



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 03:10 AM UTC

PDB ID : 4UX8 / pdb_00004ux8
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 : 2014-08-19
Resolution : 24.00 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

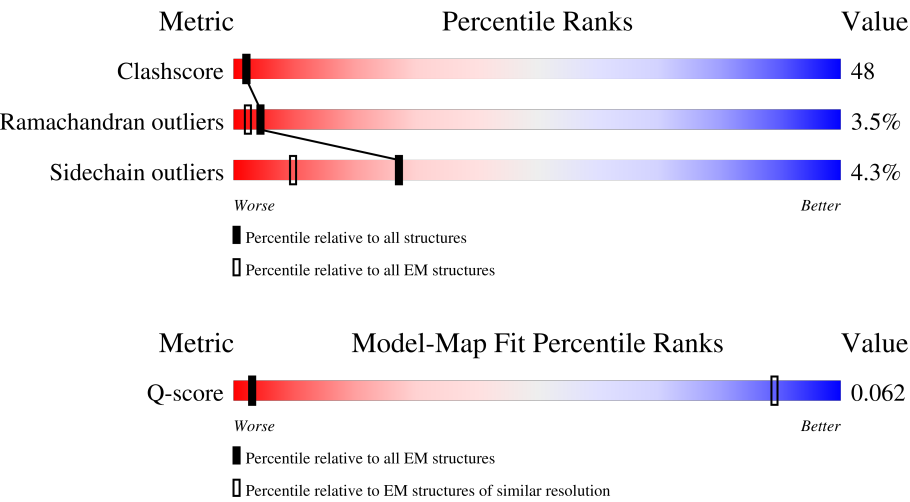
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 i

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	9 (23.50 - 24.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	607	
1	B	607	
2	C	463	
2	E	463	

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Mol	Chain	Length	Quality of chain
3	D	134	57%8%31%
3	F	134	57%8%31%
4	G	2	50%100%
4	H	2	50%100%

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 an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



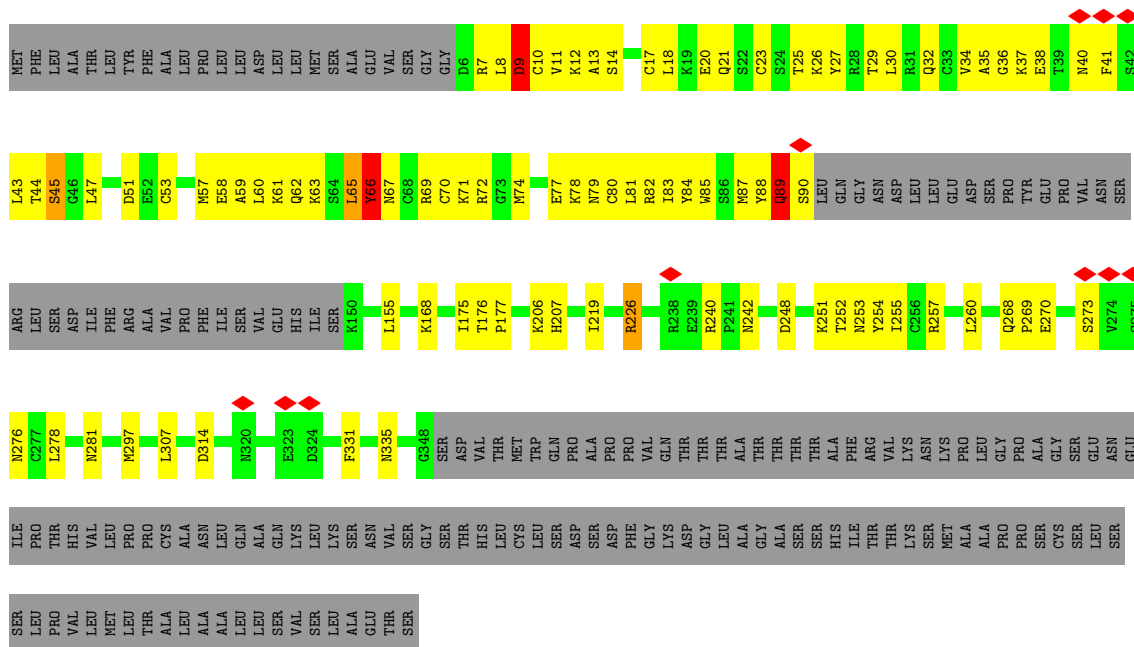
Mol	Chain	Residues	Atoms				AltConf	Trace
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	H	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

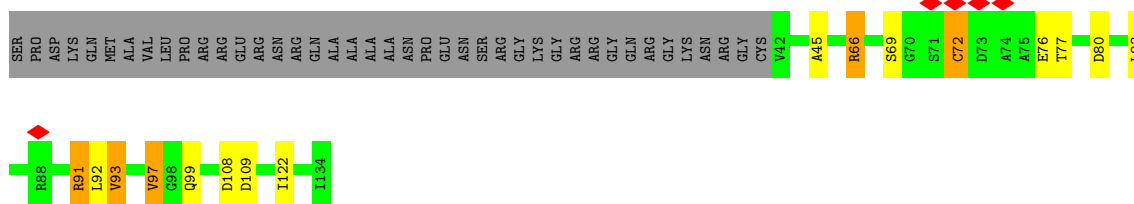
Mol	Chain	Residues	Atoms		AltConf
5	A	3	Total	Ca	0
			3	3	
5	B	3	Total	Ca	0
			3	3	



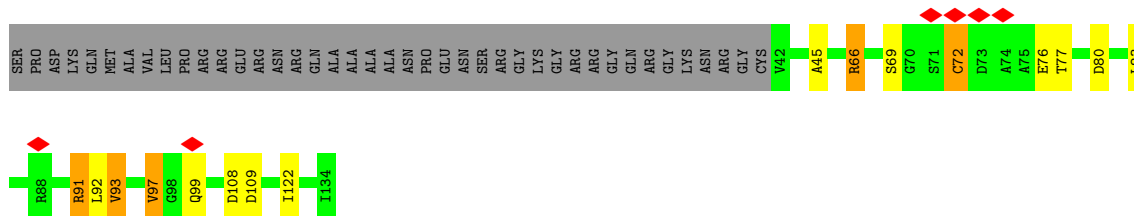
- Molecule 2: GDNF FAMILY RECEPTOR ALPHA-1



- Molecule 3: GLIAL CELL LINE-DERIVED NEUROTROPHIC FACTOR



- Molecule 3: GLIAL CELL LINE-DERIVED NEUROTROPHIC FACTOR



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	8519	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
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	
Magnification	80000	Depositor
Image detector	TVIPS TEMCAM-F415 (4k x 4k)	Depositor
Maximum map value	26.869	Depositor
Minimum map value	-19.560	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.42	Depositor
Map size ($\text{\AA}$)	416.64, 416.64, 416.64	wwPDB
Map dimensions	96, 96, 96	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	4.34, 4.34, 4.34	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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.16	93/3655 (2.5%)	2.37	204/4977 (4.1%)
1	B	2.16	92/3655 (2.5%)	2.37	203/4977 (4.1%)
2	C	0.84	0/2236	1.19	14/3005 (0.5%)
2	E	0.84	0/2236	1.19	14/3005 (0.5%)
3	D	0.45	0/730	0.77	0/985
3	F	0.45	0/730	0.77	0/985
All	All	1.68	185/13242 (1.4%)	1.91	435/17934 (2.4%)

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 (185) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	451	THR	CA-C	29.27	1.92	1.52
1	A	451	THR	CA-C	29.21	1.92	1.52
1	A	410	LEU	N-CA	24.89	1.76	1.45
1	B	410	LEU	N-CA	24.85	1.76	1.45
1	B	452	LEU	N-CA	-18.95	1.21	1.46
1	A	452	LEU	N-CA	-18.85	1.21	1.46
1	B	456	THR	N-CA	16.48	1.66	1.46
1	A	456	THR	N-CA	16.43	1.66	1.46
1	A	474	ARG	CA-C	-16.09	1.31	1.52
1	B	474	ARG	CA-C	-16.08	1.31	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	405	PRO	N-CD	15.89	1.70	1.47
1	A	405	PRO	N-CD	15.88	1.70	1.47
1	B	483	TYR	CA-C	15.72	1.71	1.52
1	A	483	TYR	CA-C	15.71	1.71	1.52
1	A	415	ARG	N-CA	15.21	1.65	1.45
1	B	415	ARG	N-CA	15.20	1.65	1.45
1	A	477	LYS	CA-C	14.43	1.72	1.52
1	B	477	LYS	CA-C	14.43	1.72	1.52
1	A	488	THR	N-CA	13.98	1.63	1.46
1	B	488	THR	N-CA	13.91	1.63	1.46
1	A	269	ALA	C-N	13.21	1.64	1.33
1	B	269	ALA	C-N	13.21	1.64	1.33
1	A	458	ALA	CA-C	-13.02	1.35	1.52
1	B	458	ALA	CA-C	-13.02	1.35	1.52
1	A	490	GLN	N-CA	12.37	1.63	1.47
1	B	490	GLN	N-CA	12.35	1.63	1.47
1	A	489	ASP	CA-C	12.31	1.69	1.52
1	B	489	ASP	CA-C	12.26	1.69	1.52
1	A	487	ALA	CA-C	-11.91	1.38	1.52
1	B	487	ALA	CA-C	-11.91	1.38	1.52
1	A	455	VAL	CA-C	-11.89	1.38	1.52
1	B	455	VAL	CA-C	-11.89	1.38	1.52
1	A	263	TYR	C-N	11.35	1.49	1.33
1	B	263	TYR	C-N	11.30	1.49	1.33
1	A	423	GLY	CA-C	11.20	1.63	1.51
1	B	423	GLY	CA-C	11.15	1.63	1.51
1	B	466	PHE	N-CA	-10.32	1.32	1.45
1	A	466	PHE	N-CA	-10.29	1.32	1.45
1	A	473	LEU	CA-C	10.21	1.66	1.52
1	B	473	LEU	CA-C	10.21	1.66	1.52
1	A	409	SER	CA-C	-9.83	1.40	1.52
1	B	409	SER	CA-C	-9.83	1.40	1.52
1	B	488	THR	CA-C	-9.81	1.41	1.52
1	A	488	THR	CA-C	-9.77	1.41	1.52
1	A	416	ALA	N-CA	9.71	1.58	1.46
1	B	416	ALA	N-CA	9.66	1.58	1.46
1	A	476	PRO	N-CD	9.52	1.61	1.47
1	B	476	PRO	N-CD	9.52	1.61	1.47
1	B	460	ASP	CA-C	-9.18	1.40	1.52
1	A	460	ASP	CA-C	-9.16	1.40	1.52
1	A	256	VAL	N-CA	8.47	1.54	1.46
1	B	256	VAL	N-CA	8.47	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	508	TYR	CA-C	8.24	1.70	1.52
1	A	431	GLN	N-CA	8.23	1.56	1.46
1	B	431	GLN	N-CA	8.23	1.56	1.46
1	A	508	TYR	CA-C	8.19	1.70	1.52
1	B	453	GLY	N-CA	8.00	1.56	1.45
1	A	453	GLY	N-CA	7.94	1.56	1.45
1	B	444	SER	N-CA	7.89	1.56	1.46
1	B	207	LEU	C-O	7.89	1.33	1.23
1	A	444	SER	N-CA	7.85	1.56	1.46
1	A	207	LEU	C-O	7.84	1.33	1.23
1	B	501	LEU	CA-C	-7.80	1.43	1.52
1	A	501	LEU	CA-C	-7.79	1.43	1.52
1	B	403	HIS	CA-C	7.70	1.61	1.52
1	A	403	HIS	CA-C	7.68	1.61	1.52
1	B	444	SER	CA-C	7.64	1.63	1.52
1	A	444	SER	CA-C	7.59	1.62	1.52
1	A	503	THR	CA-C	7.43	1.61	1.52
1	B	503	THR	CA-C	7.43	1.61	1.52
1	A	464	ILE	N-CA	7.40	1.55	1.46
1	A	475	ARG	N-CA	7.35	1.56	1.46
1	B	475	ARG	N-CA	7.33	1.56	1.46
1	B	464	ILE	N-CA	7.33	1.55	1.46
1	A	446	GLY	N-CA	7.27	1.55	1.45
1	B	446	GLY	N-CA	7.25	1.55	1.45
1	B	445	SER	CA-C	7.24	1.62	1.52
1	A	445	SER	CA-C	7.20	1.62	1.52
1	A	167	PHE	N-CA	7.18	1.52	1.45
1	B	167	PHE	N-CA	7.14	1.52	1.45
1	A	499	GLN	CA-C	7.11	1.61	1.52
1	B	499	GLN	CA-C	7.11	1.61	1.52
1	A	508	TYR	N-CA	7.09	1.59	1.46
1	B	508	TYR	N-CA	7.08	1.59	1.46
1	A	484	MET	N-CA	-7.03	1.37	1.46
1	B	441	LYS	CA-C	7.03	1.61	1.52
1	B	484	MET	N-CA	-7.02	1.37	1.46
1	A	408	TYR	CA-C	6.98	1.61	1.52
1	B	408	TYR	CA-C	6.98	1.61	1.52
1	A	441	LYS	CA-C	6.95	1.61	1.52
1	B	463	GLY	N-CA	6.69	1.55	1.45
1	B	489	ASP	N-CA	6.69	1.54	1.46
1	A	489	ASP	N-CA	6.66	1.54	1.46
1	A	476	PRO	N-CA	-6.64	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	476	PRO	N-CA	-6.64	1.38	1.47
1	A	463	GLY	N-CA	6.63	1.54	1.45
1	A	447	ALA	N-CA	6.58	1.54	1.46
1	B	447	ALA	N-CA	6.50	1.54	1.46
1	B	66	PHE	N-CA	6.44	1.54	1.46
1	A	436	ILE	N-CA	-6.39	1.40	1.46
1	B	436	ILE	N-CA	-6.39	1.40	1.46
1	A	66	PHE	N-CA	6.39	1.54	1.46
1	A	486	VAL	CA-C	6.36	1.60	1.52
1	B	433	PHE	N-CA	6.27	1.54	1.46
1	A	433	PHE	N-CA	6.25	1.54	1.46
1	B	486	VAL	CA-C	6.24	1.60	1.52
1	A	481	LEU	N-CA	6.14	1.53	1.46
1	B	481	LEU	N-CA	6.12	1.53	1.46
1	B	465	LEU	CA-C	6.00	1.60	1.52
1	B	112	ARG	CD-NE	-5.97	1.37	1.46
1	A	112	ARG	CD-NE	-5.94	1.38	1.46
1	B	126	PHE	N-CA	5.92	1.52	1.45
1	A	465	LEU	CA-C	5.92	1.59	1.52
1	A	473	LEU	N-CA	-5.89	1.38	1.46
1	B	473	LEU	N-CA	-5.86	1.38	1.46
1	A	126	PHE	N-CA	5.81	1.52	1.45
1	A	72	LEU	C-O	5.81	1.30	1.23
1	B	72	LEU	C-O	5.81	1.30	1.23
1	A	487	ALA	N-CA	-5.78	1.39	1.46
1	A	86	ILE	CA-CB	5.77	1.61	1.54
1	B	86	ILE	CA-CB	5.74	1.61	1.54
1	B	487	ALA	N-CA	-5.74	1.39	1.46
1	B	226	ARG	CA-CB	-5.73	1.45	1.54
1	A	226	ARG	CA-CB	-5.72	1.46	1.54
1	B	411	SER	CA-C	5.69	1.59	1.52
1	B	478	CYS	CA-C	-5.64	1.45	1.52
1	A	430	CYS	N-CA	5.62	1.53	1.46
1	B	430	CYS	N-CA	5.62	1.53	1.46
1	A	309	GLU	CA-C	-5.61	1.45	1.52
1	B	309	GLU	CA-C	-5.61	1.46	1.52
1	A	478	CYS	CA-C	-5.59	1.45	1.52
1	A	411	SER	CA-C	5.59	1.59	1.52
1	A	502	VAL	N-CA	5.58	1.53	1.46
1	B	502	VAL	N-CA	5.55	1.53	1.46
1	A	241	ALA	CA-CB	5.54	1.61	1.53
1	A	259	PRO	N-CA	5.54	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	259	PRO	N-CA	5.53	1.53	1.47
1	B	241	ALA	CA-CB	5.53	1.61	1.53
1	B	454	VAL	CA-C	-5.52	1.45	1.52
1	A	404	LEU	CA-C	-5.50	1.46	1.53
1	B	506	GLY	CA-C	5.50	1.61	1.52
1	A	122	TYR	N-CA	5.48	1.53	1.45
1	B	122	TYR	N-CA	5.48	1.53	1.45
1	B	205	ARG	CZ-NH1	5.47	1.40	1.32
1	A	506	GLY	CA-C	5.46	1.61	1.52
1	A	454	VAL	CA-C	-5.45	1.45	1.52
1	A	498	ALA	CA-C	-5.45	1.45	1.53
1	B	498	ALA	CA-C	-5.45	1.45	1.53
1	B	404	LEU	CA-C	-5.44	1.46	1.53
1	A	205	ARG	CZ-NH1	5.44	1.40	1.32
1	A	214	PHE	CA-CB	5.43	1.63	1.53
1	A	449	CYS	CA-C	5.42	1.58	1.52
1	B	214	PHE	CA-CB	5.40	1.62	1.53
1	B	184	THR	N-CA	5.38	1.52	1.46
1	A	184	THR	N-CA	5.35	1.52	1.46
1	B	449	CYS	CA-C	5.35	1.58	1.52
1	A	32	SER	CA-C	5.34	1.60	1.52
1	A	220	SER	C-O	5.34	1.30	1.23
1	B	500	LEU	N-CA	-5.33	1.39	1.46
1	A	111	VAL	CA-CB	5.32	1.62	1.54
1	B	32	SER	CA-C	5.32	1.59	1.52
1	A	500	LEU	N-CA	-5.31	1.39	1.46
1	B	111	VAL	CA-CB	5.28	1.62	1.54
1	A	217	ALA	CA-CB	5.27	1.60	1.53
1	A	183	GLY	CA-C	5.26	1.57	1.51
1	B	220	SER	C-O	5.24	1.30	1.23
1	A	165	LEU	CA-C	5.21	1.59	1.52
1	B	148	SER	N-CA	5.19	1.52	1.46
1	B	183	GLY	CA-C	5.19	1.57	1.51
1	B	217	ALA	CA-CB	5.18	1.60	1.53
1	A	485	VAL	CA-C	-5.17	1.46	1.52
1	B	485	VAL	CA-C	-5.17	1.46	1.52
1	B	450	SER	N-CA	5.17	1.52	1.46
1	B	165	LEU	CA-C	5.16	1.59	1.52
1	A	148	SER	N-CA	5.14	1.52	1.46
1	A	450	SER	N-CA	5.14	1.52	1.46
1	B	235	GLU	CA-C	5.14	1.59	1.52
1	B	462	SER	N-CA	-5.10	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	GLU	CA-C	5.09	1.59	1.52
1	A	251	GLU	CB-CG	-5.03	1.37	1.52
1	A	187	GLN	CB-CG	-5.03	1.37	1.52
1	B	468	ASN	N-CA	5.02	1.52	1.45
1	B	251	GLU	CB-CG	-5.01	1.37	1.52
1	A	205	ARG	CG-CD	5.00	1.67	1.52
1	A	462	SER	N-CA	-5.00	1.40	1.46

All (435) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	TYR	O-C-N	-38.05	78.17	122.68
1	B	263	TYR	O-C-N	-37.99	78.23	122.68
1	A	450	SER	CB-CA-C	-21.65	67.33	110.42
1	B	450	SER	CB-CA-C	-21.64	67.36	110.42
1	A	447	ALA	CB-CA-C	-20.93	76.65	110.14
1	B	447	ALA	CB-CA-C	-20.93	76.66	110.14
1	B	422	ILE	N-CA-C	19.16	131.89	111.58
1	A	422	ILE	N-CA-C	19.16	131.89	111.58
1	B	405	PRO	CB-CA-C	-18.21	87.97	111.46
1	A	405	PRO	CB-CA-C	-18.21	87.97	111.46
1	B	488	THR	CB-CA-C	-16.35	84.96	110.14
1	A	488	THR	CB-CA-C	-16.33	85.00	110.14
1	B	477	LYS	N-CA-CB	14.90	135.67	110.49
1	A	477	LYS	N-CA-CB	14.89	135.66	110.49
1	A	112	ARG	NE-CZ-NH1	-14.80	106.70	121.50
1	A	434	SER	N-CA-CB	14.78	135.09	111.74
1	B	434	SER	N-CA-CB	14.78	135.09	111.74
1	B	112	ARG	NE-CZ-NH1	-14.72	106.78	121.50
1	B	404	LEU	CA-C-N	14.61	134.80	119.76
1	B	404	LEU	C-N-CA	14.61	134.80	119.76
1	A	404	LEU	CA-C-N	14.56	134.75	119.76
1	A	404	LEU	C-N-CA	14.56	134.75	119.76
1	A	474	ARG	CA-C-O	-14.40	105.42	120.98
1	B	474	ARG	CA-C-O	-14.40	105.42	120.98
1	B	451	THR	N-CA-C	-14.27	80.41	110.80
1	A	451	THR	N-CA-C	-14.25	80.45	110.80
1	B	409	SER	CA-C-O	-13.48	106.48	121.58
1	A	409	SER	CA-C-O	-13.42	106.55	121.58
1	B	461	THR	CB-CA-C	-13.32	83.91	110.42
1	A	461	THR	CB-CA-C	-13.30	83.95	110.42
1	A	424	LYS	CB-CA-C	-13.11	93.73	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	424	LYS	CB-CA-C	-13.08	93.77	111.82
1	B	489	ASP	CA-C-O	13.03	139.13	120.51
1	A	489	ASP	CA-C-O	13.02	139.13	120.51
1	A	409	SER	CA-C-N	-12.96	101.03	122.81
1	A	409	SER	C-N-CA	-12.96	101.03	122.81
1	B	409	SER	CA-C-N	-12.95	101.06	122.81
1	B	409	SER	C-N-CA	-12.95	101.06	122.81
1	B	435	GLY	CA-C-O	-12.86	98.19	120.57
1	A	435	GLY	CA-C-O	-12.85	98.21	120.57
1	A	414	ARG	CA-C-N	-12.65	100.39	123.03
1	A	414	ARG	C-N-CA	-12.65	100.39	123.03
1	B	414	ARG	CA-C-N	-12.62	100.44	123.03
1	B	414	ARG	C-N-CA	-12.62	100.44	123.03
1	B	462	SER	CB-CA-C	-12.40	89.31	110.64
1	A	462	SER	CB-CA-C	-12.40	89.31	110.64
1	B	508	TYR	N-CA-CB	12.21	131.25	110.50
1	A	508	TYR	N-CA-CB	12.17	131.19	110.50
1	A	490	GLN	N-CA-C	-12.12	87.32	107.32
1	B	490	GLN	N-CA-C	-12.10	87.36	107.32
1	B	476	PRO	CB-CA-C	-11.88	91.95	111.56
1	A	476	PRO	CB-CA-C	-11.87	91.98	111.56
1	A	112	ARG	NE-CZ-NH2	11.74	129.77	119.20
1	B	490	GLN	CB-CA-C	-11.72	96.34	111.70
1	A	490	GLN	CB-CA-C	-11.70	96.38	111.70
1	B	112	ARG	NE-CZ-NH2	11.65	129.69	119.20
1	A	477	LYS	CA-C-N	-11.38	107.12	123.05
1	A	477	LYS	C-N-CA	-11.38	107.12	123.05
1	B	477	LYS	CA-C-N	-11.34	107.17	123.05
1	B	477	LYS	C-N-CA	-11.34	107.17	123.05
1	B	476	PRO	N-CA-C	-11.06	89.69	112.47
1	A	476	PRO	N-CA-C	-11.05	89.71	112.47
1	B	309	GLU	CB-CA-C	-10.82	94.17	110.95
1	A	309	GLU	CB-CA-C	-10.81	94.19	110.95
1	A	451	THR	CA-C-N	10.76	142.08	121.54
1	A	451	THR	C-N-CA	10.76	142.08	121.54
1	B	451	THR	CA-C-N	10.74	142.05	121.54
1	B	451	THR	C-N-CA	10.74	142.05	121.54
1	A	458	ALA	N-CA-CB	10.46	128.17	110.49
1	B	458	ALA	N-CA-CB	10.44	128.14	110.49
1	B	457	SER	N-CA-C	10.35	125.65	112.92
1	A	457	SER	N-CA-C	10.35	125.64	112.92
1	A	491	GLN	N-CA-CB	10.22	127.76	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	491	GLN	N-CA-CB	10.21	127.74	110.49
1	A	263	TYR	CA-C-N	10.19	139.93	122.81
1	A	263	TYR	C-N-CA	10.19	139.93	122.81
1	B	263	TYR	CA-C-N	10.18	139.90	122.81
1	B	263	TYR	C-N-CA	10.18	139.90	122.81
1	A	503	THR	CA-C-O	10.04	131.35	120.71
1	B	503	THR	CA-C-O	10.04	131.35	120.71
1	A	403	HIS	CB-CA-C	9.96	128.95	109.33
1	B	403	HIS	CB-CA-C	9.94	128.92	109.33
1	A	479	ALA	CB-CA-C	-9.86	94.67	110.94
1	B	479	ALA	CB-CA-C	-9.86	94.68	110.94
1	A	337	GLU	N-CA-C	-9.79	100.68	111.36
1	B	337	GLU	N-CA-C	-9.78	100.70	111.36
2	C	65	LEU	CA-C-N	9.70	140.06	121.54
2	C	65	LEU	C-N-CA	9.70	140.06	121.54
1	A	470	THR	N-CA-CB	-9.69	94.12	110.49
1	B	470	THR	N-CA-CB	-9.68	94.13	110.49
2	E	65	LEU	CA-C-N	9.67	140.01	121.54
2	E	65	LEU	C-N-CA	9.67	140.01	121.54
1	A	466	PHE	N-CA-C	9.62	124.70	109.50
1	B	477	LYS	N-CA-C	-9.60	90.35	110.80
1	A	477	LYS	N-CA-C	-9.60	90.35	110.80
1	B	466	PHE	N-CA-C	9.58	124.64	109.50
1	B	112	ARG	CD-NE-CZ	9.57	137.80	124.40
1	A	112	ARG	CD-NE-CZ	9.52	137.72	124.40
1	A	414	ARG	CB-CA-C	-9.47	91.57	110.42
1	B	449	CYS	CB-CA-C	-9.47	95.56	110.14
1	B	414	ARG	CB-CA-C	-9.46	91.60	110.42
1	A	449	CYS	CB-CA-C	-9.45	95.59	110.14
1	B	451	THR	N-CA-CB	9.40	126.37	110.49
1	B	478	CYS	CA-C-O	-9.40	109.98	120.32
1	A	451	THR	N-CA-CB	9.38	126.35	110.49
1	B	415	ARG	N-CA-CB	-9.36	97.00	111.05
1	A	415	ARG	N-CA-CB	-9.36	97.01	111.05
1	A	478	CYS	CA-C-O	-9.34	110.04	120.32
1	B	473	LEU	CA-C-O	9.31	133.82	120.51
1	A	473	LEU	CA-C-O	9.28	133.78	120.51
1	A	468	ASN	CB-CA-C	9.23	131.72	113.45
1	B	468	ASN	CB-CA-C	9.22	131.71	113.45
1	A	504	VAL	N-CA-C	9.20	128.48	109.34
1	B	452	LEU	N-CA-C	9.19	130.38	110.80
1	A	452	LEU	N-CA-C	9.18	130.35	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	504	VAL	N-CA-C	9.17	128.41	109.34
1	B	477	LYS	CB-CA-C	9.16	128.65	110.42
1	A	477	LYS	CB-CA-C	9.16	128.65	110.42
1	A	489	ASP	CA-C-N	-9.09	105.24	121.87
1	A	489	ASP	C-N-CA	-9.09	105.24	121.87
1	B	489	ASP	CA-C-N	-9.08	105.25	121.87
1	B	489	ASP	C-N-CA	-9.08	105.25	121.87
1	B	411	SER	CB-CA-C	-9.04	95.12	110.22
1	B	418	ARG	CB-CA-C	9.02	128.37	110.42
1	A	411	SER	CB-CA-C	-8.99	95.20	110.22
1	A	418	ARG	CB-CA-C	8.98	128.30	110.42
1	B	445	SER	N-CA-C	8.86	129.66	110.80
1	A	445	SER	N-CA-C	8.84	129.63	110.80
1	A	482	HIS	CB-CA-C	-8.70	95.71	110.16
1	B	477	LYS	CA-C-O	8.70	132.96	120.51
1	A	477	LYS	CA-C-O	8.70	132.94	120.51
1	B	482	HIS	CB-CA-C	-8.69	95.74	110.16
1	A	475	ARG	CA-C-N	8.66	130.67	119.84
1	A	475	ARG	C-N-CA	8.66	130.67	119.84
2	C	41	PHE	CA-CB-CG	-8.66	105.14	113.80
1	B	475	ARG	CA-C-N	8.65	130.65	119.84
1	B	475	ARG	C-N-CA	8.65	130.65	119.84
2	E	41	PHE	CA-CB-CG	-8.64	105.16	113.80
1	A	493	SER	CB-CA-C	-8.51	97.26	110.88
1	B	414	ARG	N-CA-C	8.51	128.93	110.80
1	B	493	SER	CB-CA-C	-8.50	97.28	110.88
1	A	414	ARG	N-CA-C	8.49	128.87	110.80
1	A	403	HIS	N-CA-C	-8.28	96.48	109.72
1	B	403	HIS	N-CA-C	-8.27	96.48	109.72
1	A	492	THR	N-CA-C	8.24	123.15	109.46
1	B	492	THR	N-CA-C	8.22	123.11	109.46
1	B	440	TYR	N-CA-C	8.17	123.68	109.96
1	A	426	CYS	N-CA-C	8.16	120.17	111.28
1	A	440	TYR	N-CA-C	8.16	123.67	109.96
1	B	426	CYS	N-CA-C	8.14	120.16	111.28
1	A	479	ALA	N-CA-C	8.10	121.95	112.72
1	B	479	ALA	N-CA-C	8.10	121.95	112.72
2	C	9	ASP	CA-CB-CG	-8.05	104.55	112.60
2	E	9	ASP	CA-CB-CG	-8.05	104.55	112.60
1	B	437	ASN	CB-CA-C	-8.00	94.50	110.42
1	A	437	ASN	CB-CA-C	-7.98	94.55	110.42
1	A	429	ASN	N-CA-C	7.93	120.62	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	429	ASN	N-CA-C	7.93	120.62	111.11
1	A	483	TYR	CA-C-O	7.90	130.08	120.60
1	B	484	MET	CB-CA-C	-7.90	97.23	110.19
1	A	484	MET	CB-CA-C	-7.88	97.27	110.19
1	B	483	TYR	CA-C-O	7.85	130.02	120.60
1	B	469	ASP	CB-CA-C	-7.84	100.00	111.91
1	A	469	ASP	CB-CA-C	-7.84	100.00	111.91
1	A	496	ALA	N-CA-C	-7.82	98.94	110.52
1	B	496	ALA	N-CA-C	-7.80	98.98	110.52
1	B	405	PRO	N-CA-CB	7.72	110.19	103.31
1	A	405	PRO	N-CA-CB	7.68	110.14	103.31
1	A	438	VAL	CA-C-O	7.67	128.85	120.64
1	A	458	ALA	N-CA-C	7.66	127.11	110.80
1	B	458	ALA	N-CA-C	7.66	127.11	110.80
1	B	269	ALA	C-N-CD	-7.65	93.65	125.00
1	A	269	ALA	C-N-CD	-7.63	93.70	125.00
1	B	438	VAL	CA-C-O	7.63	128.81	120.64
1	A	464	ILE	N-CA-C	-7.60	97.53	108.17
1	B	464	ILE	N-CA-C	-7.56	97.58	108.17
1	A	461	THR	N-CA-C	7.53	126.84	110.80
1	B	441	LYS	N-CA-C	-7.53	97.92	109.14
1	B	461	THR	N-CA-C	7.52	126.82	110.80
1	A	441	LYS	N-CA-C	-7.51	97.95	109.14
1	A	154	PHE	CA-C-N	-7.45	112.65	120.03
1	A	154	PHE	C-N-CA	-7.45	112.65	120.03
1	B	154	PHE	CA-C-N	-7.43	112.68	120.03
1	B	154	PHE	C-N-CA	-7.43	112.68	120.03
2	E	66	TYR	N-CA-C	-7.39	95.06	110.80
2	C	66	TYR	N-CA-C	-7.37	95.09	110.80
1	B	268	SER	N-CA-C	7.37	121.67	109.95
1	B	112	ARG	CG-CD-NE	-7.33	95.88	112.00
1	A	112	ARG	CG-CD-NE	-7.33	95.88	112.00
1	B	436	ILE	N-CA-C	7.32	122.13	112.98
1	A	268	SER	N-CA-C	7.32	121.58	109.95
1	A	436	ILE	N-CA-C	7.29	122.10	112.98
1	A	442	LEU	N-CA-CB	7.28	122.63	110.77
1	B	442	LEU	N-CA-CB	7.26	122.60	110.77
1	B	419	PHE	N-CA-C	7.21	126.16	110.80
1	A	419	PHE	N-CA-C	7.19	126.12	110.80
1	B	304	VAL	CB-CA-C	-7.19	106.73	114.35
1	A	442	LEU	CB-CA-C	-7.19	99.07	110.14
1	B	442	LEU	CB-CA-C	-7.18	99.08	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	446	GLY	CA-C-N	-7.18	112.65	122.77
1	A	446	GLY	C-N-CA	-7.18	112.65	122.77
1	B	505	GLU	N-CA-CB	-7.17	98.60	110.65
1	A	505	GLU	N-CA-CB	-7.17	98.61	110.65
1	A	304	VAL	CB-CA-C	-7.13	106.79	114.35
1	B	446	GLY	CA-C-N	-7.13	112.71	122.77
1	B	446	GLY	C-N-CA	-7.13	112.71	122.77
1	A	467	VAL	CA-C-N	-7.11	107.75	122.82
1	A	467	VAL	C-N-CA	-7.11	107.75	122.82
1	B	467	VAL	CA-C-N	-7.09	107.78	122.82
1	B	467	VAL	C-N-CA	-7.09	107.78	122.82
1	B	434	SER	CB-CA-C	-7.09	101.76	112.11
1	A	434	SER	CB-CA-C	-7.07	101.80	112.11
1	A	460	ASP	N-CA-C	7.06	119.97	109.59
1	B	495	GLN	CB-CA-C	7.06	122.92	110.36
1	A	495	GLN	CB-CA-C	7.05	122.91	110.36
1	B	460	ASP	N-CA-C	7.04	119.93	109.59
1	A	432	ALA	CA-C-O	7.02	128.07	120.55
1	B	416	ALA	N-CA-CB	7.02	122.36	110.49
1	A	508	TYR	CB-CA-C	7.01	123.41	110.10
1	A	418	ARG	N-CA-C	7.00	125.70	110.80
1	B	508	TYR	CB-CA-C	7.00	123.39	110.10
1	B	432	ALA	CA-C-O	6.99	128.02	120.55
1	A	416	ALA	N-CA-CB	6.98	122.29	110.49
1	B	418	ARG	N-CA-C	6.98	125.66	110.80
1	A	445	SER	CA-C-O	6.97	130.48	120.51
1	B	445	SER	CA-C-O	6.97	130.47	120.51
1	A	465	LEU	CA-C-N	6.95	133.47	122.62
1	A	465	LEU	C-N-CA	6.95	133.47	122.62
1	B	465	LEU	CA-C-N	6.94	133.45	122.62
1	B	465	LEU	C-N-CA	6.94	133.45	122.62
1	B	473	LEU	CA-C-N	6.87	133.30	122.17
1	B	473	LEU	C-N-CA	6.87	133.30	122.17
1	A	473	LEU	CA-C-N	6.83	133.24	122.17
1	A	473	LEU	C-N-CA	6.83	133.24	122.17
1	B	405	PRO	CA-N-CD	-6.77	102.53	112.00
1	A	405	PRO	CA-N-CD	-6.76	102.54	112.00
1	A	458	ALA	CA-C-O	-6.76	110.85	120.51
1	A	420	ALA	CB-CA-C	-6.73	100.44	111.68
1	B	458	ALA	CA-C-O	-6.73	110.89	120.51
1	B	420	ALA	CB-CA-C	-6.72	100.45	111.68
1	A	483	TYR	CB-CA-C	-6.71	95.75	109.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	483	TYR	CB-CA-C	-6.70	95.79	109.38
1	A	436	ILE	N-CA-CB	-6.67	93.48	111.82
1	B	436	ILE	N-CA-CB	-6.67	93.48	111.82
1	B	129	PRO	N-CA-CB	6.60	110.26	103.00
1	A	129	PRO	N-CA-CB	6.60	110.26	103.00
1	B	441	LYS	CA-C-O	6.60	128.90	121.51
1	A	441	LYS	CA-C-O	6.59	128.89	121.51
1	A	495	GLN	N-CA-CB	-6.56	100.92	110.70
1	B	403	HIS	N-CA-CB	-6.56	99.86	111.08
1	A	403	HIS	N-CA-CB	-6.55	99.89	111.08
1	B	495	GLN	N-CA-CB	-6.54	100.95	110.70
2	C	89	GLN	CA-C-N	6.51	133.43	121.70
2	C	89	GLN	C-N-CA	6.51	133.43	121.70
2	E	89	GLN	CA-C-N	6.51	133.43	121.70
2	E	89	GLN	C-N-CA	6.51	133.43	121.70
1	A	424	LYS	N-CA-C	6.51	120.85	107.37
1	B	424	LYS	N-CA-C	6.51	120.84	107.37
1	A	302	ASP	CA-CB-CG	-6.40	106.20	112.60
1	A	474	ARG	N-CA-C	6.38	119.20	108.23
1	A	451	THR	CA-C-O	6.38	129.63	120.51
1	A	289	GLU	N-CA-C	-6.37	104.25	111.07
1	B	302	ASP	CA-CB-CG	-6.37	106.23	112.60
1	B	445	SER	CA-C-N	-6.37	108.92	121.41
1	B	445	SER	C-N-CA	-6.37	108.92	121.41
1	B	451	THR	CA-C-O	6.37	129.62	120.51
1	A	445	SER	CA-C-N	-6.37	108.93	121.41
1	A	445	SER	C-N-CA	-6.37	108.93	121.41
1	B	272	PHE	CB-CA-C	-6.37	102.76	110.08
1	A	473	LEU	N-CA-C	6.37	124.36	110.80
1	B	474	ARG	N-CA-C	6.36	119.17	108.23
1	A	272	PHE	CB-CA-C	-6.34	102.78	110.08
1	A	404	LEU	N-CA-C	6.34	118.83	110.08
1	B	289	GLU	N-CA-C	-6.33	104.29	111.07
1	A	304	VAL	N-CA-CB	6.33	114.49	110.50
1	B	473	LEU	N-CA-C	6.33	124.29	110.80
1	A	439	GLN	CB-CA-C	-6.33	100.37	110.81
1	B	472	ALA	N-CA-C	6.32	123.33	113.72
1	B	304	VAL	N-CA-CB	6.32	114.48	110.50
1	B	425	VAL	N-CA-C	6.32	118.99	111.09
1	B	194	GLN	N-CA-C	-6.32	104.40	111.28
1	B	449	CYS	CA-C-O	6.31	127.90	120.20
1	A	429	ASN	CB-CA-C	6.31	120.91	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	425	VAL	N-CA-C	6.30	118.97	111.09
1	B	439	GLN	CB-CA-C	-6.30	100.41	110.81
1	A	472	ALA	N-CA-C	6.30	123.30	113.72
1	B	404	LEU	N-CA-C	6.30	118.77	110.08
1	B	429	ASN	CB-CA-C	6.29	120.88	110.81
1	A	449	CYS	CA-C-O	6.28	127.86	120.20
1	A	194	GLN	N-CA-C	-6.28	104.44	111.28
1	B	443	HIS	N-CA-C	6.27	119.71	109.06
1	A	443	HIS	N-CA-C	6.25	119.69	109.06
1	A	410	LEU	N-CA-C	-6.23	100.01	109.85
1	A	178	GLU	N-CA-CB	6.22	119.19	110.04
1	B	178	GLU	N-CA-CB	6.21	119.17	110.04
1	B	410	LEU	N-CA-C	-6.21	100.04	109.85
1	A	505	GLU	CA-C-N	6.19	130.53	121.67
1	A	505	GLU	C-N-CA	6.19	130.53	121.67
1	A	408	TYR	CA-C-O	6.19	127.17	120.43
1	A	424	LYS	CA-C-O	6.19	130.77	120.81
1	B	408	TYR	CA-C-O	6.19	127.17	120.43
1	B	505	GLU	CA-C-N	6.18	130.50	121.67
1	B	505	GLU	C-N-CA	6.18	130.50	121.67
1	B	424	LYS	CA-C-O	6.16	130.72	120.81
1	A	414	ARG	N-CA-CB	6.13	120.85	110.49
1	B	449	CYS	N-CA-C	6.12	118.42	108.26
1	A	438	VAL	CB-CA-C	-6.12	99.89	110.65
1	A	449	CYS	N-CA-C	6.11	118.40	108.26
1	B	417	ARG	N-CA-CB	6.11	120.82	110.49
1	B	414	ARG	N-CA-CB	6.10	120.81	110.49
1	B	438	VAL	CB-CA-C	-6.10	99.92	110.65
1	A	417	ARG	N-CA-CB	6.07	120.76	110.49
1	A	445	SER	CB-CA-C	6.04	122.44	110.42
1	B	456	THR	N-CA-CB	6.03	121.92	111.13
1	B	507	SER	CB-CA-C	6.03	122.42	110.42
1	B	445	SER	CB-CA-C	6.03	122.41	110.42
1	B	472	ALA	N-CA-CB	-6.03	104.79	113.65
1	A	507	SER	CB-CA-C	6.02	122.40	110.42
1	A	456	THR	N-CA-CB	6.00	121.86	111.13
1	A	423	GLY	CA-C-O	5.97	127.99	121.48
1	A	472	ALA	N-CA-CB	-5.97	104.87	113.65
1	B	423	GLY	CA-C-O	5.95	127.97	121.48
1	B	285	PHE	CA-C-N	-5.95	114.86	122.77
1	B	285	PHE	C-N-CA	-5.95	114.86	122.77
1	B	503	THR	N-CA-C	-5.94	100.03	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	PHE	CA-C-N	-5.94	114.88	122.77
1	A	285	PHE	C-N-CA	-5.94	114.88	122.77
1	B	108	LYS	N-CA-C	-5.93	104.81	111.28
1	A	503	THR	N-CA-C	-5.92	100.06	109.59
1	A	108	LYS	N-CA-C	-5.91	104.84	111.28
1	A	484	MET	CA-C-O	5.90	126.81	120.32
1	A	503	THR	CA-C-N	5.90	132.59	121.97
1	A	503	THR	C-N-CA	5.90	132.59	121.97
1	B	484	MET	CA-C-O	5.89	126.81	120.32
1	A	418	ARG	N-CA-CB	-5.89	100.53	110.49
1	B	418	ARG	N-CA-CB	-5.89	100.53	110.49
1	B	439	GLN	N-CA-C	5.87	117.86	108.41
1	B	503	THR	CA-C-N	5.87	132.53	121.97
1	B	503	THR	C-N-CA	5.87	132.53	121.97
1	A	507	SER	N-CA-CB	5.86	120.40	110.49
1	B	507	SER	N-CA-CB	5.86	120.40	110.49
1	B	414	ARG	CA-C-O	-5.85	112.14	120.51
1	A	439	GLN	N-CA-C	5.83	117.80	108.41
2	C	89	GLN	CB-CA-C	-5.83	98.83	110.42
2	E	89	GLN	CB-CA-C	-5.82	98.83	110.42
1	A	414	ARG	CA-C-O	-5.82	112.19	120.51
1	A	447	ALA	N-CA-CB	-5.81	101.65	110.77
1	A	423	GLY	N-CA-C	-5.79	100.20	111.03
1	B	447	ALA	N-CA-CB	-5.79	101.68	110.77
1	A	443	HIS	CA-C-O	5.77	127.52	120.60
1	A	285	PHE	CA-CB-CG	-5.76	108.03	113.80
1	B	443	HIS	CA-C-O	5.76	127.52	120.60
1	A	421	GLN	CA-C-N	-5.76	112.01	121.34
1	A	421	GLN	C-N-CA	-5.76	112.01	121.34
1	B	423	GLY	N-CA-C	-5.76	100.26	111.03
1	B	421	GLN	CA-C-N	-5.75	112.03	121.34
1	B	421	GLN	C-N-CA	-5.75	112.03	121.34
1	B	285	PHE	CA-CB-CG	-5.74	108.06	113.80
1	B	493	SER	N-CA-C	5.73	117.79	108.63
1	A	493	SER	N-CA-C	5.71	117.77	108.63
1	A	361	ASN	CA-CB-CG	-5.68	106.92	112.60
1	B	473	LEU	N-CA-CB	5.68	120.08	110.49
1	B	361	ASN	CA-CB-CG	-5.67	106.92	112.60
1	A	473	LEU	N-CA-CB	5.66	120.06	110.49
1	B	484	MET	CA-C-N	5.61	130.00	122.93
1	B	484	MET	C-N-CA	5.61	130.00	122.93
1	A	484	MET	CA-C-N	5.58	129.95	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	484	MET	C-N-CA	5.58	129.95	122.93
1	A	464	ILE	N-CA-CB	5.56	118.81	111.25
1	B	464	ILE	N-CA-CB	5.55	118.80	111.25
1	B	468	ASN	N-CA-CB	-5.55	99.25	109.18
1	B	336	ASN	N-CA-C	-5.55	105.85	113.56
1	A	336	ASN	N-CA-C	-5.54	105.85	113.56
1	A	468	ASN	N-CA-CB	-5.54	99.27	109.18
1	A	429	ASN	CA-C-O	5.50	126.78	120.90
1	B	429	ASN	CA-C-O	5.50	126.78	120.90
1	B	307	SER	N-CA-C	-5.48	105.85	112.54
1	A	144	ARG	NE-CZ-NH2	5.47	124.13	119.20
1	A	307	SER	N-CA-C	-5.47	105.86	112.54
1	B	144	ARG	NE-CZ-NH2	5.45	124.11	119.20
1	B	329	PHE	CA-CB-CG	-5.44	108.36	113.80
1	B	469	ASP	N-CA-C	5.44	119.13	110.70
1	B	107	GLU	N-CA-C	5.44	117.21	111.28
1	A	469	ASP	N-CA-C	5.44	119.12	110.70
1	A	409	SER	N-CA-C	5.43	118.20	107.98
1	A	326	GLN	CA-C-N	-5.43	114.86	123.23
1	A	326	GLN	C-N-CA	-5.43	114.86	123.23
1	A	107	GLU	N-CA-C	5.42	117.19	111.28
1	B	326	GLN	CA-C-N	-5.41	114.89	123.23
1	B	326	GLN	C-N-CA	-5.41	114.89	123.23
1	B	409	SER	N-CA-C	5.41	118.16	107.98
1	A	329	PHE	CA-CB-CG	-5.41	108.39	113.80
1	B	269	ALA	O-C-N	-5.40	115.11	121.32
1	A	269	ALA	O-C-N	-5.38	115.13	121.32
2	E	51	ASP	CA-CB-CG	-5.35	107.25	112.60
2	E	45	SER	N-CA-C	-5.32	100.56	109.24
2	C	51	ASP	CA-CB-CG	-5.32	107.28	112.60
1	A	487	ALA	CA-C-N	-5.31	114.53	122.39
1	A	487	ALA	C-N-CA	-5.31	114.53	122.39
2	E	66	TYR	N-CA-CB	5.31	119.46	110.49
2	C	45	SER	N-CA-C	-5.30	100.61	109.24
1	B	507	SER	CA-C-O	5.29	128.08	120.51
1	B	487	ALA	CA-C-N	-5.29	114.57	122.39
1	B	487	ALA	C-N-CA	-5.29	114.57	122.39
2	C	66	TYR	N-CA-CB	5.29	119.42	110.49
2	C	268	GLN	CA-C-N	5.27	126.42	119.84
2	C	268	GLN	C-N-CA	5.27	126.42	119.84
1	A	507	SER	CA-C-O	5.26	128.03	120.51
2	E	268	GLN	CA-C-N	5.25	126.41	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	268	GLN	C-N-CA	5.25	126.41	119.84
1	B	300	ASP	CA-CB-CG	-5.22	107.38	112.60
1	A	472	ALA	CB-CA-C	5.20	120.79	110.65
1	B	472	ALA	CB-CA-C	5.20	120.78	110.65
1	B	504	VAL	N-CA-CB	5.17	119.77	111.23
2	C	79	ASN	CA-CB-CG	-5.16	107.44	112.60
1	A	504	VAL	N-CA-CB	5.15	119.73	111.23
1	A	300	ASP	CA-CB-CG	-5.14	107.46	112.60
2	E	79	ASN	CA-CB-CG	-5.14	107.46	112.60
1	A	217	ALA	CA-C-N	-5.13	114.67	119.90
1	A	217	ALA	C-N-CA	-5.13	114.67	119.90
1	B	217	ALA	CA-C-N	-5.11	114.68	119.90
1	B	217	ALA	C-N-CA	-5.11	114.68	119.90
1	A	495	GLN	N-CA-C	5.08	117.61	110.14
1	B	485	VAL	CA-C-N	5.07	131.19	122.67
1	B	485	VAL	C-N-CA	5.07	131.19	122.67
1	A	485	VAL	CA-C-N	5.07	131.18	122.67
1	A	485	VAL	C-N-CA	5.07	131.18	122.67
1	B	278	THR	CA-C-N	-5.07	115.34	122.94
1	B	278	THR	C-N-CA	-5.07	115.34	122.94
1	B	277	ASP	CA-CB-CG	-5.06	107.54	112.60
1	A	277	ASP	CA-CB-CG	-5.06	107.54	112.60
1	B	495	GLN	N-CA-C	5.05	117.57	110.14
1	A	278	THR	CA-C-N	-5.04	115.39	122.94
1	A	278	THR	C-N-CA	-5.04	115.39	122.94
1	A	309	GLU	N-CA-CB	5.03	117.28	109.98

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	451	0
1	B	3569	0	3462	447	0
2	C	2203	0	2105	144	0
2	E	2203	0	2105	154	0
3	D	720	0	697	19	0
3	F	720	0	697	17	0
4	G	28	0	25	0	0
4	H	28	0	25	0	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0
All	All	13046	0	12576	1221	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 48.

All (1221) 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:N	1:B:410:LEU:CA	1.76	1.47
2:C:78:LYS:HE3	2:C:254:TYR:CA	1.36	1.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:LEU:N	1:A:410:LEU:CA	1.76	1.45
1:B:482:HIS:CD2	1:B:501:LEU:CD2	1.96	1.44
1:A:451:THR:C	1:A:451:THR:CA	1.91	1.43
1:B:451:THR:CA	1:B:451:THR:C	1.92	1.43
1:B:486:VAL:CG1	1:B:497:GLN:NE2	1.79	1.42
1:B:266:ASP:CG	1:B:360:ARG:HH22	1.28	1.42
1:A:405:PRO:N	1:A:405:PRO:CD	1.70	1.40
1:A:266:ASP:CG	1:A:360:ARG:HH22	1.28	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:A:269:ALA:HB2	1:A:366:GLU:OE1	1.22	1.35
1:B:405:PRO:CD	1:B:405:PRO:N	1.70	1.35
1:A:482:HIS:NE2	1:A:501:LEU:HD21	1.38	1.33
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
1:B:408:TYR:CE1	1:B:422:ILE:CG2	2.25	1.17
2:C:78:LYS:N	2:C:254:TYR:CE1	1.99	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:HG12	1:A:504:VAL:O	1.37	1.13
1:A:486:VAL:N	1:A:497:GLN:HE22	1.23	1.12
1:A:424:LYS:HE3	1:A:464:ILE:HG12	1.24	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:VAL:CG1	1:B:504:VAL:O	1.98	1.12
2:C:78:LYS:HE2	2:C:254:TYR:N	1.62	1.12
2:C:78:LYS:HE2	2:C:253:ASN:C	1.75	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:HG3	3:D:66:ARG:HH11	1.15	1.10
1:A:474:ARG:HH11	1:A:477:LYS:CD	1.63	1.10
1:A:504:VAL:CG1	1:A:504:VAL:O	1.98	1.10
1:A:360:ARG:HB3	1:A:365:SER:HB3	1.32	1.09
1:A:266:ASP:CG	1:A:360:ARG:NH2	2.10	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:HD3	1:A:477:LYS:HD2	1.33	1.08
1:A:474:ARG:NH1	1:A:477:LYS:HG3	1.67	1.08
1:B:266:ASP:CG	1:B:360:ARG:NH2	2.10	1.08
2:E:85:TRP:CZ2	2:E:257:ARG:HD2	1.87	1.08
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
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:34:VAL:HG22	2:C:53:CYS:HB2	1.07	1.06
2:C:69:ARG:HH21	2:C:81:LEU:HD23	1.16	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
1:A:269:ALA:HB2	1:A:366:GLU:CD	1.82	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
2:E:69:ARG:CD	2:E:254:TYR:CD1	2.40	1.04
1:B:445:SER:O	1:B:450:SER:O	1.74	1.04
3:F:66:ARG:HG3	3:F:66:ARG:HH11	1.15	1.04
1:A:474:ARG:HG3	1:A:476:PRO:HD2	1.40	1.04
1:B:269:ALA:HB2	1:B:366:GLU:CD	1.82	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:410:LEU:N	1:A:503:THR:O	1.90	1.03
1:A:426:CYS:HB2	1:A:462:SER:O	1.59	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: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:360:ARG:HB3	1:B:365:SER:HB3	1.32	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: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:B:486:VAL:HA	1:B:497:GLN:NE2	1.69	1.02
1:A:441:LYS:HB2	1:A:486:VAL:CG2	1.88	1.02
1:B:474:ARG:HG3	1:B:476:PRO:HD2	1.40	1.02
2:E:8:LEU:HB2	2:E:12:LYS:HB2	1.40	1.02
1:A:356:LEU:HD21	1:A:372:LEU:HD22	1.38	1.01
1:B:482:HIS:CD2	1:B:501:LEU:HD23	1.91	1.01
1:B:486:VAL:HG13	1:B:497:GLN:NE2	1.73	1.01
2:C:30:LEU:HD22	2:C:60:LEU:HD11	1.39	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:8:LEU:HB2	2:C:12:LYS:HB2	1.40	1.00
2:C:77:GLU:HB3	2:C:254:TYR:OH	1.62	1.00
1:B:451:THR:C	1:B:451:THR:N	2.20	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: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:A:451:THR:C	1:A:451:THR:N	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:ARG:HH11	1:B:477:LYS:HD2	1.28	0.96
1:B:474:ARG:NH1	1:B:477:LYS:CG	2.25	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:409:SER:C	1:A:410:LEU:CA	2.40	0.94
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
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:409:SER:C	1:B:410:LEU:CA	2.40	0.93
2:E:85:TRP:CH2	2:E:257:ARG:CD	2.51	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
1:A:302:ASP:C	1:A:309:GLU:HB2	1.96	0.90
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:450:SER:C	1:A:451:THR:C	2.41	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: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
2:C:9:ASP:CG	2:C:70:CYS:HB2	1.98	0.88
2:E:9:ASP:CG	2:E:70:CYS:HB2	1.98	0.88
1:B:302:ASP:C	1:B:309:GLU:HB2	1.96	0.88
1:B:450:SER:C	1:B:451:THR:C	2.41	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:412:VAL:CG2	1:A:504:VAL:O	2.20	0.88
1:A:474:ARG:CG	1:A:476:PRO:O	2.22	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
1:B:178:GLU:CD	1:B:231:ARG:H	1.83	0.87
1:B:283:VAL:HG23	1:B:286:LYS:HB2	1.55	0.87
1:B:293:VAL:HG21	1:B:329:PHE:CE1	2.10	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:178:GLU:CD	1:A:231:ARG:H	1.83	0.85
2:E:81:LEU:HD21	2:E:85:TRP:CE2	2.11	0.85
1:B:179:ASN:HB2	1:B:265:GLU:CD	2.00	0.84
1:A:412:VAL:CG2	1:A:504:VAL:HG12	2.06	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:275:GLY:O	1:B:370:MET:HE3	1.79	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
1:A:179:ASN:HB2	1:A:265:GLU:CD	2.01	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
2:C:78:LYS:HE3	2:C:254:TYR:HA	0.89	0.81
1:A:275:GLY:O	1:A:370:MET:HE3	1.79	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:HG3	3:D:66:ARG:NH1	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:474:ARG:NH1	1:A:477:LYS:HD2	1.90	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:70:CYS:C	2:E:254:TYR:CZ	2.46	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: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:HH11	3:D:66:ARG:CG	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
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
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:412:VAL:HG23	1:B:504:VAL:O	1.83	0.77
1:B:489:ASP:HB2	1:B:494:ARG:HD2	1.66	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:HD13	2:E:81:LEU:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:HIS:HE2	1:A:501:LEU:HD21	1.49	0.76
1:B:302:ASP:O	1:B:309:GLU:HB2	1.84	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
1:A:488:THR:O	1:A:488:THR:OG1	1.86	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
1:B:488:THR:O	1:B:488:THR:OG1	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:69:ARG:HH21	2:E:81:LEU:CD2	2.00	0.72
2:E:85:TRP:CZ2	2:E:257:ARG:CG	2.73	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
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:469:ASP:CG	1:A:469:ASP:O	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:81:LEU:HD11	2:E:85:TRP:CD2	2.24	0.71
1:A:358:LEU:O	1:A:358:LEU:HG	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:O	3:F:72:CYS:SG	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
1:B:469:ASP:CG	1:B:469:ASP:O	2.32	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
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:266:ASP:CB	1:B:360:ARG:NH2	2.50	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:410:LEU:N	1:A:410:LEU:C	2.51	0.69
1:A:429:ASN:HB2	1:A:440:TYR:OH	1.90	0.69
1:B:410:LEU:N	1:B:410:LEU:C	2.51	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:408:TYR:CZ	1:A:422:ILE:HG21	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ARG:HE	1:A:469:ASP:HB3	1.58	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:404:LEU:C	1:A:405:PRO:CD	2.66	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
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
2:E:37:LYS:HZ2	2:E:85:TRP:HB3	1.58	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: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: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:445:SER:C	1:B:449:CYS:O	2.38	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:474:ARG:HH12	1:A:477:LYS:HG3	1.60	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:412:VAL:CG1	1:A:475:ARG:H	2.07	0.66
1:A:415:ARG:O	1:A:416:ALA:CB	2.40	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
1:A:445:SER:C	1:A:449:CYS:O	2.38	0.65
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: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:C:37:LYS:HZ1	2:C:85:TRP:HE3	1.45	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
1:B:179:ASN:CB	1:B:265:GLU:CD	2.69	0.65
2:C:37:LYS:HZ2	2:C:85:TRP:HB3	1.62	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
1:A:450:SER:C	1:A:451:THR:O	2.40	0.64
1:B:450:SER:C	1:B:451:THR:O	2.40	0.64
2:E:88:TYR:CD2	2:E:89:GLN:HG3	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:LEU:C	1:B:405:PRO:CD	2.65	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:A:347:VAL:HG22	1:A:348:ARG:N	2.13	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:81:HIS:HD2	1:A:82:GLU:O	1.81	0.64
1:A:296:LEU:HD21	1:A:372:LEU:HB3	1.80	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:446:GLY:HA3	1:B:454:VAL:CG1	2.28	0.63
1:B:449:CYS:O	1:B:450:SER:CB	2.45	0.63
2:E:89:GLN:OE1	2:E:90:SER:HA	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
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:A:412:VAL:HG13	1:A:475:ARG:H	1.62	0.63
1:A:296:LEU:N	1:A:296:LEU:HD12	2.14	0.62
1:A:483:TYR:C	1:A:483:TYR:CD2	2.77	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:270:PRO:HB2	1:B:358:LEU:HD23	1.79	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:HG13	1:A:364:ILE:O	1.99	0.62
3:D:92:LEU:O	3:D:93:VAL:HB	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:40:ASN:CB	2:E:43:LEU:HD13	2.04	0.62
1:B:364:ILE:O	1:B:364:ILE:HG13	1.99	0.62
1:A:348:ARG:HD2	1:A:348:ARG:O	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:B:483:TYR:C	1:B:483:TYR:CD2	2.77	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
1:B:347:VAL:HG22	1:B:348:ARG:N	2.13	0.61
2:C:53:CYS:SG	2:C:57:MET:HE3	2.41	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:441:LYS:CB	1:B:486:VAL:CG2	2.73	0.61
1:B:483:TYR:CE2	1:B:485:VAL:HG23	2.35	0.61
2:E:53:CYS:SG	2:E:57:MET:HE3	2.40	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
2:E:37:LYS:HZ1	2:E:85:TRP:HE3	1.47	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
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:A:429:ASN:CG	1:A:440:TYR:OH	2.43	0.61
1:B:348:ARG:HD2	1:B:348:ARG:O	1.99	0.61
1:A:418:ARG:CD	1:A:469:ASP:HB2	2.31	0.61
1:A:470:THR:O	1:A:470:THR:HG22	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:ARG:CG	1:B:469:ASP:HB2	2.32	0.60
1:B:429:ASN:CG	1:B:440:TYR:OH	2.43	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:A:426:CYS:CB	1:A:462:SER:C	2.73	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:HD12	2:C:47:LEU:N	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: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:A:317:THR:HG22	1:A:318:LEU:CD1	2.32	0.59
1:A:179:ASN:CB	1:A:265:GLU:CD	2.69	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:HG3	3:D:91:ARG:HH11	1.67	0.59
1:A:199:GLN:HE21	1:A:199:GLN:N	1.94	0.59
1:B:298:VAL:CG2	1:B:358:LEU:HD13	2.32	0.59
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:B:441:LYS:C	1:B:486:VAL:HG22	2.27	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:B:426:CYS:CB	1:B:462:SER:C	2.73	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
2:C:81:LEU:HD13	2:C:81:LEU:C	2.27	0.58
2:E:81:LEU:HD13	2:E:81:LEU:C	2.27	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:448:ASN:C	1:A:452:LEU:CD2	2.77	0.58
1:B:474:ARG:HH12	1:B:477:LYS:HG3	1.60	0.58
1:A:441:LYS:C	1:A:486:VAL:HG22	2.27	0.58
1:B:298:VAL:HG21	1:B:358:LEU:HD13	1.85	0.58
3:F:91:ARG:HG3	3:F:91:ARG:HH11	1.67	0.58
1:B:436:ILE:O	1:B:436:ILE:HG22	2.01	0.58
2:C:9:ASP:OD2	2:C:72:ARG:HB2	2.04	0.58
2:C:78:LYS:CD	2:C:257:ARG:HB3	2.34	0.58
1:B:314:TYR:CE2	1:B:358:LEU:HD13	2.39	0.58
1:B:348:ARG:HD2	1:B:348:ARG:C	2.29	0.58
1:A:155:PRO:HG2	1:A:160:LEU:HD21	1.86	0.57
1:B:448:ASN:C	1:B:452:LEU:CD2	2.77	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
1:B:451:THR:CA	1:B:452:LEU:N	2.61	0.57
2:E:34:VAL:HG12	2:E:36:GLY:H	1.70	0.57
1:A:304:VAL:HG22	1:A:309:GLU:CD	2.29	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:178:GLU:OE1	1:B:230:ASP:C	2.46	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
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:A:310:LEU:C	1:A:310:LEU:HD23	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:348:ARG:HD2	1:A:348:ARG:C	2.29	0.56
1:A:356:LEU:N	1:A:356:LEU:HD22	2.20	0.56
1:B:304:VAL:HG22	1:B:309:GLU:CD	2.29	0.56
2:C:89:GLN:HE21	2:C:89:GLN:N	2.02	0.56
1:B:484:MET:HB3	1:B:497:GLN:CG	2.36	0.56
1:A:317:THR:C	1:A:318:LEU:HD12	2.31	0.56
1:B:274:ALA:CB	1:B:370:MET:HE1	2.35	0.56
1:B:410:LEU:N	1:B:410:LEU:CB	2.65	0.56
1:A:449:CYS:O	1:A:450:SER:O	2.23	0.56
1:B:486:VAL:N	1:B:497:GLN:NE2	1.88	0.56
2:E:240:ARG:HD3	2:E:314:ASP:HB3	1.88	0.56
1:A:274:ALA:CB	1:A:370:MET:HE1	2.35	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
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:B:209:GLY:O	1:B:212:LEU:HB2	2.05	0.56
1:B:310:LEU:C	1:B:310:LEU:HD23	2.31	0.55
1:B:356:LEU:N	1:B:356:LEU:HD22	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
3:D:76:GLU:CD	3:D:76:GLU:H	2.14	0.55
1:A:410:LEU:N	1:A:410:LEU:CB	2.66	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
1:B:317:THR:C	1:B:318:LEU:HD12	2.31	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:F:76:GLU:H	3:F:76:GLU:CD	2.14	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: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:178:GLU:OE1	1:A:230:ASP:C	2.46	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
2:E:85:TRP:CH2	2:E:257:ARG:HG3	2.42	0.54
1:A:151:ASN:C	1:A:152:THR:HG23	2.33	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
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
1:A:317:THR:CB	1:A:318:LEU:HD12	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:70:CYS:C	2:E:254:TYR:OH	2.47	0.53
1:A:375:LEU:C	1:A:375:LEU:HD13	2.34	0.53
1:B:308:GLY:HA2	1:B:360:ARG:CZ	2.38	0.53
1:B:474:ARG:CD	1:B:477:LYS:HD2	2.22	0.53
1:B:375:LEU:HD13	1:B:375:LEU:C	2.34	0.53
1:A:416:ALA:O	1:A:417:ARG:C	2.52	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:N	2:C:43:LEU:HD12	2.23	0.53
1:B:323:THR:HA	1:B:324:TRP:C	2.34	0.53
1:B:329:PHE:HD2	1:B:354:TYR:CE1	2.26	0.53
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:272:PHE:CG	1:A:370:MET:HB3	2.45	0.52
1:A:350:THR:HG23	1:A:351:VAL:N	2.23	0.52
1:B:416:ALA:O	1:B:417:ARG:C	2.52	0.52
2:C:61:LYS:HG2	2:C:62:GLN:HG3	1.91	0.52
1:B:296:LEU:HD23	1:B:370:MET:HE2	1.90	0.52
2:E:43:LEU:N	2:E:43:LEU:HD12	2.23	0.52
1:A:412:VAL:HG13	1:A:475:ARG:N	2.25	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: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: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:151:ASN:C	1:B:152:THR:HG23	2.33	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
1:A:296:LEU:HD23	1:A:370:MET:CE	2.40	0.52
1:A:296:LEU:HD23	1:A:370:MET:HE2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:PRO:O	1:B:336:ASN:HB2	2.10	0.51
3:F:91:ARG:HH11	3:F:91:ARG:CG	2.23	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
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:A:323:THR:HA	1:A:324:TRP:C	2.34	0.51
1:B:350:THR:C	1:B:351:VAL:HG22	2.35	0.51
1:B:470:THR:CB	1:B:473:LEU:HD21	2.41	0.51
1:B:483:TYR:HE2	1:B:485:VAL:HG23	1.74	0.51
1:B:484:MET:HB3	1:B:497:GLN:HG3	1.91	0.51
1:A:404:LEU:CA	1:A:405:PRO:CD	2.89	0.51
2:C:47:LEU:H	2:C:47:LEU:CD1	2.23	0.51
1:B:504:VAL:O	1:B:504:VAL:HG13	2.05	0.51
2:E:69:ARG:NE	2:E:257:ARG:NH2	2.56	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:350:THR:C	1:A:351:VAL:HG22	2.36	0.51
1:A:318:LEU:HD13	1:A:355:ARG:HD3	1.93	0.50
2:E:37:LYS:NZ	2:E:85:TRP:HB3	2.25	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
2:C:37:LYS:NZ	2:C:85:TRP:HB3	2.25	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: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:443:HIS:CE1	1:A:484:MET:HB2	2.47	0.50
1:A:445:SER:HA	1:A:449:CYS:O	2.12	0.50
1:A:485:VAL:CG2	1:A:500:LEU:CD1	2.90	0.50
2:C:13:ALA:HB1	2:C:67:ASN:ND2	2.27	0.50
2:C:78:LYS:CE	2:C:253:ASN:C	2.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:VAL:HG12	1:B:299:PHE:N	2.27	0.50
1:A:446:GLY:CA	1:A:454:VAL:HG12	2.42	0.50
1:B:266:ASP:CG	1:B:360:ARG:CZ	2.84	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:A:483:TYR:CD1	1:A:500:LEU:C	2.88	0.49
1:B:303:VAL:C	1:B:309:GLU:HB3	2.37	0.49
1:B:314:TYR:CE2	1:B:358:LEU:CD1	2.95	0.49
1:B:318:LEU:HD13	1:B:355:ARG:HD3	1.93	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
2:C:88:TYR:HD2	2:C:89:GLN:CD	2.20	0.49
1:A:73:TYR:CE2	2:C:41:PHE:HE2	2.30	0.49
1:A:329:PHE:CD1	1:A:340:VAL:HG22	2.46	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
2:E:88:TYR:HD2	2:E:89:GLN:CD	2.21	0.49
1:A:446:GLY:C	1:A:454:VAL:HG12	2.38	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:274:ALA:HB1	1:B:370:MET:HE1	1.94	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: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:303:VAL:C	1:A:309:GLU:HB3	2.37	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
2:C:78:LYS:C	2:C:257:ARG:NH2	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ASN:C	1:A:452:LEU:HD21	2.38	0.49
2:E:84:TYR:CD2	2:E:85:TRP:HD1	2.31	0.49
1:A:274:ALA:HB1	1:A:370:MET:HE1	1.95	0.49
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:B:483:TYR:CD1	1:B:500:LEU:C	2.88	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
2:E:88:TYR:C	2:E:89:GLN:HG3	2.39	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: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
2:C:37:LYS:O	2:C:37:LYS:HG2	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:319:LEU:HD22	1:A:354:TYR:CZ	2.49	0.48
1:A:329:PHE:HA	1:A:342:ALA:HA	1.96	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
1:B:448:ASN:C	1:B:452:LEU:HD21	2.38	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:446:GLY:C	1:B:454:VAL:HG12	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:21:GLN:O	2:C:25:THR:HG23	2.13	0.48
1:A:298:VAL:CB	1:A:358:LEU:HD22	2.43	0.47
1:A:300:ASP:OD2	1:A:302:ASP:HB2	2.12	0.47
1:A:314:TYR:CG	1:A:338:THR:CB	2.97	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:C:88:TYR:C	2:C:89:GLN:HG3	2.39	0.47
1:A:312:ARG:CB	1:A:358:LEU:HD21	2.42	0.47
1:B:271:THR:C	1:B:298:VAL:HG13	2.39	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:319:LEU:HD22	1:A:354:TYR:HH	1.77	0.47
1:B:484:MET:HE3	1:B:497:GLN:HG3	1.96	0.47
2:C:61:LYS:O	2:C:62:GLN:HB2	2.14	0.47
1:A:266:ASP:CG	1:A:360:ARG:CZ	2.84	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:271:THR:C	1:A:298:VAL:HG13	2.39	0.47
1:A:357:VAL:HG12	1:A:359:ASN:N	2.28	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:A:334:TRP:CD1	1:A:335:PRO:HD3	2.49	0.47
1:A:484:MET:HE3	1:A:497:GLN:HG3	1.96	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
2:E:251:LYS:HA	2:E:257:ARG:HB2	1.97	0.47
1:B:474:ARG:C	1:B:476:PRO:HD2	2.40	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:E:37:LYS:O	2:E:37:LYS:HG2	2.14	0.46
1:A:457:SER:CB	1:A:465:LEU:CD2	2.94	0.46
1:A:470:THR:HG22	1:A:473:LEU:HD23	1.98	0.46
1:A:474:ARG:C	1:A:476:PRO:HD2	2.40	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: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:C:88:TYR:CD2	2:C:89:GLN:CD	2.94	0.46
2:E:88:TYR:CD2	2:E:89:GLN:CD	2.94	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:HD12	1:A:318:LEU:N	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:58:ASP:HA	1:B:180:ARG: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CD2	1:A:485:VAL:HG23	2.52	0.45
2:C:176:THR:HB	2:C:177:PRO:HD3	1.99	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:483:TYR:CD2	1:B:485:VAL:HG23	2.52	0.45
1:A:73:TYR:CE2	2:C:41:PHE:CE2	3.05	0.45
1:A:187:GLN:NE2	1:A:189:ARG:H	2.15	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:B:310:LEU:HD23	1:B:310:LEU:O	2.17	0.45
1:B:457:SER:CB	1:B:465:LEU:HD23	2.47	0.45
2:C:83:ILE:O	2:C:84:TYR:HB3	2.17	0.45
2:C:206:LYS:HE2	2:C:207:HIS:NE2	2.31	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: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:E:84:TYR:HD2	2:E:85:TRP:CD1	2.35	0.44
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:CZ	2:C:82:ARG:CB	2.95	0.44
2:E:26:LYS:CG	2:E:63:LYS:HE2	2.43	0.44
2:E:37:LYS:HD2	2:E:90:SER:CB	2.48	0.44
2:E:71:LYS:O	2:E:254:TYR:CD2	2.71	0.44
1:A:284:GLU:HG2	1:A:285:PHE:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
2:C:89:GLN:CD	2:C:90:SER:N	2.76	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:NH1	3:D:66:ARG:CG	2.65	0.44
2:E:82:ARG:CZ	2:E:82:ARG:CB	2.95	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
1:A:217:ALA:O	1:A:218:PRO:C	2.61	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: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
2:E:89:GLN:CD	2:E:90:SER:N	2.76	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:42:VAL:O	1:B:43:ASP:HB2	2.18	0.43
1:B:418:ARG:HE	1:B:469:ASP:CB	2.28	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: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: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:CG2	1:B:422:ILE:O	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:242:ASN:HA	2:C:314:ASP:O	2.19	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: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
1:B:266:ASP:CG	1:B:360:ARG:HH12	2.27	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:210:GLU:CD	1:B:210:GLU:H	2.27	0.42
1:B:312:ARG:HH21	1:B:336:ASN:CB	2.30	0.42
1:A:296:LEU:HD11	1:A:372:LEU:CD1	2.44	0.42
1:A:298:VAL:CG2	1:A:314:TYR:CE2	2.95	0.42
1:A:300:ASP:HB3	1:A:309:GLU:O	2.19	0.42
1:A:310:LEU:C	1:A:310:LEU:CD2	2.92	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:210:GLU:CD	1:A:210:GLU:H	2.27	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
1:A:355:ARG:C	1:A:356:LEU:HD22	2.44	0.42
1:A:436:ILE:O	1:A:436:ILE:CG2	2.66	0.42
1:B:217:ALA:O	1:B:218:PRO:C	2.61	0.42
1:B:412:VAL:HG11	1:B:475:ARG:H	1.82	0.42
1:B:457:SER:HB2	1:B:465:LEU:HD23	1.99	0.42
1:B:507:SER:O	1:B:508:TYR:CB	2.68	0.42
2:C:13:ALA:CB	2:C:67:ASN:CG	2.93	0.42
2:E:13:ALA:CB	2:E:67:ASN:CG	2.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:PHE:CE2	1:B:298:VAL:CG2	3.02	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:292:VAL:HG13	1:B:339:SER:OG	2.20	0.42
1:B:317:THR:HB	1:B:318:LEU:HD12	2.00	0.42
1:B:355:ARG:C	1:B:356:LEU:HD22	2.44	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:HA	2:E:58:GLU:OE1	2.20	0.42
1:A:350:THR:CG2	1:A:351:VAL:N	2.82	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:296:LEU:CD1	1:A:372:LEU:HD13	2.45	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: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:56:LEU:HD23	1:B:56:LEU:HA	1.96	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:HB	1:B:473:LEU:CD2	2.50	0.42
1:B:470:THR:CB	1:B:473:LEU:CD2	2.98	0.42
1:A:266:ASP:CG	1:A:360:ARG:HH12	2.27	0.41
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:153:SER:O	1:B:154:PHE:C	2.63	0.41
1:B:285:PHE:O	1:B:285:PHE:CD2	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
1:A:320:PRO:HG2	1:A:353:ASP:HB3	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:269:ALA:CB	1:B:366:GLU:CD	2.74	0.41
1:B:296:LEU:N	1:B:296:LEU:CD1	2.82	0.41
1:B:310:LEU:C	1:B:310:LEU:CD2	2.93	0.41
1:B:312:ARG:HB2	1:B:358:LEU:CG	2.51	0.41
1:B:320:PRO:HG2	1:B:353:ASP:HB3	2.02	0.41
1:B:266:ASP:OD2	1:B:365:SER:HA	2.21	0.41
1:B:342:ALA:CB	1:B:346:PHE:CZ	3.04	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:CG	3:D:91:ARG:NH1	2.83	0.41
2:E:14:SER:HA	2:E:65:LEU:HD21	2.02	0.41
2:E:66:TYR:O	2:E:66:TYR:CG	2.71	0.41
2:E:88:TYR:C	2:E:89:GLN:CG	2.94	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:139:TRP:CG	1:A:140:PRO:HA	2.56	0.41
1:A:144:ARG:HH11	1:A:144:ARG:HD2	1.68	0.41
1:A:269:ALA:CB	1:A:366:GLU:CD	2.73	0.41
1:A:372:LEU:HD23	1:A:372:LEU:H	1.85	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
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: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:37:LYS:CE	2:E:85:TRP:CE3	2.93	0.41
2:E:270:GLU:HB2	2:E:276:ASN:O	2.21	0.41
2:E:331:PHE:O	2:E:335:ASN:HB2	2.21	0.41
1:A:266:ASP:OD2	1:A:365:SER:HA	2.21	0.41
1:B:283:VAL:HG11	1:B:494:ARG:HH22	1.86	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
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:CD2	1:A:285:PHE:O	2.73	0.40
1:A:297:ARG:NH1	1:A:297:ARG:HB2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:E:29:THR:C	2:E:32:GLN:HG2	2.46	0.40
2:E:69:ARG:HD2	2:E:69:ARG:C	2.46	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:348:ARG:C	1:A:348:ARG:CD	2.95	0.40
1:A:443:HIS:NE2	1:A:484:MET:HB2	2.36	0.40
1:B:274:ALA:HB3	1:B:370:MET:HE1	2.02	0.40
1:B:300:ASP:C	1:B:309:GLU:HG3	2.45	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:81:LEU:CD2	2:E:85:TRP:CE2	2.95	0.40
2:E:83:ILE:CG2	2:E:84:TYR:N	2.83	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%)	1	16
1	B	440/607 (72%)	385 (88%)	33 (8%)	22 (5%)	1	16
2	C	280/463 (60%)	260 (93%)	15 (5%)	5 (2%)	6	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	280/463 (60%)	260 (93%)	15 (5%)	5 (2%)	6	34
3	D	91/134 (68%)	84 (92%)	6 (7%)	1 (1%)	11	46
3	F	91/134 (68%)	84 (92%)	6 (7%)	1 (1%)	11	46
All	All	1622/2408 (67%)	1458 (90%)	108 (7%)	56 (4%)	4	20

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%)	371 (95%)	19 (5%)	22	43
1	B	390/528 (74%)	371 (95%)	19 (5%)	22	43
2	C	247/408 (60%)	239 (97%)	8 (3%)	34	56
2	E	247/408 (60%)	239 (97%)	8 (3%)	34	56
3	D	78/113 (69%)	74 (95%)	4 (5%)	21	42
3	F	78/113 (69%)	74 (95%)	4 (5%)	21	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1430/2098 (68%)	1368 (96%)	62 (4%)	27	47

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	GLU
1	A	101	LEU
1	A	112	ARG
1	A	127	LEU
1	A	180	ARG
1	A	199	GLN
1	A	216	SER
1	A	235	GLU
1	A	238	GLU
1	A	267	ASP
1	A	286	LYS
1	A	414	ARG
1	A	415	ARG
1	A	417	ARG
1	A	422	ILE
1	A	431	GLN
1	A	473	LEU
1	A	477	LYS
1	A	494	ARG
1	B	90	GLU
1	B	101	LEU
1	B	112	ARG
1	B	127	LEU
1	B	180	ARG
1	B	199	GLN
1	B	216	SER
1	B	235	GLU
1	B	238	GLU
1	B	267	ASP
1	B	286	LYS
1	B	414	ARG
1	B	415	ARG
1	B	417	ARG
1	B	422	ILE
1	B	431	GLN
1	B	473	LEU
1	B	477	LYS

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Mol	Chain	Res	Type
1	B	494	ARG
2	C	66	TYR
2	C	89	GLN
2	C	155	LEU
2	C	219	ILE
2	C	226	ARG
2	C	248	ASP
2	C	273	SER
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	219	ILE
2	E	226	ARG
2	E	248	ASP
2	E	273	SER
2	E	307	LEU
3	F	66	ARG
3	F	72	CYS
3	F	91	ARG
3	F	97	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) 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	468	ASN
1	A	482	HIS
1	A	490	GLN
1	A	495	GLN
1	A	497	GLN
1	B	81	HIS
1	B	187	GLN

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Mol	Chain	Res	Type
1	B	199	GLN
1	B	246	HIS
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	330	ASN
2	C	340	ASN
2	E	89	GLN
2	E	281	ASN
2	E	330	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 ⓘ

4 monosaccharides 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
4	NAG	G	1	4,3	14,14,15	0.55	0	17,19,21	1.14	1 (5%)
4	NAG	G	2	4	14,14,15	0.79	1 (7%)	17,19,21	1.39	2 (11%)
4	NAG	H	1	4,3	14,14,15	0.57	0	17,19,21	1.15	1 (5%)
4	NAG	H	2	4	14,14,15	0.78	1 (7%)	17,19,21	1.38	2 (11%)

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
4	NAG	G	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	NAG	H	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	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)
4	G	2	NAG	C1-C2	2.18	1.55	1.52
4	H	2	NAG	C1-C2	2.16	1.55	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	NAG	C1-O5-C5	3.45	116.81	112.19
4	H	2	NAG	C4-C3-C2	3.42	116.03	111.02
4	G	2	NAG	C4-C3-C2	3.40	116.00	111.02
4	G	1	NAG	C1-O5-C5	3.38	116.71	112.19
4	G	2	NAG	O5-C1-C2	2.24	114.76	111.29
4	H	2	NAG	O5-C1-C2	2.16	114.64	111.29

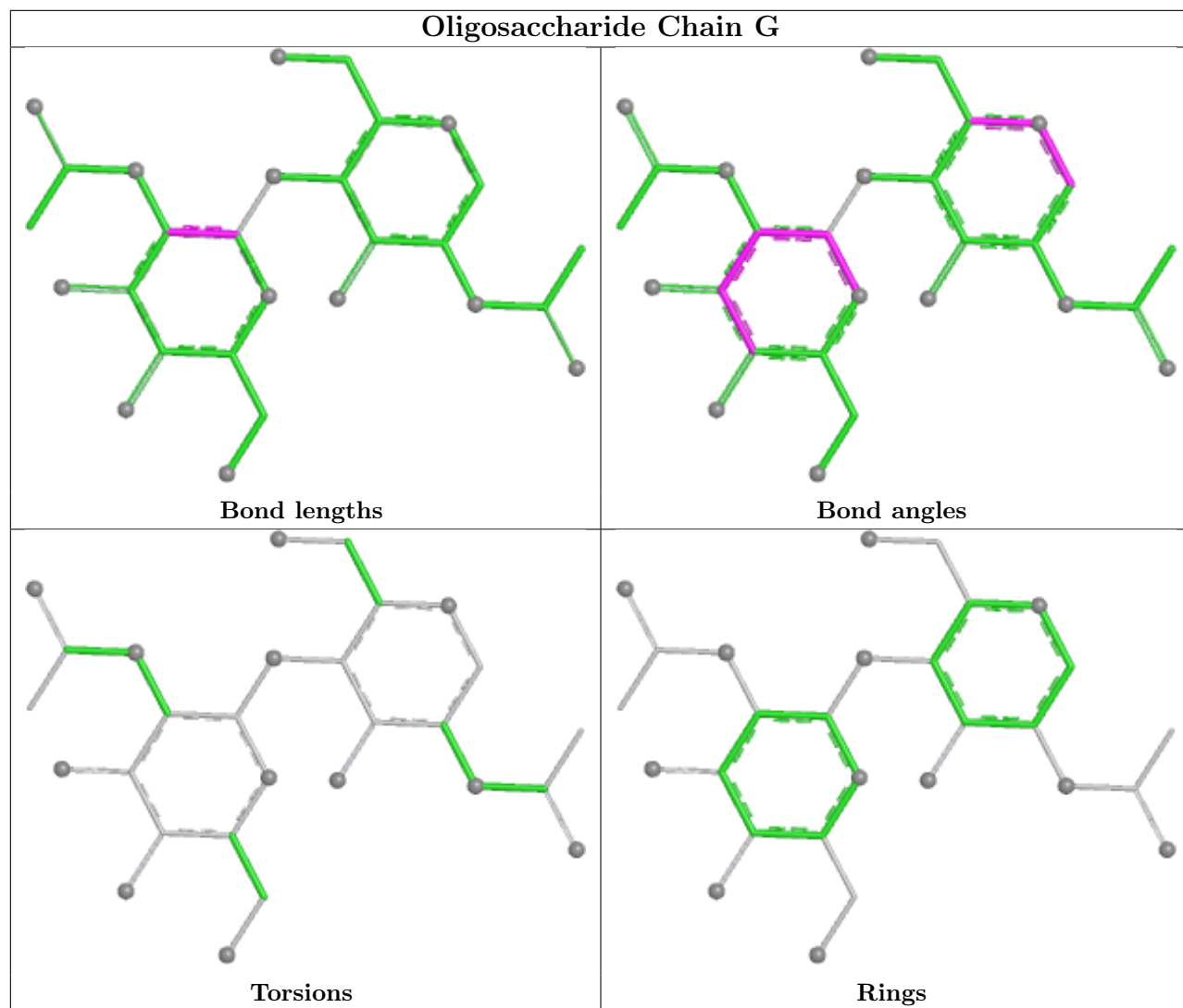
There are no chirality outliers.

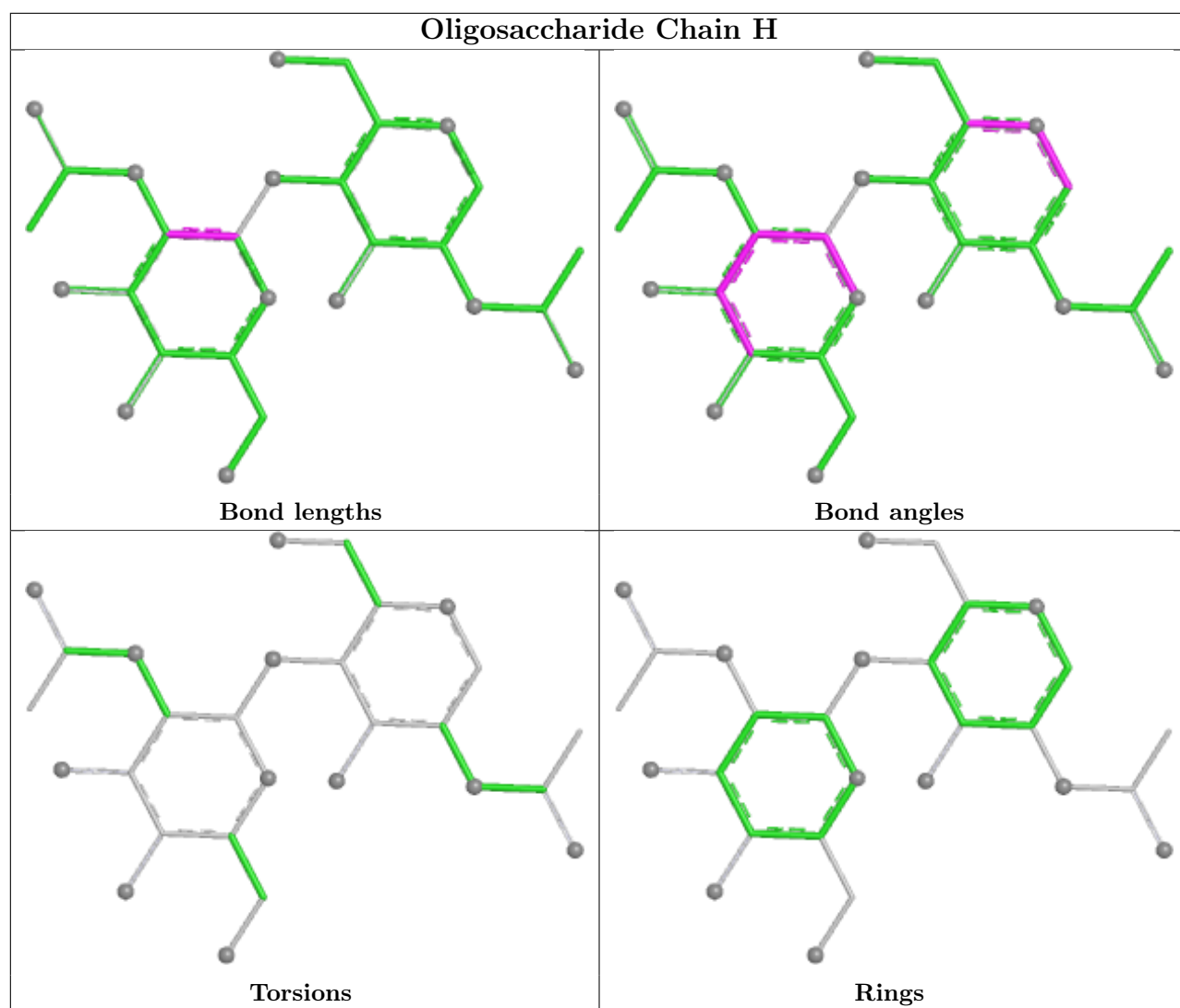
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	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

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2712. These allow visual inspection of the internal detail of the map and identification of artifacts.

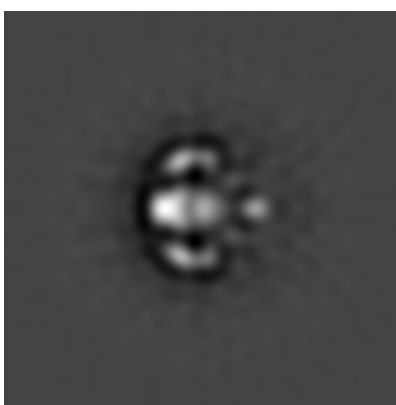
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

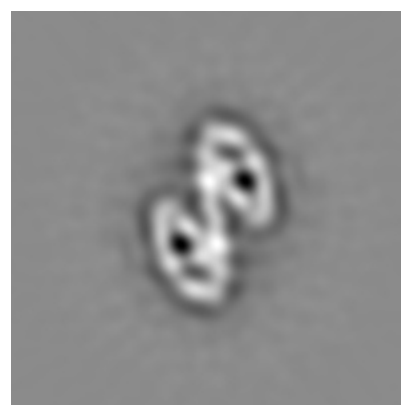
6.1.1 Primary map



X



Y



Z

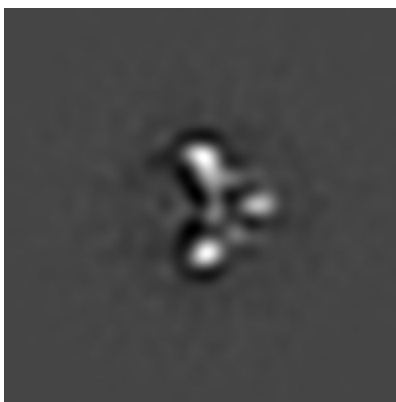
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

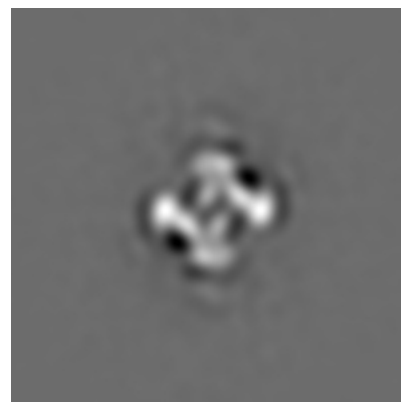
6.2.1 Primary map



X Index: 48



Y Index: 48



Z Index: 48

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 48



Y Index: 47

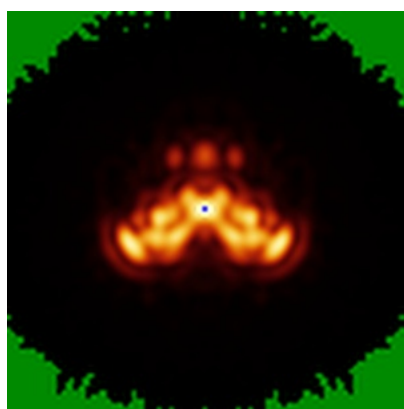


Z Index: 41

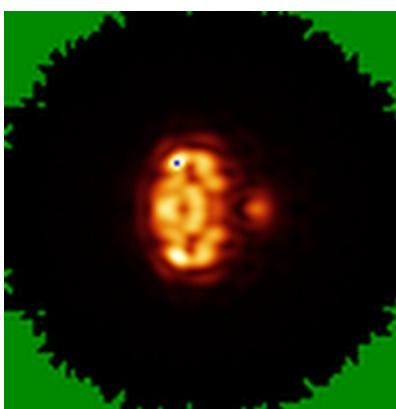
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

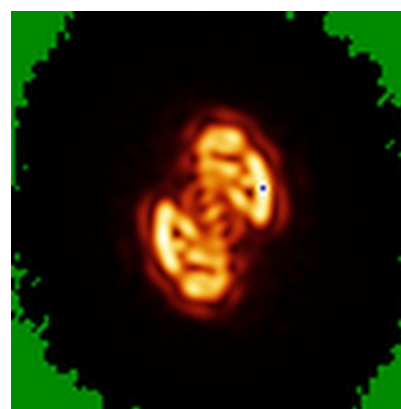
6.4.1 Primary map



X



Y

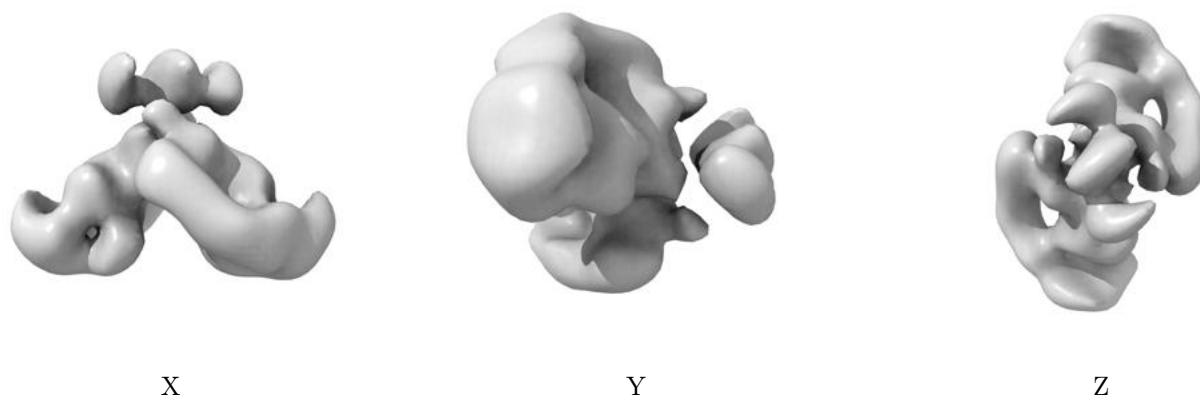


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.42. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

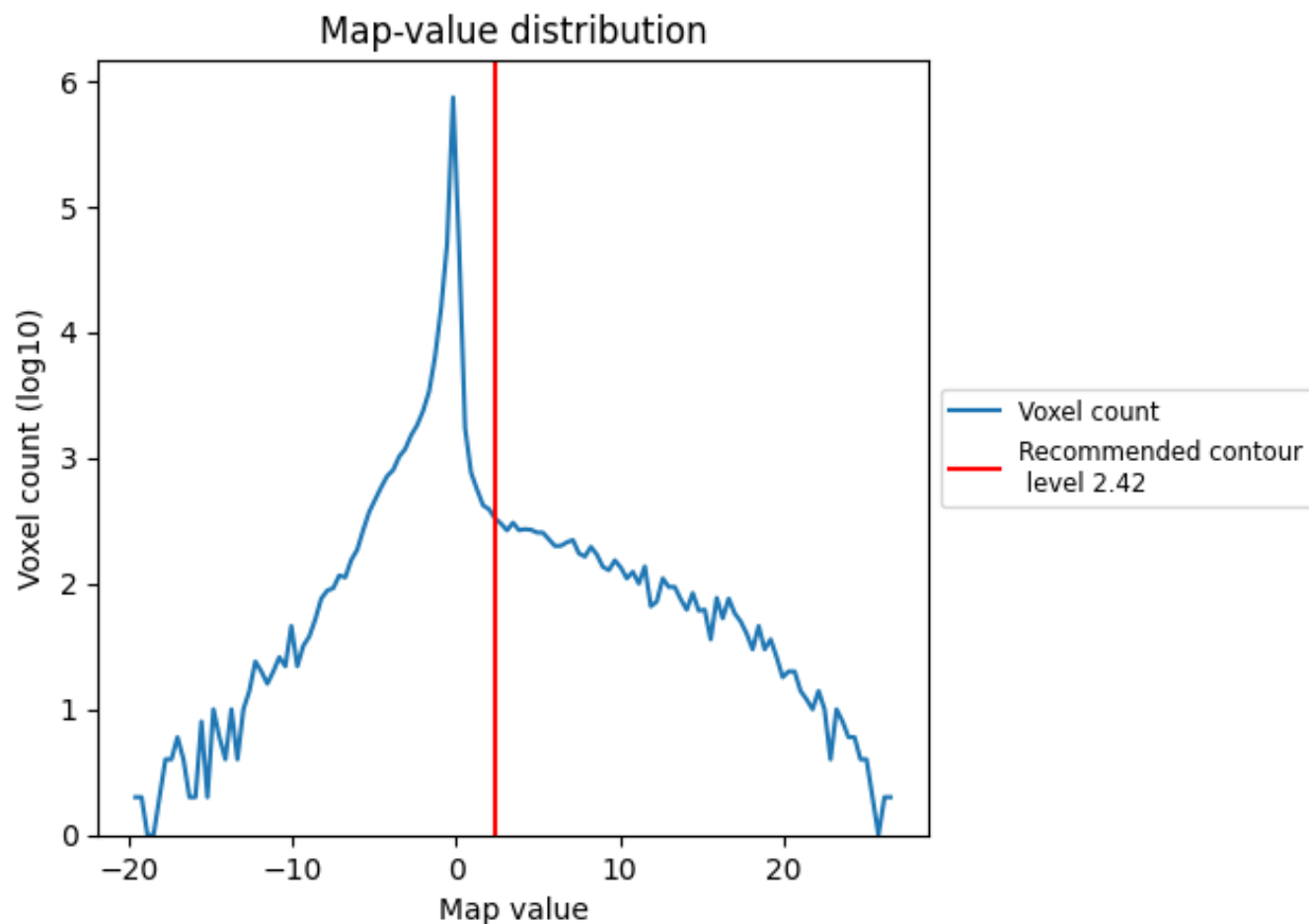
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

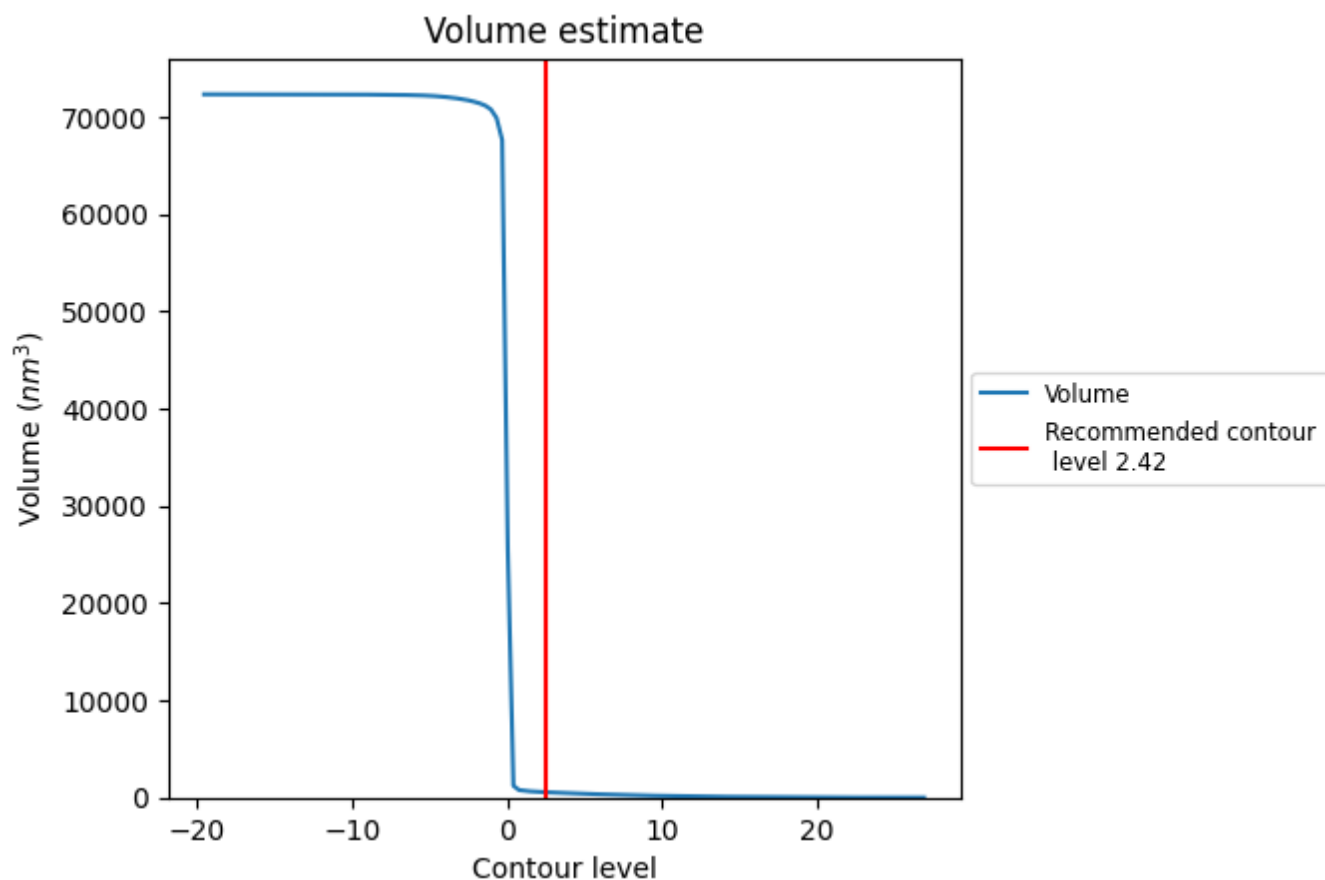
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

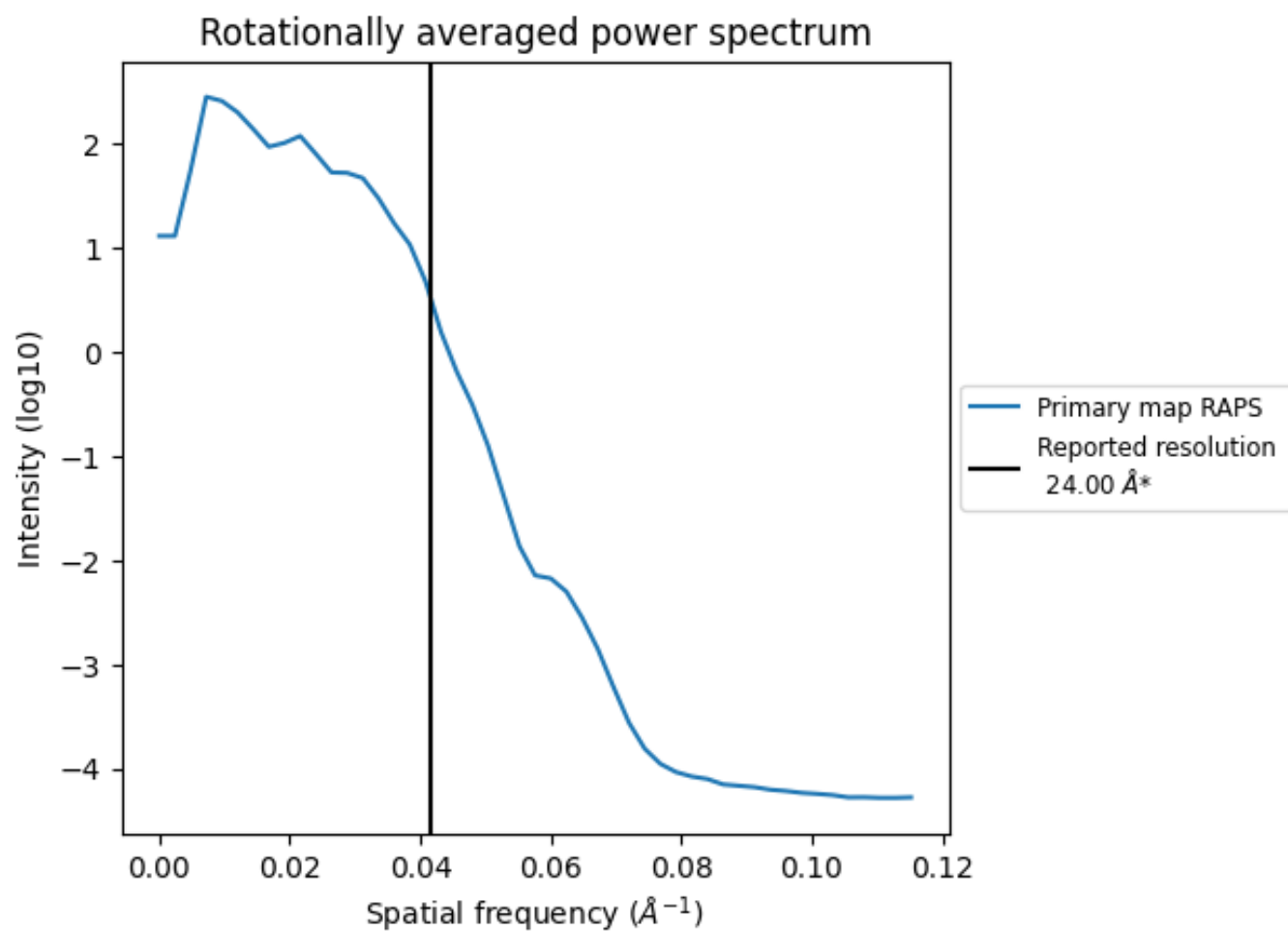
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 552 nm³; this corresponds to an approximate mass of 499 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.042 Å⁻¹

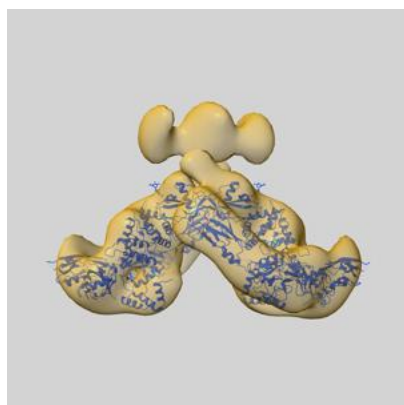
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

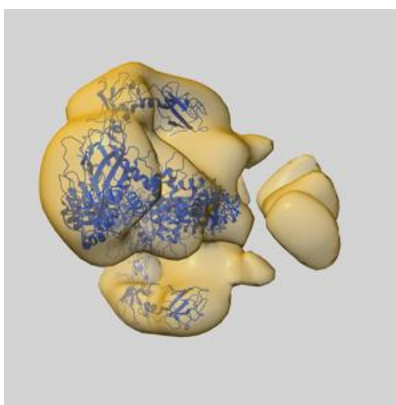
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2712 and PDB model 4UX8. Per-residue inclusion information can be found in section [3](#) on page [6](#).

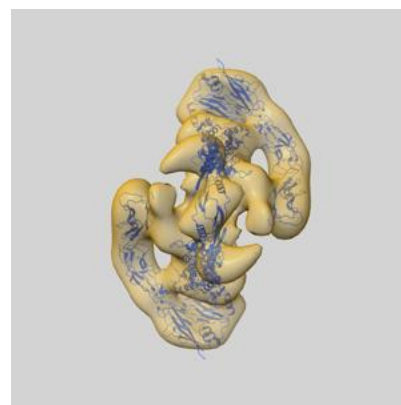
9.1 Map-model overlay [i](#)



X



Y



Z

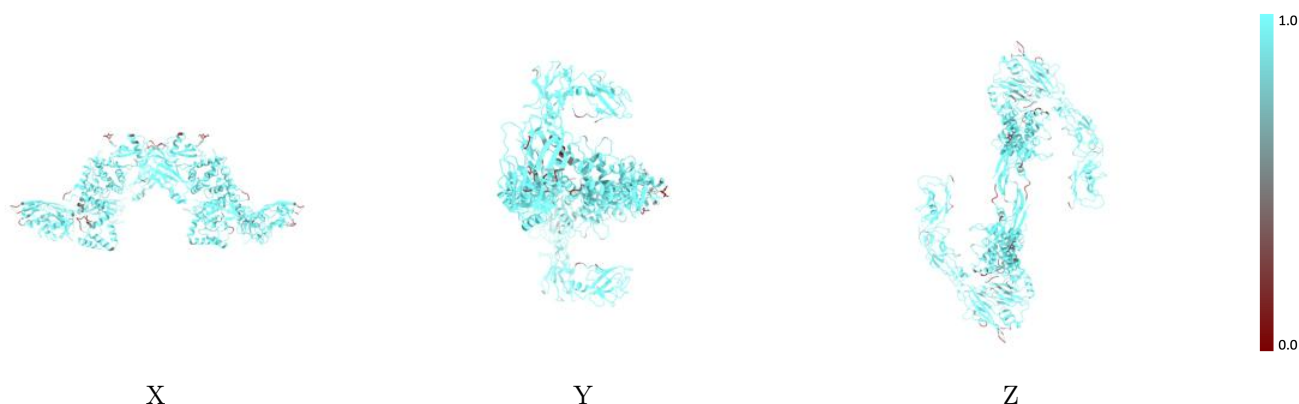
The images above show the 3D surface view of the map at the recommended contour level 2.42 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



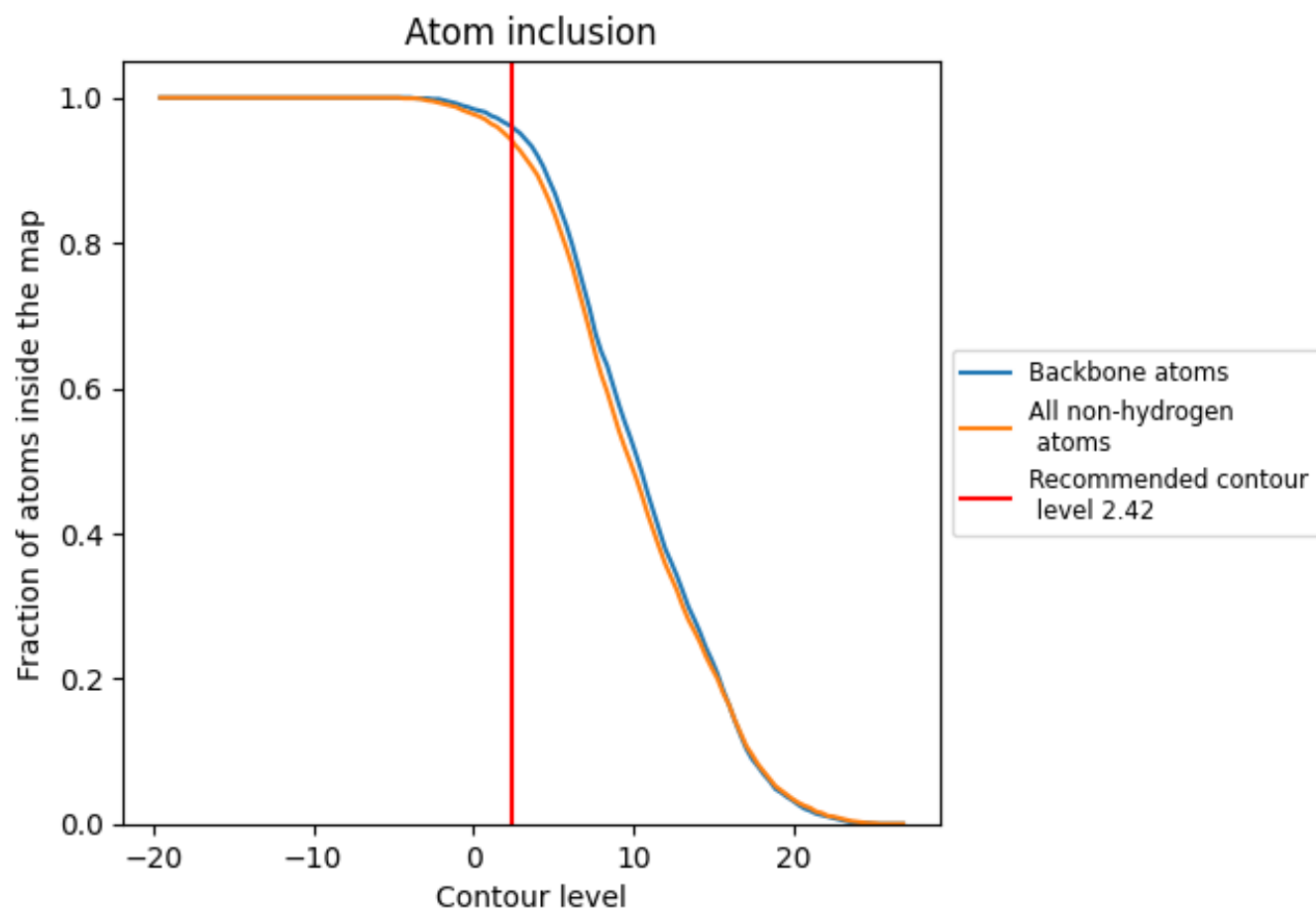
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.42).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (2.42) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9410	0.0620
A	0.9470	0.0710
B	0.9460	0.0700
C	0.9330	0.0470
D	0.9300	0.0560
E	0.9520	0.0550
F	0.9260	0.0590
G	0.3570	0.0490
H	0.3570	0.0390

1.0

0.0

<0.0