-NH1	10.89	125.74	120.30
1	B	205	ARG	NE-CZ-NH1	10.85	125.72	120.30
1	A	468	ASN	CB-CA-C	10.66	131.72	110.40
1	B	468	ASN	CB-CA-C	10.66	131.71	110.40
1	A	479	ALA	CB-CA-C	-10.29	94.67	110.10
1	B	479	ALA	CB-CA-C	-10.28	94.68	110.10
1	B	461	THR	CB-CA-C	-10.26	83.91	111.60
1	A	461	THR	CB-CA-C	-10.24	83.95	111.60
1	B	112	ARG	CD-NE-CZ	10.14	137.80	123.60
1	A	112	ARG	CD-NE-CZ	10.09	137.72	123.60
1	B	488	THR	CB-CA-C	-9.87	84.96	111.60
1	A	488	THR	CB-CA-C	-9.85	85.00	111.60
1	B	435	GLY	CA-C-N	9.76	138.66	117.20
1	A	435	GLY	CA-C-N	9.75	138.64	117.20
1	A	405	PRO	CB-CA-C	-9.61	87.97	112.00
1	B	405	PRO	CB-CA-C	-9.61	87.97	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	491	GLN	N-CA-CB	9.53	127.76	110.60
1	B	491	GLN	N-CA-CB	9.52	127.74	110.60
1	A	414	ARG	CB-CA-C	-9.41	91.57	110.40
1	B	414	ARG	CB-CA-C	-9.40	91.60	110.40
1	A	403	HIS	CB-CA-C	9.28	128.95	110.40
1	B	403	HIS	CB-CA-C	9.26	128.92	110.40
1	B	477	LYS	CB-CA-C	9.12	128.65	110.40
1	A	477	LYS	CB-CA-C	9.12	128.65	110.40
1	A	489	ASP	CA-C-O	9.06	139.13	120.10
1	B	489	ASP	CA-C-O	9.06	139.13	120.10
1	B	418	ARG	CB-CA-C	8.98	128.37	110.40
1	A	418	ARG	CB-CA-C	8.95	128.30	110.40
1	A	490	GLN	N-CA-C	-8.77	87.32	111.00
1	B	416	ALA	N-CA-CB	8.76	122.36	110.10
1	B	490	GLN	N-CA-C	-8.75	87.36	111.00
1	A	416	ALA	N-CA-CB	8.71	122.29	110.10
1	A	489	ASP	CA-C-N	-8.66	98.14	117.20
1	B	489	ASP	CA-C-N	-8.66	98.14	117.20
1	B	476	PRO	N-CA-C	-8.62	89.69	112.10
1	A	436	ILE	CB-CA-C	-8.61	94.37	111.60
1	A	476	PRO	N-CA-C	-8.61	89.71	112.10
1	B	436	ILE	CB-CA-C	-8.60	94.40	111.60
1	A	414	ARG	C-N-CA	-8.53	100.39	121.70
1	A	470	THR	N-CA-CB	-8.52	94.12	110.30
1	B	470	THR	N-CA-CB	-8.51	94.13	110.30
1	B	414	ARG	C-N-CA	-8.51	100.44	121.70
1	B	451	THR	N-CA-CB	8.46	126.37	110.30
1	A	451	THR	N-CA-CB	8.45	126.35	110.30
1	A	424	LYS	CB-CA-C	-8.34	93.73	110.40
1	B	424	LYS	CB-CA-C	-8.32	93.77	110.40
1	A	409	SER	C-N-CA	-8.27	101.03	121.70
1	B	409	SER	C-N-CA	-8.26	101.06	121.70
1	B	189	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	A	189	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	A	451	THR	C-N-CA	8.15	142.08	121.70
1	B	451	THR	C-N-CA	8.14	142.05	121.70
1	B	309	GLU	CB-CA-C	-8.11	94.17	110.40
1	A	309	GLU	CB-CA-C	-8.11	94.19	110.40
1	B	230	ASP	CB-CG-OD1	8.02	125.52	118.30
1	B	476	PRO	CB-CA-C	-8.02	91.95	112.00
1	A	476	PRO	CB-CA-C	-8.01	91.98	112.00
1	A	230	ASP	CB-CG-OD1	7.98	125.48	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	437	ASN	CB-CA-C	-7.95	94.50	110.40
1	A	437	ASN	CB-CA-C	-7.93	94.55	110.40
1	B	411	SER	CB-CA-C	-7.88	95.12	110.10
1	A	411	SER	CB-CA-C	-7.84	95.20	110.10
1	B	422	ILE	N-CA-C	7.74	131.89	111.00
1	A	422	ILE	N-CA-C	7.74	131.89	111.00
1	A	144	ARG	NE-CZ-NH2	7.66	124.13	120.30
1	B	477	LYS	N-CA-C	-7.65	90.35	111.00
1	A	427	VAL	CB-CA-C	-7.65	96.87	111.40
1	A	477	LYS	N-CA-C	-7.65	90.35	111.00
1	B	427	VAL	CB-CA-C	-7.63	96.90	111.40
1	B	144	ARG	NE-CZ-NH2	7.61	124.11	120.30
1	A	112	ARG	CG-CD-NE	-7.58	95.88	111.80
1	B	112	ARG	CG-CD-NE	-7.58	95.88	111.80
1	B	189	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	B	415	ARG	N-CA-CB	-7.55	97.00	110.60
1	A	415	ARG	N-CA-CB	-7.55	97.01	110.60
1	A	436	ILE	N-CA-CB	-7.53	93.48	110.80
1	B	436	ILE	N-CA-CB	-7.53	93.48	110.80
1	A	189	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	B	449	CYS	CB-CA-C	-7.42	95.56	110.40
1	A	449	CYS	CB-CA-C	-7.41	95.59	110.40
2	C	65	LEU	C-N-CA	7.34	140.06	121.70
1	A	482	HIS	CB-CA-C	-7.34	95.71	110.40
1	B	482	HIS	CB-CA-C	-7.33	95.74	110.40
1	A	483	TYR	CB-CA-C	-7.33	95.75	110.40
2	E	65	LEU	C-N-CA	7.33	140.01	121.70
1	B	483	TYR	CB-CA-C	-7.31	95.79	110.40
1	A	263	TYR	C-N-CA	7.29	139.93	121.70
1	B	263	TYR	C-N-CA	7.28	139.90	121.70
1	B	452	LEU	N-CA-C	7.18	130.38	111.00
1	A	452	LEU	N-CA-C	7.17	130.35	111.00
1	A	472	ALA	CB-CA-C	7.13	120.79	110.10
1	B	472	ALA	CB-CA-C	7.12	120.78	110.10
1	A	205	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	B	490	GLN	CB-CA-C	-7.03	96.34	110.40
1	A	490	GLN	CB-CA-C	-7.01	96.38	110.40
1	B	205	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	A	474	ARG	CA-C-O	-6.99	105.42	120.10
1	B	474	ARG	CA-C-O	-6.99	105.42	120.10
1	B	445	SER	N-CA-C	6.91	129.66	111.00
1	A	445	SER	N-CA-C	6.90	129.63	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	473	LEU	CA-C-N	-6.83	102.17	117.20
1	B	473	LEU	CA-C-N	-6.83	102.17	117.20
1	A	493	SER	CB-CA-C	-6.76	97.26	110.10
1	B	493	SER	CB-CA-C	-6.75	97.28	110.10
1	B	505	GLU	N-CA-CB	-6.67	98.60	110.60
1	A	505	GLU	N-CA-CB	-6.66	98.61	110.60
1	B	414	ARG	N-CA-C	6.64	128.93	111.00
1	A	414	ARG	N-CA-C	6.62	128.87	111.00
1	A	507	SER	N-CA-CB	6.60	120.40	110.50
1	B	507	SER	N-CA-CB	6.60	120.40	110.50
1	A	489	ASP	C-N-CA	-6.58	105.24	121.70
1	B	484	MET	CB-CA-C	-6.58	97.23	110.40
1	B	489	ASP	C-N-CA	-6.58	105.25	121.70
1	A	484	MET	CB-CA-C	-6.57	97.27	110.40
1	B	473	LEU	CA-C-O	6.53	133.82	120.10
1	A	473	LEU	CA-C-O	6.51	133.78	120.10
1	A	508	TYR	CB-CA-C	6.50	123.41	110.40
1	B	508	TYR	CB-CA-C	6.50	123.39	110.40
1	A	445	SER	CB-CA-C	6.49	122.44	110.10
1	B	409	SER	CA-C-O	-6.48	106.48	120.10
1	B	507	SER	CB-CA-C	6.48	122.42	110.10
1	B	445	SER	CB-CA-C	6.48	122.41	110.10
1	A	504	VAL	N-CA-C	6.47	128.48	111.00
1	A	507	SER	CB-CA-C	6.47	122.40	110.10
1	A	409	SER	CA-C-O	-6.45	106.55	120.10
1	B	504	VAL	N-CA-C	6.45	128.41	111.00
1	A	420	ALA	CB-CA-C	-6.44	100.44	110.10
1	B	420	ALA	CB-CA-C	-6.43	100.45	110.10
1	B	409	SER	CA-C-N	6.42	131.33	117.20
1	B	405	PRO	CA-N-CD	-6.41	102.53	111.50
1	A	409	SER	CA-C-N	6.41	131.29	117.20
1	A	405	PRO	CA-N-CD	-6.40	102.54	111.50
1	B	445	SER	C-N-CA	-6.37	108.92	122.30
1	A	445	SER	C-N-CA	-6.37	108.93	122.30
1	B	468	ASN	N-CA-CB	-6.31	99.25	110.60
1	A	468	ASN	N-CA-CB	-6.30	99.27	110.60
1	A	474	ARG	CA-C-N	6.28	131.01	117.20
1	B	495	GLN	CB-CA-C	6.26	122.92	110.40
1	B	474	ARG	CA-C-N	6.26	130.97	117.20
1	A	495	GLN	CB-CA-C	6.26	122.91	110.40
1	B	477	LYS	CA-C-O	6.12	132.96	120.10
1	B	456	THR	N-CA-CB	6.12	121.92	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	442	LEU	N-CA-CB	6.12	122.63	110.40
1	A	477	LYS	CA-C-O	6.12	132.94	120.10
1	B	442	LEU	N-CA-CB	6.10	122.60	110.40
1	A	456	THR	N-CA-CB	6.08	121.86	110.30
1	A	438	VAL	CB-CA-C	-6.06	99.89	111.40
1	A	226	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	B	438	VAL	CB-CA-C	-6.04	99.92	111.40
1	B	416	ALA	CB-CA-C	-6.04	101.04	110.10
1	A	447	ALA	N-CA-CB	-6.04	101.65	110.10
1	A	416	ALA	CB-CA-C	-6.02	101.07	110.10
1	B	447	ALA	N-CA-CB	-6.01	101.68	110.10
1	A	477	LYS	CA-C-N	-6.00	103.99	117.20
1	B	477	LYS	CA-C-N	-6.00	103.99	117.20
1	A	458	ALA	N-CA-C	5.96	127.11	111.00
1	B	403	HIS	N-CA-CB	-5.96	99.86	110.60
1	B	458	ALA	N-CA-C	5.96	127.11	111.00
1	A	458	ALA	CB-CA-C	-5.96	101.16	110.10
1	A	403	HIS	N-CA-CB	-5.95	99.89	110.60
1	B	458	ALA	CB-CA-C	-5.95	101.18	110.10
1	B	226	ARG	NE-CZ-NH1	-5.94	117.33	120.30
2	E	66	TYR	N-CA-C	-5.90	95.06	111.00
2	C	66	TYR	N-CA-C	-5.89	95.09	111.00
1	A	461	THR	N-CA-C	5.87	126.84	111.00
1	A	442	LEU	CB-CA-C	-5.86	99.07	110.20
1	B	461	THR	N-CA-C	5.86	126.82	111.00
1	B	442	LEU	CB-CA-C	-5.85	99.08	110.20
1	A	477	LYS	C-N-CA	-5.83	107.12	121.70
1	B	477	LYS	C-N-CA	-5.81	107.17	121.70
1	B	129	PRO	N-CA-CB	5.80	110.26	103.30
1	A	129	PRO	N-CA-CB	5.80	110.26	103.30
2	C	89	GLN	CB-CA-C	-5.79	98.83	110.40
1	A	114	ARG	NE-CZ-NH2	5.78	123.19	120.30
2	E	89	GLN	CB-CA-C	-5.78	98.83	110.40
1	B	114	ARG	NE-CZ-NH2	5.75	123.17	120.30
1	B	405	PRO	N-CA-CB	5.74	110.19	103.30
1	A	405	PRO	N-CA-CB	5.70	110.14	103.30
1	A	414	ARG	N-CA-CB	5.70	120.85	110.60
1	B	417	ARG	N-CA-CB	5.67	120.82	110.60
1	B	414	ARG	N-CA-CB	5.67	120.81	110.60
1	A	417	ARG	N-CA-CB	5.64	120.76	110.60
1	B	29	LEU	CA-CB-CG	5.63	128.24	115.30
1	B	419	PHE	N-CA-C	5.62	126.16	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	LEU	CA-CB-CG	5.61	128.20	115.30
1	A	419	PHE	N-CA-C	5.60	126.12	111.00
1	A	144	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	A	418	ARG	N-CA-CB	-5.59	100.53	110.60
1	B	418	ARG	N-CA-CB	-5.59	100.53	110.60
1	A	467	VAL	C-N-CA	-5.58	107.75	121.70
1	B	467	VAL	C-N-CA	-5.57	107.78	121.70
1	B	503	THR	CA-C-N	-5.51	105.09	117.20
1	B	144	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	A	503	THR	CA-C-N	-5.49	105.12	117.20
1	A	354	TYR	CB-CG-CD2	-5.45	117.73	121.00
1	A	418	ARG	N-CA-C	5.45	125.70	111.00
1	B	33	ARG	NE-CZ-NH1	-5.43	117.58	120.30
1	B	418	ARG	N-CA-C	5.43	125.66	111.00
1	A	457	SER	N-CA-C	5.42	125.64	111.00
1	B	457	SER	N-CA-C	5.42	125.65	111.00
1	A	483	TYR	CA-C-N	-5.38	105.35	117.20
1	A	77	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	A	403	HIS	N-CA-C	-5.38	96.48	111.00
1	A	495	GLN	N-CA-CB	-5.38	100.92	110.60
1	A	99	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	403	HIS	N-CA-C	-5.38	96.48	111.00
1	B	495	GLN	N-CA-CB	-5.36	100.95	110.60
1	B	483	TYR	CA-C-N	-5.36	105.41	117.20
1	A	503	THR	CA-C-O	5.36	131.35	120.10
1	B	503	THR	CA-C-O	5.36	131.35	120.10
1	A	33	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	B	99	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	B	354	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	B	451	THR	CA-C-N	-5.32	105.49	117.20
1	A	451	THR	CA-C-N	-5.30	105.53	117.20
1	A	478	CYS	CA-C-N	5.26	128.78	117.20
1	B	77	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	B	478	CYS	CA-C-N	5.26	128.77	117.20
1	A	429	ASN	CB-CA-C	5.25	120.91	110.40
1	B	429	ASN	CB-CA-C	5.24	120.88	110.40
1	B	469	ASP	CB-CA-C	-5.20	100.00	110.40
1	A	469	ASP	CB-CA-C	-5.20	100.00	110.40
1	B	266	ASP	CB-CG-OD2	5.16	122.95	118.30
1	A	423	GLY	N-CA-C	-5.16	100.20	113.10
1	B	423	GLY	N-CA-C	-5.13	100.26	113.10
1	A	266	ASP	CB-CG-OD2	5.12	122.91	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	424	LYS	CA-C-N	-5.09	106.00	117.20
1	B	43	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	A	424	LYS	CA-C-O	5.08	130.77	120.10
1	A	466	PHE	N-CA-C	5.08	124.70	111.00
1	B	424	LYS	CA-C-N	-5.07	106.05	117.20
1	B	424	LYS	CA-C-O	5.06	130.72	120.10
1	B	466	PHE	N-CA-C	5.05	124.64	111.00
1	A	43	ASP	CB-CG-OD2	-5.04	113.77	118.30
1	A	57	ARG	NE-CZ-NH1	-5.03	117.78	120.30
1	A	439	GLN	CB-CA-C	-5.02	100.37	110.40

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	445	SER	CA
1	A	452	LEU	CA
1	A	491	GLN	CA
1	A	507	SER	CA
1	B	445	SER	CA
1	B	452	LEU	CA
1	B	491	GLN	CA
1	B	507	SER	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	ARG	Sidechain
1	A	263	TYR	Peptide
1	B	112	ARG	Sidechain
1	B	263	TYR	Peptide

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	3569	0	3460	442	0
1	B	3569	0	3462	437	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2203	0	2105	143	0
2	E	2203	0	2105	148	0
3	D	720	0	697	19	0
3	F	720	0	697	17	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
5	D	28	0	25	0	0
5	F	28	0	25	0	0
All	All	13046	0	12576	1195	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 47.

All (1195) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:VAL:CA	1:A:497:GLN:HE22	1.06	1.65
1:B:486:VAL:CA	1:B:497:GLN:HE22	1.06	1.62
1:A:482:HIS:CD2	1:A:501:LEU:HD21	1.37	1.60
2:C:78:LYS:CE	2:C:254:TYR:CA	1.75	1.59
1:B:482:HIS:CD2	1:B:501:LEU:HD21	1.37	1.59
1:B:486:VAL:CG1	1:B:497:GLN:HE21	1.19	1.53
1:A:486:VAL:CG1	1:A:497:GLN:HE21	1.19	1.51
1:A:482:HIS:CD2	1:A:501:LEU:CD2	1.96	1.48
1:B:410:LEU:CA	1:B:410:LEU:N	1.76	1.47
2:C:78:LYS:HE3	2:C:254:TYR:CA	1.36	1.46
1:A:410:LEU:CA	1:A:410:LEU:N	1.76	1.45
1:B:482:HIS:CD2	1:B:501:LEU:CD2	1.96	1.44
1:B:486:VAL:CG1	1:B:497:GLN:NE2	1.79	1.42
1:A:405:PRO:N	1:A:405:PRO:CD	1.70	1.40
1:A:451:THR:CA	1:A:451:THR:C	1.91	1.39
1:B:451:THR:CA	1:B:451:THR:C	1.92	1.39
1:A:486:VAL:CG1	1:A:497:GLN:NE2	1.79	1.38
1:B:486:VAL:CA	1:B:497:GLN:NE2	1.84	1.38
1:B:482:HIS:NE2	1:B:501:LEU:HD21	1.38	1.38
1:A:486:VAL:CA	1:A:497:GLN:NE2	1.84	1.37
1:B:266:ASP:CG	1:B:360:ARG:HH22	1.28	1.37
1:A:269:ALA:HB2	1:A:366:GLU:OE1	1.22	1.35
1:B:405:PRO:N	1:B:405:PRO:CD	1.70	1.35
1:A:266:ASP:CG	1:A:360:ARG:HH22	1.28	1.35
1:A:482:HIS:NE2	1:A:501:LEU:HD21	1.38	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:78:LYS:CE	2:C:254:TYR:HA	0.88	1.33
2:E:71:LYS:HD2	2:E:254:TYR:CD2	1.62	1.32
1:B:269:ALA:HB2	1:B:366:GLU:OE1	1.22	1.31
1:B:408:TYR:CE1	1:B:422:ILE:HG23	1.68	1.29
2:E:85:TRP:CH2	2:E:257:ARG:HD2	1.66	1.28
1:A:178:GLU:OE1	1:A:231:ARG:N	1.67	1.28
1:A:408:TYR:CE1	1:A:422:ILE:HG23	1.68	1.26
1:B:178:GLU:OE1	1:B:231:ARG:N	1.67	1.26
1:A:474:ARG:HG2	1:A:476:PRO:O	1.35	1.25
1:B:442:LEU:CD2	1:B:485:VAL:HG22	1.67	1.24
1:A:442:LEU:CD2	1:A:485:VAL:HG22	1.67	1.23
1:B:474:ARG:HG2	1:B:476:PRO:O	1.35	1.21
1:A:408:TYR:CE1	1:A:422:ILE:CG2	2.25	1.20
2:C:78:LYS:HE3	2:C:254:TYR:CB	1.70	1.20
1:A:474:ARG:CG	1:A:476:PRO:HD2	1.73	1.18
2:C:78:LYS:HE2	2:C:254:TYR:CA	1.50	1.18
2:C:78:LYS:N	2:C:254:TYR:CE1	1.99	1.17
1:B:408:TYR:CE1	1:B:422:ILE:CG2	2.25	1.17
1:B:474:ARG:CG	1:B:476:PRO:HD2	1.73	1.16
1:B:424:LYS:HE3	1:B:464:ILE:HG12	1.24	1.15
1:A:412:VAL:HG22	1:A:504:VAL:CG1	1.77	1.14
2:C:78:LYS:CD	2:C:254:TYR:HA	1.76	1.14
1:B:412:VAL:HG22	1:B:504:VAL:CG1	1.77	1.13
1:A:504:VAL:O	1:A:504:VAL:HG12	1.37	1.13
1:A:486:VAL:N	1:A:497:GLN:HE22	1.23	1.12
1:B:504:VAL:O	1:B:504:VAL:CG1	1.98	1.12
1:A:424:LYS:HE3	1:A:464:ILE:HG12	1.24	1.12
2:C:78:LYS:HE2	2:C:254:TYR:N	1.62	1.12
1:A:266:ASP:OD2	1:A:360:ARG:NH2	1.84	1.10
1:B:266:ASP:OD2	1:B:360:ARG:NH2	1.84	1.10
3:D:66:ARG:HH11	3:D:66:ARG:HG3	1.15	1.10
1:A:474:ARG:HH11	1:A:477:LYS:CD	1.63	1.10
1:A:504:VAL:O	1:A:504:VAL:CG1	1.98	1.10
1:A:360:ARG:HB3	1:A:365:SER:HB3	1.32	1.09
1:B:474:ARG:HH11	1:B:477:LYS:CD	1.63	1.09
1:B:474:ARG:NH1	1:B:477:LYS:HG3	1.67	1.09
1:B:486:VAL:N	1:B:497:GLN:HE22	1.23	1.09
1:B:504:VAL:O	1:B:504:VAL:HG12	1.37	1.09
1:A:474:ARG:NH1	1:A:477:LYS:HG3	1.67	1.08
1:A:474:ARG:HD3	1:A:477:LYS:HD2	1.33	1.08
2:E:85:TRP:CZ2	2:E:257:ARG:HD2	1.87	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:486:VAL:CB	1:B:497:GLN:NE2	2.16	1.08
1:B:412:VAL:HG22	1:B:504:VAL:HG12	1.36	1.08
1:A:474:ARG:NH1	1:A:477:LYS:CD	2.17	1.07
1:A:486:VAL:CB	1:A:497:GLN:NE2	2.16	1.07
2:C:78:LYS:HE2	2:C:253:ASN:C	1.75	1.07
1:A:486:VAL:HA	1:A:497:GLN:NE2	1.69	1.07
1:B:474:ARG:NH1	1:B:477:LYS:CD	2.17	1.06
2:C:69:ARG:HH21	2:C:81:LEU:HD23	1.16	1.06
2:C:34:VAL:HG22	2:C:53:CYS:HB2	1.07	1.06
1:B:474:ARG:HD3	1:B:477:LYS:HD2	1.33	1.06
1:A:482:HIS:CD2	1:A:501:LEU:HD23	1.91	1.06
2:E:34:VAL:HG22	2:E:53:CYS:HB2	1.07	1.06
2:E:69:ARG:HH21	2:E:81:LEU:HD23	1.16	1.06
1:A:412:VAL:HG22	1:A:504:VAL:HG12	1.36	1.05
2:E:40:ASN:HB2	2:E:43:LEU:HD13	1.07	1.05
1:A:474:ARG:HH11	1:A:477:LYS:CG	1.70	1.05
1:B:442:LEU:HD11	1:B:465:LEU:HD22	1.38	1.05
2:C:40:ASN:HB2	2:C:43:LEU:HD13	1.07	1.05
1:A:266:ASP:CG	1:A:360:ARG:NH2	2.10	1.04
2:E:69:ARG:CD	2:E:254:TYR:CD1	2.40	1.04
3:F:66:ARG:HG3	3:F:66:ARG:HH11	1.15	1.04
1:B:445:SER:O	1:B:450:SER:O	1.74	1.04
1:A:474:ARG:HG3	1:A:476:PRO:HD2	1.40	1.04
1:B:266:ASP:CG	1:B:360:ARG:NH2	2.10	1.04
1:B:410:LEU:N	1:B:503:THR:O	1.90	1.03
2:E:30:LEU:HD22	2:E:60:LEU:HD11	1.39	1.03
1:A:426:CYS:HB2	1:A:462:SER:O	1.59	1.03
1:A:410:LEU:N	1:A:503:THR:O	1.90	1.03
1:B:419:PHE:CD1	1:B:468:ASN:OD1	2.12	1.03
1:A:445:SER:O	1:A:450:SER:O	1.74	1.03
1:B:360:ARG:HB3	1:B:365:SER:HB3	1.32	1.03
1:A:419:PHE:CD1	1:A:468:ASN:OD1	2.12	1.03
1:A:442:LEU:HD11	1:A:465:LEU:HD22	1.38	1.03
1:B:474:ARG:HH11	1:B:477:LYS:CG	1.70	1.03
1:B:356:LEU:HD21	1:B:372:LEU:HD22	1.38	1.03
1:B:441:LYS:HB2	1:B:486:VAL:CG2	1.88	1.02
1:B:486:VAL:HA	1:B:497:GLN:NE2	1.69	1.02
1:A:486:VAL:CB	1:A:497:GLN:HE22	1.72	1.02
1:B:426:CYS:HB2	1:B:462:SER:O	1.59	1.02
1:A:441:LYS:HB2	1:A:486:VAL:CG2	1.88	1.02
2:E:8:LEU:HB2	2:E:12:LYS:HB2	1.40	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:ARG:HG3	1:B:476:PRO:HD2	1.40	1.02
1:A:356:LEU:HD21	1:A:372:LEU:HD22	1.38	1.01
1:B:486:VAL:HG13	1:B:497:GLN:NE2	1.73	1.01
1:B:482:HIS:CD2	1:B:501:LEU:HD23	1.91	1.01
2:C:30:LEU:HD22	2:C:60:LEU:HD11	1.39	1.00
1:A:269:ALA:HB2	1:A:366:GLU:CD	1.82	1.00
1:A:445:SER:O	1:A:451:THR:O	1.80	1.00
1:A:474:ARG:HG2	1:A:476:PRO:HD2	1.43	1.00
1:B:445:SER:O	1:B:451:THR:O	1.80	1.00
2:C:77:GLU:HB3	2:C:254:TYR:OH	1.62	1.00
2:C:8:LEU:HB2	2:C:12:LYS:HB2	1.40	1.00
2:E:71:LYS:N	2:E:254:TYR:OH	1.92	1.00
1:B:474:ARG:HG2	1:B:476:PRO:HD2	1.43	0.99
1:A:474:ARG:NH1	1:A:477:LYS:CG	2.25	0.99
2:E:69:ARG:CD	2:E:254:TYR:CE1	2.42	0.99
1:A:474:ARG:HH11	1:A:477:LYS:HD2	1.28	0.99
1:A:486:VAL:HG12	1:A:497:GLN:NE2	1.57	0.99
1:B:269:ALA:HB2	1:B:366:GLU:CD	1.82	0.99
1:B:298:VAL:HG23	1:B:314:TYR:HE2	1.28	0.98
1:B:323:THR:HB	1:B:324:TRP:HA	1.46	0.97
1:B:482:HIS:NE2	1:B:501:LEU:CD2	2.17	0.97
1:A:419:PHE:HD1	1:A:468:ASN:OD1	1.47	0.97
1:A:486:VAL:HG13	1:A:497:GLN:NE2	1.73	0.97
1:A:442:LEU:HD21	1:A:485:VAL:HG22	1.46	0.96
1:B:474:ARG:NH1	1:B:477:LYS:CG	2.25	0.96
1:B:474:ARG:HH11	1:B:477:LYS:HD2	1.28	0.96
1:B:442:LEU:HD23	1:B:485:VAL:HG22	1.47	0.96
1:B:486:VAL:HG12	1:B:497:GLN:NE2	1.57	0.96
1:B:486:VAL:CB	1:B:497:GLN:HE22	1.72	0.96
2:E:69:ARG:HD2	2:E:254:TYR:CE1	2.01	0.96
2:E:85:TRP:CZ2	2:E:257:ARG:CD	2.48	0.96
1:B:293:VAL:HG21	1:B:329:PHE:HE1	1.31	0.95
2:C:78:LYS:HE2	2:C:254:TYR:HA	0.98	0.95
1:A:298:VAL:HG23	1:A:314:TYR:HE2	1.28	0.95
1:A:482:HIS:NE2	1:A:501:LEU:CD2	2.17	0.95
1:A:298:VAL:CG1	1:A:358:LEU:HD22	1.97	0.95
1:A:323:THR:HB	1:A:324:TRP:HA	1.46	0.94
1:B:298:VAL:CG1	1:B:358:LEU:HD22	1.97	0.94
1:A:293:VAL:HG21	1:A:329:PHE:HE1	1.31	0.94
1:B:199:GLN:H	1:B:199:GLN:HE21	1.14	0.94
2:E:71:LYS:CD	2:E:254:TYR:CD2	2.50	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:GLN:H	1:A:199:GLN:HE21	1.14	0.93
1:A:442:LEU:HD23	1:A:485:VAL:HG22	1.47	0.93
1:B:266:ASP:CB	1:B:360:ARG:HH22	1.82	0.93
1:B:451:THR:N	1:B:451:THR:C	2.20	0.93
2:E:85:TRP:CH2	2:E:257:ARG:CD	2.51	0.93
1:A:451:THR:C	1:A:451:THR:N	2.20	0.93
1:B:442:LEU:HD21	1:B:485:VAL:HG22	1.46	0.93
1:A:319:LEU:HD13	1:A:354:TYR:CE1	2.04	0.93
1:B:319:LEU:HD13	1:B:354:TYR:CE1	2.04	0.93
1:B:357:VAL:HG22	1:B:369:THR:HG22	1.51	0.93
2:E:69:ARG:NE	2:E:254:TYR:HD1	1.52	0.93
2:E:69:ARG:NE	2:E:254:TYR:CD1	2.09	0.92
1:A:357:VAL:HG22	1:A:369:THR:HG22	1.51	0.92
1:B:269:ALA:CB	1:B:366:GLU:OE1	2.16	0.92
1:A:266:ASP:CB	1:A:360:ARG:HH22	1.82	0.91
1:B:416:ALA:O	1:B:417:ARG:O	1.88	0.91
2:C:78:LYS:CE	2:C:254:TYR:N	2.28	0.91
2:E:71:LYS:HD2	2:E:254:TYR:HD2	1.14	0.90
1:A:416:ALA:O	1:A:417:ARG:O	1.88	0.90
1:B:419:PHE:HD1	1:B:468:ASN:OD1	1.47	0.90
2:C:81:LEU:HD11	2:C:85:TRP:CE3	2.07	0.90
1:A:409:SER:C	1:A:410:LEU:CA	2.40	0.90
1:B:412:VAL:CG2	1:B:504:VAL:O	2.20	0.90
1:A:429:ASN:CB	1:A:440:TYR:OH	2.20	0.90
2:E:81:LEU:HD11	2:E:85:TRP:CE3	2.06	0.90
2:E:40:ASN:HB2	2:E:43:LEU:CD1	2.01	0.89
1:A:303:VAL:HG12	1:A:305:PRO:HD2	1.52	0.89
2:C:78:LYS:N	2:C:254:TYR:HE1	1.62	0.89
2:E:30:LEU:HD22	2:E:60:LEU:CD1	2.03	0.89
1:B:429:ASN:CB	1:B:440:TYR:OH	2.20	0.89
1:A:486:VAL:HG12	1:A:497:GLN:HE21	0.72	0.89
1:B:409:SER:C	1:B:410:LEU:CA	2.40	0.89
1:B:486:VAL:HG12	1:B:497:GLN:HE21	0.72	0.89
1:B:303:VAL:HG12	1:B:305:PRO:HD2	1.52	0.88
1:B:474:ARG:CG	1:B:476:PRO:O	2.22	0.88
2:C:30:LEU:HD22	2:C:60:LEU:CD1	2.03	0.88
1:A:269:ALA:CB	1:A:366:GLU:OE1	2.16	0.88
1:A:474:ARG:CG	1:A:476:PRO:O	2.22	0.88
1:A:412:VAL:CG2	1:A:504:VAL:O	2.20	0.88
1:A:408:TYR:CE1	1:A:422:ILE:HG21	2.08	0.87
1:A:293:VAL:HG21	1:A:329:PHE:CE1	2.10	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:VAL:HG23	1:B:286:LYS:HB2	1.55	0.87
1:B:298:VAL:HG11	1:B:358:LEU:HD22	1.55	0.87
1:B:304:VAL:HB	1:B:305:PRO:HD3	1.56	0.87
1:B:293:VAL:HG21	1:B:329:PHE:CE1	2.10	0.87
2:C:78:LYS:HE2	2:C:253:ASN:O	1.74	0.87
1:A:298:VAL:HG11	1:A:358:LEU:HD22	1.55	0.86
1:A:441:LYS:HB2	1:A:486:VAL:HG21	1.56	0.86
1:A:283:VAL:HG23	1:A:286:LYS:HB2	1.55	0.86
2:C:78:LYS:HE3	2:C:254:TYR:HB2	1.55	0.86
1:B:489:ASP:HB2	1:B:494:ARG:CD	2.05	0.86
1:B:408:TYR:CE1	1:B:422:ILE:HG21	2.08	0.86
1:B:441:LYS:HB2	1:B:486:VAL:HG21	1.56	0.86
1:A:302:ASP:C	1:A:309:GLU:HB2	1.96	0.86
2:C:26:LYS:HD2	2:C:59:ALA:HB1	1.58	0.86
2:C:81:LEU:HD21	2:C:85:TRP:CE2	2.11	0.85
1:B:178:GLU:HG3	1:B:265:GLU:CB	2.06	0.85
1:A:360:ARG:HB3	1:A:365:SER:CB	2.06	0.85
1:B:360:ARG:HB3	1:B:365:SER:CB	2.06	0.85
1:A:178:GLU:HG3	1:A:265:GLU:CB	2.06	0.85
1:A:489:ASP:HB2	1:A:494:ARG:CD	2.05	0.85
1:B:412:VAL:CG2	1:B:504:VAL:HG12	2.06	0.85
1:A:304:VAL:HB	1:A:305:PRO:HD3	1.56	0.85
1:B:424:LYS:HE3	1:B:464:ILE:CG1	2.06	0.85
2:E:81:LEU:HD21	2:E:85:TRP:CE2	2.11	0.85
1:A:412:VAL:CG2	1:A:504:VAL:HG12	2.06	0.84
1:B:302:ASP:C	1:B:309:GLU:HB2	1.96	0.84
2:E:9:ASP:CG	2:E:70:CYS:HB2	1.98	0.84
1:B:300:ASP:OD2	1:B:309:GLU:HA	1.76	0.84
1:A:300:ASP:OD2	1:A:309:GLU:HA	1.77	0.84
2:C:40:ASN:HB2	2:C:43:LEU:CD1	2.01	0.84
2:E:26:LYS:HD2	2:E:59:ALA:HB1	1.58	0.84
2:E:34:VAL:HG22	2:E:53:CYS:CB	2.02	0.83
1:A:424:LYS:HE3	1:A:464:ILE:CG1	2.06	0.83
1:B:298:VAL:HG23	1:B:314:TYR:CE2	2.13	0.83
1:A:314:TYR:CE2	1:A:338:THR:HG21	2.14	0.83
1:A:354:TYR:HB2	1:A:372:LEU:CD2	2.09	0.82
2:C:9:ASP:CG	2:C:70:CYS:HB2	1.98	0.82
1:B:178:GLU:CD	1:B:231:ARG:H	1.83	0.82
1:A:486:VAL:N	1:A:497:GLN:NE2	1.88	0.82
1:B:354:TYR:HB2	1:B:372:LEU:CD2	2.09	0.82
1:A:298:VAL:HG23	1:A:314:TYR:CE2	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:78:LYS:HE3	2:C:254:TYR:HA	0.89	0.81
1:A:426:CYS:CB	1:A:462:SER:O	2.27	0.81
1:B:314:TYR:CE2	1:B:338:THR:HG21	2.14	0.81
1:B:474:ARG:HH11	1:B:477:LYS:HG3	1.33	0.81
3:D:66:ARG:NH1	3:D:66:ARG:HG3	1.95	0.81
1:B:275:GLY:O	1:B:370:MET:HB2	1.81	0.81
1:A:275:GLY:O	1:A:370:MET:HB2	1.81	0.81
1:B:426:CYS:CB	1:B:462:SER:O	2.27	0.81
2:E:78:LYS:HA	2:E:252:THR:O	1.81	0.81
1:A:470:THR:CG2	1:A:473:LEU:CD2	2.59	0.81
1:A:474:ARG:HH11	1:A:477:LYS:HG3	1.33	0.81
1:B:354:TYR:HB2	1:B:372:LEU:HD21	1.63	0.81
3:F:66:ARG:HH11	3:F:66:ARG:CG	1.94	0.81
1:B:470:THR:CG2	1:B:473:LEU:CD2	2.59	0.80
1:A:354:TYR:HB2	1:A:372:LEU:HD21	1.63	0.80
1:A:456:THR:OG1	1:A:468:ASN:ND2	2.14	0.80
1:B:272:PHE:CD2	1:B:298:VAL:HG22	2.16	0.80
1:A:272:PHE:CD2	1:A:298:VAL:HG22	2.16	0.80
1:A:178:GLU:CD	1:A:231:ARG:H	1.83	0.80
1:A:474:ARG:NH1	1:A:477:LYS:HD2	1.90	0.80
1:B:450:SER:C	1:B:451:THR:C	2.41	0.80
1:A:450:SER:C	1:A:451:THR:C	2.41	0.80
2:E:34:VAL:CG2	2:E:53:CYS:HB2	2.03	0.80
1:A:300:ASP:HB3	1:A:309:GLU:HG3	1.65	0.79
1:A:412:VAL:HG21	1:A:475:ARG:HB2	1.64	0.79
2:E:69:ARG:CG	2:E:80:CYS:HB3	2.12	0.79
1:A:412:VAL:HG23	1:A:504:VAL:O	1.83	0.79
1:B:412:VAL:HG21	1:B:475:ARG:HB2	1.64	0.79
1:B:456:THR:OG1	1:B:468:ASN:ND2	2.14	0.79
1:B:300:ASP:HB3	1:B:309:GLU:HG3	1.65	0.79
1:A:179:ASN:HB2	1:A:265:GLU:CD	2.01	0.79
1:A:408:TYR:CD1	1:A:422:ILE:CG2	2.65	0.79
2:C:34:VAL:HG22	2:C:53:CYS:CB	2.02	0.79
2:C:34:VAL:CG2	2:C:53:CYS:HB2	2.02	0.79
1:B:408:TYR:CD1	1:B:422:ILE:CG2	2.65	0.79
2:C:69:ARG:CG	2:C:80:CYS:HB3	2.12	0.78
3:F:66:ARG:HG3	3:F:66:ARG:NH1	1.95	0.78
1:B:474:ARG:NH1	1:B:477:LYS:HD2	1.90	0.78
3:D:66:ARG:CG	3:D:66:ARG:HH11	1.94	0.78
2:E:85:TRP:CZ3	2:E:257:ARG:HD2	2.18	0.78
1:A:296:LEU:HD11	1:A:372:LEU:HD13	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:GLN:OE1	1:B:464:ILE:HG21	1.84	0.77
1:A:302:ASP:O	1:A:309:GLU:HB2	1.84	0.77
1:A:421:GLN:OE1	1:A:464:ILE:HG21	1.84	0.77
1:B:179:ASN:HB2	1:B:265:GLU:CD	2.00	0.77
1:B:302:ASP:O	1:B:309:GLU:HB2	1.84	0.77
2:E:26:LYS:HG3	2:E:63:LYS:HE2	1.66	0.77
1:A:296:LEU:O	1:A:338:THR:HG23	1.85	0.77
1:A:474:ARG:NH1	1:A:477:LYS:CE	2.48	0.77
1:B:489:ASP:HB2	1:B:494:ARG:HD2	1.66	0.77
1:B:412:VAL:HG23	1:B:504:VAL:O	1.83	0.77
2:C:35:ALA:O	2:C:38:GLU:HG2	1.85	0.77
1:A:359:ASN:HB2	1:A:367:ASN:OD1	1.85	0.77
1:B:470:THR:HG21	1:B:473:LEU:CD2	2.15	0.76
1:A:408:TYR:CZ	1:A:422:ILE:CG2	2.69	0.76
1:A:443:HIS:O	1:A:444:SER:OG	2.03	0.76
1:B:296:LEU:O	1:B:338:THR:HG23	1.85	0.76
2:C:26:LYS:HG3	2:C:63:LYS:HE2	1.67	0.76
2:E:81:LEU:O	2:E:81:LEU:HD13	1.86	0.76
1:B:296:LEU:HD11	1:B:372:LEU:HD13	1.66	0.76
2:E:37:LYS:HD3	2:E:89:GLN:O	1.86	0.76
2:C:37:LYS:HD3	2:C:89:GLN:O	1.86	0.76
1:A:474:ARG:HG2	1:A:476:PRO:CD	2.16	0.76
1:B:359:ASN:HB2	1:B:367:ASN:OD1	1.85	0.76
1:A:470:THR:HG21	1:A:473:LEU:CD2	2.15	0.76
1:A:482:HIS:HE2	1:A:501:LEU:HD21	1.49	0.76
2:E:70:CYS:C	2:E:254:TYR:CZ	2.46	0.76
2:E:35:ALA:O	2:E:38:GLU:HG2	1.85	0.76
1:A:445:SER:O	1:A:449:CYS:O	2.04	0.75
1:B:482:HIS:HE2	1:B:501:LEU:HD21	1.49	0.75
1:B:474:ARG:NH1	1:B:477:LYS:CE	2.48	0.75
2:E:9:ASP:OD2	2:E:70:CYS:HB2	1.86	0.75
1:B:178:GLU:HG3	1:B:265:GLU:HB2	1.69	0.75
1:B:408:TYR:CZ	1:B:422:ILE:CG2	2.69	0.75
1:B:443:HIS:O	1:B:444:SER:OG	2.03	0.75
1:B:445:SER:O	1:B:449:CYS:O	2.04	0.75
2:E:10:CYS:HB2	2:E:69:ARG:HA	1.69	0.75
1:A:284:GLU:HB2	1:A:377:ASN:O	1.87	0.75
1:A:489:ASP:HB2	1:A:494:ARG:HD2	1.66	0.75
2:C:81:LEU:HD13	2:C:81:LEU:O	1.86	0.75
1:A:303:VAL:CG1	1:A:305:PRO:HD2	2.17	0.74
1:B:442:LEU:HD11	1:B:457:SER:HB2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:488:THR:OG1	1:B:488:THR:O	1.86	0.74
1:A:178:GLU:HG3	1:A:265:GLU:HB3	1.69	0.74
1:A:314:TYR:CZ	1:A:338:THR:HG21	2.22	0.74
2:C:10:CYS:HB2	2:C:69:ARG:HA	1.69	0.74
1:A:319:LEU:HD13	1:A:354:TYR:CD1	2.22	0.74
1:B:474:ARG:CG	1:B:476:PRO:CD	2.62	0.74
2:C:9:ASP:OD2	2:C:70:CYS:HB2	1.86	0.74
1:B:303:VAL:CG1	1:B:305:PRO:HD2	2.17	0.74
1:A:319:LEU:HB2	1:A:354:TYR:CE2	2.21	0.74
1:B:199:GLN:H	1:B:199:GLN:NE2	1.85	0.74
1:B:284:GLU:HB2	1:B:377:ASN:O	1.87	0.74
1:A:199:GLN:H	1:A:199:GLN:NE2	1.85	0.74
1:B:266:ASP:CB	1:B:360:ARG:NH2	2.50	0.74
2:E:71:LYS:HD2	2:E:254:TYR:CE2	2.22	0.74
1:B:314:TYR:CZ	1:B:338:THR:HG21	2.22	0.74
1:B:474:ARG:HG2	1:B:476:PRO:CD	2.16	0.74
1:A:442:LEU:HD11	1:A:457:SER:HB2	1.69	0.74
1:B:319:LEU:HB2	1:B:354:TYR:CE2	2.21	0.74
1:A:356:LEU:HD21	1:A:372:LEU:CD2	2.16	0.74
2:E:69:ARG:HD3	2:E:254:TYR:CD1	2.22	0.74
1:A:270:PRO:CB	1:A:358:LEU:HD23	2.18	0.73
1:A:302:ASP:HB2	1:A:309:GLU:HA	1.70	0.73
1:A:507:SER:O	1:A:508:TYR:HD1	1.71	0.73
1:B:178:GLU:HG3	1:B:265:GLU:HB3	1.69	0.73
1:B:304:VAL:HG22	1:B:309:GLU:OE2	1.89	0.73
1:B:441:LYS:HB2	1:B:486:VAL:HG22	1.71	0.73
1:B:319:LEU:HD13	1:B:354:TYR:CD1	2.22	0.73
2:E:71:LYS:CD	2:E:254:TYR:CE2	2.71	0.73
1:A:302:ASP:HB2	1:A:309:GLU:CA	2.18	0.73
1:A:304:VAL:HG22	1:A:309:GLU:OE2	1.89	0.73
1:A:441:LYS:HB2	1:A:486:VAL:HG22	1.71	0.73
1:B:302:ASP:HB2	1:B:309:GLU:CA	2.18	0.73
1:B:302:ASP:HB2	1:B:309:GLU:HA	1.70	0.73
1:B:507:SER:O	1:B:508:TYR:HD1	1.71	0.73
2:C:69:ARG:NH2	2:C:81:LEU:HD23	2.00	0.72
1:A:266:ASP:CB	1:A:360:ARG:NH2	2.50	0.72
1:B:270:PRO:CB	1:B:358:LEU:HD23	2.18	0.72
1:A:178:GLU:HG3	1:A:265:GLU:HB2	1.69	0.72
1:A:474:ARG:CG	1:A:476:PRO:CD	2.62	0.72
1:A:300:ASP:O	1:A:309:GLU:HG3	1.90	0.72
1:B:356:LEU:HD21	1:B:372:LEU:CD2	2.16	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:81:LEU:HD11	2:C:85:TRP:CD2	2.25	0.72
1:B:418:ARG:HG3	1:B:469:ASP:HB2	1.70	0.72
1:B:300:ASP:O	1:B:309:GLU:HG3	1.90	0.72
2:C:69:ARG:HB2	2:C:84:TYR:HB2	1.70	0.72
2:E:85:TRP:CZ2	2:E:257:ARG:CG	2.73	0.72
2:E:69:ARG:HH21	2:E:81:LEU:CD2	2.00	0.72
1:A:137:CYS:N	2:C:42:SER:O	2.22	0.72
2:C:37:LYS:HE3	2:C:85:TRP:CE3	2.24	0.72
1:A:418:ARG:HG3	1:A:469:ASP:HB2	1.70	0.71
1:A:488:THR:OG1	1:A:488:THR:O	1.86	0.71
2:C:69:ARG:HH21	2:C:81:LEU:CD2	2.00	0.71
1:B:408:TYR:CD1	1:B:422:ILE:HG21	2.26	0.71
1:B:429:ASN:HB2	1:B:440:TYR:OH	1.90	0.71
1:B:442:LEU:CD1	1:B:457:SER:HB2	2.20	0.71
2:E:37:LYS:HE3	2:E:85:TRP:CE3	2.24	0.71
1:A:408:TYR:CD1	1:A:422:ILE:HG21	2.26	0.71
2:E:69:ARG:HB2	2:E:84:TYR:HB2	1.70	0.71
1:A:300:ASP:HB3	1:A:309:GLU:CG	2.21	0.71
2:E:69:ARG:HG3	2:E:80:CYS:HB3	1.72	0.71
1:A:319:LEU:HB2	1:A:354:TYR:CZ	2.25	0.71
1:B:319:LEU:HB2	1:B:354:TYR:CZ	2.26	0.71
1:B:317:THR:HG22	1:B:318:LEU:HD12	1.73	0.71
1:A:442:LEU:CD1	1:A:457:SER:HB2	2.20	0.71
1:B:329:PHE:HB3	1:B:340:VAL:CG2	2.20	0.71
2:E:81:LEU:HD11	2:E:85:TRP:CD2	2.24	0.71
1:A:358:LEU:HG	1:A:358:LEU:O	1.91	0.70
1:B:293:VAL:HB	1:B:340:VAL:HG13	1.73	0.70
2:E:69:ARG:HE	2:E:257:ARG:NH2	1.89	0.70
1:A:329:PHE:HB3	1:A:340:VAL:CG2	2.20	0.70
2:E:78:LYS:CA	2:E:252:THR:O	2.40	0.70
1:A:266:ASP:HB2	1:A:360:ARG:NH2	2.06	0.70
3:D:69:SER:HB3	3:F:97:VAL:HG13	1.73	0.70
1:B:266:ASP:HB2	1:B:360:ARG:NH2	2.06	0.70
2:C:69:ARG:HG3	2:C:80:CYS:HB3	1.72	0.70
3:D:45:ALA:HB2	3:D:66:ARG:HD3	1.73	0.70
3:F:72:CYS:SG	3:F:72:CYS:O	2.49	0.70
1:B:300:ASP:HB3	1:B:309:GLU:CG	2.21	0.70
1:B:361:ASN:H	1:B:365:SER:HB2	1.57	0.70
2:E:78:LYS:HD3	2:E:252:THR:HB	1.72	0.70
3:D:72:CYS:SG	3:D:72:CYS:O	2.49	0.70
1:A:317:THR:HG22	1:A:318:LEU:HD12	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:VAL:HB	1:A:340:VAL:HG13	1.73	0.69
2:E:37:LYS:HE3	2:E:85:TRP:HE3	1.57	0.69
1:B:314:TYR:CD1	1:B:338:THR:HB	2.27	0.69
1:B:357:VAL:HG22	1:B:369:THR:CG2	2.21	0.69
3:D:97:VAL:HG13	3:F:69:SER:HB3	1.73	0.69
1:B:356:LEU:CD2	1:B:372:LEU:HD22	2.19	0.69
1:B:482:HIS:HD2	1:B:501:LEU:HD21	1.49	0.69
1:A:357:VAL:HG22	1:A:369:THR:CG2	2.21	0.69
1:B:312:ARG:HH21	1:B:336:ASN:HB3	1.57	0.69
1:B:347:VAL:HG22	1:B:348:ARG:H	1.58	0.69
1:A:361:ASN:H	1:A:365:SER:HB2	1.57	0.69
1:B:269:ALA:HA	1:B:366:GLU:HB2	1.75	0.69
2:C:8:LEU:HB2	2:C:12:LYS:CB	2.22	0.69
1:A:314:TYR:CD1	1:A:338:THR:HB	2.27	0.69
1:B:273:PRO:HD2	1:B:297:ARG:O	1.93	0.69
1:A:429:ASN:HB2	1:A:440:TYR:OH	1.90	0.69
1:B:358:LEU:O	1:B:358:LEU:HG	1.91	0.69
1:B:408:TYR:CZ	1:B:422:ILE:HG21	2.28	0.68
1:B:408:TYR:HE1	1:B:422:ILE:HG23	1.54	0.68
1:A:418:ARG:HE	1:A:469:ASP:HB3	1.58	0.68
1:A:408:TYR:CZ	1:A:422:ILE:HG21	2.28	0.68
1:A:273:PRO:HD2	1:A:297:ARG:O	1.93	0.68
2:C:69:ARG:HB2	2:C:84:TYR:CB	2.24	0.68
2:E:69:ARG:NH2	2:E:81:LEU:HD23	2.00	0.68
1:A:347:VAL:HG22	1:A:348:ARG:H	1.58	0.68
2:C:37:LYS:HE3	2:C:85:TRP:HE3	1.57	0.68
3:F:45:ALA:HB2	3:F:66:ARG:HD3	1.73	0.68
2:C:29:THR:O	2:C:32:GLN:HG2	1.94	0.68
1:A:283:VAL:CG2	1:A:286:LYS:HB2	2.24	0.68
1:A:303:VAL:HG12	1:A:305:PRO:CD	2.23	0.68
2:E:20:GLU:OE2	2:E:23:CYS:HB2	1.94	0.68
1:A:482:HIS:HD2	1:A:501:LEU:CD2	1.97	0.68
1:B:415:ARG:O	1:B:416:ALA:CB	2.40	0.68
1:A:269:ALA:HA	1:A:366:GLU:HB2	1.75	0.68
1:A:303:VAL:O	1:A:309:GLU:HB3	1.94	0.68
1:A:314:TYR:CE1	1:A:336:ASN:HA	2.29	0.68
1:A:429:ASN:ND2	1:A:440:TYR:OH	2.27	0.68
1:A:457:SER:HB2	1:A:465:LEU:CD2	2.24	0.68
1:B:429:ASN:ND2	1:B:440:TYR:OH	2.27	0.68
1:A:312:ARG:HH21	1:A:336:ASN:HB3	1.57	0.68
1:A:319:LEU:HD22	1:A:354:TYR:OH	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:ARG:HE	1:B:469:ASP:HB3	1.58	0.68
2:C:20:GLU:OE2	2:C:23:CYS:HB2	1.94	0.68
2:C:30:LEU:CD2	2:C:60:LEU:HD11	2.22	0.68
1:B:283:VAL:CG2	1:B:286:LYS:HB2	2.24	0.67
1:B:319:LEU:HD22	1:B:354:TYR:OH	1.94	0.67
1:B:332:GLU:HB3	1:B:335:PRO:HG2	1.76	0.67
1:B:457:SER:HB2	1:B:465:LEU:CD2	2.24	0.67
1:B:482:HIS:HD2	1:B:501:LEU:CD2	1.97	0.67
1:B:303:VAL:O	1:B:309:GLU:HB3	1.94	0.67
1:A:409:SER:O	1:A:410:LEU:CA	2.43	0.67
1:B:314:TYR:CE1	1:B:336:ASN:HA	2.29	0.67
2:C:37:LYS:HZ1	2:C:85:TRP:HE3	1.42	0.67
2:C:88:TYR:HB3	2:C:89:GLN:HE21	1.60	0.67
2:E:29:THR:O	2:E:32:GLN:HG2	1.94	0.67
2:E:69:ARG:HB2	2:E:84:TYR:CB	2.24	0.67
1:A:356:LEU:CD2	1:A:372:LEU:HD22	2.19	0.67
1:B:486:VAL:N	1:B:497:GLN:NE2	1.88	0.67
1:A:475:ARG:N	1:A:476:PRO:CD	2.58	0.67
1:B:412:VAL:CG1	1:B:475:ARG:H	2.07	0.67
1:B:303:VAL:HG12	1:B:305:PRO:CD	2.24	0.67
1:B:444:SER:HB2	1:B:483:TYR:HA	1.76	0.67
1:A:469:ASP:O	1:A:469:ASP:CG	2.32	0.66
1:A:474:ARG:HH12	1:A:477:LYS:HG3	1.60	0.66
2:E:37:LYS:HZ1	2:E:85:TRP:HE3	1.40	0.66
2:E:88:TYR:HB3	2:E:89:GLN:HE21	1.60	0.66
1:A:350:THR:O	1:A:351:VAL:HG13	1.96	0.66
1:A:415:ARG:O	1:A:416:ALA:CB	2.40	0.66
1:A:412:VAL:CG1	1:A:475:ARG:H	2.07	0.66
1:A:419:PHE:CE1	1:A:468:ASN:OD1	2.49	0.66
2:E:88:TYR:HB3	2:E:89:GLN:NE2	2.09	0.66
1:B:412:VAL:HG22	1:B:504:VAL:O	1.96	0.66
2:C:11:VAL:HG23	2:C:80:CYS:SG	2.36	0.66
1:A:332:GLU:HB3	1:A:335:PRO:HG2	1.76	0.66
1:B:475:ARG:N	1:B:476:PRO:CD	2.58	0.66
2:C:88:TYR:HB3	2:C:89:GLN:NE2	2.09	0.66
1:B:350:THR:O	1:B:351:VAL:HG13	1.96	0.66
1:A:443:HIS:O	1:A:444:SER:CB	2.43	0.66
1:A:457:SER:HB2	1:A:465:LEU:HD22	1.78	0.66
1:B:409:SER:O	1:B:410:LEU:CA	2.43	0.66
1:B:465:LEU:CD1	1:B:500:LEU:CD1	2.73	0.66
1:A:293:VAL:HB	1:A:340:VAL:CG1	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:LEU:CD1	1:A:500:LEU:CD1	2.73	0.65
1:A:507:SER:O	1:A:508:TYR:CD1	2.49	0.65
1:B:507:SER:O	1:B:508:TYR:CD1	2.49	0.65
1:A:444:SER:HB2	1:A:483:TYR:HA	1.76	0.65
1:B:469:ASP:CG	1:B:469:ASP:O	2.32	0.65
1:B:457:SER:HB2	1:B:465:LEU:HD22	1.78	0.65
1:A:408:TYR:HE1	1:A:422:ILE:HG23	1.54	0.65
2:E:30:LEU:CD2	2:E:60:LEU:HD11	2.22	0.65
1:B:419:PHE:CE1	1:B:468:ASN:OD1	2.49	0.65
2:E:69:ARG:HH21	2:E:257:ARG:NH2	1.94	0.65
3:F:80:ASP:O	3:F:99:GLN:NE2	2.30	0.65
2:E:11:VAL:HG23	2:E:80:CYS:SG	2.36	0.65
1:A:312:ARG:HB2	1:A:358:LEU:HD21	1.79	0.65
2:C:88:TYR:CD2	2:C:89:GLN:HG3	2.32	0.65
2:C:47:LEU:HD12	2:C:47:LEU:H	1.62	0.64
2:E:88:TYR:CD2	2:E:89:GLN:HG3	2.32	0.64
2:C:40:ASN:CB	2:C:43:LEU:HD13	2.04	0.64
1:A:70:GLN:OE1	2:C:54:ARG:NH2	2.31	0.64
1:B:451:THR:CA	1:B:452:LEU:N	2.61	0.64
1:A:347:VAL:HG22	1:A:348:ARG:N	2.13	0.64
1:A:410:LEU:N	1:A:410:LEU:C	2.51	0.64
1:B:412:VAL:HG13	1:B:475:ARG:H	1.62	0.64
2:E:37:LYS:CE	2:E:85:TRP:HE3	2.10	0.64
1:B:293:VAL:HB	1:B:340:VAL:CG1	2.27	0.64
1:B:296:LEU:HD21	1:B:372:LEU:HB3	1.80	0.64
2:C:37:LYS:CE	2:C:85:TRP:HE3	2.10	0.64
2:E:47:LEU:HD12	2:E:47:LEU:H	1.62	0.64
1:A:296:LEU:HD21	1:A:372:LEU:HB3	1.80	0.64
1:A:81:HIS:HD2	1:A:82:GLU:O	1.81	0.64
1:B:443:HIS:O	1:B:444:SER:CB	2.43	0.64
1:A:307:SER:O	1:A:360:ARG:HD2	1.98	0.63
1:A:412:VAL:HG22	1:A:504:VAL:O	1.96	0.63
1:B:449:CYS:O	1:B:450:SER:CB	2.45	0.63
1:B:446:GLY:HA3	1:B:454:VAL:CG1	2.28	0.63
2:E:89:GLN:OE1	2:E:90:SER:HA	1.98	0.63
3:D:92:LEU:O	3:D:93:VAL:HB	1.98	0.63
1:A:270:PRO:HB2	1:A:358:LEU:HD23	1.79	0.63
1:B:81:HIS:HD2	1:B:82:GLU:O	1.81	0.63
2:C:83:ILE:HG22	2:C:84:TYR:N	2.13	0.63
3:D:80:ASP:O	3:D:99:GLN:NE2	2.30	0.63
2:E:83:ILE:HG22	2:E:84:TYR:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:CYS:SG	1:A:436:ILE:HA	2.38	0.63
1:A:485:VAL:HG21	1:A:500:LEU:HD11	1.81	0.63
2:C:89:GLN:OE1	2:C:90:SER:HA	1.98	0.63
1:B:307:SER:O	1:B:360:ARG:HD2	1.98	0.63
1:B:312:ARG:HB2	1:B:358:LEU:HD21	1.79	0.63
1:B:364:ILE:O	1:B:364:ILE:HG13	1.99	0.63
1:A:412:VAL:HG13	1:A:475:ARG:H	1.62	0.63
1:A:296:LEU:HD12	1:A:296:LEU:N	2.14	0.62
1:B:296:LEU:HD12	1:B:296:LEU:N	2.14	0.62
2:C:77:GLU:HB3	2:C:254:TYR:CZ	2.33	0.62
2:E:78:LYS:CB	2:E:252:THR:O	2.46	0.62
1:A:446:GLY:HA3	1:A:454:VAL:CG1	2.28	0.62
1:B:347:VAL:HG22	1:B:348:ARG:N	2.13	0.62
1:B:270:PRO:HB2	1:B:358:LEU:HD23	1.79	0.62
1:A:470:THR:HG22	1:A:470:THR:O	2.00	0.62
1:B:430:CYS:SG	1:B:436:ILE:HA	2.38	0.62
1:A:178:GLU:OE1	1:A:230:ASP:HA	2.00	0.62
1:A:350:THR:O	1:A:351:VAL:HG22	1.99	0.62
1:A:364:ILE:O	1:A:364:ILE:HG13	1.99	0.62
3:F:92:LEU:O	3:F:93:VAL:HB	1.99	0.62
1:A:449:CYS:O	1:A:450:SER:CB	2.45	0.62
1:B:442:LEU:CD2	1:B:485:VAL:CG2	2.62	0.62
1:B:445:SER:C	1:B:449:CYS:O	2.38	0.62
2:E:40:ASN:CB	2:E:43:LEU:HD13	2.04	0.62
1:A:348:ARG:O	1:A:348:ARG:HD2	1.99	0.62
1:B:350:THR:O	1:B:351:VAL:HG22	1.99	0.62
1:B:446:GLY:O	1:B:454:VAL:HG12	2.00	0.62
1:A:357:VAL:HG12	1:A:359:ASN:H	1.65	0.61
1:A:421:GLN:OE1	1:A:464:ILE:CG2	2.47	0.61
1:A:441:LYS:CB	1:A:486:VAL:CG2	2.73	0.61
1:A:317:THR:CG2	1:A:318:LEU:HD12	2.30	0.61
1:A:483:TYR:CE2	1:A:485:VAL:HG23	2.35	0.61
2:C:78:LYS:HD2	2:C:257:ARG:HB3	1.81	0.61
2:E:85:TRP:CH2	2:E:257:ARG:CG	2.83	0.61
1:B:483:TYR:CE2	1:B:485:VAL:HG23	2.35	0.61
1:B:441:LYS:CB	1:B:486:VAL:CG2	2.73	0.61
1:B:178:GLU:OE1	1:B:230:ASP:HA	2.00	0.61
2:E:8:LEU:HB2	2:E:12:LYS:CB	2.22	0.61
1:B:178:GLU:HB2	1:B:230:ASP:HA	1.83	0.61
1:B:317:THR:CG2	1:B:318:LEU:HD12	2.30	0.61
1:B:354:TYR:HB2	1:B:372:LEU:HD23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:GLN:OE1	1:B:464:ILE:CG2	2.47	0.61
1:B:485:VAL:HG21	1:B:500:LEU:HD11	1.81	0.61
1:B:357:VAL:HG12	1:B:359:ASN:H	1.65	0.61
1:B:348:ARG:O	1:B:348:ARG:HD2	1.99	0.61
1:A:418:ARG:CD	1:A:469:ASP:HB2	2.31	0.61
1:B:314:TYR:CG	1:B:338:THR:HB	2.36	0.61
1:B:418:ARG:CD	1:B:469:ASP:HB2	2.31	0.61
1:A:354:TYR:HB2	1:A:372:LEU:HD23	1.82	0.60
1:A:451:THR:CA	1:A:452:LEU:N	2.61	0.60
1:B:470:THR:HG22	1:B:470:THR:O	2.00	0.60
1:B:474:ARG:HG3	1:B:476:PRO:CD	2.23	0.60
1:A:304:VAL:O	1:A:310:LEU:HB2	2.01	0.60
1:A:445:SER:C	1:A:449:CYS:O	2.38	0.60
1:B:418:ARG:CG	1:B:469:ASP:HB2	2.32	0.60
1:B:465:LEU:CD1	1:B:500:LEU:HD11	2.32	0.60
1:A:446:GLY:O	1:A:454:VAL:HG12	2.00	0.60
1:A:178:GLU:HB2	1:A:230:ASP:HA	1.83	0.60
1:A:474:ARG:CD	1:A:477:LYS:HD2	2.22	0.60
1:B:410:LEU:C	1:B:410:LEU:N	2.51	0.60
1:A:418:ARG:CG	1:A:469:ASP:HB2	2.31	0.60
1:B:450:SER:O	1:B:451:THR:O	2.20	0.60
2:C:47:LEU:N	2:C:47:LEU:HD12	2.16	0.60
2:E:47:LEU:HD12	2:E:47:LEU:N	2.16	0.60
1:A:465:LEU:CD1	1:A:500:LEU:HD11	2.31	0.60
1:B:317:THR:HG22	1:B:318:LEU:CD1	2.32	0.60
2:E:32:GLN:O	2:E:47:LEU:HD22	2.02	0.60
1:A:450:SER:C	1:A:451:THR:O	2.40	0.60
1:B:179:ASN:CB	1:B:265:GLU:CD	2.69	0.60
1:A:302:ASP:HB2	1:A:309:GLU:N	2.17	0.59
1:A:436:ILE:HG22	1:A:436:ILE:O	2.01	0.59
1:A:450:SER:O	1:A:451:THR:O	2.20	0.59
1:B:450:SER:C	1:B:451:THR:O	2.40	0.59
1:A:317:THR:HG22	1:A:318:LEU:CD1	2.32	0.59
1:B:404:LEU:C	1:B:405:PRO:CD	2.65	0.59
1:A:298:VAL:CG2	1:A:358:LEU:HD13	2.32	0.59
1:B:302:ASP:HB2	1:B:309:GLU:N	2.17	0.59
1:B:360:ARG:CB	1:B:365:SER:HB3	2.22	0.59
2:C:32:GLN:O	2:C:47:LEU:HD22	2.02	0.59
3:D:91:ARG:HH11	3:D:91:ARG:HG3	1.67	0.59
1:A:199:GLN:N	1:A:199:GLN:HE21	1.94	0.59
1:B:298:VAL:CG2	1:B:358:LEU:HD13	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:VAL:CG2	1:A:329:PHE:HE1	2.09	0.59
1:B:293:VAL:CG2	1:B:329:PHE:HE1	2.09	0.59
1:A:314:TYR:CG	1:A:338:THR:HB	2.36	0.59
1:A:332:GLU:OE1	1:A:335:PRO:HG2	2.03	0.59
1:A:474:ARG:NH1	1:A:477:LYS:HE2	2.16	0.59
1:A:151:ASN:O	1:A:152:THR:CG2	2.51	0.58
1:A:442:LEU:CD2	1:A:485:VAL:CG2	2.62	0.58
2:C:37:LYS:NZ	2:C:85:TRP:HE3	2.01	0.58
2:C:53:CYS:O	2:C:57:MET:HG3	2.03	0.58
2:E:53:CYS:O	2:E:57:MET:HG3	2.03	0.58
1:B:151:ASN:O	1:B:152:THR:CG2	2.51	0.58
1:A:474:ARG:HG3	1:A:476:PRO:CD	2.23	0.58
1:B:290:ASP:HB2	1:B:341:GLN:HB3	1.86	0.58
1:B:304:VAL:O	1:B:310:LEU:HB2	2.01	0.58
1:B:474:ARG:NH1	1:B:477:LYS:HE2	2.16	0.58
2:E:78:LYS:HB2	2:E:252:THR:O	2.03	0.58
1:A:151:ASN:O	1:A:152:THR:HG23	2.04	0.58
1:B:474:ARG:HH12	1:B:477:LYS:HG3	1.60	0.58
1:A:404:LEU:C	1:A:405:PRO:CD	2.66	0.58
1:A:483:TYR:CD2	1:A:483:TYR:C	2.77	0.58
1:B:298:VAL:HG21	1:B:358:LEU:HD13	1.85	0.58
3:F:91:ARG:HH11	3:F:91:ARG:HG3	1.67	0.58
1:B:436:ILE:O	1:B:436:ILE:HG22	2.01	0.58
2:C:78:LYS:CD	2:C:257:ARG:HB3	2.34	0.58
2:C:9:ASP:OD2	2:C:72:ARG:HB2	2.04	0.58
1:B:314:TYR:CE2	1:B:358:LEU:HD13	2.39	0.58
1:A:155:PRO:HG2	1:A:160:LEU:HD21	1.86	0.57
2:E:37:LYS:NZ	2:E:85:TRP:HE3	2.01	0.57
1:A:314:TYR:HE1	1:A:336:ASN:HA	1.69	0.57
1:B:155:PRO:HG2	1:B:160:LEU:HD21	1.86	0.57
2:E:34:VAL:HG12	2:E:36:GLY:H	1.70	0.57
1:B:151:ASN:O	1:B:152:THR:HG23	2.04	0.57
1:B:332:GLU:OE1	1:B:335:PRO:HG2	2.03	0.57
1:B:449:CYS:O	1:B:450:SER:O	2.23	0.57
2:C:81:LEU:HD21	2:C:85:TRP:CZ2	2.39	0.57
1:B:295:THR:HA	1:B:339:SER:HA	1.87	0.57
2:E:9:ASP:OD2	2:E:72:ARG:HB2	2.04	0.57
1:B:283:VAL:HA	1:B:377:ASN:HB3	1.86	0.57
1:A:290:ASP:HB2	1:A:341:GLN:HB3	1.86	0.57
1:A:298:VAL:HG21	1:A:358:LEU:HD13	1.85	0.57
1:B:483:TYR:CD2	1:B:483:TYR:C	2.77	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:89:GLN:HE21	2:E:89:GLN:N	2.02	0.57
1:A:283:VAL:HA	1:A:377:ASN:HB3	1.86	0.57
1:A:314:TYR:CE2	1:A:358:LEU:HD13	2.39	0.57
1:A:408:TYR:CZ	1:A:422:ILE:HG23	2.32	0.57
1:B:314:TYR:HE1	1:B:336:ASN:HA	1.69	0.57
2:E:81:LEU:HD21	2:E:85:TRP:CZ2	2.39	0.57
1:B:199:GLN:HE21	1:B:199:GLN:N	1.94	0.56
2:C:34:VAL:HG12	2:C:36:GLY:H	1.69	0.56
1:B:266:ASP:OD2	1:B:360:ARG:CZ	2.53	0.56
1:A:209:GLY:O	1:A:212:LEU:HB2	2.05	0.56
1:A:356:LEU:HD22	1:A:356:LEU:N	2.20	0.56
2:C:89:GLN:N	2:C:89:GLN:HE21	2.02	0.56
1:A:429:ASN:CG	1:A:440:TYR:OH	2.43	0.56
1:B:484:MET:HB3	1:B:497:GLN:CG	2.36	0.56
1:B:410:LEU:CB	1:B:410:LEU:N	2.65	0.56
1:A:449:CYS:O	1:A:450:SER:O	2.23	0.56
2:E:240:ARG:HD3	2:E:314:ASP:HB3	1.88	0.56
1:A:295:THR:HA	1:A:339:SER:HA	1.87	0.56
1:A:438:VAL:HG11	1:A:487:ALA:HB1	1.88	0.56
1:B:438:VAL:HG11	1:B:487:ALA:HB1	1.88	0.56
2:C:37:LYS:HZ2	2:C:85:TRP:HB3	1.71	0.56
1:A:280:SER:HB2	1:A:374:VAL:HA	1.87	0.56
1:B:280:SER:HB2	1:B:374:VAL:HA	1.87	0.56
2:C:240:ARG:HD3	2:C:314:ASP:HB3	1.87	0.56
1:A:179:ASN:CB	1:A:265:GLU:CD	2.69	0.56
1:B:209:GLY:O	1:B:212:LEU:HB2	2.05	0.56
1:B:429:ASN:CG	1:B:440:TYR:OH	2.43	0.56
1:B:356:LEU:HD22	1:B:356:LEU:N	2.20	0.55
2:C:27:TYR:HB2	2:C:65:LEU:HD12	1.88	0.55
2:E:20:GLU:HG3	2:E:23:CYS:H	1.70	0.55
1:B:361:ASN:H	1:B:365:SER:CB	2.19	0.55
1:A:320:PRO:HD2	1:A:353:ASP:O	2.06	0.55
1:A:446:GLY:CA	1:A:454:VAL:CG1	2.85	0.55
1:A:484:MET:HB3	1:A:497:GLN:CG	2.36	0.55
2:C:20:GLU:HG3	2:C:23:CYS:H	1.70	0.55
1:A:410:LEU:N	1:A:410:LEU:CB	2.66	0.55
1:A:426:CYS:CB	1:A:462:SER:C	2.73	0.55
1:B:470:THR:CG2	1:B:473:LEU:HD21	2.36	0.55
1:B:320:PRO:HD2	1:B:353:ASP:O	2.06	0.55
2:E:27:TYR:HB2	2:E:65:LEU:HD12	1.88	0.55
1:B:314:TYR:O	1:B:333:HIS:HA	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:VAL:CG2	1:B:475:ARG:HB2	2.35	0.55
2:C:175:ILE:HG22	3:D:122:ILE:HD11	1.89	0.55
1:A:314:TYR:O	1:A:333:HIS:HA	2.06	0.55
1:A:412:VAL:CG2	1:A:504:VAL:CG1	2.68	0.55
1:B:415:ARG:O	1:B:416:ALA:HB2	2.07	0.55
1:A:266:ASP:OD2	1:A:360:ARG:CZ	2.53	0.54
1:B:441:LYS:C	1:B:486:VAL:HG22	2.27	0.54
1:B:470:THR:HG21	1:B:473:LEU:HD21	1.88	0.54
1:A:409:SER:O	1:A:410:LEU:HA	2.06	0.54
1:A:412:VAL:CG2	1:A:475:ARG:HB2	2.35	0.54
1:B:446:GLY:CA	1:B:454:VAL:CG1	2.85	0.54
1:B:474:ARG:CZ	1:B:476:PRO:HB2	2.37	0.54
1:A:412:VAL:HG22	1:A:504:VAL:HG13	1.80	0.54
1:B:271:THR:O	1:B:298:VAL:HG13	2.08	0.54
2:E:278:LEU:H	2:E:281:ASN:HD22	1.56	0.54
1:A:465:LEU:HD11	1:A:500:LEU:HD11	1.90	0.54
1:B:465:LEU:HD11	1:B:500:LEU:HD11	1.90	0.54
1:A:271:THR:O	1:A:298:VAL:HG13	2.08	0.54
1:B:426:CYS:CB	1:B:462:SER:C	2.73	0.54
2:E:85:TRP:CH2	2:E:257:ARG:HG3	2.42	0.54
1:A:308:GLY:HA2	1:A:360:ARG:CZ	2.38	0.54
1:A:415:ARG:O	1:A:416:ALA:HB2	2.07	0.54
1:A:474:ARG:CZ	1:A:476:PRO:HB2	2.37	0.54
1:B:357:VAL:HG11	1:B:367:ASN:OD1	2.08	0.54
1:A:323:THR:CB	1:A:324:TRP:HA	2.25	0.54
1:A:361:ASN:H	1:A:365:SER:CB	2.19	0.54
2:C:81:LEU:HD13	2:C:81:LEU:C	2.27	0.54
2:E:81:LEU:C	2:E:81:LEU:HD13	2.27	0.54
1:A:276:VAL:O	1:A:276:VAL:HG13	2.07	0.54
1:A:433:PHE:HE2	1:A:495:GLN:HG3	1.73	0.54
1:B:409:SER:O	1:B:410:LEU:HA	2.06	0.54
1:B:444:SER:O	1:B:447:ALA:N	2.38	0.54
1:B:489:ASP:H	1:B:494:ARG:HG3	1.73	0.54
1:B:433:PHE:HE2	1:B:495:GLN:HG3	1.73	0.53
2:C:17:CYS:SG	2:C:65:LEU:HG	2.49	0.53
1:B:276:VAL:HG13	1:B:276:VAL:O	2.07	0.53
1:B:329:PHE:CD2	1:B:354:TYR:CE1	2.96	0.53
2:E:175:ILE:HG22	3:F:122:ILE:HD11	1.89	0.53
1:A:489:ASP:H	1:A:494:ARG:HG3	1.73	0.53
2:C:278:LEU:H	2:C:281:ASN:HD22	1.56	0.53
2:E:17:CYS:SG	2:E:65:LEU:HG	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:THR:CB	1:A:318:LEU:HD12	2.39	0.53
1:A:441:LYS:C	1:A:486:VAL:HG22	2.27	0.53
1:A:446:GLY:HA3	1:A:454:VAL:HG11	1.90	0.53
2:C:78:LYS:HD3	2:C:254:TYR:O	2.08	0.53
1:A:329:PHE:CD2	1:A:354:TYR:CE1	2.96	0.53
1:A:329:PHE:HD2	1:A:354:TYR:CE1	2.26	0.53
1:A:445:SER:CA	1:A:449:CYS:O	2.56	0.53
1:A:357:VAL:HG11	1:A:367:ASN:OD1	2.08	0.53
1:B:348:ARG:C	1:B:348:ARG:HD2	2.29	0.53
1:B:308:GLY:HA2	1:B:360:ARG:CZ	2.38	0.53
1:B:448:ASN:C	1:B:452:LEU:CD2	2.77	0.53
1:B:474:ARG:CD	1:B:477:LYS:HD2	2.22	0.53
1:A:470:THR:HG21	1:A:473:LEU:HD21	1.88	0.53
1:B:317:THR:CB	1:B:318:LEU:HD12	2.39	0.53
1:B:445:SER:CA	1:B:449:CYS:O	2.56	0.53
2:C:43:LEU:HD12	2:C:43:LEU:N	2.23	0.53
1:B:329:PHE:HD2	1:B:354:TYR:CE1	2.26	0.53
1:A:348:ARG:HD2	1:A:348:ARG:C	2.29	0.52
1:A:275:GLY:O	1:A:370:MET:HE3	2.09	0.52
1:A:448:ASN:C	1:A:452:LEU:CD2	2.77	0.52
1:B:489:ASP:HB2	1:B:494:ARG:CG	2.39	0.52
2:E:61:LYS:HG2	2:E:62:GLN:HG3	1.91	0.52
1:A:350:THR:HG23	1:A:351:VAL:N	2.23	0.52
1:A:272:PHE:CG	1:A:370:MET:HB3	2.45	0.52
2:C:61:LYS:HG2	2:C:62:GLN:HG3	1.91	0.52
2:E:43:LEU:HD12	2:E:43:LEU:N	2.23	0.52
1:A:444:SER:O	1:A:447:ALA:N	2.38	0.52
1:A:470:THR:HB	1:A:473:LEU:HD21	1.91	0.52
1:A:412:VAL:HG13	1:A:475:ARG:N	2.25	0.52
1:A:484:MET:HB3	1:A:497:GLN:HG3	1.91	0.52
2:C:168:LYS:HE3	3:D:109:ASP:HB2	1.92	0.52
2:E:47:LEU:H	2:E:47:LEU:CD1	2.23	0.52
1:A:429:ASN:HB3	1:A:440:TYR:OH	2.08	0.52
1:B:335:PRO:O	1:B:336:ASN:HB2	2.10	0.52
1:B:350:THR:HG23	1:B:351:VAL:N	2.23	0.52
3:D:91:ARG:HH11	3:D:91:ARG:CG	2.23	0.52
1:A:470:THR:CG2	1:A:473:LEU:HD21	2.36	0.52
1:B:272:PHE:CG	1:B:370:MET:HB3	2.44	0.52
1:B:446:GLY:HA3	1:B:454:VAL:HG11	1.90	0.52
1:A:296:LEU:HD23	1:A:370:MET:SD	2.50	0.52
1:B:412:VAL:HG13	1:B:475:ARG:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:VAL:HG22	1:B:309:GLU:CD	2.29	0.52
1:A:304:VAL:HG22	1:A:309:GLU:CD	2.29	0.52
1:A:296:LEU:HD23	1:A:370:MET:CE	2.40	0.52
1:B:275:GLY:O	1:B:370:MET:HE3	2.09	0.52
2:E:37:LYS:NZ	2:E:85:TRP:HB3	2.25	0.52
3:F:91:ARG:HH11	3:F:91:ARG:CG	2.23	0.51
1:A:310:LEU:C	1:A:310:LEU:HD23	2.30	0.51
1:B:296:LEU:HD23	1:B:370:MET:SD	2.50	0.51
1:A:489:ASP:HB2	1:A:494:ARG:CG	2.39	0.51
1:B:470:THR:HB	1:B:473:LEU:HD21	1.91	0.51
2:C:37:LYS:NZ	2:C:85:TRP:HB3	2.25	0.51
1:B:296:LEU:HD23	1:B:370:MET:CE	2.40	0.51
2:E:168:LYS:HE3	3:F:109:ASP:HB2	1.91	0.51
1:B:470:THR:CB	1:B:473:LEU:HD21	2.41	0.51
1:B:484:MET:HB3	1:B:497:GLN:HG3	1.91	0.51
1:B:483:TYR:HE2	1:B:485:VAL:HG23	1.74	0.51
1:A:404:LEU:CA	1:A:405:PRO:CD	2.89	0.51
2:C:47:LEU:CD1	2:C:47:LEU:H	2.23	0.51
3:D:76:GLU:H	3:D:76:GLU:CD	2.14	0.51
1:B:310:LEU:C	1:B:310:LEU:HD23	2.31	0.51
1:B:504:VAL:HG13	1:B:504:VAL:O	2.05	0.51
2:E:69:ARG:NE	2:E:257:ARG:NH2	2.56	0.51
1:A:317:THR:C	1:A:318:LEU:HD12	2.31	0.51
1:A:335:PRO:O	1:A:336:ASN:HB2	2.10	0.51
1:A:470:THR:CB	1:A:473:LEU:HD21	2.41	0.51
1:B:329:PHE:CZ	1:B:346:PHE:HE1	2.29	0.51
1:A:318:LEU:HD13	1:A:355:ARG:HD3	1.93	0.50
1:B:312:ARG:HB2	1:B:358:LEU:CD2	2.42	0.50
1:B:336:ASN:O	1:B:338:THR:HG22	2.11	0.50
2:C:260:LEU:HD13	2:C:297:MET:HG2	1.93	0.50
1:A:336:ASN:O	1:A:338:THR:HG22	2.11	0.50
1:B:329:PHE:CD1	1:B:340:VAL:HG22	2.46	0.50
1:B:470:THR:HG21	1:B:473:LEU:HD22	1.93	0.50
1:A:312:ARG:HB2	1:A:358:LEU:CD2	2.42	0.50
1:B:272:PHE:CD2	1:B:298:VAL:CG2	2.92	0.50
1:B:317:THR:C	1:B:318:LEU:HD12	2.31	0.50
1:B:474:ARG:CZ	1:B:477:LYS:HE2	2.41	0.50
2:C:88:TYR:CD2	2:C:89:GLN:CG	2.94	0.50
1:A:445:SER:HA	1:A:449:CYS:O	2.12	0.50
1:A:443:HIS:CE1	1:A:484:MET:HB2	2.47	0.50
1:A:485:VAL:CG2	1:A:500:LEU:CD1	2.90	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:13:ALA:HB1	2:C:67:ASN:ND2	2.27	0.50
2:E:88:TYR:CD2	2:E:89:GLN:CG	2.94	0.50
1:A:474:ARG:CZ	1:A:477:LYS:HE2	2.41	0.50
1:A:483:TYR:HE2	1:A:485:VAL:HG23	1.74	0.50
1:B:298:VAL:HG12	1:B:299:PHE:N	2.27	0.50
3:F:76:GLU:H	3:F:76:GLU:CD	2.14	0.50
1:A:446:GLY:CA	1:A:454:VAL:HG12	2.42	0.50
1:A:426:CYS:SG	1:A:462:SER:O	2.65	0.50
1:B:274:ALA:HB3	1:B:370:MET:CE	2.42	0.50
1:B:404:LEU:CA	1:B:405:PRO:CD	2.89	0.50
2:E:13:ALA:HB1	2:E:67:ASN:ND2	2.27	0.50
1:A:360:ARG:CB	1:A:365:SER:HB3	2.22	0.50
1:B:412:VAL:HG22	1:B:504:VAL:HG13	1.80	0.50
2:C:81:LEU:CD1	2:C:85:TRP:CD2	2.95	0.50
2:E:81:LEU:CD1	2:E:85:TRP:CD2	2.95	0.50
1:A:329:PHE:CZ	1:A:346:PHE:HE1	2.29	0.49
1:B:318:LEU:HD13	1:B:355:ARG:HD3	1.93	0.49
1:B:314:TYR:CE2	1:B:358:LEU:CD1	2.95	0.49
1:B:443:HIS:CE1	1:B:484:MET:HB2	2.47	0.49
1:B:485:VAL:CG2	1:B:500:LEU:CD1	2.90	0.49
1:A:178:GLU:OE1	1:A:230:ASP:C	2.46	0.49
1:A:329:PHE:CD1	1:A:340:VAL:HG22	2.46	0.49
1:A:73:TYR:CE2	2:C:41:PHE:HE2	2.30	0.49
1:B:332:GLU:HB3	1:B:335:PRO:CG	2.42	0.49
1:B:489:ASP:HB2	1:B:494:ARG:NE	2.27	0.49
1:A:357:VAL:CG1	1:A:359:ASN:H	2.25	0.49
1:A:404:LEU:HA	1:A:405:PRO:CD	2.42	0.49
1:B:300:ASP:OD2	1:B:302:ASP:HB2	2.12	0.49
1:B:449:CYS:O	1:B:450:SER:HB3	2.12	0.49
1:A:151:ASN:C	1:A:152:THR:HG23	2.33	0.49
1:A:274:ALA:HB3	1:A:370:MET:CE	2.42	0.49
2:E:260:LEU:HD13	2:E:297:MET:HG2	1.94	0.49
1:A:449:CYS:O	1:A:450:SER:HB3	2.12	0.49
1:A:470:THR:HG21	1:A:473:LEU:HD22	1.93	0.49
1:B:270:PRO:HB2	1:B:358:LEU:CD2	2.42	0.49
1:B:357:VAL:CG1	1:B:359:ASN:H	2.25	0.49
1:A:298:VAL:HG12	1:A:299:PHE:N	2.27	0.49
1:A:314:TYR:CE2	1:A:358:LEU:CD1	2.95	0.49
1:B:470:THR:CG2	1:B:473:LEU:HD23	2.41	0.49
1:A:270:PRO:HB2	1:A:358:LEU:CD2	2.42	0.49
2:E:84:TYR:CD2	2:E:85:TRP:HD1	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:SER:O	1:B:457:SER:OG	2.28	0.49
1:A:304:VAL:HG12	1:A:310:LEU:HD12	1.95	0.49
1:A:478:CYS:SG	1:A:480:GLU:O	2.71	0.49
1:B:404:LEU:HA	1:B:405:PRO:CD	2.42	0.49
1:B:429:ASN:HB3	1:B:440:TYR:OH	2.08	0.49
1:A:489:ASP:HB2	1:A:494:ARG:NE	2.27	0.48
1:B:298:VAL:CB	1:B:358:LEU:HD22	2.42	0.48
2:E:69:ARG:NH2	2:E:257:ARG:NH2	2.61	0.48
1:A:332:GLU:HB3	1:A:335:PRO:CG	2.42	0.48
1:B:446:GLY:CA	1:B:454:VAL:HG12	2.42	0.48
1:B:478:CYS:SG	1:B:480:GLU:O	2.71	0.48
1:B:304:VAL:HG12	1:B:310:LEU:HD12	1.95	0.48
2:E:21:GLN:O	2:E:25:THR:HG23	2.13	0.48
2:E:83:ILE:HG22	2:E:84:TYR:H	1.77	0.48
1:A:322:ASP:O	1:A:326:GLN:HA	2.13	0.48
1:B:322:ASP:O	1:B:326:GLN:HA	2.13	0.48
1:B:357:VAL:HG12	1:B:359:ASN:N	2.28	0.48
1:B:445:SER:HA	1:B:449:CYS:O	2.12	0.48
1:B:375:LEU:HD13	1:B:375:LEU:C	2.34	0.48
1:A:457:SER:O	1:A:457:SER:OG	2.28	0.48
1:A:475:ARG:N	1:A:476:PRO:HD3	2.29	0.48
1:B:314:TYR:CG	1:B:338:THR:CB	2.97	0.48
1:B:466:PHE:CD2	1:B:468:ASN:OD1	2.67	0.48
1:A:466:PHE:CD2	1:A:468:ASN:OD1	2.67	0.48
1:B:323:THR:HA	1:B:324:TRP:C	2.34	0.48
1:B:274:ALA:HB3	1:B:370:MET:HE3	1.95	0.48
2:C:37:LYS:HG2	2:C:37:LYS:O	2.14	0.48
2:E:61:LYS:O	2:E:62:GLN:HB2	2.14	0.48
1:A:295:THR:HG23	1:A:337:GLU:O	2.14	0.48
1:A:329:PHE:HA	1:A:342:ALA:HA	1.96	0.48
1:A:319:LEU:HD22	1:A:354:TYR:CZ	2.49	0.48
1:B:295:THR:HG23	1:B:337:GLU:O	2.14	0.48
1:B:323:THR:CB	1:B:324:TRP:HA	2.25	0.48
1:B:442:LEU:CD1	1:B:465:LEU:HD22	2.27	0.48
2:C:77:GLU:HB3	2:C:254:TYR:HH	1.76	0.48
3:D:77:THR:HG23	3:D:80:ASP:H	1.79	0.48
3:F:77:THR:HG23	3:F:80:ASP:H	1.79	0.48
1:B:319:LEU:HD22	1:B:354:TYR:CZ	2.49	0.48
1:B:416:ALA:O	1:B:417:ARG:C	2.52	0.48
2:C:21:GLN:O	2:C:25:THR:HG23	2.13	0.48
1:A:300:ASP:OD2	1:A:302:ASP:HB2	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:TYR:CG	1:A:338:THR:CB	2.97	0.47
1:A:298:VAL:CB	1:A:358:LEU:HD22	2.43	0.47
1:B:312:ARG:CB	1:B:358:LEU:HD21	2.43	0.47
1:A:404:LEU:HA	1:A:405:PRO:HD3	1.96	0.47
2:C:81:LEU:HD11	2:C:85:TRP:CZ3	2.49	0.47
2:C:83:ILE:HG22	2:C:84:TYR:H	1.77	0.47
2:E:37:LYS:HZ2	2:E:85:TRP:HB3	1.80	0.47
1:A:312:ARG:CB	1:A:358:LEU:HD21	2.42	0.47
1:A:323:THR:HA	1:A:324:TRP:C	2.34	0.47
1:B:334:TRP:CD1	1:B:335:PRO:HD3	2.49	0.47
1:B:404:LEU:HA	1:B:405:PRO:HD3	1.96	0.47
2:C:29:THR:HA	2:C:32:GLN:HG2	1.97	0.47
1:A:274:ALA:HB3	1:A:370:MET:HE3	1.95	0.47
2:C:61:LYS:O	2:C:62:GLN:HB2	2.14	0.47
1:B:151:ASN:C	1:B:152:THR:HG23	2.33	0.47
2:C:17:CYS:HB2	2:C:65:LEU:HG	1.96	0.47
2:C:84:TYR:CD2	2:C:85:TRP:HD1	2.31	0.47
1:A:357:VAL:HG12	1:A:359:ASN:N	2.28	0.47
1:A:375:LEU:HD13	1:A:375:LEU:C	2.34	0.47
1:A:470:THR:CG2	1:A:473:LEU:HD23	2.41	0.47
2:E:8:LEU:CB	2:E:12:LYS:HB2	2.30	0.47
1:A:319:LEU:HD12	1:A:353:ASP:O	2.15	0.47
1:B:319:LEU:HD12	1:B:353:ASP:O	2.15	0.47
2:C:251:LYS:HA	2:C:257:ARG:HB2	1.97	0.47
1:A:334:TRP:CD1	1:A:335:PRO:HD3	2.49	0.47
2:E:251:LYS:HA	2:E:257:ARG:HB2	1.97	0.47
1:B:475:ARG:N	1:B:476:PRO:HD3	2.29	0.47
2:E:29:THR:HA	2:E:32:GLN:HG2	1.97	0.47
2:E:70:CYS:C	2:E:254:TYR:OH	2.47	0.47
1:A:299:PHE:CD1	1:A:300:ASP:N	2.83	0.47
1:B:329:PHE:HA	1:B:342:ALA:HA	1.96	0.47
2:E:37:LYS:CD	2:E:90:SER:HB2	2.45	0.47
2:C:17:CYS:SG	2:C:65:LEU:CD1	3.03	0.47
2:C:78:LYS:CE	2:C:253:ASN:C	2.66	0.47
2:C:37:LYS:CD	2:C:90:SER:HB2	2.45	0.47
2:E:69:ARG:N	2:E:84:TYR:CD1	2.83	0.47
2:E:81:LEU:HD11	2:E:85:TRP:CZ3	2.49	0.47
1:A:304:VAL:CG1	1:A:310:LEU:HD12	2.45	0.46
1:A:355:ARG:HE	1:A:371:GLN:HE21	1.63	0.46
1:A:489:ASP:CB	1:A:494:ARG:HD2	2.41	0.46
1:B:304:VAL:HB	1:B:305:PRO:CD	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:TYR:CZ	1:B:422:ILE:HG23	2.32	0.46
1:B:465:LEU:HD13	1:B:500:LEU:CD1	2.45	0.46
2:E:17:CYS:HB2	2:E:65:LEU:HG	1.96	0.46
1:A:465:LEU:HD13	1:A:500:LEU:CD1	2.45	0.46
1:B:350:THR:C	1:B:351:VAL:HG22	2.35	0.46
2:E:37:LYS:HG2	2:E:37:LYS:O	2.14	0.46
1:A:457:SER:CB	1:A:465:LEU:CD2	2.94	0.46
1:B:266:ASP:CG	1:B:360:ARG:CZ	2.84	0.46
1:A:470:THR:HG22	1:A:473:LEU:HD23	1.98	0.46
1:B:304:VAL:CG1	1:B:310:LEU:HD12	2.45	0.46
2:E:17:CYS:SG	2:E:65:LEU:CD1	3.03	0.46
1:B:298:VAL:HB	1:B:358:LEU:HD22	1.98	0.46
2:C:82:ARG:HB2	2:C:82:ARG:NH1	2.31	0.46
1:A:350:THR:C	1:A:351:VAL:HG22	2.36	0.46
1:A:311:VAL:O	1:A:360:ARG:HG3	2.15	0.46
1:B:361:ASN:N	1:B:365:SER:CB	2.79	0.46
2:E:206:LYS:HE2	2:E:207:HIS:NE2	2.31	0.46
1:A:304:VAL:CB	1:A:305:PRO:HD3	2.37	0.46
1:B:299:PHE:CD1	1:B:300:ASP:N	2.83	0.46
1:B:355:ARG:HE	1:B:371:GLN:HE21	1.63	0.46
1:B:408:TYR:HD2	1:B:410:LEU:HG	1.57	0.46
1:A:445:SER:OG	1:A:450:SER:CB	2.64	0.46
1:A:368:ARG:HG3	1:A:369:THR:N	2.31	0.45
1:B:311:VAL:O	1:B:360:ARG:HG3	2.15	0.45
1:B:445:SER:OG	1:B:450:SER:CB	2.64	0.45
1:A:318:LEU:N	1:A:318:LEU:HD12	2.32	0.45
2:C:69:ARG:HG2	2:C:80:CYS:HB3	1.95	0.45
2:E:176:THR:HB	2:E:177:PRO:HD3	1.99	0.45
1:B:357:VAL:CG2	1:B:369:THR:HG22	2.36	0.45
1:B:489:ASP:CB	1:B:494:ARG:HD2	2.41	0.45
1:B:58:ASP:HA	1:B:180:ARG:HD3	1.99	0.45
1:A:433:PHE:CE2	1:A:495:GLN:OE1	2.70	0.45
2:C:69:ARG:N	2:C:84:TYR:CD1	2.83	0.45
2:E:85:TRP:CE2	2:E:257:ARG:HD2	2.46	0.45
1:B:368:ARG:HG3	1:B:369:THR:N	2.31	0.45
1:B:442:LEU:HD23	1:B:485:VAL:CG2	2.34	0.45
1:B:470:THR:HG22	1:B:473:LEU:HD23	1.98	0.45
2:C:226:ARG:O	2:C:226:ARG:HG3	2.16	0.45
2:E:82:ARG:HB2	2:E:82:ARG:NH1	2.31	0.45
1:A:475:ARG:O	1:A:475:ARG:HG2	2.17	0.45
1:A:483:TYR:CD1	1:A:500:LEU:C	2.88	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:TYR:CD2	1:A:485:VAL:HG23	2.52	0.45
1:B:303:VAL:C	1:B:309:GLU:HB3	2.37	0.45
2:C:176:THR:HB	2:C:177:PRO:HD3	1.99	0.45
2:C:88:TYR:HD2	2:C:89:GLN:CD	2.20	0.45
3:F:83:LEU:HB2	3:F:99:GLN:HE21	1.82	0.45
1:A:58:ASP:HA	1:A:180:ARG:HD3	1.99	0.45
1:A:504:VAL:O	1:A:504:VAL:HG13	2.05	0.45
1:B:187:GLN:NE2	1:B:189:ARG:H	2.15	0.45
1:B:274:ALA:CB	1:B:370:MET:HE3	2.47	0.45
1:B:483:TYR:CD2	1:B:485:VAL:HG23	2.52	0.45
2:E:88:TYR:HD2	2:E:89:GLN:CD	2.21	0.45
1:A:187:GLN:NE2	1:A:189:ARG:H	2.15	0.45
1:A:274:ALA:CB	1:A:370:MET:HE3	2.47	0.45
1:A:278:THR:HG23	1:A:279:ALA:N	2.31	0.45
1:A:310:LEU:HD23	1:A:310:LEU:O	2.17	0.45
1:A:446:GLY:C	1:A:454:VAL:HG12	2.38	0.45
1:B:310:LEU:O	1:B:310:LEU:HD23	2.17	0.45
1:B:457:SER:CB	1:B:465:LEU:HD23	2.47	0.45
2:C:206:LYS:HE2	2:C:207:HIS:NE2	2.31	0.45
1:A:73:TYR:CE2	2:C:41:PHE:CE2	3.05	0.45
2:C:83:ILE:O	2:C:84:TYR:HB3	2.17	0.45
2:E:226:ARG:O	2:E:226:ARG:HG3	2.16	0.45
1:A:298:VAL:HB	1:A:358:LEU:HD22	1.98	0.45
1:B:296:LEU:HD11	1:B:372:LEU:CD1	2.43	0.45
2:C:8:LEU:O	2:C:9:ASP:HB2	2.17	0.45
3:D:83:LEU:HB2	3:D:99:GLN:HE21	1.82	0.45
1:A:361:ASN:N	1:A:365:SER:CB	2.79	0.44
1:B:318:LEU:HD12	1:B:318:LEU:N	2.32	0.44
2:C:27:TYR:CD1	2:C:65:LEU:HD13	2.52	0.44
2:E:89:GLN:HB2	2:E:90:SER:H	0.96	0.44
1:A:303:VAL:C	1:A:309:GLU:HB3	2.37	0.44
1:B:412:VAL:CG2	1:B:504:VAL:CG1	2.68	0.44
2:C:37:LYS:CE	2:C:85:TRP:CE3	2.93	0.44
2:C:84:TYR:HD2	2:C:85:TRP:CD1	2.35	0.44
2:E:77:GLU:OE1	2:E:253:ASN:OD1	2.35	0.44
1:A:42:VAL:O	1:A:43:ASP:HB2	2.18	0.44
1:B:485:VAL:HG21	1:B:500:LEU:CD1	2.47	0.44
2:C:78:LYS:C	2:C:257:ARG:NH2	2.69	0.44
2:E:84:TYR:HD2	2:E:85:TRP:CD1	2.35	0.44
1:A:284:GLU:HG2	1:A:285:PHE:N	2.33	0.44
1:A:448:ASN:C	1:A:452:LEU:HD21	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:THR:HG22	1:B:473:LEU:CD2	2.46	0.44
2:C:84:TYR:HD2	2:C:85:TRP:HD1	1.64	0.44
1:B:433:PHE:CE2	1:B:495:GLN:OE1	2.70	0.44
2:C:82:ARG:CB	2:C:82:ARG:CZ	2.95	0.44
2:E:26:LYS:CG	2:E:63:LYS:HE2	2.43	0.44
2:E:71:LYS:O	2:E:254:TYR:CD2	2.71	0.44
2:E:37:LYS:HD2	2:E:90:SER:CB	2.48	0.44
1:A:457:SER:CB	1:A:465:LEU:HD23	2.47	0.44
1:B:278:THR:HG23	1:B:279:ALA:N	2.31	0.44
1:B:483:TYR:CD1	1:B:500:LEU:C	2.88	0.44
1:A:272:PHE:CD2	1:A:298:VAL:CG2	2.92	0.44
1:A:272:PHE:CE1	1:A:369:THR:CA	3.00	0.44
1:A:329:PHE:CD2	1:A:354:TYR:HE1	2.36	0.44
1:B:272:PHE:CE1	1:B:369:THR:CA	3.00	0.44
2:E:8:LEU:O	2:E:9:ASP:HB2	2.17	0.44
1:A:332:GLU:CB	1:A:335:PRO:HG2	2.47	0.44
1:B:178:GLU:OE1	1:B:230:ASP:C	2.46	0.44
1:B:284:GLU:HG2	1:B:285:PHE:N	2.33	0.44
1:B:448:ASN:O	1:B:452:LEU:HD21	2.18	0.44
2:C:30:LEU:HD13	2:C:57:MET:HA	2.00	0.44
1:A:178:GLU:OE1	1:A:230:ASP:CA	2.66	0.44
2:C:37:LYS:HD2	2:C:90:SER:CB	2.48	0.44
3:D:66:ARG:CG	3:D:66:ARG:NH1	2.65	0.44
2:E:82:ARG:CZ	2:E:82:ARG:CB	2.95	0.44
2:E:88:TYR:C	2:E:89:GLN:HG3	2.39	0.44
1:A:448:ASN:O	1:A:452:LEU:HD21	2.18	0.43
1:B:410:LEU:HD22	1:B:422:ILE:CD1	2.47	0.43
1:B:475:ARG:O	1:B:475:ARG:HG2	2.17	0.43
2:C:14:SER:O	2:C:18:LEU:HG	2.18	0.43
2:E:14:SER:O	2:E:18:LEU:HG	2.18	0.43
2:E:27:TYR:CD1	2:E:65:LEU:HD13	2.52	0.43
2:E:83:ILE:O	2:E:84:TYR:HB3	2.17	0.43
1:A:266:ASP:CG	1:A:360:ARG:CZ	2.84	0.43
1:A:357:VAL:CG2	1:A:369:THR:HG22	2.35	0.43
1:A:408:TYR:HD2	1:A:410:LEU:HG	1.57	0.43
1:A:410:LEU:HD22	1:A:422:ILE:CD1	2.47	0.43
1:A:418:ARG:HE	1:A:469:ASP:CB	2.28	0.43
2:E:74:MET:SD	2:E:255:ILE:HD11	2.59	0.43
1:A:433:PHE:HE2	1:A:495:GLN:OE1	2.02	0.43
1:A:485:VAL:HG21	1:A:500:LEU:CD1	2.47	0.43
1:B:418:ARG:HE	1:B:469:ASP:CB	2.28	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:VAL:O	1:B:43:ASP:HB2	2.18	0.43
2:C:89:GLN:HB2	2:C:90:SER:H	0.96	0.43
2:E:30:LEU:HD13	2:E:57:MET:HA	2.00	0.43
1:B:436:ILE:O	1:B:436:ILE:CG2	2.66	0.43
1:A:442:LEU:CD1	1:A:457:SER:CB	2.96	0.43
1:B:350:THR:CG2	1:B:351:VAL:N	2.82	0.43
2:C:88:TYR:C	2:C:89:GLN:HG3	2.39	0.43
2:E:30:LEU:HD21	2:E:87:MET:SD	2.58	0.43
1:B:304:VAL:CB	1:B:305:PRO:HD3	2.37	0.43
1:B:422:ILE:O	1:B:422:ILE:CG2	2.66	0.43
1:B:448:ASN:C	1:B:452:LEU:HD21	2.38	0.43
1:B:446:GLY:C	1:B:454:VAL:HG12	2.38	0.43
2:C:242:ASN:HA	2:C:314:ASP:O	2.19	0.43
1:A:350:THR:CG2	1:A:351:VAL:N	2.82	0.43
2:E:242:ASN:HA	2:E:314:ASP:O	2.18	0.43
1:A:375:LEU:HD13	1:A:376:VAL:O	2.19	0.43
1:B:271:THR:C	1:B:298:VAL:HG13	2.39	0.43
1:B:329:PHE:CD2	1:B:354:TYR:HE1	2.36	0.43
2:C:26:LYS:CG	2:C:63:LYS:HE2	2.43	0.43
2:E:69:ARG:HG2	2:E:80:CYS:HB3	1.95	0.43
1:A:304:VAL:HB	1:A:305:PRO:CD	2.38	0.43
1:A:319:LEU:HD11	1:A:352:HIS:HD2	1.84	0.43
3:F:66:ARG:NH1	3:F:108:ASP:OD2	2.52	0.43
1:A:137:CYS:N	2:C:43:LEU:HA	2.34	0.42
1:A:422:ILE:CG2	1:A:422:ILE:O	2.66	0.42
1:B:37:TRP:HA	1:B:146:TYR:O	2.19	0.42
1:B:312:ARG:HH21	1:B:336:ASN:CB	2.30	0.42
1:A:271:THR:C	1:A:298:VAL:HG13	2.39	0.42
1:A:296:LEU:HD11	1:A:372:LEU:CD1	2.44	0.42
1:A:300:ASP:HB3	1:A:309:GLU:O	2.19	0.42
1:A:298:VAL:CG2	1:A:314:TYR:CE2	2.95	0.42
1:B:319:LEU:HD11	1:B:352:HIS:HD2	1.84	0.42
1:B:457:SER:CB	1:B:465:LEU:CD2	2.94	0.42
2:C:10:CYS:SG	2:C:83:ILE:CG2	3.07	0.42
2:C:30:LEU:HD21	2:C:87:MET:SD	2.58	0.42
1:A:457:SER:HB2	1:A:465:LEU:HD23	1.99	0.42
2:C:65:LEU:HD23	2:C:65:LEU:HA	1.87	0.42
1:A:278:THR:CG2	1:A:279:ALA:N	2.82	0.42
2:C:14:SER:HA	2:C:65:LEU:HD21	2.01	0.42
2:E:84:TYR:HD2	2:E:85:TRP:HD1	1.64	0.42
1:A:272:PHE:CE2	1:A:298:VAL:CG2	3.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:ILE:CG2	1:A:436:ILE:O	2.66	0.42
1:B:457:SER:HB2	1:B:465:LEU:HD23	1.99	0.42
1:B:412:VAL:HG11	1:B:475:ARG:H	1.82	0.42
1:B:507:SER:O	1:B:508:TYR:CB	2.68	0.42
2:C:53:CYS:SG	2:C:57:MET:HE3	2.59	0.42
1:A:37:TRP:HA	1:A:146:TYR:O	2.19	0.42
1:A:331:VAL:O	1:A:331:VAL:HG23	2.19	0.42
1:A:428:GLU:CA	1:A:431:GLN:HG3	2.46	0.42
1:B:272:PHE:CE2	1:B:298:VAL:CG2	3.02	0.42
1:B:474:ARG:C	1:B:476:PRO:HD2	2.40	0.42
1:B:484:MET:HB3	1:B:497:GLN:HG2	2.01	0.42
1:A:334:TRP:CD1	1:A:335:PRO:CD	3.03	0.42
1:A:507:SER:O	1:A:508:TYR:CB	2.68	0.42
1:B:278:THR:CG2	1:B:279:ALA:N	2.82	0.42
1:B:317:THR:HB	1:B:318:LEU:HD12	2.00	0.42
1:B:292:VAL:HG13	1:B:339:SER:OG	2.20	0.42
1:B:442:LEU:HD21	1:B:485:VAL:CG2	2.34	0.42
2:E:10:CYS:SG	2:E:83:ILE:CG2	3.07	0.42
2:E:58:GLU:OE1	2:E:58:GLU:HA	2.20	0.42
2:E:66:TYR:CG	2:E:66:TYR:O	2.71	0.42
1:A:416:ALA:O	1:A:417:ARG:C	2.52	0.42
1:B:187:GLN:HE22	1:B:189:ARG:HB3	1.85	0.42
1:A:442:LEU:CD1	1:A:465:LEU:HD22	2.27	0.42
1:B:372:LEU:HD23	1:B:372:LEU:H	1.85	0.42
1:B:485:VAL:CG2	1:B:500:LEU:HD12	2.50	0.42
1:A:317:THR:HB	1:A:318:LEU:HD12	2.00	0.42
1:A:347:VAL:CG2	1:A:348:ARG:N	2.82	0.42
1:A:296:LEU:CD1	1:A:372:LEU:HD13	2.45	0.42
1:A:457:SER:OG	1:A:465:LEU:HD23	2.20	0.42
1:A:470:THR:CB	1:A:473:LEU:CD2	2.98	0.42
1:B:300:ASP:HB3	1:B:309:GLU:O	2.19	0.42
1:B:375:LEU:HD13	1:B:376:VAL:O	2.19	0.42
1:B:470:THR:CB	1:B:473:LEU:CD2	2.98	0.42
1:B:470:THR:HB	1:B:473:LEU:CD2	2.50	0.42
1:B:56:LEU:HD23	1:B:56:LEU:HA	1.96	0.42
1:A:484:MET:HB3	1:A:497:GLN:HG2	2.01	0.41
1:A:485:VAL:CG2	1:A:500:LEU:HD12	2.50	0.41
1:B:285:PHE:CD2	1:B:285:PHE:O	2.73	0.41
1:B:329:PHE:HB3	1:B:340:VAL:HG22	2.02	0.41
1:B:334:TRP:CD1	1:B:335:PRO:CD	3.03	0.41
1:B:433:PHE:HE2	1:B:495:GLN:OE1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:PRO:HG2	1:A:353:ASP:HB3	2.02	0.41
1:A:474:ARG:C	1:A:476:PRO:HD2	2.40	0.41
2:C:78:LYS:HD2	2:C:257:ARG:CD	2.37	0.41
2:E:71:LYS:HD3	2:E:255:ILE:HA	1.36	0.41
1:A:312:ARG:HB2	1:A:358:LEU:CG	2.51	0.41
1:A:433:PHE:CE2	1:A:495:GLN:HG3	2.54	0.41
1:B:178:GLU:OE1	1:B:230:ASP:CA	2.66	0.41
1:B:272:PHE:CE2	1:B:298:VAL:HG21	2.55	0.41
2:C:58:GLU:OE1	2:C:58:GLU:HA	2.20	0.41
1:A:272:PHE:CE2	1:A:298:VAL:HG21	2.55	0.41
1:B:296:LEU:CD1	1:B:296:LEU:N	2.82	0.41
1:B:320:PRO:HG2	1:B:353:ASP:HB3	2.02	0.41
1:B:312:ARG:HB2	1:B:358:LEU:CG	2.51	0.41
1:B:342:ALA:CB	1:B:346:PHE:CZ	3.04	0.41
1:B:266:ASP:OD2	1:B:365:SER:HA	2.21	0.41
2:C:88:TYR:CD2	2:C:89:GLN:CD	2.94	0.41
3:D:66:ARG:NH1	3:D:108:ASP:OD2	2.51	0.41
1:A:292:VAL:HG13	1:A:339:SER:OG	2.20	0.41
1:A:470:THR:HB	1:A:473:LEU:CD2	2.50	0.41
2:C:270:GLU:HB2	2:C:276:ASN:O	2.21	0.41
3:D:91:ARG:NH1	3:D:91:ARG:CG	2.83	0.41
2:E:14:SER:HA	2:E:65:LEU:HD21	2.02	0.41
1:A:272:PHE:CE1	1:A:369:THR:HA	2.56	0.41
1:B:317:THR:CG2	1:B:318:LEU:CD1	2.95	0.41
2:C:331:PHE:O	2:C:335:ASN:HB2	2.21	0.41
1:A:144:ARG:HH11	1:A:144:ARG:HD2	1.68	0.41
1:A:413:SER:O	1:A:415:ARG:HG2	2.21	0.41
1:A:438:VAL:CG1	1:A:487:ALA:HB1	2.51	0.41
2:C:66:TYR:O	2:C:66:TYR:CG	2.71	0.41
2:C:83:ILE:CG2	2:C:84:TYR:N	2.83	0.41
2:E:331:PHE:O	2:E:335:ASN:HB2	2.21	0.41
1:A:139:TRP:CG	1:A:140:PRO:HA	2.56	0.41
1:A:372:LEU:HD23	1:A:372:LEU:H	1.85	0.41
1:B:331:VAL:O	1:B:331:VAL:HG23	2.19	0.41
1:B:465:LEU:CD1	1:B:500:LEU:HD13	2.51	0.41
2:E:270:GLU:HB2	2:E:276:ASN:O	2.21	0.41
2:E:37:LYS:CE	2:E:85:TRP:CE3	2.93	0.41
1:A:266:ASP:OD2	1:A:365:SER:HA	2.21	0.41
1:B:428:GLU:CA	1:B:431:GLN:HG3	2.46	0.41
1:B:443:HIS:NE2	1:B:484:MET:HB2	2.36	0.41
1:B:283:VAL:HG11	1:B:494:ARG:HH22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:43:LEU:O	2:E:45:SER:N	2.54	0.41
1:A:187:GLN:HE22	1:A:189:ARG:HB3	1.85	0.40
1:A:285:PHE:O	1:A:285:PHE:CD2	2.73	0.40
1:A:297:ARG:HB2	1:A:297:ARG:NH1	2.37	0.40
1:A:342:ALA:CB	1:A:346:PHE:CZ	3.04	0.40
1:B:329:PHE:HD2	1:B:354:TYR:HE1	1.68	0.40
1:B:413:SER:O	1:B:415:ARG:HG2	2.21	0.40
1:B:457:SER:OG	1:B:465:LEU:HD23	2.20	0.40
2:C:88:TYR:O	2:C:89:GLN:CB	2.69	0.40
2:E:7:ARG:HB2	2:E:72:ARG:HD3	2.03	0.40
2:E:88:TYR:CD2	2:E:89:GLN:CD	2.94	0.40
1:A:299:PHE:CZ	1:A:309:GLU:OE2	2.75	0.40
1:B:314:TYR:HE1	1:B:336:ASN:OD1	2.04	0.40
2:C:212:LEU:HD23	2:C:213:PHE:CZ	2.56	0.40
1:A:314:TYR:HE1	1:A:336:ASN:OD1	2.04	0.40
1:A:442:LEU:HD23	1:A:485:VAL:CG2	2.34	0.40
2:C:34:VAL:HG12	2:C:36:GLY:N	2.35	0.40
1:A:443:HIS:NE2	1:A:484:MET:HB2	2.36	0.40
1:B:438:VAL:CG1	1:B:487:ALA:HB1	2.51	0.40
2:C:43:LEU:O	2:C:45:SER:N	2.54	0.40
2:E:83:ILE:CG2	2:E:84:TYR:N	2.83	0.40
2:E:81:LEU:CD2	2:E:85:TRP:CE2	2.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	440/607 (72%)	385 (88%)	33 (8%)	22 (5%)	2	27
1	B	440/607 (72%)	385 (88%)	33 (8%)	22 (5%)	2	27
2	C	280/463 (60%)	260 (93%)	15 (5%)	5 (2%)	10	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles		
2	E	280/463 (60%)	260 (93%)	15 (5%)	5 (2%)	10	49	
3	D	91/134 (68%)	84 (92%)	6 (7%)	1 (1%)	17	60	
3	F	91/134 (68%)	84 (92%)	6 (7%)	1 (1%)	17	60	
All	All	1622/2408 (67%)	1458 (90%)	108 (7%)	56 (4%)	7	34	

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	349	ALA
1	A	351	VAL
1	A	414	ARG
1	A	416	ALA
1	A	417	ARG
1	A	418	ARG
1	A	444	SER
1	A	445	SER
1	A	450	SER
1	A	451	THR
1	A	458	ALA
1	A	461	THR
1	A	473	LEU
1	A	477	LYS
1	A	489	ASP
1	B	349	ALA
1	B	351	VAL
1	B	414	ARG
1	B	416	ALA
1	B	417	ARG
1	B	418	ARG
1	B	444	SER
1	B	445	SER
1	B	450	SER
1	B	451	THR
1	B	458	ALA
1	B	461	THR
1	B	473	LEU
1	B	477	LYS
1	B	489	ASP
2	C	9	ASP
2	C	44	THR
2	C	66	TYR

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Mol	Chain	Res	Type
2	C	89	GLN
2	E	9	ASP
2	E	44	THR
2	E	66	TYR
2	E	89	GLN
1	A	363	SER
1	A	421	GLN
1	B	363	SER
1	B	421	GLN
3	D	93	VAL
3	F	93	VAL
1	A	359	ASN
1	B	359	ASN
1	A	270	PRO
1	A	352	HIS
1	A	491	GLN
1	B	270	PRO
1	B	352	HIS
1	B	491	GLN
1	A	452	LEU
1	B	452	LEU
2	C	269	PRO
2	E	269	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 PDB entries followed by that with respect to all EM entries.

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	390/528 (74%)	372 (95%)	18 (5%)	31	62
1	B	390/528 (74%)	372 (95%)	18 (5%)	31	62
2	C	247/408 (60%)	236 (96%)	11 (4%)	32	63
2	E	247/408 (60%)	236 (96%)	11 (4%)	32	63
3	D	78/113 (69%)	74 (95%)	4 (5%)	28	60
3	F	78/113 (69%)	74 (95%)	4 (5%)	28	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1430/2098 (68%)	1364 (95%)	66 (5%)	36 62

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLU
1	A	89	GLN
1	A	90	GLU
1	A	101	LEU
1	A	112	ARG
1	A	127	LEU
1	A	171	ARG
1	A	180	ARG
1	A	199	GLN
1	A	205	ARG
1	A	216	SER
1	A	238	GLU
1	A	267	ASP
1	A	417	ARG
1	A	445	SER
1	A	473	LEU
1	A	477	LYS
1	A	494	ARG
1	B	38	GLU
1	B	89	GLN
1	B	90	GLU
1	B	101	LEU
1	B	112	ARG
1	B	127	LEU
1	B	171	ARG
1	B	180	ARG
1	B	199	GLN
1	B	205	ARG
1	B	216	SER
1	B	238	GLU
1	B	267	ASP
1	B	417	ARG
1	B	445	SER
1	B	473	LEU
1	B	477	LYS
1	B	494	ARG
2	C	66	TYR

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Mol	Chain	Res	Type
2	C	89	GLN
2	C	155	LEU
2	C	174	TYR
2	C	214	CYS
2	C	219	ILE
2	C	226	ARG
2	C	248	ASP
2	C	273	SER
2	C	277	CYS
2	C	307	LEU
3	D	66	ARG
3	D	72	CYS
3	D	91	ARG
3	D	97	VAL
2	E	66	TYR
2	E	89	GLN
2	E	155	LEU
2	E	174	TYR
2	E	214	CYS
2	E	219	ILE
2	E	226	ARG
2	E	248	ASP
2	E	273	SER
2	E	277	CYS
2	E	307	LEU
3	F	66	ARG
3	F	72	CYS
3	F	91	ARG
3	F	97	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	HIS
1	A	187	GLN
1	A	199	GLN
1	A	352	HIS
1	A	359	ASN
1	A	361	ASN
1	A	371	GLN
1	A	437	ASN
1	A	468	ASN

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Mol	Chain	Res	Type
1	A	482	HIS
1	A	490	GLN
1	A	495	GLN
1	A	497	GLN
1	B	81	HIS
1	B	187	GLN
1	B	199	GLN
1	B	352	HIS
1	B	359	ASN
1	B	361	ASN
1	B	437	ASN
1	B	468	ASN
1	B	482	HIS
1	B	490	GLN
1	B	495	GLN
1	B	497	GLN
2	C	89	GLN
2	C	281	ASN
2	C	340	ASN
2	E	89	GLN
2	E	281	ASN
2	E	340	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.

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
5	NAG	D	1135	3,5	14,14,15	0.53	0	15,19,21	1.18	1 (6%)
5	NAG	D	1136	5	14,14,15	0.76	1 (7%)	15,19,21	1.34	2 (13%)
5	NAG	F	1135	3,5	14,14,15	0.55	0	15,19,21	1.19	1 (6%)
5	NAG	F	1136	5	14,14,15	0.75	1 (7%)	15,19,21	1.34	2 (13%)

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
5	NAG	D	1135	3,5	-	0/6/23/26	0/1/1/1
5	NAG	D	1136	5	-	0/6/23/26	0/1/1/1
5	NAG	F	1135	3,5	-	0/6/23/26	0/1/1/1
5	NAG	F	1136	5	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	1136	NAG	C1-C2	2.06	1.55	1.52
5	D	1136	NAG	C1-C2	2.09	1.55	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	1136	NAG	O5-C1-C2	2.27	114.64	111.47
5	D	1136	NAG	O5-C1-C2	2.36	114.76	111.47
5	D	1135	NAG	C1-O5-C5	3.30	116.71	112.17
5	F	1135	NAG	C1-O5-C5	3.37	116.81	112.17
5	D	1136	NAG	C4-C3-C2	3.40	116.00	111.02
5	F	1136	NAG	C4-C3-C2	3.42	116.03	111.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	269:ALA	C	270:PRO	N	1.64
1	B	269:ALA	C	270:PRO	N	1.64