Full wwPDB EM Validation Report ⓘ

Jun 9, 2025 – 08:36 PM JST

PDB ID	:	8Y45 / pdb_00008y45
EMDB ID	:	EMD-38909
Title	:	Cryo-EM structure of opioid receptor with biased agonist
Authors	:	Lin, C.; Chang, Z.
Deposited on	:	2024-01-30
Resolution	:	3.45 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:

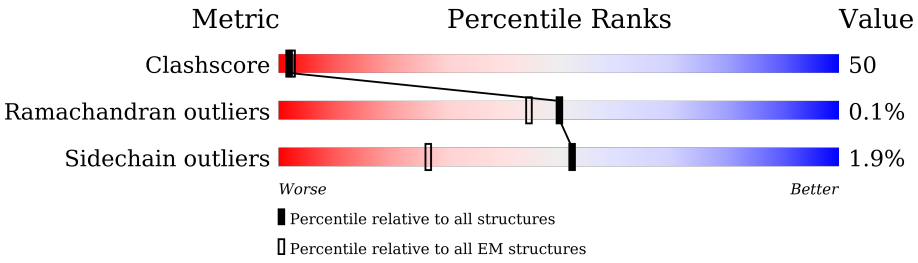
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 3.45 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	325	22% 37% 29% · 12%
2	B	358	30% 43% 22% 5%
3	D	355	25% 27% 12% 37%
4	S	266	29% 42% 17% 13%
5	C	71	28% 30% 23% 20%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8867 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 Delta-type opioid receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	286	2244	1486	367	370	21	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	ASP	-	expression tag	UNP P41143
A	29	TYR	-	expression tag	UNP P41143
A	30	LYS	-	expression tag	UNP P41143
A	31	ASP	-	expression tag	UNP P41143
A	32	ASP	-	expression tag	UNP P41143
A	33	ASP	-	expression tag	UNP P41143
A	34	ASP	-	expression tag	UNP P41143
A	35	ALA	-	expression tag	UNP P41143

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	340	2603	1606	469	508	20	0	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	MET	-	initiating methionine	UNP P62873
B	-16	PRO	-	expression tag	UNP P62873
B	-15	PRO	-	expression tag	UNP P62873
B	-14	HIS	-	expression tag	UNP P62873
B	-13	HIS	-	expression tag	UNP P62873
B	-12	HIS	-	expression tag	UNP P62873
B	-11	HIS	-	expression tag	UNP P62873
B	-10	LEU	-	expression tag	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	GLU	-	expression tag	UNP P62873
B	-8	VAL	-	expression tag	UNP P62873
B	-7	LEU	-	expression tag	UNP P62873
B	-6	PHE	-	expression tag	UNP P62873
B	-5	GLN	-	expression tag	UNP P62873
B	-4	GLY	-	expression tag	UNP P62873
B	-3	PRO	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	GLY	-	expression tag	UNP P62873

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(i) subunit alpha-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	223	Total	C	N	O	S	0	0
			1786	1138	297	339	12		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	5	LEU	VAL	variant	UNP P04899
D	47	ASN	SER	conflict	UNP P04899
D	204	ALA	GLY	conflict	UNP P04899
D	246	ALA	GLU	conflict	UNP P04899
D	327	SER	ALA	conflict	UNP P04899

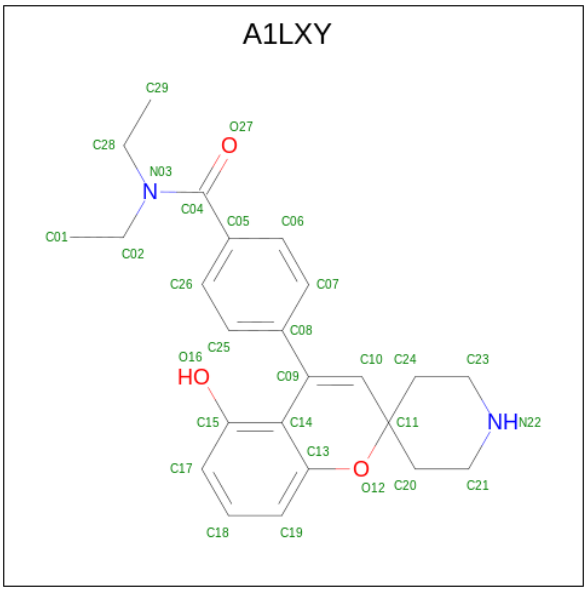
- Molecule 4 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	232	Total	C	N	O	S	0	0
			1767	1121	291	346	9		

- Molecule 5 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	57	Total	C	N	O	S	0	0
			438	274	77	84	3		

- Molecule 6 is {N}, {N}-diethyl-4-(5-oxidanylspiro[chromene-2,4'-piperidine]-4-yl)benzamide (CCD ID: A1LXY) (formula: $C_{24}H_{28}N_2O_3$).



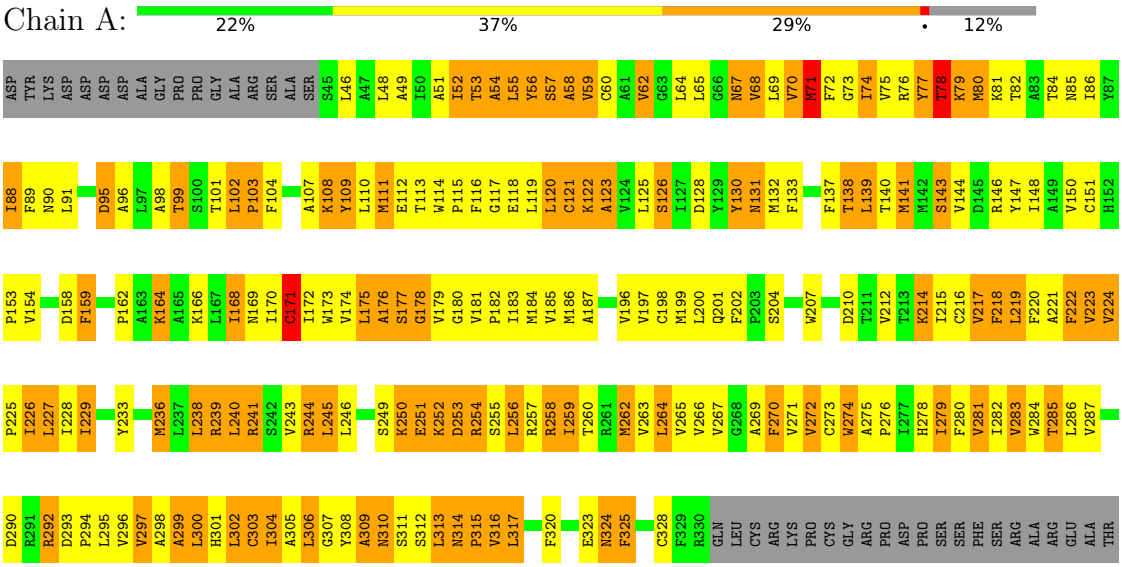
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	A	1	29	24	2	3	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

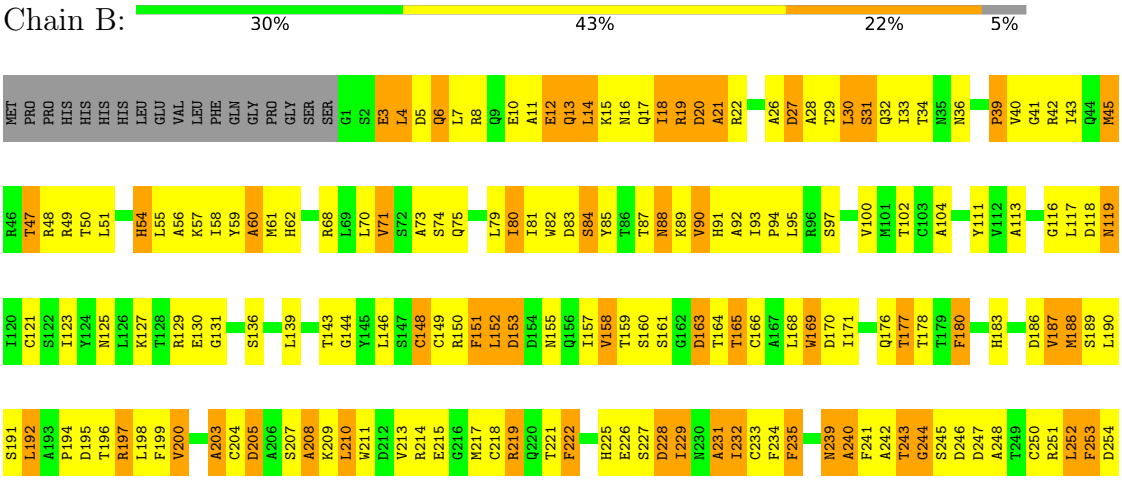
• Molecule 1: Delta-type opioid receptor

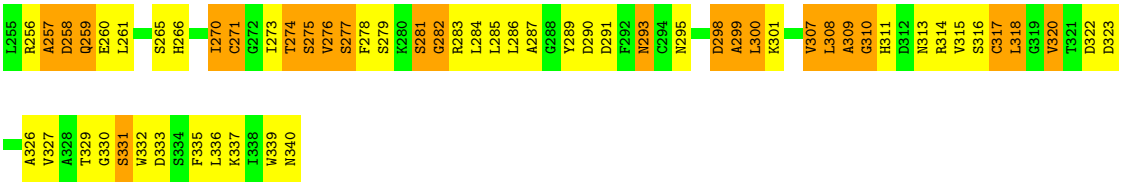
Chain A:



• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

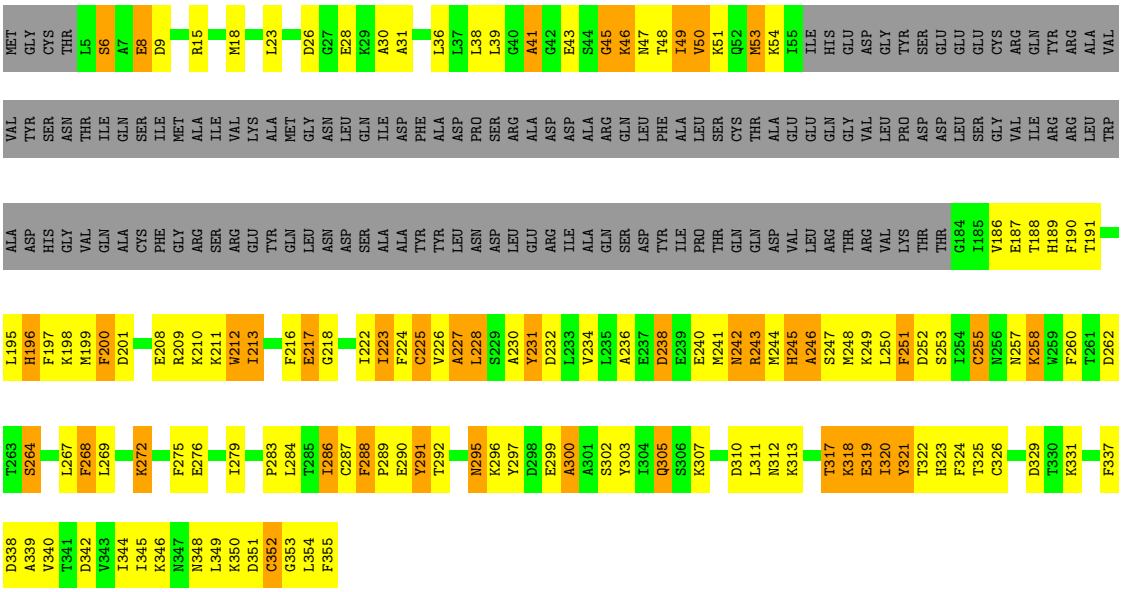
Chain B:





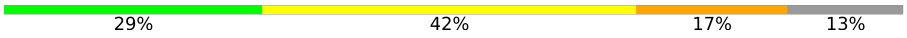
• Molecule 3: Guanine nucleotide-binding protein G(i) subunit alpha-2

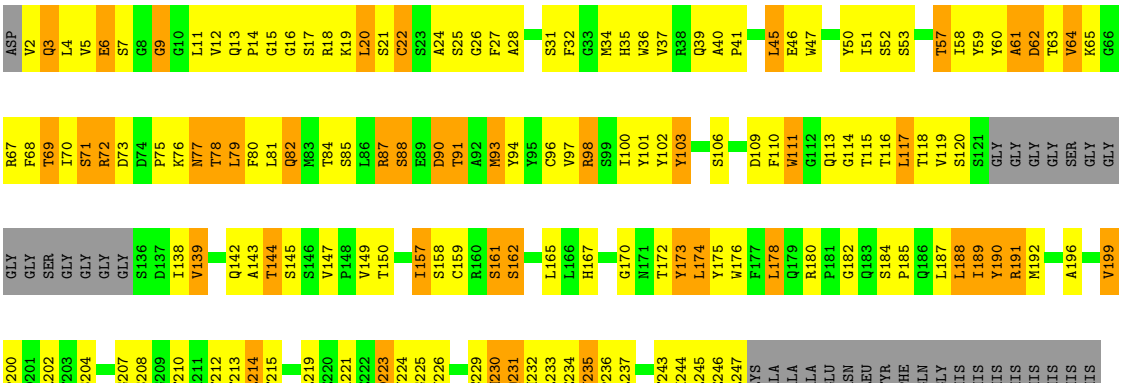
Chain D:



• Molecule 4: scFv16

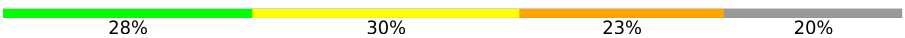
Chain S:

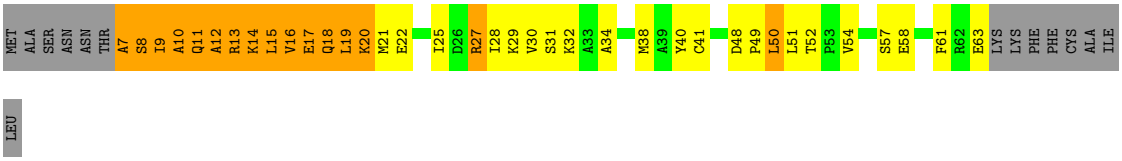




• Molecule 5: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain C:




MET
ALA
SER
ASN
ASN
THR
A7
S8
I9
A10
Q11
A12
R13
K14
L15
V16
E17
Q18
L19
K20
M21
E22
I25
D26
R27
I28
K29
V30
S31
K32
A33
A34
M38
A39
Y40
C41
D48
P49
L50
L51
T52
P53
V54
S57
E58
F61
R62
E63
LYS
LYS
PHE
PHE
CYS
ALA
ILE
LEU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	676428	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI SPIRIT	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	65	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.707	Depositor
Minimum map value	-3.056	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.080	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	217.6, 217.6, 217.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1LXY

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	1.82	85/2297 (3.7%)	2.13	145/3132 (4.6%)
2	B	1.83	87/2650 (3.3%)	1.73	92/3592 (2.6%)
3	D	1.71	69/1817 (3.8%)	1.40	32/2438 (1.3%)
4	S	1.92	71/1811 (3.9%)	1.60	46/2458 (1.9%)
5	C	2.32	24/444 (5.4%)	2.67	54/599 (9.0%)
All	All	1.85	336/9019 (3.7%)	1.82	369/12219 (3.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
4	S	0	1
All	All	0	3

All (336) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	93	ILE	C-N	20.99	1.58	1.33
1	A	54	ALA	C-N	20.89	1.58	1.33
2	B	21	ALA	C-N	20.11	1.59	1.33
4	S	7	SER	C-N	18.43	1.60	1.33
1	A	159	PHE	C-N	18.34	1.56	1.33
2	B	18	ILE	C-N	17.41	1.57	1.33
5	C	9	ILE	C-N	16.11	1.55	1.33
2	B	188	MET	C-N	15.65	1.52	1.33
4	S	91	THR	C-N	14.82	1.51	1.33
5	C	14	LYS	C-N	14.53	1.52	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	225	CYS	C-N	14.45	1.51	1.33
4	S	90	ASP	C-N	14.22	1.53	1.33
2	B	205	ASP	C-N	14.12	1.51	1.33
2	B	14	LEU	C-N	13.87	1.52	1.33
3	D	307	LYS	C-N	13.87	1.53	1.33
2	B	253	PHE	C-N	13.71	1.53	1.33
3	D	350	LYS	C-N	13.57	1.51	1.33
4	S	188	LEU	C-N	13.18	1.51	1.33
4	S	3	GLN	C-N	13.16	1.50	1.33
4	S	18	ARG	C-N	12.97	1.52	1.33
3	D	292	THR	C-N	12.78	1.47	1.33
4	S	61	ALA	C-N	12.76	1.50	1.33
1	A	180	GLY	C-N	12.52	1.50	1.34
5	C	13	ARG	C-N	12.48	1.50	1.33
2	B	243	THR	C-N	12.46	1.50	1.33
4	S	185	PRO	C-N	12.39	1.48	1.33
4	S	100	ILE	C-N	12.15	1.49	1.33
1	A	292	ARG	C-N	11.89	1.49	1.33
4	S	230	MET	C-N	11.83	1.50	1.33
5	C	11	GLN	C-N	11.75	1.48	1.33
2	B	59	TYR	C-N	11.67	1.48	1.33
1	A	314	ASN	C-N	-11.66	1.23	1.33
5	C	17	GLU	C-N	11.65	1.49	1.33
4	S	71	SER	C-N	11.64	1.49	1.33
4	S	5	VAL	C-N	11.51	1.49	1.33
4	S	147	VAL	C-N	11.47	1.47	1.33
2	B	204	CYS	C-N	11.33	1.48	1.33
4	S	28	ALA	C-N	11.31	1.49	1.33
1	A	52	ILE	C-N	11.20	1.48	1.33
5	C	27	ARG	C-N	11.11	1.43	1.33
4	S	191	ARG	C-N	10.94	1.47	1.33
2	B	117	LEU	C-N	10.93	1.50	1.33
1	A	316	VAL	C-N	10.90	1.48	1.33
1	A	219	LEU	C-N	10.83	1.49	1.34
4	S	64	VAL	C-N	10.73	1.47	1.33
5	C	49	PRO	C-N	10.61	1.49	1.33
2	B	169	TRP	C-N	-10.59	1.20	1.33
3	D	310	ASP	C-N	10.48	1.49	1.33
1	A	315	PRO	C-N	-10.48	1.20	1.33
4	S	213	THR	C-N	10.37	1.47	1.33
4	S	20	LEU	C-N	10.30	1.47	1.33
2	B	41	GLY	C-N	10.24	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	289	PRO	C-N	10.24	1.50	1.33
3	D	288	PHE	C-N	-10.16	1.21	1.33
3	D	300	ALA	C-N	-10.13	1.20	1.33
2	B	153	ASP	C-N	-10.10	1.21	1.33
5	C	12	ALA	C-N	10.06	1.47	1.33
5	C	8	SER	C-N	10.04	1.46	1.33
1	A	164	LYS	C-N	10.02	1.46	1.33
3	D	216	PHE	C-N	10.00	1.46	1.33
2	B	208	ALA	C-N	9.98	1.47	1.33
1	A	323	GLU	C-N	9.97	1.47	1.33
2	B	92	ALA	C-N	9.94	1.42	1.33
2	B	277	SER	C-N	-9.86	1.21	1.33
3	D	319	GLU	C-N	9.85	1.47	1.33
3	D	339	ALA	C-N	-9.80	1.22	1.33
2	B	50	THR	C-N	9.75	1.49	1.33
1	A	317	LEU	C-N	9.72	1.50	1.33
2	B	285	LEU	C-N	9.71	1.47	1.33
1	A	214	LYS	C-N	9.70	1.46	1.33
4	S	199	VAL	C-N	9.64	1.45	1.33
1	A	262	MET	C-N	-9.61	1.23	1.34
4	S	224	VAL	C-N	9.56	1.42	1.33
2	B	47	THR	C-N	-9.55	1.21	1.33
4	S	143	ALA	C-N	-9.54	1.20	1.33
2	B	271	CYS	C-N	9.51	1.50	1.33
3	D	217	GLU	C-N	9.51	1.48	1.33
2	B	323	ASP	C-N	9.49	1.45	1.33
4	S	111	TRP	C-N	9.48	1.47	1.33
1	A	70	VAL	C-N	-9.46	1.21	1.33
3	D	228	LEU	C-N	9.46	1.45	1.33
1	A	59	VAL	C-N	9.45	1.45	1.33
3	D	321	TYR	C-N	9.39	1.47	1.33
4	S	225	GLY	C-N	9.34	1.45	1.33
4	S	45	LEU	C-N	9.30	1.45	1.33
3	D	253	SER	C-N	-9.28	1.21	1.33
2	B	178	THR	C-N	9.27	1.46	1.33
5	C	10	ALA	C-N	9.25	1.46	1.33
1	A	185	VAL	C-N	-9.25	1.21	1.33
2	B	226	GLU	C-N	9.24	1.41	1.33
1	A	148	ILE	C-N	9.23	1.46	1.33
1	A	222	PHE	C-N	9.19	1.44	1.33
2	B	326	ALA	C-N	-9.03	1.22	1.33
2	B	240	ALA	C-N	-9.02	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	PRO	C-N	-8.91	1.22	1.33
3	D	226	VAL	C-N	-8.89	1.20	1.33
2	B	274	THR	C-N	8.88	1.44	1.33
1	A	89	PHE	C-N	-8.86	1.22	1.33
1	A	141	MET	C-N	-8.85	1.22	1.33
1	A	154	VAL	C-N	8.84	1.47	1.33
1	A	296	VAL	C-N	-8.83	1.22	1.33
5	C	28	ILE	C-N	8.80	1.45	1.33
1	A	223	VAL	C-N	8.75	1.45	1.34
4	S	67	ARG	C-N	-8.67	1.21	1.33
5	C	25	ILE	C-N	8.67	1.45	1.33
4	S	98	ARG	C-N	-8.66	1.22	1.33
2	B	71	VAL	C-N	-8.65	1.21	1.33
5	C	40	TYR	C-N	-8.65	1.22	1.34
2	B	282	GLY	C-N	-8.57	1.22	1.33
4	S	158	SER	C-N	8.54	1.45	1.33
2	B	318	LEU	C-N	8.51	1.46	1.33
5	C	57	SER	C-N	8.51	1.45	1.34
3	D	223	ILE	C-N	-8.48	1.22	1.33
1	A	241	ARG	C-N	8.40	1.46	1.33
5	C	29	LYS	C-N	8.36	1.44	1.33
2	B	309	ALA	C-N	-8.35	1.21	1.33
2	B	192	LEU	C-N	8.34	1.48	1.33
2	B	209	LYS	C-N	-8.30	1.21	1.33
4	S	34	MET	C-N	-8.30	1.21	1.33
4	S	78	THR	C-N	-8.29	1.23	1.33
1	A	168	ILE	C-N	-8.25	1.23	1.33
2	B	322	ASP	C-N	-8.21	1.22	1.33
3	D	195	LEU	C-N	-8.20	1.22	1.33
2	B	159	THR	C-N	8.18	1.44	1.33
1	A	285	THR	C-N	8.11	1.44	1.33
3	D	305	GLN	C-N	8.10	1.45	1.33
2	B	194	PRO	C-N	-8.08	1.23	1.33
1	A	62	VAL	C-N	8.08	1.45	1.33
3	D	302	SER	C-N	-8.06	1.23	1.33
1	A	166	LYS	C-N	-8.05	1.23	1.33
1	A	218	PHE	C-N	8.00	1.43	1.33
3	D	272	LYS	C-N	-7.88	1.23	1.33
3	D	46	LYS	C-N	-7.79	1.23	1.33
1	A	280	PHE	C-N	-7.75	1.24	1.33
2	B	222	PHE	C-N	7.75	1.44	1.33
3	D	317	THR	C-N	7.75	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	287	ALA	C-N	7.74	1.38	1.33
1	A	144	VAL	C-N	-7.72	1.23	1.33
3	D	36	LEU	C-N	-7.67	1.22	1.33
2	B	127	LYS	C-N	-7.65	1.23	1.33
1	A	176	ALA	C-N	-7.63	1.23	1.33
2	B	293	ASN	C-N	-7.62	1.23	1.33
1	A	103	PRO	C-N	-7.60	1.24	1.33
2	B	197	ARG	C-N	7.56	1.45	1.33
2	B	290	ASP	C-N	7.55	1.44	1.33
3	D	238	ASP	C-N	7.55	1.45	1.33
3	D	287	CYS	C-N	7.54	1.49	1.33
5	C	16	VAL	C-N	7.53	1.43	1.33
4	S	69	THR	C-N	-7.53	1.25	1.33
4	S	187	LEU	C-N	7.48	1.44	1.33
2	B	265	SER	C-N	-7.44	1.23	1.33
4	S	24	ALA	C-N	7.42	1.43	1.33
3	D	320	ILE	C-N	-7.37	1.22	1.33
3	D	41	ALA	C-N	7.37	1.44	1.33
4	S	47	TRP	C-N	7.37	1.44	1.33
1	A	252	LYS	C-N	7.36	1.44	1.34
1	A	303	CYS	C-N	7.34	1.43	1.34
4	S	53	SER	C-N	-7.34	1.22	1.33
4	S	178	LEU	C-N	-7.33	1.23	1.33
4	S	62	ASP	C-N	7.28	1.44	1.33
4	S	145	SER	C-N	7.28	1.42	1.33
1	A	253	ASP	C-N	7.26	1.43	1.34
4	S	231	GLN	C-N	7.24	1.43	1.33
3	D	200	PHE	C-N	-7.24	1.23	1.33
4	S	200	PRO	C-N	7.23	1.44	1.33
1	A	290	ASP	C-N	7.21	1.42	1.33
3	D	353	GLY	C-N	7.20	1.42	1.33
1	A	82	THR	C-N	-7.18	1.24	1.34
2	B	170	ASP	C-N	7.17	1.43	1.33
3	D	227	ALA	C-N	7.16	1.43	1.33
3	D	240	GLU	C-N	-7.14	1.24	1.33
1	A	187	ALA	C-N	7.14	1.43	1.33
3	D	191	THR	C-N	-7.14	1.23	1.33
2	B	229	ILE	C-N	-7.13	1.24	1.33
2	B	58	ILE	C-N	7.11	1.43	1.33
4	S	235	TYR	C-N	-7.10	1.25	1.33
3	D	213	ILE	C-N	7.09	1.43	1.33
3	D	323	HIS	C-N	-7.08	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	306	LEU	C-N	7.06	1.41	1.33
3	D	311	LEU	C-N	-7.05	1.23	1.33
4	S	196	ALA	C-N	7.05	1.43	1.33
4	S	17	SER	C-N	7.05	1.42	1.33
4	S	52	SER	CA-CB	-7.03	1.42	1.53
3	D	6	SER	C-N	-6.97	1.24	1.33
5	C	32	LYS	C-N	6.97	1.43	1.34
2	B	131	GLY	C-N	6.95	1.43	1.33
2	B	311	HIS	C-N	-6.95	1.24	1.33
3	D	234	VAL	C-N	-6.93	1.24	1.33
1	A	281	VAL	C-N	-6.92	1.25	1.33
4	S	192	MET	C-N	6.90	1.43	1.33
2	B	327	VAL	C-N	6.87	1.43	1.33
3	D	258	LYS	C-N	-6.87	1.23	1.33
3	D	290	GLU	C-N	-6.84	1.23	1.33
1	A	74	ILE	C-N	-6.83	1.25	1.33
3	D	53	MET	C-N	-6.82	1.24	1.33
3	D	232	ASP	C-N	6.81	1.41	1.33
1	A	244	ARG	C-N	-6.79	1.24	1.33
1	A	86	ILE	C-N	-6.78	1.24	1.33
3	D	318	LYS	C-N	-6.77	1.23	1.33
2	B	195	ASP	C-N	6.77	1.43	1.33
2	B	100	VAL	C-N	-6.75	1.22	1.33
1	A	99	THR	C-N	-6.74	1.24	1.33
1	A	320	PHE	C-N	6.74	1.44	1.33
1	A	227	LEU	C-N	6.72	1.42	1.33
2	B	219	ARG	C-N	-6.70	1.25	1.33
1	A	80	MET	C-N	-6.70	1.24	1.33
4	S	167	HIS	C-N	-6.69	1.25	1.33
1	A	178	GLY	C-N	-6.68	1.25	1.33
3	D	313	LYS	C-N	-6.66	1.24	1.33
3	D	245	HIS	C-N	-6.63	1.25	1.33
2	B	331	SER	C-N	-6.58	1.24	1.33
2	B	36	ASN	C-N	6.57	1.43	1.33
3	D	337	PHE	C-N	6.56	1.42	1.33
3	D	231	TYR	C-N	6.51	1.42	1.33
4	S	60	TYR	C-N	-6.51	1.24	1.33
5	C	15	LEU	C-N	6.44	1.42	1.33
2	B	119	ASN	C-N	-6.42	1.25	1.33
1	A	104	PHE	C-N	-6.39	1.24	1.33
2	B	55	LEU	C-N	-6.39	1.23	1.33
3	D	243	ARG	C-N	-6.37	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	196	HIS	C-N	6.37	1.42	1.33
4	S	32	PHE	C-N	-6.37	1.21	1.33
1	A	264	LEU	C-N	6.35	1.41	1.33
5	C	58	GLU	C-N	-6.34	1.22	1.33
3	D	286	ILE	C-N	-6.33	1.24	1.33
4	S	150	THR	C-N	-6.25	1.25	1.33
1	A	84	THR	C-N	6.25	1.42	1.33
4	S	144	THR	C-N	6.24	1.42	1.33
2	B	310	GLY	C-N	-6.23	1.24	1.33
1	A	53	THR	C-N	6.21	1.41	1.33
2	B	177	THR	C-N	-6.21	1.25	1.33
4	S	170	GLY	C-N	-6.18	1.26	1.33
1	A	98	ALA	C-N	6.17	1.42	1.33
3	D	295	ASN	C-N	-6.17	1.25	1.33
2	B	152	LEU	C-N	6.12	1.42	1.33
1	A	115	PRO	C-N	-6.12	1.24	1.33
4	S	173	TYR	C-N	6.10	1.41	1.33
2	B	87	THR	C-N	6.10	1.41	1.33
2	B	125	ASN	C-N	-6.10	1.25	1.33
2	B	221	THR	C-N	6.09	1.42	1.33
2	B	176	GLN	C-N	-6.08	1.25	1.33
3	D	296	LYS	C-N	6.03	1.41	1.33
5	C	18	GLN	C-N	6.02	1.42	1.33
1	A	68	VAL	C-N	-6.01	1.26	1.33
3	D	268	PHE	C-N	-5.99	1.25	1.33
1	A	196	VAL	C-N	-5.97	1.25	1.33
4	S	75	PRO	C-N	5.96	1.42	1.33
2	B	228	ASP	C-N	-5.93	1.25	1.33
2	B	84	SER	CA-CB	-5.90	1.44	1.53
4	S	207	GLY	C-N	5.89	1.40	1.33
1	A	102	LEU	C-N	5.88	1.42	1.34
1	A	245	LEU	C-N	-5.84	1.24	1.33
2	B	90	VAL	C-N	-5.82	1.26	1.33
3	D	338	ASP	C-N	-5.82	1.26	1.33
2	B	218	CYS	C-N	-5.80	1.25	1.33
4	S	190	TYR	C-N	-5.80	1.25	1.33
2	B	75	GLN	C-N	5.80	1.42	1.33
3	D	260	PHE	C-N	5.74	1.41	1.34
3	D	352	CYS	C-N	-5.74	1.25	1.33
4	S	215	THR	C-N	5.73	1.40	1.33
3	D	30	ALA	C-N	5.68	1.42	1.33
1	A	140	THR	C-N	5.68	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	52	THR	C-N	-5.65	1.26	1.33
3	D	264	SER	C-N	5.63	1.40	1.33
1	A	171	CYS	C-N	5.63	1.41	1.33
2	B	56	ALA	C-N	-5.63	1.26	1.33
3	D	251	PHE	C-N	5.62	1.41	1.33
2	B	276	VAL	C-N	5.61	1.41	1.33
2	B	333	ASP	C-N	5.60	1.41	1.33
3	D	31	ALA	C-N	-5.59	1.23	1.33
1	A	76	ARG	C-N	5.59	1.42	1.33
1	A	138	THR	C-N	-5.59	1.26	1.34
4	S	21	SER	C-N	-5.57	1.26	1.33
4	S	6	GLU	C-N	5.57	1.40	1.33
3	D	255	CYS	C-N	5.57	1.41	1.33
1	A	137	PHE	C-N	-5.56	1.26	1.33
4	S	189	ILE	C-N	-5.54	1.25	1.33
2	B	19	ARG	C-N	-5.52	1.26	1.33
1	A	270	PHE	C-N	5.52	1.40	1.33
1	A	79	LYS	C-N	-5.51	1.25	1.33
4	S	162	SER	C-N	5.49	1.40	1.33
2	B	335	PHE	C-N	-5.49	1.25	1.33
3	D	26	ASP	C-N	-5.49	1.27	1.34
1	A	77	TYR	C-N	-5.48	1.26	1.33
4	S	22	CYS	C-N	5.47	1.41	1.33
3	D	211	LYS	C-N	-5.45	1.25	1.33
4	S	223	ASP	C-N	-5.45	1.27	1.33
2	B	232	ILE	C-N	5.44	1.40	1.33
4	S	208	SER	C-N	-5.44	1.25	1.33
1	A	120	LEU	C-N	-5.42	1.26	1.34
1	A	269	ALA	C-N	-5.42	1.26	1.34
1	A	310	ASN	C-O	-5.41	1.17	1.24
1	A	121	CYS	C-N	-5.40	1.25	1.33
3	D	28	GLU	C-N	5.39	1.41	1.34
1	A	88	ILE	C-N	-5.39	1.26	1.33
2	B	45	MET	C-N	-5.37	1.26	1.33
2	B	316	SER	CA-CB	-5.35	1.44	1.53
4	S	117	LEU	C-N	-5.35	1.26	1.33
3	D	218	GLY	C-N	-5.33	1.21	1.33
2	B	136	SER	CA-CB	-5.33	1.46	1.53
1	A	139	LEU	C-O	-5.32	1.17	1.24
5	C	7	ALA	C-N	5.32	1.41	1.33
4	S	174	LEU	C-N	-5.31	1.25	1.33
2	B	42	ARG	C-N	-5.30	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	78	THR	C-N	-5.29	1.26	1.33
3	D	236	ALA	C-N	-5.29	1.26	1.33
2	B	116	GLY	C-N	-5.28	1.26	1.33
2	B	80	ILE	C-N	5.28	1.40	1.33
1	A	308	TYR	C-N	-5.27	1.25	1.33
2	B	81	ILE	C-N	-5.26	1.27	1.33
2	B	299	ALA	C-N	-5.25	1.26	1.33
4	S	161	SER	C-N	-5.25	1.26	1.33
4	S	15	GLY	C-N	-5.24	1.24	1.33
2	B	308	LEU	C-N	5.23	1.40	1.33
1	A	81	LYS	C-N	-5.23	1.25	1.33
5	C	54	VAL	C-N	5.22	1.40	1.33
4	S	214	LEU	C-N	5.22	1.41	1.33
2	B	235	PHE	C-N	-5.20	1.27	1.33
1	A	111	MET	C-N	5.20	1.41	1.33
2	B	129	ARG	C-N	-5.19	1.27	1.34
1	A	304	ILE	C-O	5.19	1.30	1.24
4	S	103	TYR	C-N	-5.18	1.26	1.33
5	C	50	LEU	C-N	5.17	1.41	1.33
2	B	88	ASN	C-N	5.17	1.40	1.33
4	S	35	HIS	C-N	5.14	1.40	1.33
3	D	230	ALA	C-N	-5.12	1.26	1.33
4	S	31	SER	C-N	5.12	1.40	1.33
1	A	238	LEU	C-N	5.12	1.41	1.34
4	S	159	CYS	C-N	5.11	1.41	1.33
3	D	39	LEU	C-N	5.11	1.39	1.33
1	A	95	ASP	C-N	-5.09	1.27	1.33
1	A	220	PHE	C-N	-5.05	1.26	1.33
2	B	143	THR	C-N	5.05	1.38	1.32
3	D	15	ARG	C-N	-5.05	1.27	1.33
1	A	67	ASN	C-N	-5.04	1.26	1.33
1	A	71	MET	C-N	-5.03	1.27	1.33

All (369) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	52	ILE	O-C-N	20.90	142.37	121.89
1	A	52	ILE	CA-C-N	-17.45	97.76	120.44
1	A	52	ILE	C-N-CA	-17.45	97.76	120.44
1	A	53	THR	O-C-N	15.88	138.42	122.07
1	A	130	TYR	CB-CA-C	-15.09	86.39	110.08
4	S	77	ASN	O-C-N	14.10	140.04	122.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	177	SER	CA-C-N	-14.02	104.33	120.03
1	A	177	SER	C-N-CA	-14.02	104.33	120.03
5	C	12	ALA	O-C-N	13.94	136.59	122.09
5	C	11	GLN	O-C-N	13.58	136.51	122.12
2	B	14	LEU	O-C-N	13.38	136.30	122.12
5	C	8	SER	O-C-N	13.20	136.11	122.12
2	B	244	GLY	O-C-N	-12.65	111.80	123.57
4	S	77	ASN	CA-C-N	-12.57	103.08	122.81
4	S	77	ASN	C-N-CA	-12.57	103.08	122.81
1	A	223	VAL	CA-C-N	-12.34	112.47	120.24
1	A	223	VAL	C-N-CA	-12.34	112.47	120.24
1	A	53	THR	CA-C-N	-12.05	104.27	120.54
1	A	53	THR	C-N-CA	-12.05	104.27	120.54
2	B	192	LEU	O-C-N	-11.75	111.82	123.46
5	C	9	ILE	O-C-N	11.66	133.18	121.87
5	C	15	LEU	O-C-N	11.65	134.07	122.07
5	C	16	VAL	O-C-N	11.48	133.00	121.87
1	A	269	ALA	O-C-N	11.42	133.83	122.07
5	C	10	ALA	O-C-N	11.17	133.96	122.12
1	A	56	TYR	N-CA-C	-10.86	99.44	111.28
5	C	13	ARG	O-C-N	10.69	133.45	122.12
1	A	283	VAL	O-C-N	10.48	132.80	121.90
3	D	226	VAL	O-C-N	-10.48	112.28	123.18
4	S	67	ARG	O-C-N	10.41	137.14	122.36
4	S	67	ARG	CA-C-N	-10.34	104.72	122.92
4	S	67	ARG	C-N-CA	-10.34	104.72	122.92
1	A	216	CYS	CB-CA-C	-10.33	94.67	110.88
2	B	20	ASP	O-C-N	10.32	133.06	122.12
2	B	14	LEU	CA-C-N	-10.29	106.49	120.28
2	B	14	LEU	C-N-CA	-10.29	106.49	120.28
1	A	58	ALA	O-C-N	10.28	132.65	122.07
4	S	187	LEU	O-C-N	10.21	134.81	123.27
2	B	18	ILE	O-C-N	10.01	131.58	121.87
5	C	14	LYS	O-C-N	9.98	132.87	122.09
1	A	269	ALA	CA-C-N	-9.91	105.24	120.31
1	A	269	ALA	C-N-CA	-9.91	105.24	120.31
5	C	10	ALA	CA-C-N	-9.86	107.06	120.28
5	C	10	ALA	C-N-CA	-9.86	107.06	120.28
3	D	228	LEU	O-C-N	9.86	132.57	122.12
1	A	54	ALA	O-C-N	9.79	132.27	122.09
5	C	7	ALA	CA-C-N	-9.57	107.46	120.28
5	C	7	ALA	C-N-CA	-9.57	107.46	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	52	THR	CA-C-N	-9.45	110.31	119.85
5	C	52	THR	C-N-CA	-9.45	110.31	119.85
1	A	55	LEU	O-C-N	9.36	132.09	122.08
4	S	79	LEU	O-C-N	9.27	134.12	123.27
3	D	320	ILE	O-C-N	-9.19	113.26	123.18
2	B	204	CYS	O-C-N	-9.11	111.77	122.15
2	B	286	LEU	O-C-N	-9.02	113.07	123.27
1	A	117	GLY	O-C-N	8.97	134.36	122.70
1	A	224	VAL	O-C-N	8.94	126.42	120.07
1	A	57	SER	O-C-N	8.93	131.64	122.08
2	B	243	THR	CA-C-N	-8.90	112.18	121.35
2	B	243	THR	C-N-CA	-8.90	112.18	121.35
2	B	320	VAL	O-C-N	-8.89	113.50	122.93
5	C	7	ALA	O-C-N	8.88	137.20	123.00
5	C	13	ARG	CA-C-N	-8.86	108.39	120.44
5	C	13	ARG	C-N-CA	-8.86	108.39	120.44
1	A	279	ILE	O-C-N	-8.53	113.60	121.87
4	S	101	TYR	O-C-N	-8.50	113.41	123.27
1	A	309	ALA	CB-CA-C	-8.42	94.11	110.11
3	D	50	VAL	O-C-N	8.42	130.04	121.87
2	B	298	ASP	O-C-N	-8.41	112.97	123.06
3	D	49	ILE	N-CA-C	-8.40	101.54	110.36
5	C	8	SER	CA-C-N	-8.36	109.01	120.46
5	C	8	SER	C-N-CA	-8.36	109.01	120.46
2	B	190	LEU	O-C-N	8.20	132.91	123.31
2	B	210	LEU	O-C-N	8.20	132.79	123.19
5	C	17	GLU	O-C-N	8.17	130.78	122.12
3	D	291	TYR	O-C-N	-8.15	113.51	123.04
1	A	54	ALA	CA-C-N	-8.14	109.47	120.79
1	A	54	ALA	C-N-CA	-8.14	109.47	120.79
1	A	310	ASN	N-CA-C	-8.14	100.74	111.24
1	A	308	TYR	N-CA-C	-8.06	102.54	112.38
5	C	12	ALA	CA-C-N	-8.02	109.53	120.28
5	C	12	ALA	C-N-CA	-8.02	109.53	120.28
2	B	266	HIS	O-C-N	-8.00	114.00	123.27
1	A	299	ALA	O-C-N	7.99	130.66	122.03
1	A	315	PRO	CA-C-N	-7.85	109.27	120.42
1	A	315	PRO	C-N-CA	-7.85	109.27	120.42
2	B	163	ASP	O-C-N	7.83	131.33	122.32
3	D	228	LEU	CA-C-N	-7.78	110.70	122.21
3	D	228	LEU	C-N-CA	-7.78	110.70	122.21
2	B	257	ALA	N-CA-C	-7.76	100.08	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	S	115	THR	O-C-N	7.75	131.74	123.06
1	A	229	ILE	O-C-N	-7.74	113.05	121.80
4	S	79	LEU	CA-C-N	-7.65	112.25	123.11
4	S	79	LEU	C-N-CA	-7.65	112.25	123.11
1	A	173	TRP	O-C-N	7.64	130.91	122.20
5	C	18	GLN	O-C-N	7.64	130.21	122.12
5	C	11	GLN	CA-C-N	-7.60	110.28	120.54
5	C	11	GLN	C-N-CA	-7.60	110.28	120.54
4	S	113	GLN	CA-C-N	-7.60	113.58	122.77
4	S	113	GLN	C-N-CA	-7.60	113.58	122.77
1	A	283	VAL	CA-C-N	-7.58	110.12	120.28
1	A	283	VAL	C-N-CA	-7.58	110.12	120.28
2	B	27	ASP	N-CA-C	-7.54	104.22	113.19
2	B	20	ASP	CA-C-N	-7.53	109.60	120.29
2	B	20	ASP	C-N-CA	-7.53	109.60	120.29
1	A	58	ALA	CA-C-N	-7.51	109.75	120.42
1	A	58	ALA	C-N-CA	-7.51	109.75	120.42
1	A	325	PHE	O-C-N	-7.50	113.05	122.27
1	A	254	ARG	O-C-N	7.50	130.99	122.22
1	A	293	ASP	O-C-N	-7.49	114.98	121.35
2	B	60	ALA	O-C-N	-7.45	115.13	123.48
5	C	9	ILE	CA-C-N	-7.45	110.30	120.28
5	C	9	ILE	C-N-CA	-7.45	110.30	120.28
3	D	213	ILE	O-C-N	7.43	132.14	122.26
5	C	15	LEU	CA-C-N	-7.33	110.42	120.46
5	C	15	LEU	C-N-CA	-7.33	110.42	120.46
2	B	13	GLN	O-C-N	7.30	129.86	122.12
2	B	243	THR	O-C-N	7.30	132.64	123.15
1	A	222	PHE	CA-C-N	-7.27	112.01	120.88
1	A	222	PHE	C-N-CA	-7.27	112.01	120.88
1	A	123	ALA	O-C-N	7.25	129.81	122.12
1	A	300	LEU	O-C-N	7.25	130.45	122.11
2	B	229	ILE	O-C-N	7.20	130.69	122.99
2	B	252	LEU	O-C-N	-7.17	114.84	123.29
5	C	16	VAL	CA-C-N	-7.16	110.68	120.28
5	C	16	VAL	C-N-CA	-7.16	110.68	120.28
3	D	213	ILE	CA-C-N	-7.14	110.80	122.65
3	D	213	ILE	C-N-CA	-7.14	110.80	122.65
1	A	284	TRP	O-C-N	7.06	129.60	122.12
3	D	226	VAL	CA-C-N	7.04	131.94	121.72
3	D	226	VAL	C-N-CA	7.04	131.94	121.72
1	A	226	ILE	O-C-N	7.02	128.68	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	272	VAL	CB-CA-C	-7.02	102.82	111.87
1	A	144	VAL	O-C-N	-6.98	115.10	121.87
5	C	54	VAL	O-C-N	6.93	129.00	121.10
1	A	256	LEU	N-CA-C	-6.92	103.74	111.28
4	S	61	ALA	O-C-N	6.91	130.80	121.74
1	A	300	LEU	CA-C-N	-6.91	109.81	120.31
1	A	300	LEU	C-N-CA	-6.91	109.81	120.31
2	B	244	GLY	CA-C-N	6.91	133.65	122.53
2	B	244	GLY	C-N-CA	6.91	133.65	122.53
1	A	224	VAL	CA-C-N	-6.85	111.45	119.05
1	A	224	VAL	C-N-CA	-6.85	111.45	119.05
1	A	264	LEU	CA-C-N	-6.80	111.86	120.56
1	A	264	LEU	C-N-CA	-6.80	111.86	120.56
3	D	286	ILE	O-C-N	-6.79	115.24	121.89
2	B	207	SER	O-C-N	-6.77	115.54	123.25
1	A	315	PRO	O-C-N	6.72	133.28	122.52
1	A	222	PHE	O-C-N	6.69	130.15	122.25
1	A	253	ASP	O-C-N	6.69	130.50	122.27
2	B	203	ALA	CA-C-N	6.66	129.75	120.29
2	B	203	ALA	C-N-CA	6.66	129.75	120.29
1	A	325	PHE	CA-C-N	6.66	129.09	120.44
1	A	325	PHE	C-N-CA	6.66	129.09	120.44
2	B	300	LEU	N-CA-C	-6.65	105.17	113.55
1	A	126	SER	CB-CA-C	-6.62	99.79	110.79
4	S	187	LEU	CA-C-N	-6.61	110.56	122.46
4	S	187	LEU	C-N-CA	-6.61	110.56	122.46
2	B	286	LEU	CA-C-N	6.60	132.31	123.00
2	B	286	LEU	C-N-CA	6.60	132.31	123.00
2	B	307	VAL	CA-C-N	-6.60	112.18	122.08
2	B	307	VAL	C-N-CA	-6.60	112.18	122.08
1	A	117	GLY	CA-C-N	-6.58	110.32	122.09
1	A	117	GLY	C-N-CA	-6.58	110.32	122.09
1	A	185	VAL	O-C-N	6.57	130.51	121.84
5	C	41	CYS	O-C-N	-6.53	114.24	122.27
1	A	229	ILE	CA-C-N	6.51	129.29	120.44
1	A	229	ILE	C-N-CA	6.51	129.29	120.44
1	A	223	VAL	O-C-N	6.50	129.87	121.94
5	C	54	VAL	CA-C-N	-6.46	113.12	119.78
5	C	54	VAL	C-N-CA	-6.46	113.12	119.78
5	C	20	LYS	O-C-N	-6.45	115.29	122.12
2	B	231	ALA	O-C-N	-6.44	115.50	123.36
1	A	324	ASN	O-C-N	-6.42	115.32	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	91	HIS	CA-C-N	6.41	131.60	121.72
2	B	91	HIS	C-N-CA	6.41	131.60	121.72
3	D	291	TYR	CA-C-N	6.40	132.17	122.95
3	D	291	TYR	C-N-CA	6.40	132.17	122.95
4	S	101	TYR	CA-C-N	6.39	133.82	122.45
4	S	101	TYR	C-N-CA	6.39	133.82	122.45
2	B	91	HIS	CA-CB-CG	6.37	120.17	113.80
1	A	126	SER	N-CA-C	6.37	118.22	111.28
2	B	266	HIS	CA-C-N	6.35	129.96	120.31
2	B	266	HIS	C-N-CA	6.35	129.96	120.31
1	A	315	PRO	N-CA-C	-6.34	105.80	114.80
3	D	252	ASP	O-C-N	-6.32	114.94	122.15
2	B	45	MET	O-C-N	6.30	130.05	122.68
1	A	299	ALA	CA-C-N	-6.29	111.39	120.82
1	A	299	ALA	C-N-CA	-6.29	111.39	120.82
2	B	18	ILE	CA-C-N	-6.28	111.38	120.29
2	B	18	ILE	C-N-CA	-6.28	111.38	120.29
2	B	75	GLN	O-C-N	-6.25	113.74	122.37
1	A	240	LEU	N-CA-C	-6.25	105.14	112.89
4	S	221	ALA	O-C-N	6.25	128.74	122.12
2	B	198	LEU	O-C-N	-6.24	115.56	123.24
2	B	158	VAL	O-C-N	-6.21	114.33	122.47
5	C	14	LYS	CA-C-N	-6.15	112.44	120.44
5	C	14	LYS	C-N-CA	-6.15	112.44	120.44
1	A	175	LEU	O-C-N	-6.15	115.19	122.20
2	B	203	ALA	O-C-N	-6.14	113.97	121.83
2	B	30	LEU	N-CA-C	-6.13	106.20	113.38
2	B	60	ALA	CA-C-N	6.12	130.71	121.40
2	B	60	ALA	C-N-CA	6.12	130.71	121.40
2	B	178	THR	O-C-N	-6.12	115.63	122.91
1	A	272	VAL	N-CA-C	6.12	116.17	110.42
2	B	13	GLN	CA-C-N	-6.12	112.08	120.28
2	B	13	GLN	C-N-CA	-6.12	112.08	120.28
4	S	7	SER	O-C-N	-6.11	116.64	123.48
2	B	210	LEU	CA-C-N	-6.10	112.56	122.81
2	B	210	LEU	C-N-CA	-6.10	112.56	122.81
1	A	62	VAL	O-C-N	-6.09	115.96	121.87
3	D	242	ASN	CA-C-N	-6.08	111.69	120.82
3	D	242	ASN	C-N-CA	-6.08	111.69	120.82
3	D	320	ILE	CA-C-N	6.08	132.35	122.81
3	D	320	ILE	C-N-CA	6.08	132.35	122.81
3	D	227	ALA	O-C-N	6.07	130.49	123.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	52	THR	O-C-N	6.04	131.50	121.59
4	S	93	MET	N-CA-C	-6.00	102.44	110.55
2	B	54	HIS	O-C-N	-6.00	115.66	122.68
5	C	20	LYS	CA-C-N	6.00	129.43	120.31
5	C	20	LYS	C-N-CA	6.00	129.43	120.31
1	A	250	LYS	N-CA-C	-5.96	105.10	112.38
1	A	251	GLU	CA-C-N	-5.96	113.19	122.67
1	A	251	GLU	C-N-CA	-5.96	113.19	122.67
2	B	180	PHE	O-C-N	5.92	129.59	122.85
1	A	253	ASP	CA-C-N	-5.91	111.76	120.28
1	A	253	ASP	C-N-CA	-5.91	111.76	120.28
1	A	293	ASP	CA-C-N	5.90	127.00	120.45
1	A	293	ASP	C-N-CA	5.90	127.00	120.45
2	B	39	PRO	CB-CA-C	-5.89	103.85	111.39
1	A	259	ILE	N-CA-C	-5.89	104.61	110.62
4	S	57	THR	N-CA-C	5.88	118.79	108.56
1	A	183	ILE	CB-CA-C	-5.87	104.36	111.88
2	B	151	PHE	O-C-N	-5.87	115.60	123.23
1	A	109	TYR	N-CA-C	-5.86	104.24	111.33
1	A	216	CYS	N-CA-C	5.85	117.33	111.07
1	A	254	ARG	CA-C-N	-5.84	111.43	120.31
1	A	254	ARG	C-N-CA	-5.84	111.43	120.31
1	A	226	ILE	CA-C-N	-5.84	112.50	120.44
1	A	226	ILE	C-N-CA	-5.84	112.50	120.44
1	A	55	LEU	N-CA-C	5.82	118.12	111.02
4	S	52	SER	CA-C-O	-5.82	115.45	122.03
1	A	304	ILE	O-C-N	5.82	127.78	121.90
3	D	212	TRP	O-C-N	5.82	129.53	122.20
2	B	192	LEU	CA-C-N	5.82	133.35	121.48
2	B	192	LEU	C-N-CA	5.82	133.35	121.48
4	S	71	SER	O-C-N	5.81	129.71	122.92
3	D	246	ALA	N-CA-C	-5.75	105.03	112.68
2	B	97	SER	O-C-N	-5.75	116.17	122.84
5	C	18	GLN	CA-C-N	-5.74	112.14	120.29
5	C	18	GLN	C-N-CA	-5.74	112.14	120.29
2	B	163	ASP	CA-C-N	-5.72	111.79	121.18
2	B	163	ASP	C-N-CA	-5.72	111.79	121.18
1	A	262	MET	O-C-N	5.72	127.97	122.07
4	S	139	VAL	O-C-N	5.72	128.87	122.75
3	D	53	MET	N-CA-C	-5.72	106.26	113.18
2	B	232	ILE	O-C-N	5.70	129.02	123.03
4	S	157	ILE	O-C-N	-5.70	117.05	122.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	143	SER	O-C-N	-5.68	115.67	122.15
2	B	228	ASP	CA-C-N	-5.67	115.53	123.13
2	B	228	ASP	C-N-CA	-5.67	115.53	123.13
1	A	236	MET	CA-C-N	-5.66	111.70	120.31
1	A	236	MET	C-N-CA	-5.66	111.70	120.31
1	A	297	VAL	O-C-N	5.66	127.36	121.87
1	A	123	ALA	CA-C-N	-5.66	113.32	120.56
1	A	123	ALA	C-N-CA	-5.66	113.32	120.56
4	S	87	ARG	N-CA-C	-5.65	104.98	112.94
1	A	279	ILE	CA-C-N	5.62	128.26	120.29
1	A	279	ILE	C-N-CA	5.62	128.26	120.29
3	D	45	GLY	O-C-N	-5.62	115.49	122.34
2	B	31	SER	N-CA-C	-5.61	105.22	112.68
5	C	22	GLU	O-C-N	-5.60	115.38	122.27
1	A	266	VAL	CA-C-N	-5.60	113.38	120.60
1	A	266	VAL	C-N-CA	-5.60	113.38	120.60
4	S	115	THR	CA-C-N	-5.59	114.52	122.41
4	S	115	THR	C-N-CA	-5.59	114.52	122.41
4	S	182	GLY	O-C-N	5.58	129.02	122.38
4	S	15	GLY	CA-C-N	-5.56	115.41	122.19
4	S	15	GLY	C-N-CA	-5.56	115.41	122.19
5	C	21	MET	O-C-N	-5.55	115.44	122.27
1	A	266	VAL	O-C-N	5.54	127.32	121.89
2	B	317	CYS	O-C-N	-5.54	116.84	123.27
2	B	12	GLU	N-CA-C	-5.53	105.33	111.36
4	S	72	ARG	O-C-N	-5.53	116.86	123.27
4	S	224	VAL	O-C-N	-5.51	116.66	122.67
1	A	186	MET	CA-C-N	-5.51	114.43	122.19
1	A	186	MET	C-N-CA	-5.51	114.43	122.19
5	C	32	LYS	O-C-N	-5.48	115.90	122.15
4	S	188	LEU	O-C-N	5.48	128.83	122.09
2	B	239	ASN	O-C-N	5.46	128.75	122.25
1	A	55	LEU	CB-CA-C	-5.46	102.24	110.92
1	A	185	VAL	CA-C-N	-5.45	113.77	122.66
1	A	185	VAL	C-N-CA	-5.45	113.77	122.66
1	A	158	ASP	O-C-N	5.44	130.44	122.39
1	A	144	VAL	CA-C-N	5.43	127.56	120.28
1	A	144	VAL	C-N-CA	5.43	127.56	120.28
2	B	160	SER	O-C-N	5.43	129.81	122.96
1	A	214	LYS	CA-C-N	5.42	128.12	120.42
1	A	214	LYS	C-N-CA	5.42	128.12	120.42
1	A	262	MET	CA-C-N	-5.42	111.80	120.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	262	MET	C-N-CA	-5.42	111.80	120.86
2	B	93	ILE	O-C-N	5.42	125.69	121.46
1	A	265	VAL	N-CA-C	5.41	115.62	110.53
4	S	184	SER	CA-C-N	5.41	125.40	120.21
4	S	184	SER	C-N-CA	5.41	125.40	120.21
1	A	173	TRP	CA-C-N	-5.40	113.02	120.74
1	A	173	TRP	C-N-CA	-5.40	113.02	120.74
2	B	45	MET	CA-C-N	-5.39	113.40	122.29
2	B	45	MET	C-N-CA	-5.39	113.40	122.29
1	A	217	VAL	CA-C-N	-5.38	113.45	120.44
1	A	217	VAL	C-N-CA	-5.38	113.45	120.44
2	B	8	ARG	N-CA-C	-5.38	105.50	111.36
2	B	204	CYS	CA-C-N	5.38	130.75	120.97
2	B	204	CYS	C-N-CA	5.38	130.75	120.97
2	B	281	SER	O-C-N	-5.37	115.24	122.43
4	S	60	TYR	O-C-N	5.32	129.14	122.92
1	A	57	SER	CA-C-N	-5.31	113.53	120.44
1	A	57	SER	C-N-CA	-5.31	113.53	120.44
4	S	214	LEU	O-C-N	-5.29	117.00	123.30
4	S	75	PRO	O-C-N	5.29	129.05	122.22
5	C	19	LEU	O-C-N	5.29	128.18	122.15
1	A	302	LEU	O-C-N	5.28	127.72	122.12
3	D	227	ALA	CA-C-N	-5.28	113.21	120.28
3	D	227	ALA	C-N-CA	-5.28	113.21	120.28
1	A	158	ASP	CA-C-N	-5.27	113.96	122.24
1	A	158	ASP	C-N-CA	-5.27	113.96	122.24
1	A	207	TRP	O-C-N	5.27	128.12	121.64
3	D	30	ALA	O-C-N	-5.27	115.75	122.34
2	B	228	ASP	O-C-N	5.25	129.22	122.23
1	A	121	CYS	N-CA-C	-5.24	105.69	111.71
5	C	17	GLU	CA-C-N	-5.19	113.33	120.28
5	C	17	GLU	C-N-CA	-5.19	113.33	120.28
3	D	8	GLU	O-C-N	5.17	128.46	122.25
3	D	252	ASP	CA-C-N	5.17	127.62	120.29
3	D	252	ASP	C-N-CA	5.17	127.62	120.29
1	A	239	ARG	CA-C-N	-5.16	112.11	121.14
1	A	239	ARG	C-N-CA	-5.16	112.11	121.14
1	A	258	ARG	CA-C-N	-5.16	113.39	120.46
1	A	258	ARG	C-N-CA	-5.16	113.39	120.46
1	A	313	LEU	N-CA-C	-5.16	105.84	111.82
1	A	131	ASN	N-CA-C	-5.15	104.93	111.11
5	C	22	GLU	CA-C-N	5.15	127.61	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	22	GLU	C-N-CA	5.15	127.61	120.29
1	A	323	GLU	CA-C-N	-5.15	113.38	120.28
1	A	323	GLU	C-N-CA	-5.15	113.38	120.28
4	S	15	GLY	O-C-N	5.14	128.34	122.23
4	S	61	ALA	CA-C-N	-5.13	112.96	122.60
4	S	61	ALA	C-N-CA	-5.13	112.96	122.60
1	A	118	GLU	CA-C-N	-5.11	113.80	120.44
1	A	118	GLU	C-N-CA	-5.11	113.80	120.44
2	B	208	ALA	CA-C-N	-5.10	115.28	122.94
2	B	208	ALA	C-N-CA	-5.10	115.28	122.94
1	A	122	LYS	CA-C-N	-5.10	113.44	120.28
1	A	122	LYS	C-N-CA	-5.10	113.44	120.28
1	A	214	LYS	O-C-N	-5.10	115.11	122.36
4	S	9	GLY	O-C-N	-5.09	118.43	122.81
5	C	21	MET	CA-C-N	5.09	128.04	120.31
5	C	21	MET	C-N-CA	5.09	128.04	120.31
2	B	178	THR	CA-C-N	5.06	129.56	121.66
2	B	178	THR	C-N-CA	5.06	129.56	121.66
2	B	320	VAL	CA-C-N	5.06	130.18	120.97
2	B	320	VAL	C-N-CA	5.06	130.18	120.97
4	S	57	THR	CA-C-O	-5.04	116.57	122.37
2	B	118	ASP	CA-C-N	5.03	131.14	121.54
2	B	118	ASP	C-N-CA	5.03	131.14	121.54
2	B	275	SER	CA-C-N	-5.02	115.48	122.71
2	B	275	SER	C-N-CA	-5.02	115.48	122.71
1	A	108	LYS	CA-C-N	-5.01	113.52	120.38
1	A	108	LYS	C-N-CA	-5.01	113.52	120.38

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	171	CYS	Mainchain
2	B	148	CYS	Mainchain
4	S	82	GLN	Mainchain

5.2 Too-close contacts (i)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2244	0	2363	352	0
2	B	2603	0	2506	261	0
3	D	1786	0	1772	143	0
4	S	1767	0	1686	116	0
5	C	438	0	443	69	0
6	A	29	0	0	3	0
All	All	8867	0	8770	875	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 50.

All (875) 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:126:SER:HB3	1:A:184:MET:SD	1.43	1.56
2:B:283:ARG:NE	2:B:300:LEU:HD12	1.29	1.44
1:A:126:SER:CB	1:A:184:MET:SD	2.04	1.44
2:B:22:ARG:CG	5:C:30:VAL:HG11	1.51	1.36
3:D:275:PHE:O	3:D:279:ILE:HG23	1.25	1.35
2:B:34:THR:HG22	5:C:38:MET:SD	1.67	1.32
5:C:8:SER:O	5:C:12:ALA:N	1.57	1.32
2:B:22:ARG:HG3	5:C:30:VAL:CG1	1.61	1.28
2:B:281:SER:HB3	5:C:48:ASP:CB	1.59	1.26
1:A:312:SER:O	1:A:316:VAL:HG23	1.33	1.25
2:B:250:CYS:SG	2:B:273:ILE:HD13	1.81	1.20
5:C:12:ALA:O	5:C:16:VAL:N	1.74	1.19
3:D:275:PHE:O	3:D:279:ILE:CG2	1.94	1.15
2:B:26:ALA:HB1	2:B:33:ILE:HD11	1.23	1.15
4:S:91:THR:HG23	4:S:118:THR:HA	1.29	1.14
2:B:281:SER:CB	5:C:48:ASP:HB2	1.77	1.14
3:D:48:THR:HA	3:D:51:LYS:CB	1.79	1.13
5:C:14:LYS:O	5:C:18:GLN:N	1.82	1.12
2:B:26:ALA:CB	2:B:33:ILE:HD11	1.78	1.12
1:A:313:LEU:HA	1:A:316:VAL:HB	1.30	1.11
1:A:52:ILE:CG2	1:A:56:TYR:CE1	2.35	1.09
4:S:70:ILE:HD12	4:S:81:LEU:HD12	1.26	1.09
1:A:116:PHE:CD2	1:A:120:LEU:HB2	1.88	1.08
2:B:15:LYS:HZ1	2:B:258:ASP:HB2	1.07	1.07
4:S:11:LEU:HD11	4:S:120:SER:HB2	1.30	1.07
5:C:15:LEU:O	5:C:19:LEU:N	1.87	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:250:CYS:SG	2:B:273:ILE:CD1	2.44	1.05
5:C:9:ILE:HA	5:C:12:ALA:HB3	1.32	1.05
1:A:245:LEU:CD1	3:D:342:ASP:OD1	2.03	1.05
1:A:246:LEU:HD13	3:D:355:PHE:HE1	1.18	1.05
3:D:48:THR:HA	3:D:51:LYS:HB2	1.11	1.05
4:S:70:ILE:HA	4:S:81:LEU:HA	1.39	1.05
1:A:77:TYR:CE2	1:A:328:CYS:SG	2.50	1.05
4:S:71:SER:O	4:S:79:LEU:HD12	1.58	1.04
2:B:26:ALA:HB1	2:B:33:ILE:CD1	1.87	1.03
1:A:257:ARG:O	1:A:260:THR:HG22	1.60	1.02
3:D:49:ILE:HG22	3:D:53:MET:HE3	1.40	1.02
4:S:71:SER:N	4:S:80:PHE:O	1.94	1.01
2:B:283:ARG:CD	2:B:300:LEU:HD12	1.89	1.00
3:D:186:VAL:HB	3:D:201:ASP:HB3	1.43	1.00
3:D:224:PHE:CE2	3:D:251:PHE:HD2	1.79	1.00
3:D:349:LEU:HG	3:D:355:PHE:HB2	1.01	1.00
4:S:142:GLN:NE2	4:S:229:CYS:SG	2.35	1.00
1:A:67:ASN:ND2	1:A:95:ASP:HB3	1.77	1.00
1:A:299:ALA:HA	1:A:302:LEU:HB2	1.37	1.00
2:B:15:LYS:NZ	2:B:258:ASP:HB2	1.76	0.99
1:A:52:ILE:CG2	1:A:56:TYR:CZ	2.47	0.98
4:S:70:ILE:HD12	4:S:81:LEU:CD1	1.91	0.98
2:B:283:ARG:NE	2:B:300:LEU:CD1	2.26	0.98
1:A:245:LEU:HD11	3:D:342:ASP:OD1	1.61	0.98
2:B:197:ARG:HE	2:B:214:ARG:NH2	1.61	0.98
1:A:313:LEU:HA	1:A:316:VAL:CB	1.93	0.97
1:A:150:VAL:HG21	1:A:236:MET:HG3	1.45	0.97
4:S:138:ILE:HB	4:S:231:GLN:OE1	1.64	0.97
3:D:349:LEU:CG	3:D:355:PHE:HB2	1.93	0.97
1:A:313:LEU:CA	1:A:316:VAL:HB	1.95	0.96
3:D:272:LYS:HB2	3:D:326:CYS:SG	2.06	0.96
3:D:228:LEU:HD21	3:D:269:LEU:HD13	1.45	0.95
1:A:116:PHE:HE2	1:A:120:LEU:N	1.65	0.95
5:C:16:VAL:O	5:C:20:LYS:N	1.99	0.95
1:A:125:LEU:HD11	1:A:198:CYS:SG	2.05	0.95
2:B:22:ARG:HA	5:C:30:VAL:HG12	1.46	0.94
5:C:13:ARG:O	5:C:17:GLU:HB2	1.69	0.93
1:A:126:SER:HB2	1:A:184:MET:SD	2.07	0.93
2:B:340:ASN:HD22	5:C:61:PHE:HB2	1.34	0.92
3:D:349:LEU:HG	3:D:355:PHE:CB	1.96	0.92
1:A:52:ILE:O	1:A:56:TYR:N	2.03	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:9:ILE:HA	5:C:12:ALA:CB	2.00	0.92
3:D:269:LEU:O	3:D:325:THR:OG1	1.88	0.92
1:A:246:LEU:HD13	3:D:355:PHE:CE1	2.05	0.92
3:D:53:MET:SD	3:D:199:MET:SD	2.67	0.91
4:S:70:ILE:HG13	4:S:81:LEU:HB2	1.52	0.90
1:A:312:SER:O	1:A:316:VAL:CG2	2.18	0.90
4:S:64:VAL:CG1	4:S:68:PHE:CD2	2.55	0.90
2:B:283:ARG:HE	2:B:300:LEU:HD12	1.08	0.89
5:C:7:ALA:O	5:C:11:GLN:N	2.05	0.89
4:S:64:VAL:HG11	4:S:68:PHE:CD2	2.08	0.88
1:A:56:TYR:CE1	1:A:305:ALA:HB2	2.08	0.88
1:A:54:ALA:O	1:A:58:ALA:N	2.05	0.87
1:A:74:ILE:HD13	1:A:88:ILE:HG23	1.56	0.87
1:A:102:LEU:HD23	1:A:103:PRO:HD3	1.57	0.87
2:B:250:CYS:HG	2:B:273:ILE:HD13	1.37	0.87
1:A:176:ALA:O	1:A:179:VAL:N	2.07	0.87
1:A:119:LEU:HA	1:A:122:LYS:HZ3	1.40	0.86
1:A:202:PHE:CD2	1:A:210:ASP:HB2	2.10	0.86
1:A:52:ILE:HG23	1:A:56:TYR:CE1	2.10	0.86
2:B:256:ARG:H	2:B:256:ARG:HD2	1.39	0.86
1:A:108:LYS:O	1:A:112:GLU:N	2.08	0.86
2:B:283:ARG:HE	2:B:300:LEU:CD1	1.89	0.85
1:A:299:ALA:O	1:A:302:LEU:N	2.09	0.85
1:A:146:ARG:HD2	3:D:354:LEU:HD12	1.58	0.85
2:B:340:ASN:ND2	5:C:61:PHE:HB2	1.91	0.85
1:A:53:THR:O	1:A:57:SER:N	2.08	0.85
4:S:71:SER:O	4:S:80:PHE:N	2.09	0.85
1:A:52:ILE:HG22	1:A:56:TYR:CE1	2.11	0.84
3:D:48:THR:CA	3:D:51:LYS:HB2	2.03	0.84
1:A:91:LEU:HD22	1:A:138:THR:HG21	1.60	0.84
2:B:15:LYS:HG2	5:C:27:ARG:HH22	1.42	0.83
4:S:64:VAL:HG12	4:S:68:PHE:CG	2.12	0.83
1:A:306:LEU:O	1:A:309:ALA:HB3	1.79	0.83
2:B:310:GLY:O	2:B:337:LYS:NZ	2.12	0.83
2:B:119:ASN:ND2	2:B:144:GLY:O	2.11	0.83
2:B:47:THR:HG22	2:B:339:TRP:CD1	2.14	0.83
1:A:52:ILE:HG21	1:A:56:TYR:CZ	2.13	0.82
2:B:227:SER:OG	2:B:246:ASP:HB3	1.79	0.82
2:B:281:SER:CB	5:C:48:ASP:CB	2.43	0.82
2:B:3:GLU:HG2	5:C:16:VAL:HG11	1.60	0.82
2:B:26:ALA:CA	2:B:33:ILE:HD11	2.10	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:161:SER:HB3	2:B:187:VAL:HG21	1.60	0.81
2:B:278:PHE:HE2	2:B:282:GLY:HA2	1.43	0.81
2:B:15:LYS:HG2	5:C:27:ARG:NH2	1.94	0.81
1:A:64:LEU:HA	1:A:99:THR:HG21	1.62	0.81
3:D:224:PHE:CE2	3:D:251:PHE:CD2	2.68	0.81
3:D:49:ILE:CG2	3:D:53:MET:HE3	2.10	0.81
1:A:260:THR:O	1:A:263:VAL:HG22	1.80	0.81
1:A:153:PRO:HG3	3:D:345:ILE:HD11	1.63	0.80
3:D:264:SER:OG	3:D:319:GLU:OE2	2.00	0.80
1:A:54:ALA:O	1:A:57:SER:HB3	1.82	0.80
2:B:26:ALA:CB	2:B:33:ILE:CD1	2.53	0.80
1:A:56:TYR:HA	1:A:59:VAL:CG1	2.12	0.79
1:A:146:ARG:HD2	3:D:354:LEU:CD1	2.11	0.79
1:A:133:PHE:CE2	1:A:179:VAL:HG11	2.17	0.79
2:B:281:SER:HB3	5:C:48:ASP:HB2	0.84	0.79
1:A:313:LEU:HA	1:A:316:VAL:CG2	2.12	0.79
1:A:299:ALA:CA	1:A:302:LEU:HB2	2.12	0.79
1:A:72:PHE:O	1:A:75:VAL:N	2.15	0.79
1:A:245:LEU:CG	3:D:342:ASP:OD1	2.31	0.79
1:A:272:VAL:O	1:A:276:PRO:HD3	1.82	0.78
1:A:311:SER:O	1:A:315:PRO:HD2	1.84	0.78
1:A:52:ILE:HA	1:A:55:LEU:HB3	1.66	0.78
4:S:138:ILE:HG13	4:S:231:GLN:HE22	1.47	0.78
4:S:64:VAL:HG11	4:S:68:PHE:CE2	2.18	0.78
1:A:202:PHE:HD2	1:A:210:ASP:HB2	1.47	0.78
5:C:9:ILE:CA	5:C:12:ALA:HB3	2.13	0.78
1:A:313:LEU:O	1:A:316:VAL:N	2.17	0.77
1:A:51:ALA:O	1:A:55:LEU:N	2.16	0.77
2:B:278:PHE:CE2	2:B:282:GLY:HA2	2.19	0.77
2:B:228:ASP:O	2:B:245:SER:HA	1.85	0.77
4:S:98:ARG:HD3	4:S:110:PHE:HB3	1.66	0.77
4:S:6:GLU:OE2	4:S:96:CYS:SG	2.43	0.77
2:B:18:ILE:O	2:B:22:ARG:N	2.17	0.76
1:A:56:TYR:HA	1:A:59:VAL:HG12	1.66	0.76
3:D:272:LYS:HD3	3:D:324:PHE:HB3	1.66	0.76
1:A:67:ASN:HD21	1:A:95:ASP:HB3	1.49	0.76
1:A:130:TYR:HE1	1:A:177:SER:N	1.82	0.76
2:B:283:ARG:CD	2:B:300:LEU:CD1	2.64	0.76
4:S:64:VAL:CG1	4:S:68:PHE:CG	2.67	0.76
3:D:227:ALA:O	3:D:244:MET:HE2	1.86	0.76
3:D:54:LYS:HD2	3:D:190:PHE:HB3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:PHE:HB2	1:A:210:ASP:OD2	1.86	0.75
3:D:245:HIS:HA	3:D:248:MET:SD	2.27	0.75
4:S:244:LYS:C	4:S:245:LEU:HD12	2.11	0.75
1:A:302:LEU:O	1:A:305:ALA:HB3	1.86	0.75
2:B:48:ARG:HG2	2:B:340:ASN:HB3	1.68	0.75
3:D:6:SER:OG	3:D:9:ASP:OD1	2.03	0.75
3:D:47:ASN:O	3:D:51:LYS:N	2.20	0.75
1:A:78:THR:HG21	1:A:85:ASN:ND2	2.02	0.75
3:D:188:THR:O	3:D:198:LYS:HA	1.87	0.75
1:A:51:ALA:O	1:A:54:ALA:HB3	1.86	0.75
4:S:70:ILE:CD1	4:S:81:LEU:HD12	2.10	0.75
1:A:245:LEU:HD13	3:D:346:LYS:HB2	1.68	0.75
4:S:2:VAL:HG12	4:S:26:GLY:O	1.86	0.74
1:A:141:MET:HE2	1:A:168:ILE:HD13	1.69	0.74
1:A:52:ILE:HG22	1:A:56:TYR:CZ	2.22	0.74
1:A:72:PHE:O	1:A:75:VAL:HB	1.88	0.74
1:A:257:ARG:C	1:A:260:THR:HG22	2.12	0.74
3:D:272:LYS:CD	3:D:324:PHE:HB3	2.18	0.74
3:D:272:LYS:HG3	3:D:325:THR:O	1.88	0.74
1:A:56:TYR:HE1	1:A:305:ALA:HB2	1.52	0.74
1:A:224:VAL:HA	1:A:227:LEU:HG	1.68	0.74
1:A:56:TYR:CA	1:A:59:VAL:HG12	2.16	0.73
2:B:283:ARG:O	2:B:299:ALA:N	2.18	0.73
4:S:244:LYS:O	4:S:245:LEU:HD12	1.86	0.73
1:A:176:ALA:O	1:A:177:SER:C	2.28	0.73
4:S:90:ASP:OD1	4:S:119:VAL:HG21	1.87	0.73
1:A:170:ILE:O	1:A:174:VAL:HG22	1.89	0.73
1:A:67:ASN:ND2	1:A:96:ALA:N	2.36	0.73
2:B:47:THR:HG22	2:B:339:TRP:NE1	2.03	0.73
2:B:318:LEU:HG	2:B:329:THR:HG22	1.71	0.73
1:A:243:VAL:HG12	1:A:245:LEU:H	1.53	0.73
1:A:245:LEU:HG	3:D:342:ASP:OD1	1.88	0.73
1:A:246:LEU:CD2	1:A:259:ILE:HD12	2.19	0.73
2:B:22:ARG:CG	5:C:30:VAL:CG1	2.41	0.73
1:A:313:LEU:O	1:A:316:VAL:HB	1.88	0.73
5:C:14:LYS:O	5:C:17:GLU:HB3	1.88	0.73
1:A:91:LEU:HD22	1:A:138:THR:CG2	2.20	0.72
1:A:299:ALA:O	1:A:303:CYS:N	2.23	0.72
2:B:15:LYS:NZ	2:B:258:ASP:O	2.23	0.72
1:A:116:PHE:HD2	1:A:120:LEU:HB2	1.49	0.72
2:B:161:SER:HB3	2:B:187:VAL:CG2	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:10:ALA:O	5:C:14:LYS:N	2.23	0.72
2:B:34:THR:CG2	5:C:38:MET:SD	2.64	0.71
4:S:71:SER:C	4:S:79:LEU:HD12	2.13	0.71
1:A:311:SER:O	1:A:314:ASN:HB2	1.89	0.71
2:B:197:ARG:HE	2:B:214:ARG:CZ	2.02	0.71
1:A:90:ASN:OD1	1:A:169:ASN:ND2	2.24	0.71
3:D:187:GLU:OE1	3:D:200:PHE:HD1	1.74	0.71
2:B:61:MET:SD	2:B:70:LEU:HD11	2.31	0.71
2:B:283:ARG:HD2	2:B:300:LEU:CD1	2.20	0.71
3:D:255:CYS:SG	3:D:318:LYS:NZ	2.63	0.71
5:C:16:VAL:O	5:C:20:LYS:HG3	1.91	0.71
2:B:22:ARG:CB	5:C:30:VAL:HG11	2.21	0.70
1:A:246:LEU:HD21	1:A:259:ILE:HD12	1.73	0.70
1:A:243:VAL:HG12	1:A:244:ARG:N	2.06	0.70
1:A:56:TYR:CE1	1:A:305:ALA:CB	2.74	0.70
1:A:130:TYR:OH	1:A:177:SER:HB3	1.92	0.70
1:A:132:MET:HE2	6:A:401:A1LXY:C19	2.22	0.70
1:A:52:ILE:O	1:A:55:LEU:HB3	1.93	0.69
2:B:26:ALA:HB2	5:C:31:SER:HB2	1.73	0.69
2:B:314:ARG:C	2:B:331:SER:HG	1.99	0.69
4:S:226:VAL:HG22	4:S:244:LYS:HD3	1.75	0.69
1:A:51:ALA:O	1:A:54:ALA:N	2.26	0.69
4:S:70:ILE:CG1	4:S:81:LEU:HB2	2.23	0.69
2:B:15:LYS:NZ	2:B:258:ASP:C	2.51	0.69
2:B:22:ARG:CA	5:C:30:VAL:HG12	2.23	0.68
3:D:224:PHE:HE1	3:D:250:LEU:HD22	1.58	0.68
2:B:60:ALA:HB3	2:B:73:ALA:HB3	1.75	0.68
1:A:197:VAL:HB	1:A:199:MET:HE3	1.75	0.68
1:A:251:GLU:HG2	1:A:252:LYS:HE3	1.76	0.68
2:B:82:TRP:HB3	2:B:89:LYS:HA	1.75	0.68
2:B:248:ALA:HB2	2:B:271:CYS:O	1.92	0.68
3:D:188:THR:HB	3:D:199:MET:HB2	1.76	0.68
1:A:313:LEU:C	1:A:316:VAL:HB	2.17	0.68
2:B:15:LYS:NZ	2:B:258:ASP:CB	2.56	0.68
4:S:202:ARG:NH2	4:S:223:ASP:OD1	2.27	0.68
1:A:299:ALA:O	1:A:300:LEU:C	2.38	0.67
3:D:209:ARG:HA	3:D:212:TRP:NE1	2.09	0.67
5:C:13:ARG:O	5:C:17:GLU:CB	2.40	0.67
1:A:55:LEU:O	1:A:59:VAL:HG12	1.94	0.67
1:A:257:ARG:O	1:A:260:THR:CG2	2.39	0.67
4:S:72:ARG:HA	4:S:79:LEU:HA	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:TRP:CB	2:B:89:LYS:HA	2.24	0.67
4:S:19:LYS:HB3	4:S:82:GLN:NE2	2.10	0.67
1:A:52:ILE:HA	1:A:55:LEU:CB	2.25	0.67
1:A:273:CYS:HB3	1:A:310:ASN:HB3	1.75	0.67
4:S:64:VAL:CG1	4:S:68:PHE:CE2	2.77	0.67
3:D:224:PHE:CD2	3:D:251:PHE:CD2	2.83	0.67
1:A:56:TYR:O	1:A:60:CYS:N	2.13	0.67
1:A:282:ILE:HA	1:A:285:THR:OG1	1.94	0.67
2:B:257:ALA:HB1	2:B:259:GLN:NE2	2.10	0.67
1:A:146:ARG:HH11	3:D:354:LEU:HD11	1.60	0.67
1:A:78:THR:CG2	1:A:85:ASN:ND2	2.57	0.66
3:D:54:LYS:CD	3:D:190:PHE:HB3	2.25	0.66
3:D:305:GLN:HG2	3:D:322:THR:HG21	1.78	0.66
1:A:244:ARG:NH2	3:D:321:TYR:CE1	2.64	0.66
2:B:168:LEU:HB3	2:B:177:THR:O	1.96	0.66
4:S:139:VAL:CG1	4:S:162:SER:OG	2.43	0.66
2:B:3:GLU:CG	5:C:16:VAL:HG11	2.26	0.66
2:B:253:PHE:HD1	2:B:260:GLU:HA	1.59	0.66
1:A:314:ASN:HB2	1:A:315:PRO:HD3	1.78	0.66
1:A:125:LEU:CD1	1:A:198:CYS:SG	2.82	0.66
1:A:74:ILE:HG12	1:A:325:PHE:HZ	1.61	0.66
1:A:257:ARG:HA	1:A:260:THR:HG22	1.78	0.66
4:S:12:VAL:HG12	4:S:13:GLN:H	1.59	0.66
4:S:138:ILE:CG1	4:S:231:GLN:HE22	2.09	0.66
1:A:70:VAL:O	1:A:71:MET:C	2.39	0.65
1:A:159:PHE:HA	1:A:164:LYS:HE3	1.77	0.65
2:B:30:LEU:HD13	5:C:34:ALA:HB2	1.78	0.65
2:B:26:ALA:C	2:B:28:ALA:H	2.05	0.65
2:B:163:ASP:O	2:B:186:ASP:HA	1.96	0.65
2:B:215:GLU:HG3	2:B:217:MET:HE2	1.78	0.65
2:B:43:ILE:HD13	2:B:284:LEU:HD11	1.77	0.65
1:A:225:PRO:O	1:A:229:ILE:HG22	1.96	0.65
2:B:314:ARG:O	2:B:331:SER:OG	2.10	0.65
3:D:246:ALA:O	3:D:249:LYS:N	2.30	0.65
3:D:187:GLU:OE1	3:D:200:PHE:CD1	2.50	0.65
1:A:78:THR:HG21	1:A:85:ASN:HD21	1.62	0.64
2:B:3:GLU:OE1	2:B:7:LEU:HD12	1.97	0.64
3:D:244:MET:HA	3:D:247:SER:HB2	1.79	0.64
1:A:95:ASP:OD2	1:A:315:PRO:CG	2.45	0.64
2:B:215:GLU:HG3	2:B:217:MET:SD	2.37	0.64
1:A:258:ARG:NH2	3:D:355:PHE:OXT	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:ILE:HD11	5:C:27:ARG:HB2	1.79	0.64
1:A:116:PHE:CE2	1:A:120:LEU:HB2	2.32	0.64
2:B:189:SER:OG	2:B:232:ILE:HG12	1.98	0.64
2:B:48:ARG:NH1	5:C:63:GLU:OE2	2.28	0.63
1:A:116:PHE:CD2	1:A:120:LEU:CB	2.74	0.63
2:B:113:ALA:HB2	2:B:151:PHE:HE1	1.64	0.63
2:B:199:PHE:HE1	2:B:213:VAL:HG22	1.62	0.63
1:A:222:PHE:O	1:A:226:ILE:HD12	1.98	0.63
3:D:46:LYS:O	3:D:50:VAL:HG23	1.98	0.63
3:D:224:PHE:CD2	3:D:251:PHE:HD2	2.16	0.63
1:A:223:VAL:HG12	1:A:227:LEU:HD23	1.78	0.63
2:B:48:ARG:CG	2:B:340:ASN:HB3	2.28	0.63
3:D:187:GLU:OE2	3:D:200:PHE:CE1	2.51	0.63
4:S:70:ILE:HG13	4:S:81:LEU:CB	2.26	0.63
2:B:232:ILE:HG22	2:B:243:THR:OG1	1.98	0.63
4:S:94:TYR:O	4:S:114:GLY:HA3	1.98	0.63
2:B:30:LEU:HD23	2:B:33:ILE:HD12	1.81	0.63
2:B:200:VAL:HA	2:B:210:LEU:HA	1.81	0.63
4:S:139:VAL:HG13	4:S:162:SER:CB	2.28	0.63
2:B:22:ARG:CB	5:C:30:VAL:CG1	2.77	0.63
2:B:11:ALA:O	2:B:15:LYS:N	2.29	0.62
3:D:49:ILE:HD12	3:D:225:CYS:SG	2.39	0.62
1:A:56:TYR:HE1	1:A:305:ALA:CB	2.12	0.62
1:A:77:TYR:CZ	1:A:328:CYS:SG	2.92	0.62
2:B:82:TRP:HB2	2:B:88:ASN:O	2.00	0.62
1:A:116:PHE:CE2	1:A:120:LEU:HG	2.33	0.62
1:A:250:LYS:HA	1:A:253:ASP:HB2	1.82	0.62
1:A:133:PHE:CD2	1:A:179:VAL:HG11	2.33	0.62
1:A:300:LEU:HD21	6:A:401:A1LXY:O27	2.00	0.62
1:A:219:LEU:HD12	1:A:223:VAL:HG21	1.81	0.62
1:A:218:PHE:CE1	1:A:278:HIS:HB3	2.34	0.62
2:B:27:ASP:C	2:B:29:THR:H	2.07	0.62
3:D:48:THR:HA	3:D:51:LYS:HB3	1.78	0.62
4:S:176:TRP:CD1	4:S:189:ILE:HB	2.33	0.62
2:B:29:THR:C	2:B:31:SER:H	2.08	0.61
1:A:71:MET:O	1:A:75:VAL:HG23	2.00	0.61
1:A:108:LYS:O	1:A:109:TYR:C	2.38	0.61
1:A:170:ILE:O	1:A:174:VAL:HG13	2.00	0.61
1:A:270:PHE:HD1	1:A:274:TRP:CE3	2.19	0.61
2:B:3:GLU:O	2:B:6:GLN:HG3	2.00	0.61
2:B:54:HIS:ND1	2:B:74:SER:HB2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:PHE:HE2	1:A:120:LEU:H	0.81	0.61
1:A:271:VAL:O	1:A:275:ALA:HB2	2.01	0.61
3:D:45:GLY:O	3:D:48:THR:HG22	2.01	0.61
1:A:214:LYS:HE2	1:A:281:VAL:HB	1.83	0.60
1:A:225:PRO:HA	1:A:228:ILE:HG22	1.82	0.60
1:A:243:VAL:CG1	1:A:244:ARG:N	2.64	0.60
4:S:139:VAL:HG13	4:S:162:SER:HB3	1.84	0.60
1:A:219:LEU:HD12	1:A:223:VAL:CG2	2.31	0.60
2:B:200:VAL:HG22	2:B:210:LEU:HD12	1.83	0.60
3:D:38:LEU:HD21	3:D:50:VAL:CG2	2.30	0.60
4:S:37:VAL:HA	4:S:46:GLU:O	2.02	0.60
4:S:173:TYR:HD2	4:S:233:LEU:HA	1.66	0.60
4:S:51:ILE:HD13	4:S:79:LEU:HD11	1.82	0.60
4:S:174:LEU:HD12	4:S:230:MET:O	2.02	0.60
3:D:275:PHE:O	3:D:279:ILE:HG21	1.97	0.60
1:A:126:SER:OG	1:A:184:MET:SD	2.59	0.60
2:B:187:VAL:HA	2:B:203:ALA:HA	1.82	0.60
2:B:277:SER:OG	2:B:278:PHE:N	2.32	0.60
1:A:310:ASN:OD1	1:A:311:SER:N	2.35	0.60
2:B:102:THR:HG21	2:B:148:CYS:HA	1.84	0.60
2:B:130:GLU:OE2	4:S:27:PHE:HA	2.01	0.60
3:D:187:GLU:OE2	3:D:200:PHE:HE1	1.83	0.60
1:A:49:ALA:O	1:A:53:THR:HG23	2.02	0.59
1:A:52:ILE:CA	1:A:55:LEU:HB3	2.31	0.59
1:A:120:LEU:HA	1:A:123:ALA:HB3	1.83	0.59
1:A:257:ARG:CA	1:A:260:THR:HG22	2.32	0.59
1:A:311:SER:O	1:A:315:PRO:CD	2.49	0.59
2:B:121:CYS:HB2	2:B:146:LEU:CD2	2.32	0.59
5:C:12:ALA:O	5:C:16:VAL:CB	2.50	0.59
1:A:52:ILE:HG22	1:A:56:TYR:CD1	2.38	0.59
1:A:77:TYR:CD2	1:A:328:CYS:SG	2.88	0.59
1:A:244:ARG:NH2	3:D:321:TYR:HE1	2.00	0.59
1:A:314:ASN:HB2	1:A:315:PRO:CD	2.32	0.59
2:B:28:ALA:O	2:B:30:LEU:HG	2.02	0.59
2:B:228:ASP:O	2:B:245:SER:CB	2.51	0.59
3:D:242:ASN:O	3:D:243:ARG:C	2.42	0.59
1:A:74:ILE:HD13	1:A:88:ILE:CG2	2.30	0.59
1:A:298:ALA:O	1:A:302:LEU:N	2.34	0.59
2:B:340:ASN:HD22	5:C:61:PHE:CB	2.11	0.59
2:B:30:LEU:HD11	5:C:30:VAL:HG22	1.83	0.59
1:A:116:PHE:CE2	1:A:120:LEU:CB	2.86	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:GLU:O	2:B:16:ASN:N	2.33	0.59
2:B:274:THR:HG23	2:B:315:VAL:O	2.03	0.59
1:A:245:LEU:CD1	3:D:346:LYS:HB2	2.33	0.59
1:A:272:VAL:O	1:A:276:PRO:CD	2.50	0.59
1:A:267:VAL:O	1:A:271:VAL:HG23	2.02	0.58
2:B:33:ILE:HG22	2:B:33:ILE:O	2.02	0.58
1:A:79:LYS:NZ	1:A:80:MET:HE1	2.18	0.58
2:B:49:ARG:HH12	5:C:61:PHE:HD1	1.49	0.58
1:A:67:ASN:ND2	1:A:95:ASP:CB	2.60	0.58
2:B:14:LEU:O	2:B:18:ILE:HG12	2.02	0.58
2:B:231:ALA:CB	2:B:275:SER:HA	2.32	0.58
2:B:258:ASP:N	2:B:258:ASP:OD2	2.35	0.58
2:B:200:VAL:HG22	2:B:210:LEU:HG	1.84	0.58
2:B:228:ASP:O	2:B:245:SER:CA	2.51	0.58
2:B:234:PHE:HA	2:B:241:PHE:HA	1.86	0.58
1:A:257:ARG:HD3	1:A:260:THR:HG21	1.85	0.58
1:A:298:ALA:O	1:A:302:LEU:HG	2.03	0.58
1:A:65:LEU:O	1:A:68:VAL:HB	2.04	0.58
1:A:181:VAL:HG23	1:A:182:PRO:HD3	1.86	0.58
2:B:200:VAL:HG23	2:B:234:PHE:CZ	2.39	0.58
1:A:171:CYS:HA	1:A:174:VAL:HG22	1.85	0.58
1:A:176:ALA:C	1:A:178:GLY:N	2.61	0.58
1:A:299:ALA:O	1:A:302:LEU:HB2	2.04	0.58
4:S:139:VAL:HG12	4:S:162:SER:OG	2.03	0.58
2:B:200:VAL:HG22	2:B:210:LEU:CG	2.34	0.58
1:A:119:LEU:HA	1:A:122:LYS:NZ	2.16	0.57
1:A:257:ARG:HD3	1:A:260:THR:CG2	2.33	0.57
2:B:199:PHE:CZ	2:B:211:TRP:HB2	2.39	0.57
3:D:248:MET:CE	3:D:288:PHE:HZ	2.17	0.57
4:S:139:VAL:HG13	4:S:162:SER:OG	2.03	0.57
1:A:72:PHE:O	1:A:73:GLY:C	2.45	0.57
2:B:90:VAL:HG13	4:S:102:TYR:HB2	1.86	0.57
3:D:188:THR:O	3:D:199:MET:N	2.35	0.57
2:B:317:CYS:SG	2:B:330:GLY:HA3	2.44	0.57
1:A:91:LEU:CD2	1:A:138:THR:CG2	2.82	0.57
2:B:200:VAL:HG22	2:B:210:LEU:CD1	2.34	0.57
1:A:67:ASN:ND2	1:A:95:ASP:C	2.62	0.57
3:D:47:ASN:O	3:D:51:LYS:HB2	2.04	0.57
1:A:168:ILE:O	1:A:172:ILE:HG13	2.04	0.57
2:B:274:THR:CG2	2:B:315:VAL:O	2.53	0.57
1:A:111:MET:C	1:A:113:THR:H	2.13	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:144:THR:HG22	4:S:243:THR:HG23	1.87	0.57
1:A:139:LEU:CD2	1:A:229:ILE:HD12	2.34	0.57
4:S:4:LEU:HD21	4:S:27:PHE:CZ	2.40	0.57
1:A:58:ALA:O	1:A:62:VAL:HG23	2.05	0.57
1:A:60:CYS:HB2	1:A:102:LEU:HD11	1.86	0.57
3:D:272:LYS:HE2	3:D:326:CYS:SG	2.44	0.57
2:B:39:PRO:HG3	2:B:301:LYS:NZ	2.20	0.56
4:S:39:GLN:HB2	4:S:45:LEU:HD23	1.87	0.56
3:D:189:HIS:CG	3:D:198:LYS:HG2	2.39	0.56
4:S:9:GLY:HA2	4:S:117:LEU:CD1	2.34	0.56
1:A:91:LEU:CD2	1:A:138:THR:HG22	2.35	0.56
1:A:300:LEU:O	1:A:304:ILE:HG13	2.05	0.56
2:B:228:ASP:O	2:B:245:SER:OG	2.16	0.56
3:D:224:PHE:HE1	3:D:250:LEU:CD2	2.18	0.56
3:D:262:ASP:OD1	3:D:317:THR:OG1	2.18	0.56
4:S:98:ARG:HD3	4:S:110:PHE:CB	2.34	0.56
2:B:47:THR:HG22	2:B:339:TRP:HE1	1.69	0.56
2:B:30:LEU:CD2	2:B:33:ILE:HD12	2.36	0.56
4:S:40:ALA:HB1	4:S:41:PRO:HD2	1.86	0.56
1:A:259:ILE:O	1:A:263:VAL:HG13	2.06	0.56
2:B:161:SER:CB	2:B:187:VAL:HG21	2.35	0.56
2:B:233:CYS:O	2:B:241:PHE:HB2	2.06	0.56
4:S:12:VAL:HG12	4:S:13:GLN:N	2.20	0.56
1:A:51:ALA:C	1:A:53:THR:N	2.61	0.56
3:D:340:VAL:O	3:D:344:ILE:HG13	2.06	0.56
1:A:224:VAL:HA	1:A:227:LEU:CG	2.35	0.56
1:A:130:TYR:HH	1:A:177:SER:HB3	1.71	0.56
2:B:26:ALA:C	2:B:28:ALA:N	2.63	0.56
2:B:308:LEU:O	2:B:339:TRP:CH2	2.58	0.56
1:A:212:VAL:HG12	1:A:212:VAL:O	2.06	0.56
1:A:275:ALA:HB3	1:A:276:PRO:HD3	1.88	0.55
2:B:29:THR:C	2:B:31:SER:N	2.62	0.55
2:B:191:SER:O	2:B:199:PHE:HB2	2.06	0.55
1:A:270:PHE:CD1	1:A:274:TRP:CE3	2.95	0.55
4:S:71:SER:O	4:S:79:LEU:CD1	2.45	0.55
1:A:74:ILE:HG12	1:A:325:PHE:CZ	2.40	0.55
1:A:240:LEU:HD21	1:A:246:LEU:CD2	2.36	0.55
4:S:11:LEU:HD11	4:S:120:SER:CB	2.21	0.55
1:A:54:ALA:C	1:A:57:SER:HB3	2.31	0.55
1:A:95:ASP:OD2	1:A:315:PRO:HG2	2.07	0.55
2:B:104:ALA:HB2	2:B:149:CYS:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:ASP:OD2	2:B:196:THR:HG23	2.07	0.55
1:A:119:LEU:HD12	1:A:122:LYS:NZ	2.22	0.55
2:B:139:LEU:HD23	2:B:169:TRP:CD2	2.42	0.55
1:A:313:LEU:C	1:A:316:VAL:H	2.15	0.55
1:A:146:ARG:NH1	3:D:354:LEU:HG	2.21	0.55
1:A:74:ILE:CD1	1:A:88:ILE:HG12	2.37	0.54
1:A:75:VAL:O	1:A:79:LYS:HD3	2.07	0.54
2:B:3:GLU:CG	5:C:16:VAL:CG1	2.85	0.54
4:S:9:GLY:HA2	4:S:117:LEU:HD13	1.89	0.54
4:S:62:ASP:OD1	4:S:63:THR:N	2.40	0.54
3:D:47:ASN:O	3:D:51:LYS:HE2	2.08	0.54
1:A:249:SER:C	1:A:251:GLU:N	2.65	0.54
1:A:310:ASN:O	1:A:311:SER:C	2.50	0.54
1:A:119:LEU:HD12	1:A:122:LYS:HE2	1.90	0.54
1:A:146:ARG:HD3	3:D:352:CYS:SG	2.47	0.54
1:A:146:ARG:O	1:A:150:VAL:HG22	2.07	0.54
1:A:77:TYR:O	1:A:79:LYS:N	2.40	0.54
3:D:190:PHE:HE2	3:D:199:MET:HE2	1.71	0.54
4:S:61:ALA:O	4:S:65:LYS:HB2	2.08	0.54
1:A:107:ALA:HA	1:A:110:LEU:HB3	1.88	0.54
1:A:297:VAL:HG13	1:A:301:HIS:CD2	2.42	0.54
1:A:313:LEU:O	1:A:316:VAL:CB	2.56	0.54
1:A:53:THR:O	1:A:57:SER:CB	2.56	0.54
1:A:53:THR:O	1:A:54:ALA:C	2.48	0.54
4:S:71:SER:OG	4:S:80:PHE:HB2	2.07	0.54
1:A:56:TYR:C	1:A:59:VAL:HG12	2.31	0.54
1:A:171:CYS:O	1:A:175:LEU:HD13	2.07	0.54
2:B:273:ILE:HG22	2:B:289:TYR:CD2	2.43	0.54
1:A:181:VAL:CG2	1:A:182:PRO:HD3	2.37	0.54
1:A:313:LEU:CA	1:A:316:VAL:CG2	2.85	0.54
2:B:43:ILE:HD12	2:B:284:LEU:HD21	1.89	0.54
2:B:183:HIS:NE2	2:B:211:TRP:HZ2	2.06	0.54
2:B:197:ARG:HE	2:B:214:ARG:HH22	1.48	0.54
1:A:303:CYS:SG	1:A:304:ILE:N	2.81	0.53
3:D:188:THR:HG21	3:D:199:MET:HE3	1.89	0.53
4:S:20:LEU:HD12	4:S:36:TRP:HZ3	1.72	0.53
1:A:69:LEU:O	1:A:70:VAL:C	2.50	0.53
2:B:80:ILE:HD11	3:D:23:LEU:HD11	1.89	0.53
3:D:244:MET:O	3:D:247:SER:HB2	2.07	0.53
1:A:177:SER:O	1:A:178:GLY:C	2.43	0.53
5:C:12:ALA:O	5:C:16:VAL:CA	2.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:12:ALA:HA	5:C:15:LEU:HB3	1.89	0.53
1:A:305:ALA:C	1:A:307:GLY:N	2.67	0.53
1:A:313:LEU:O	1:A:316:VAL:CA	2.56	0.53
2:B:168:LEU:HD23	2:B:169:TRP:N	2.23	0.53
2:B:215:GLU:HG3	2:B:217:MET:CE	2.37	0.53
3:D:228:LEU:O	3:D:244:MET:CE	2.57	0.53
3:D:349:LEU:HD21	3:D:355:PHE:HD1	1.73	0.53
1:A:79:LYS:HZ3	1:A:80:MET:HE1	1.72	0.53
3:D:49:ILE:CG2	3:D:53:MET:CE	2.84	0.53
1:A:250:LYS:H	1:A:250:LYS:HD2	1.73	0.53
3:D:238:ASP:HB3	3:D:241:MET:HG2	1.89	0.53
5:C:11:GLN:HA	5:C:14:LYS:HB3	1.89	0.53
1:A:299:ALA:HA	1:A:302:LEU:CB	2.26	0.53
1:A:91:LEU:HD21	1:A:138:THR:HG22	1.91	0.53
3:D:228:LEU:HG	3:D:269:LEU:HB3	1.91	0.53
4:S:172:THR:O	4:S:191:ARG:HG2	2.08	0.53
1:A:243:VAL:CG1	1:A:244:ARG:H	2.22	0.52
3:D:209:ARG:O	3:D:213:ILE:HB	2.10	0.52
4:S:190:TYR:O	4:S:191:ARG:C	2.50	0.52
1:A:171:CYS:CA	1:A:174:VAL:HG22	2.39	0.52
2:B:61:MET:HA	2:B:71:VAL:O	2.09	0.52
2:B:68:ARG:HG2	4:S:103:TYR:CZ	2.45	0.52
2:B:168:LEU:C	2:B:169:TRP:CD1	2.87	0.52
2:B:278:PHE:O	2:B:320:VAL:HG11	2.09	0.52
4:S:97:VAL:HG22	4:S:111:TRP:CD2	2.44	0.52
1:A:246:LEU:HD22	1:A:259:ILE:HD12	1.92	0.52
3:D:54:LYS:HD2	3:D:190:PHE:CB	2.38	0.52
3:D:267:LEU:HB3	3:D:321:TYR:O	2.09	0.52
1:A:54:ALA:HA	1:A:57:SER:HB3	1.92	0.52
1:A:219:LEU:HD12	1:A:223:VAL:HB	1.92	0.52
2:B:27:ASP:O	2:B:29:THR:N	2.41	0.52
2:B:163:ASP:OD1	2:B:164:THR:N	2.42	0.52
2:B:273:ILE:HG22	2:B:289:TYR:CE2	2.43	0.52
3:D:224:PHE:CE1	3:D:250:LEU:HD22	2.43	0.52
1:A:294:PRO:HG2	1:A:295:LEU:HD12	1.90	0.52
2:B:186:ASP:O	2:B:188:MET:HG3	2.09	0.52
1:A:116:PHE:CE2	1:A:120:LEU:N	2.53	0.52
1:A:171:CYS:HA	1:A:174:VAL:CG2	2.40	0.52
1:A:257:ARG:HA	1:A:260:THR:CG2	2.38	0.52
2:B:15:LYS:HZ1	2:B:258:ASP:CB	1.99	0.52
2:B:199:PHE:CE2	2:B:211:TRP:CD1	2.98	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:HIS:NE2	2:B:251:ARG:HG3	2.24	0.52
3:D:43:GLU:C	3:D:243:ARG:HH22	2.18	0.52
3:D:48:THR:CA	3:D:51:LYS:CB	2.70	0.52
3:D:49:ILE:HG22	3:D:53:MET:CE	2.27	0.52
1:A:171:CYS:O	1:A:175:LEU:HB2	2.09	0.52
2:B:43:ILE:CD1	2:B:284:LEU:HD11	2.40	0.52
1:A:146:ARG:NH1	3:D:354:LEU:CG	2.73	0.52
2:B:19:ARG:HA	2:B:22:ARG:HB3	1.92	0.52
2:B:295:ASN:OD1	2:B:307:VAL:HG13	2.09	0.52
3:D:305:GLN:CG	3:D:322:THR:HG21	2.39	0.52
1:A:282:ILE:HA	1:A:285:THR:HG1	1.73	0.51
4:S:51:ILE:HG23	4:S:58:ILE:HG13	1.92	0.51
1:A:219:LEU:HD12	1:A:223:VAL:CB	2.41	0.51
4:S:93:MET:HE3	4:S:116:THR:HG23	1.92	0.51
1:A:101:THR:HG21	1:A:128:ASP:CG	2.36	0.51
1:A:51:ALA:O	1:A:54:ALA:CB	2.57	0.51
2:B:13:GLN:O	2:B:17:GLN:N	2.38	0.51
2:B:22:ARG:HG3	5:C:30:VAL:HG11	0.65	0.51
2:B:104:ALA:HB3	2:B:113:ALA:HB3	1.92	0.51
2:B:233:CYS:O	2:B:242:ALA:N	2.42	0.51
2:B:26:ALA:HA	2:B:33:ILE:HD11	1.90	0.51
2:B:251:ARG:NH1	2:B:260:GLU:OE1	2.43	0.51
2:B:121:CYS:HB2	2:B:146:LEU:HD22	1.91	0.51
4:S:4:LEU:HD21	4:S:27:PHE:HZ	1.76	0.51
2:B:315:VAL:HA	2:B:331:SER:HA	1.93	0.51
1:A:139:LEU:HD21	1:A:229:ILE:CD1	2.41	0.51
1:A:214:LYS:CE	1:A:281:VAL:HB	2.40	0.51
1:A:307:GLY:C	1:A:309:ALA:N	2.60	0.51
1:A:72:PHE:C	1:A:75:VAL:H	2.18	0.51
3:D:48:THR:C	3:D:51:LYS:H	2.20	0.51
1:A:201:GLN:N	1:A:201:GLN:OE1	2.43	0.50
2:B:40:VAL:HG21	5:C:51:LEU:HD11	1.93	0.50
1:A:314:ASN:CB	1:A:315:PRO:HD3	2.40	0.50
3:D:283:PRO:HG2	3:D:286:ILE:HG13	1.93	0.50
1:A:199:MET:C	1:A:200:LEU:HD12	2.36	0.50
2:B:18:ILE:HG13	5:C:27:ARG:HD3	1.92	0.50
2:B:29:THR:HG21	2:B:32:GLN:HE21	1.76	0.50
2:B:84:SER:O	2:B:85:TYR:C	2.54	0.50
3:D:228:LEU:O	3:D:244:MET:HE1	2.11	0.50
2:B:215:GLU:HG3	2:B:217:MET:HG2	1.94	0.50
2:B:152:LEU:HD23	2:B:157:ILE:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:183:HIS:HE2	2:B:211:TRP:HZ2	1.60	0.50
3:D:47:ASN:O	3:D:51:LYS:CA	2.59	0.50
1:A:215:ILE:O	1:A:218:PHE:HB3	2.12	0.50
4:S:139:VAL:CG1	4:S:162:SER:CB	2.90	0.50
4:S:144:THR:CG2	4:S:243:THR:HG23	2.41	0.50
4:S:20:LEU:HD12	4:S:36:TRP:CZ3	2.47	0.49
4:S:58:ILE:HD12	4:S:58:ILE:H	1.77	0.49
5:C:12:ALA:O	5:C:16:VAL:HB	2.12	0.49
1:A:283:VAL:O	1:A:287:VAL:N	2.40	0.49
1:A:314:ASN:CB	1:A:315:PRO:CD	2.90	0.49
2:B:4:LEU:HA	5:C:19:LEU:CD2	2.41	0.49
2:B:283:ARG:HD2	2:B:300:LEU:HD11	1.93	0.49
3:D:48:THR:O	3:D:51:LYS:HB3	2.12	0.49
4:S:72:ARG:HB3	4:S:79:LEU:HD13	1.93	0.49
4:S:73:ASP:O	4:S:77:ASN:N	2.45	0.49
1:A:52:ILE:C	1:A:55:LEU:HB3	2.37	0.49
1:A:170:ILE:O	1:A:174:VAL:CG2	2.60	0.49
1:A:297:VAL:CG1	1:A:301:HIS:HD2	2.26	0.49
2:B:241:PHE:O	2:B:252:LEU:HD12	2.12	0.49
3:D:38:LEU:HD21	3:D:50:VAL:HG22	1.95	0.49
1:A:130:TYR:O	1:A:131:ASN:C	2.54	0.49
2:B:68:ARG:NE	2:B:83:ASP:OD1	2.42	0.49
2:B:232:ILE:HG22	2:B:243:THR:CB	2.42	0.49
3:D:246:ALA:O	3:D:247:SER:C	2.56	0.49
1:A:52:ILE:C	1:A:55:LEU:N	2.70	0.49
1:A:204:SER:HB2	1:A:210:ASP:CG	2.38	0.49
2:B:256:ARG:HD2	2:B:256:ARG:N	2.17	0.49
3:D:272:LYS:HD2	3:D:324:PHE:HB3	1.94	0.49
4:S:84:THR:OG1	4:S:85:SER:N	2.43	0.49
1:A:262:MET:O	1:A:263:VAL:C	2.52	0.48
2:B:17:GLN:O	2:B:21:ALA:N	2.40	0.48
4:S:157:ILE:HG23	4:S:243:THR:HG21	1.94	0.48
1:A:198:CYS:C	1:A:199:MET:HE2	2.38	0.48
1:A:274:TRP:CH2	1:A:314:ASN:OD1	2.66	0.48
2:B:57:LYS:NZ	3:D:217:GLU:OE2	2.47	0.48
2:B:166:CYS:HB2	2:B:180:PHE:HD2	1.77	0.48
1:A:119:LEU:HD12	1:A:122:LYS:CE	2.43	0.48
1:A:313:LEU:HA	1:A:316:VAL:HG21	1.92	0.48
1:A:67:ASN:HD22	1:A:96:ALA:N	2.11	0.48
1:A:299:ALA:C	1:A:302:LEU:HB2	2.38	0.48
1:A:324:ASN:OD1	1:A:325:PHE:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:LEU:HB2	2:B:336:LEU:HB2	1.94	0.48
1:A:72:PHE:O	1:A:75:VAL:CB	2.61	0.48
1:A:297:VAL:CG1	1:A:301:HIS:CD2	2.96	0.48
2:B:80:ILE:HG22	2:B:82:TRP:HE3	1.77	0.48
4:S:88:SER:HA	4:S:119:VAL:CG1	2.44	0.48
1:A:67:ASN:HD21	1:A:96:ALA:N	2.09	0.48
1:A:67:ASN:O	1:A:68:VAL:C	2.55	0.48
1:A:111:MET:C	1:A:113:THR:N	2.72	0.48
1:A:116:PHE:CE2	1:A:120:LEU:CG	2.96	0.48
2:B:4:LEU:HA	5:C:19:LEU:HD23	1.96	0.48
2:B:32:GLN:C	2:B:34:THR:H	2.21	0.48
2:B:199:PHE:CE2	2:B:211:TRP:HB2	2.49	0.48
3:D:189:HIS:HA	3:D:197:PHE:O	2.14	0.48
1:A:240:LEU:CD2	1:A:246:LEU:HD23	2.44	0.48
3:D:222:ILE:O	3:D:223:ILE:C	2.56	0.48
4:S:6:GLU:HG3	4:S:22:CYS:SG	2.54	0.48
2:B:45:MET:SD	2:B:308:LEU:HD21	2.54	0.48
3:D:190:PHE:CE2	3:D:199:MET:HE2	2.48	0.48
1:A:130:TYR:CE1	1:A:177:SER:CA	2.97	0.48
1:A:252:LYS:O	1:A:255:SER:HB2	2.13	0.48
1:A:299:ALA:O	1:A:302:LEU:CA	2.62	0.48
1:A:303:CYS:C	1:A:305:ALA:N	2.70	0.48
3:D:53:MET:SD	3:D:199:MET:CE	3.02	0.47
2:B:22:ARG:HH21	2:B:259:GLN:CD	2.22	0.47
4:S:98:ARG:CD	4:S:110:PHE:HB3	2.41	0.47
2:B:215:GLU:HG3	2:B:217:MET:CG	2.44	0.47
4:S:246:GLU:C	4:S:247:LEU:HD12	2.39	0.47
1:A:305:ALA:C	1:A:307:GLY:H	2.22	0.47
2:B:153:ASP:OD2	2:B:196:THR:CG2	2.63	0.47
1:A:70:VAL:HG13	1:A:71:MET:N	2.30	0.47
1:A:258:ARG:O	1:A:259:ILE:C	2.53	0.47
1:A:307:GLY:C	1:A:309:ALA:H	2.21	0.47
2:B:27:ASP:C	2:B:29:THR:N	2.70	0.47
5:C:8:SER:O	5:C:11:GLN:HB2	2.14	0.47
1:A:283:VAL:C	1:A:286:LEU:H	2.23	0.47
2:B:16:ASN:O	2:B:20:ASP:N	2.33	0.47
2:B:22:ARG:CA	5:C:30:VAL:CG1	2.93	0.47
2:B:51:LEU:HD23	2:B:82:TRP:CZ2	2.50	0.47
2:B:250:CYS:SG	2:B:273:ILE:HD12	2.50	0.47
3:D:349:LEU:HD21	3:D:355:PHE:CD1	2.49	0.47
4:S:88:SER:HA	4:S:119:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:12:ALA:O	5:C:16:VAL:HG23	2.14	0.47
1:A:218:PHE:HE1	1:A:278:HIS:HB3	1.75	0.47
1:A:297:VAL:HG12	1:A:301:HIS:HD2	1.80	0.47
1:A:311:SER:HA	1:A:314:ASN:OD1	2.15	0.47
2:B:123:ILE:HG13	2:B:171:ILE:HD12	1.97	0.47
2:B:208:ALA:N	2:B:222:PHE:O	2.48	0.47
2:B:331:SER:HG	2:B:332:TRP:H	1.63	0.47
3:D:6:SER:C	3:D:8:GLU:H	2.21	0.47
3:D:188:THR:HG21	3:D:199:MET:CE	2.45	0.47
1:A:102:LEU:CD2	1:A:103:PRO:HD3	2.36	0.47
1:A:130:TYR:CE1	1:A:177:SER:N	2.73	0.47
1:A:243:VAL:HG12	1:A:245:LEU:N	2.26	0.47
2:B:18:ILE:CD1	5:C:27:ARG:HB2	2.44	0.47
3:D:49:ILE:HD13	3:D:268:PHE:CD2	2.50	0.47
1:A:48:LEU:O	1:A:51:ALA:HB3	2.15	0.47
3:D:349:LEU:CD2	3:D:355:PHE:CD1	2.98	0.47
4:S:232:HIS:CD2	4:S:237:LEU:HD21	2.50	0.47
1:A:67:ASN:HD22	1:A:95:ASP:C	2.23	0.46
1:A:74:ILE:HD11	1:A:88:ILE:HG12	1.96	0.46
2:B:119:ASN:ND2	2:B:144:GLY:C	2.74	0.46
4:S:50:TYR:C	4:S:51:ILE:HG13	2.40	0.46
1:A:64:LEU:HA	1:A:99:THR:CG2	2.37	0.46
1:A:108:LYS:O	1:A:111:MET:N	2.46	0.46
4:S:64:VAL:HG13	4:S:68:PHE:CE1	2.50	0.46
5:C:9:ILE:O	5:C:12:ALA:HB3	2.14	0.46
1:A:172:ILE:C	1:A:174:VAL:N	2.71	0.46
1:A:299:ALA:C	1:A:302:LEU:H	2.22	0.46
1:A:313:LEU:O	1:A:317:LEU:N	2.47	0.46
4:S:73:ASP:O	4:S:78:THR:N	2.36	0.46
1:A:130:TYR:CE1	1:A:177:SER:HA	2.51	0.46
1:A:243:VAL:HG12	1:A:244:ARG:H	1.79	0.46
2:B:191:SER:OG	2:B:192:LEU:N	2.49	0.46
1:A:279:ILE:O	1:A:282:ILE:HG22	2.16	0.46
2:B:239:ASN:HB2	2:B:256:ARG:CZ	2.45	0.46
4:S:70:ILE:HB	4:S:81:LEU:HD12	1.97	0.46
1:A:251:GLU:O	1:A:252:LYS:HE2	2.16	0.46
4:S:64:VAL:CG1	4:S:68:PHE:CD1	2.98	0.46
4:S:243:THR:O	4:S:245:LEU:CD1	2.64	0.46
1:A:218:PHE:CD1	1:A:278:HIS:HB3	2.51	0.46
1:A:52:ILE:HG21	1:A:56:TYR:OH	2.15	0.46
2:B:231:ALA:HB3	2:B:275:SER:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:49:ILE:O	3:D:53:MET:HB2	2.16	0.46
1:A:74:ILE:HD11	1:A:88:ILE:CD1	2.45	0.46
1:A:143:SER:HB2	1:A:233:TYR:CE2	2.51	0.46
1:A:171:CYS:C	1:A:174:VAL:HG22	2.41	0.46
1:A:198:CYS:O	1:A:199:MET:HE2	2.15	0.46
1:A:227:LEU:HD12	1:A:228:ILE:N	2.30	0.46
3:D:312:ASN:HB2	3:D:320:ILE:HD11	1.97	0.46
1:A:270:PHE:HD1	1:A:274:TRP:HE3	1.62	0.46
2:B:18:ILE:CG2	2:B:259:GLN:HE22	2.28	0.46
3:D:329:ASP:C	3:D:331:LYS:H	2.24	0.46
1:A:307:GLY:O	1:A:310:ASN:CG	2.59	0.45
2:B:217:MET:HE3	2:B:219:ARG:NH2	2.31	0.45
1:A:250:LYS:HD2	1:A:250:LYS:N	2.30	0.45
2:B:165:THR:HG23	2:B:180:PHE:O	2.16	0.45
2:B:254:ASP:O	2:B:257:ALA:O	2.35	0.45
4:S:70:ILE:CD1	4:S:81:LEU:HB2	2.47	0.45
4:S:138:ILE:HB	4:S:231:GLN:CD	2.39	0.45
1:A:72:PHE:HA	1:A:75:VAL:CG2	2.47	0.45
1:A:256:LEU:C	1:A:256:LEU:HD23	2.41	0.45
2:B:22:ARG:O	2:B:26:ALA:HB3	2.16	0.45
2:B:39:PRO:HG3	2:B:301:LYS:HZ1	1.81	0.45
4:S:188:LEU:HA	4:S:199:VAL:HG11	1.99	0.45
1:A:299:ALA:C	1:A:301:HIS:N	2.71	0.45
4:S:2:VAL:HA	4:S:26:GLY:HA3	1.98	0.45
4:S:161:SER:H	4:S:210:THR:HG23	1.81	0.45
1:A:119:LEU:O	1:A:122:LYS:HG2	2.17	0.45
5:C:14:LYS:O	5:C:17:GLU:CB	2.62	0.45
5:C:9:ILE:C	5:C:12:ALA:HB3	2.41	0.45
2:B:18:ILE:HG13	5:C:27:ARG:CD	2.47	0.45
3:D:208:GLU:OE2	3:D:210:LYS:NZ	2.41	0.45
5:C:10:ALA:C	5:C:14:LYS:H	2.23	0.45
2:B:3:GLU:C	2:B:3:GLU:CD	2.85	0.45
2:B:51:LEU:N	2:B:336:LEU:O	2.38	0.45
4:S:149:VAL:HG11	4:S:219:LEU:HD13	1.99	0.45
4:S:175:TYR:HD1	4:S:190:TYR:HA	1.81	0.45
4:S:244:LYS:HZ2	4:S:246:GLU:HG3	1.82	0.45
1:A:46:LEU:O	1:A:49:ALA:HB3	2.17	0.45
1:A:273:CYS:O	1:A:276:PRO:HD2	2.17	0.45
2:B:48:ARG:HA	2:B:48:ARG:HD3	1.65	0.45
2:B:293:ASN:HB2	2:B:309:ALA:HB2	1.99	0.45
3:D:189:HIS:CG	3:D:198:LYS:CG	3.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:93:MET:HE3	4:S:116:THR:CG2	2.46	0.45
1:A:54:ALA:CA	1:A:57:SER:HB3	2.46	0.44
2:B:233:CYS:SG	2:B:276:VAL:O	2.66	0.44
2:B:235:PHE:CB	2:B:240:ALA:HB3	2.47	0.44
4:S:64:VAL:HG13	4:S:68:PHE:CZ	2.53	0.44
1:A:146:ARG:HH11	3:D:354:LEU:CD1	2.27	0.44
3:D:43:GLU:O	3:D:243:ARG:NH2	2.49	0.44
1:A:119:LEU:HD12	1:A:122:LYS:HZ1	1.82	0.44
2:B:22:ARG:HA	5:C:30:VAL:CG1	2.32	0.44
2:B:200:VAL:CG2	2:B:210:LEU:HD12	2.46	0.44
3:D:231:TYR:CE1	3:D:275:PHE:CE1	3.05	0.44
4:S:73:ASP:OD1	4:S:76:LYS:HG2	2.18	0.44
1:A:240:LEU:HD21	1:A:246:LEU:HD22	2.00	0.44
1:A:311:SER:OG	1:A:312:SER:N	2.50	0.44
2:B:243:THR:HG22	2:B:251:ARG:O	2.16	0.44
2:B:254:ASP:HB3	2:B:261:LEU:HD11	1.99	0.44
3:D:189:HIS:ND1	3:D:198:LYS:CG	2.80	0.44
3:D:248:MET:HE2	3:D:288:PHE:HZ	1.82	0.44
3:D:276:GLU:HG2	3:D:297:TYR:HB2	1.99	0.44
3:D:291:TYR:OH	3:D:299:GLU:HG2	2.17	0.44
5:C:17:GLU:HA	5:C:20:LYS:HB2	1.98	0.44
5:C:17:GLU:O	5:C:20:LYS:HB2	2.18	0.44
1:A:56:TYR:O	1:A:59:VAL:CG1	2.66	0.44
1:A:56:TYR:OH	1:A:301:HIS:O	2.28	0.44
1:A:130:TYR:HE1	1:A:177:SER:CA	2.30	0.44
1:A:239:ARG:O	1:A:243:VAL:HG23	2.17	0.44
2:B:168:LEU:O	2:B:169:TRP:CG	2.70	0.44
2:B:3:GLU:O	2:B:4:LEU:C	2.61	0.44
2:B:4:LEU:HG	2:B:5:ASP:N	2.32	0.44
4:S:88:SER:HA	4:S:119:VAL:HB	1.99	0.44
1:A:56:TYR:HH	1:A:301:HIS:C	2.22	0.44
1:A:294:PRO:HG2	1:A:295:LEU:CD1	2.48	0.44
1:A:255:SER:O	1:A:256:LEU:C	2.61	0.44
1:A:292:ARG:HD2	1:A:292:ARG:O	2.17	0.44
1:A:238:LEU:O	1:A:241:ARG:HB3	2.17	0.44
2:B:289:TYR:O	2:B:315:VAL:HG22	2.17	0.44
3:D:348:ASN:HA	3:D:351:ASP:OD1	2.17	0.44
4:S:235:TYR:HB2	4:S:236:PRO:HD3	2.00	0.44
2:B:82:TRP:HB2	2:B:88:ASN:C	2.43	0.43
2:B:22:ARG:NH2	2:B:259:GLN:CD	2.76	0.43
2:B:277:SER:OG	2:B:320:VAL:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:188:THR:CG2	3:D:199:MET:HE3	2.48	0.43
1:A:224:VAL:O	1:A:227:LEU:HG	2.18	0.43
2:B:28:ALA:O	2:B:29:THR:C	2.61	0.43
2:B:139:LEU:HD12	2:B:139:LEU:N	2.32	0.43
3:D:49:ILE:CD1	3:D:268:PHE:HD2	2.31	0.43
4:S:50:TYR:O	4:S:58:ILE:HA	2.18	0.43
1:A:217:VAL:O	1:A:221:ALA:HB3	2.18	0.43
2:B:274:THR:O	2:B:274:THR:OG1	2.33	0.43
3:D:284:LEU:CD1	3:D:300:ALA:HB1	2.48	0.43
1:A:139:LEU:C	1:A:139:LEU:HD23	2.43	0.43
1:A:262:MET:C	1:A:264:LEU:N	2.66	0.43
3:D:49:ILE:CD1	3:D:268:PHE:CD2	3.02	0.43
1:A:254:ARG:O	1:A:257:ARG:HB3	2.19	0.43
6:A:401:A1LXY:C08	6:A:401:A1LXY:O16	2.67	0.43
1:A:283:VAL:HA	1:A:286:LEU:HB2	2.01	0.43
2:B:279:SER:HB2	5:C:50:LEU:HD12	2.01	0.43
2:B:33:ILE:O	2:B:33:ILE:CG2	2.67	0.43
2:B:111:TYR:CD2	2:B:155:ASN:HB2	2.54	0.43
2:B:253:PHE:CD1	2:B:260:GLU:HA	2.48	0.43
2:B:313:ASN:C	2:B:331:SER:OG	2.61	0.43
3:D:231:TYR:OH	3:D:279:ILE:HG22	2.19	0.43
1:A:146:ARG:NH1	3:D:354:LEU:HD21	2.34	0.43
2:B:10:GLU:O	2:B:13:GLN:HB3	2.18	0.43
2:B:163:ASP:CG	2:B:164:THR:N	2.77	0.43
3:D:283:PRO:HA	3:D:295:ASN:HD21	1.83	0.42
4:S:69:THR:HG22	4:S:82:GLN:O	2.19	0.42
2:B:215:GLU:CG	2:B:217:MET:HG2	2.48	0.42
4:S:70:ILE:HD12	4:S:81:LEU:HD13	1.91	0.42
4:S:165:LEU:HD12	4:S:212:PHE:CE2	2.54	0.42
1:A:56:TYR:O	1:A:59:VAL:HG12	2.20	0.42
1:A:282:ILE:O	1:A:286:LEU:N	2.52	0.42
2:B:200:VAL:HG23	2:B:234:PHE:HZ	1.82	0.42
2:B:229:ILE:HD13	2:B:244:GLY:O	2.19	0.42
3:D:188:THR:O	3:D:198:LYS:CA	2.61	0.42
1:A:69:LEU:O	1:A:72:PHE:N	2.52	0.42
1:A:262:MET:C	1:A:262:MET:SD	3.02	0.42
4:S:204:SER:O	4:S:214:LEU:HD12	2.18	0.42
1:A:77:TYR:O	1:A:79:LYS:HB2	2.20	0.42
1:A:114:TRP:CH2	1:A:121:CYS:HA	2.55	0.42
2:B:119:ASN:HA	2:B:144:GLY:O	2.18	0.42
2:B:205:ASP:OD1	2:B:205:ASP:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:7:ALA:N	5:C:10:ALA:HB3	2.35	0.42
3:D:50:VAL:O	3:D:51:LYS:C	2.62	0.42
4:S:70:ILE:HG13	4:S:81:LEU:CA	2.50	0.42
1:A:108:LYS:C	1:A:110:LEU:N	2.74	0.42
1:A:141:MET:HE2	1:A:168:ILE:HG21	2.02	0.42
1:A:170:ILE:O	1:A:174:VAL:CG1	2.67	0.42
2:B:153:ASP:CG	2:B:196:THR:CG2	2.92	0.42
2:B:314:ARG:C	2:B:331:SER:OG	2.62	0.42
4:S:73:ASP:N	4:S:78:THR:O	2.29	0.42
1:A:78:THR:HG23	1:A:85:ASN:ND2	2.35	0.41
2:B:80:ILE:HD11	3:D:23:LEU:CD1	2.50	0.41
1:A:224:VAL:CA	1:A:227:LEU:HG	2.44	0.41
2:B:94:PRO:C	2:B:95:LEU:HD12	2.46	0.41
3:D:53:MET:HG2	3:D:190:PHE:CE2	2.55	0.41
4:S:178:LEU:HD21	4:S:180:ARG:HH11	1.85	0.41
1:A:139:LEU:HD23	1:A:229:ILE:HD12	2.01	0.41
4:S:3:GLN:O	4:S:25:SER:O	2.39	0.41
1:A:116:PHE:CG	1:A:120:LEU:HD12	2.55	0.41
1:A:222:PHE:O	1:A:226:ILE:CD1	2.68	0.41
3:D:41:ALA:HB2	3:D:250:LEU:HD13	2.02	0.41
3:D:48:THR:C	3:D:51:LYS:N	2.78	0.41
1:A:306:LEU:C	1:A:309:ALA:HB3	2.44	0.41
2:B:208:ALA:O	2:B:222:PHE:N	2.39	0.41
2:B:313:ASN:HB3	2:B:331:SER:OG	2.20	0.41
3:D:257:ASN:OD1	3:D:258:LYS:N	2.53	0.41
4:S:106:SER:OG	4:S:109:ASP:OD2	2.37	0.41
2:B:298:ASP:OD2	2:B:301:LYS:HB2	2.20	0.41
5:C:8:SER:O	5:C:12:ALA:CA	2.57	0.41
1:A:53:THR:O	1:A:57:SER:HB2	2.21	0.41
2:B:60:ALA:HB3	2:B:73:ALA:CB	2.47	0.41
2:B:314:ARG:HD3	2:B:332:TRP:CZ3	2.56	0.41
3:D:189:HIS:HE2	3:D:196:HIS:HB3	1.85	0.41
4:S:4:LEU:HD11	4:S:27:PHE:CE1	2.56	0.41
1:A:102:LEU:HD23	1:A:102:LEU:H	1.84	0.41
1:A:146:ARG:CG	3:D:354:LEU:HD11	2.50	0.41
1:A:295:LEU:HD12	1:A:295:LEU:N	2.36	0.41
1:A:304:ILE:HG13	1:A:304:ILE:H	1.73	0.41
2:B:22:ARG:NH2	2:B:259:GLN:HG3	2.36	0.41
2:B:197:ARG:NE	2:B:214:ARG:NH2	2.47	0.41
2:B:271:CYS:HB2	2:B:291:ASP:OD1	2.21	0.41
4:S:14:PRO:C	4:S:16:GLY:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:14:LYS:O	5:C:17:GLU:CA	2.68	0.41
2:B:13:GLN:HA	2:B:16:ASN:HB2	2.03	0.41
2:B:15:LYS:O	2:B:19:ARG:N	2.49	0.41
4:S:12:VAL:CG1	4:S:13:GLN:H	2.32	0.41
1:A:56:TYR:CA	1:A:59:VAL:CG1	2.85	0.40
1:A:146:ARG:HD2	3:D:354:LEU:HD11	2.00	0.40
1:A:299:ALA:O	1:A:302:LEU:CB	2.69	0.40
2:B:18:ILE:HG22	2:B:259:GLN:HE22	1.85	0.40
2:B:130:GLU:O	4:S:27:PHE:HB2	2.21	0.40
2:B:239:ASN:HB3	2:B:256:ARG:NH2	2.36	0.40
4:S:93:MET:HE2	4:S:114:GLY:C	2.47	0.40
1:A:71:MET:C	1:A:71:MET:SD	3.04	0.40
2:B:62:HIS:O	2:B:70:LEU:HD12	2.22	0.40
2:B:279:SER:OG	5:C:50:LEU:HD12	2.22	0.40
1:A:53:THR:OG1	1:A:54:ALA:N	2.55	0.40
2:B:199:PHE:O	2:B:211:TRP:N	2.22	0.40
2:B:283:ARG:HE	2:B:300:LEU:HB2	1.87	0.40
3:D:48:THR:O	3:D:49:ILE:C	2.60	0.40
3:D:291:TYR:CD1	3:D:303:TYR:CD2	3.09	0.40
1:A:85:ASN:O	1:A:88:ILE:HG22	2.21	0.40
1:A:147:TYR:HD1	1:A:151:CYS:HG	1.65	0.40
2:B:168:LEU:C	2:B:169:TRP:CG	3.00	0.40
1:A:107:ALA:O	1:A:110:LEU:HB3	2.21	0.40
1:A:283:VAL:O	1:A:286:LEU:N	2.53	0.40
2:B:150:ARG:O	2:B:158:VAL:CG2	2.70	0.40
2:B:163:ASP:CG	2:B:164:THR:H	2.29	0.40
2:B:270:ILE:HD12	2:B:270:ILE:HA	1.82	0.40
3:D:18:MET:HE2	3:D:18:MET:HB3	1.97	0.40
5:C:7:ALA:O	5:C:10:ALA:HB3	2.22	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	284/325 (87%)	245 (86%)	38 (13%)	1 (0%)	30 64
2	B	338/358 (94%)	300 (89%)	38 (11%)	0	100 100
3	D	219/355 (62%)	199 (91%)	20 (9%)	0	100 100
4	S	228/266 (86%)	207 (91%)	21 (9%)	0	100 100
5	C	55/71 (78%)	54 (98%)	1 (2%)	0	100 100
All	All	1124/1375 (82%)	1005 (89%)	118 (10%)	1 (0%)	50 79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	THR

5.3.2 Protein sidechains (i)

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	247/278 (89%)	245 (99%)	2 (1%)	79 87
2	B	279/298 (94%)	268 (96%)	11 (4%)	27 58
3	D	195/309 (63%)	195 (100%)	0	100 100
4	S	193/215 (90%)	188 (97%)	5 (3%)	41 68
5	C	46/58 (79%)	46 (100%)	0	100 100
All	All	960/1158 (83%)	942 (98%)	18 (2%)	52 74

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	MET
1	A	274	TRP
2	B	3	GLU
2	B	4	LEU
2	B	6	GLN
2	B	79	LEU
2	B	165	THR

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Mol	Chain	Res	Type
2	B	187	VAL
2	B	200	VAL
2	B	247	ASP
2	B	258	ASP
2	B	259	GLN
2	B	270	ILE
4	S	57	THR
4	S	59	TYR
4	S	87	ARG
4	S	88	SER
4	S	234	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	301	HIS
1	A	314	ASN
2	B	9	GLN
2	B	32	GLN
2	B	91	HIS
2	B	110	ASN
2	B	237	ASN
2	B	259	GLN
2	B	311	HIS
2	B	340	ASN
3	D	47	ASN
3	D	205	GLN
4	S	35	HIS
4	S	194	ASN
4	S	231	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
6	A1LXY	A	401	-	31,32,32	2.15	7 (22%)	38,46,46	1.99	12 (31%)

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
6	A1LXY	A	401	-	-	5/16/40/40	1/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	401	A1LXY	C10-C09	6.01	1.40	1.34
6	A	401	A1LXY	C24-C11	5.59	1.59	1.52
6	A	401	A1LXY	C04-N03	5.44	1.46	1.34
6	A	401	A1LXY	C14-C15	3.52	1.47	1.41
6	A	401	A1LXY	C19-C13	3.04	1.45	1.39
6	A	401	A1LXY	C05-C04	2.15	1.53	1.50
6	A	401	A1LXY	C26-C25	2.10	1.42	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	401	A1LXY	C24-C11-C20	-5.91	103.30	109.69
6	A	401	A1LXY	C23-C24-C11	4.05	115.40	111.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	401	A1LXY	O12-C13-C19	3.41	121.82	116.61
6	A	401	A1LXY	C08-C09-C10	3.39	124.39	119.94
6	A	401	A1LXY	O12-C11-C10	-3.27	104.98	109.83
6	A	401	A1LXY	C21-C20-C11	2.93	114.45	111.98
6	A	401	A1LXY	C05-C04-N03	2.88	122.37	118.72
6	A	401	A1LXY	C25-C08-C09	2.55	124.27	120.98
6	A	401	A1LXY	C17-C15-C14	2.33	123.17	120.17
6	A	401	A1LXY	O27-C04-N03	-2.32	118.50	122.34
6	A	401	A1LXY	C14-C09-C08	-2.22	118.80	122.97
6	A	401	A1LXY	C25-C08-C07	-2.18	115.48	118.59

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	401	A1LXY	C01-C02-N03-C04
6	A	401	A1LXY	C01-C02-N03-C28
6	A	401	A1LXY	C07-C08-C09-C10
6	A	401	A1LXY	C25-C08-C09-C10
6	A	401	A1LXY	C25-C08-C09-C14

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	401	A1LXY	C11-C20-C21-C23-C24-N22

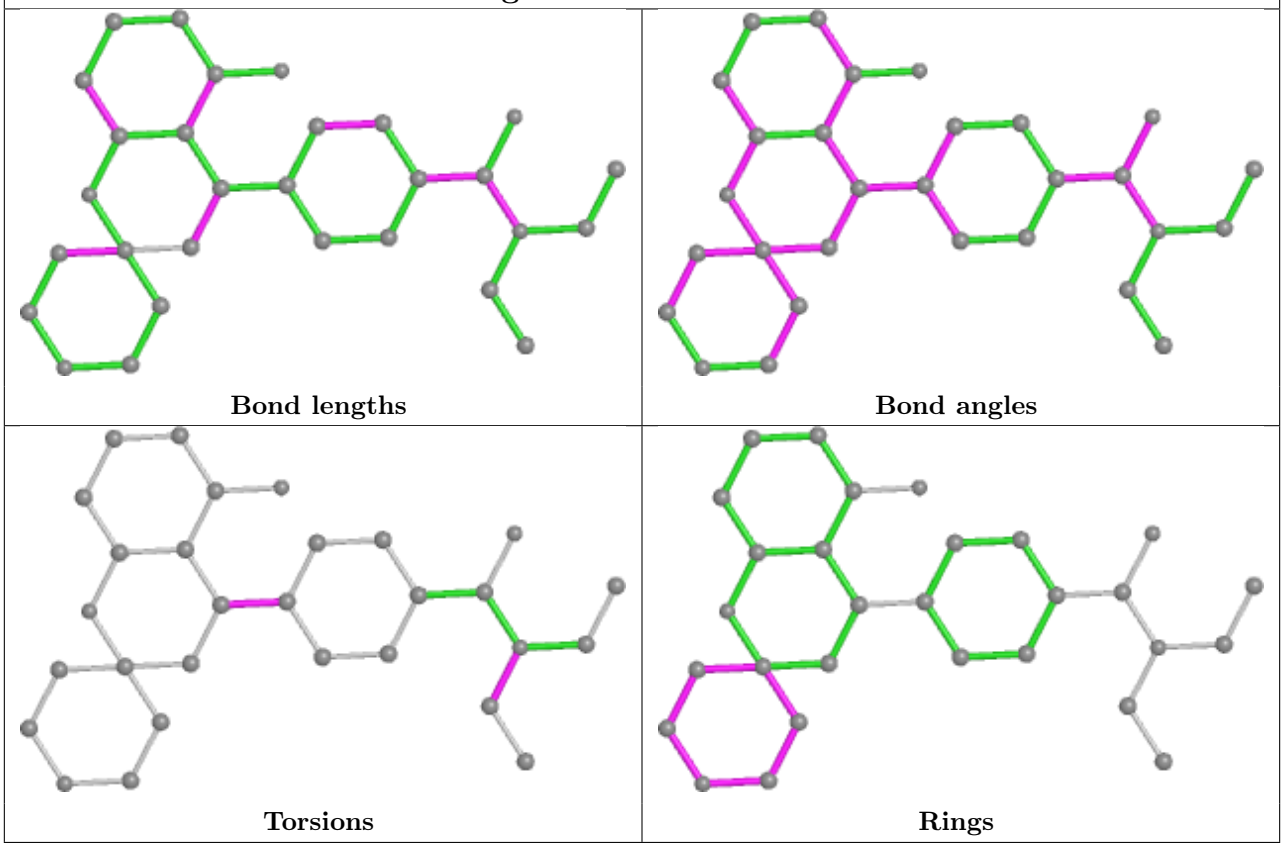
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	401	A1LXY	3	0

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

equivalents in the CSD to analyse the geometry.

Ligand A1LXY A 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

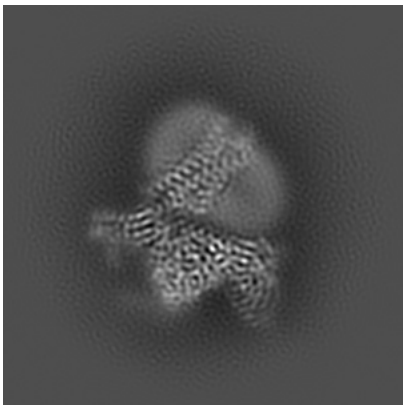
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38909. These allow visual inspection of the internal detail of the map and identification of artifacts.

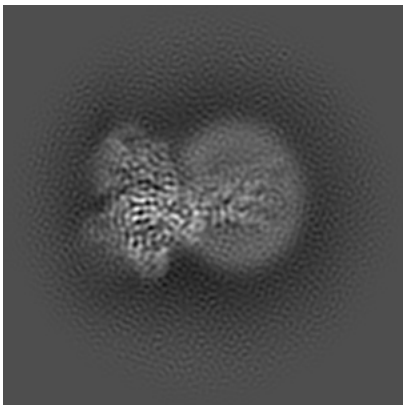
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

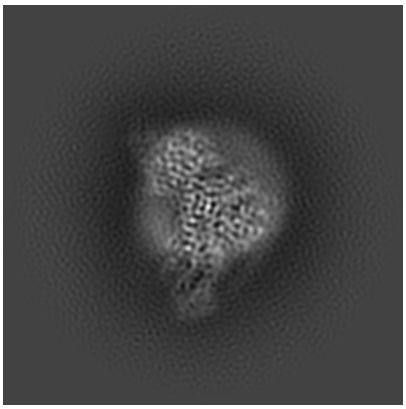
6.1.1 Primary map



X

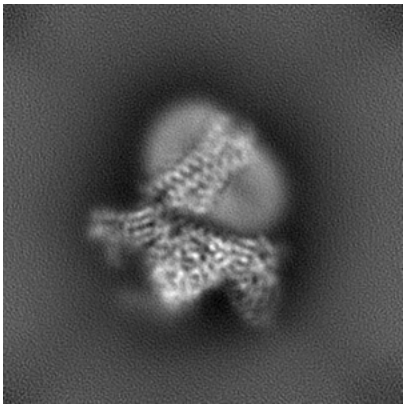


Y

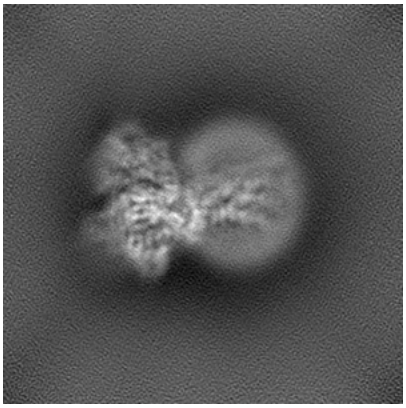


Z

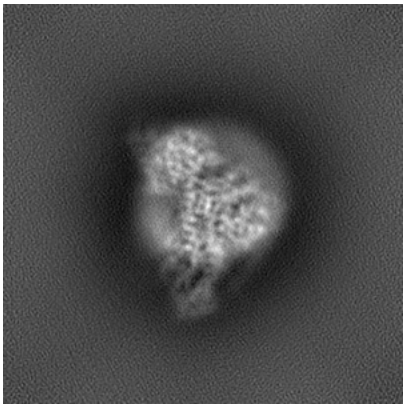
6.1.2 Raw map



X



Y

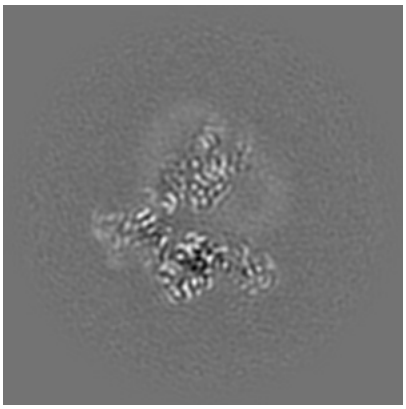


Z

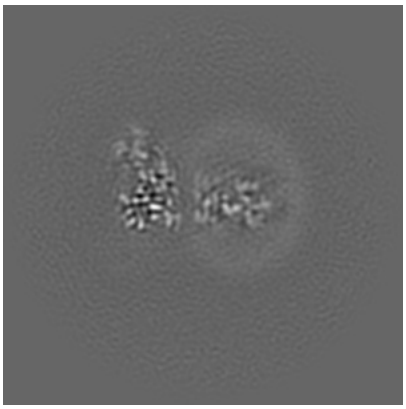
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

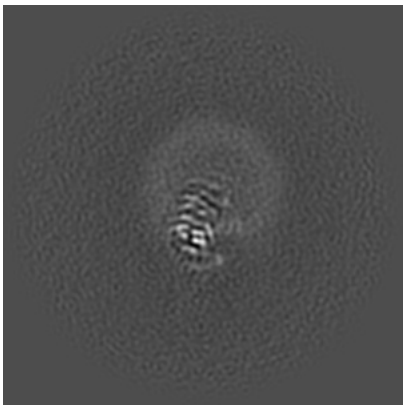
6.2.1 Primary map



X Index: 128

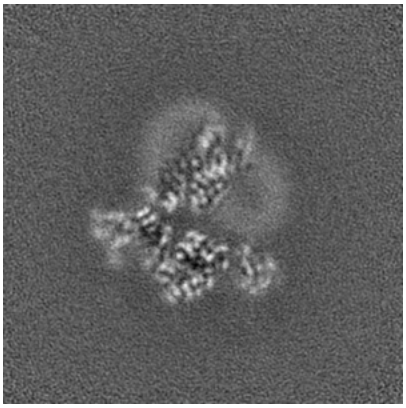


Y Index: 128

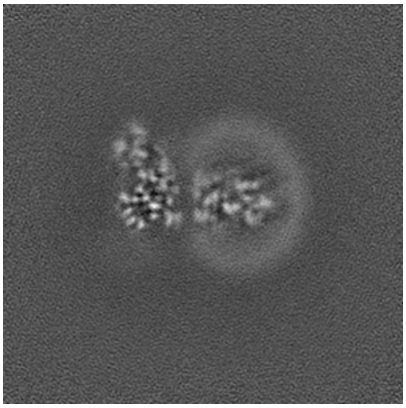


Z Index: 128

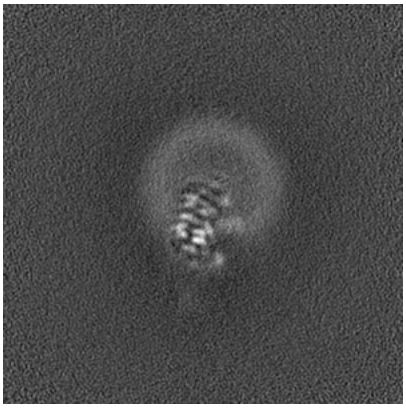
6.2.2 Raw map



X Index: 128



Y Index: 128

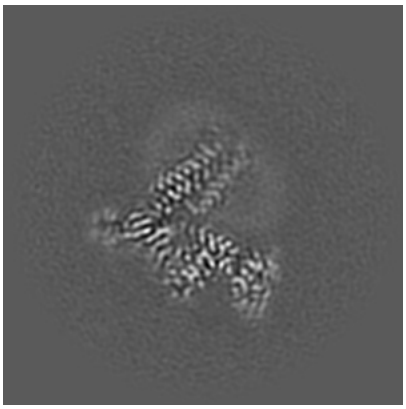


Z Index: 128

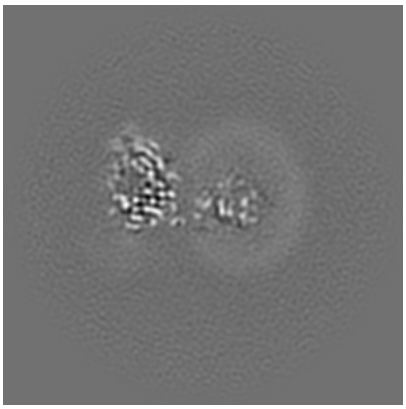
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

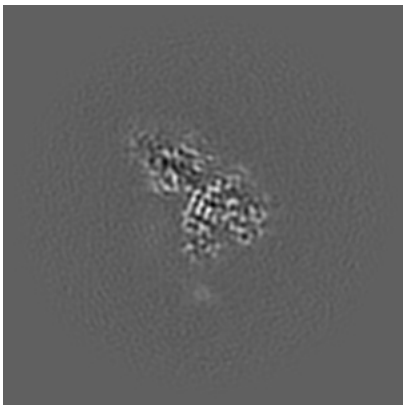
6.3.1 Primary map



X Index: 120

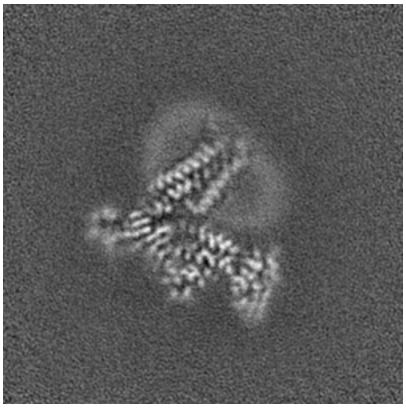


Y Index: 122

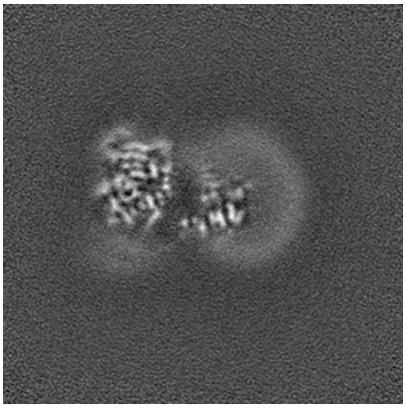


Z Index: 95

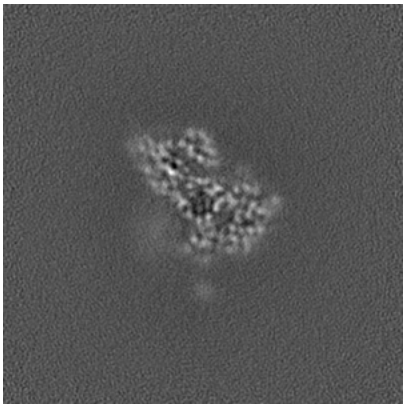
6.3.2 Raw map



X Index: 120



Y Index: 112

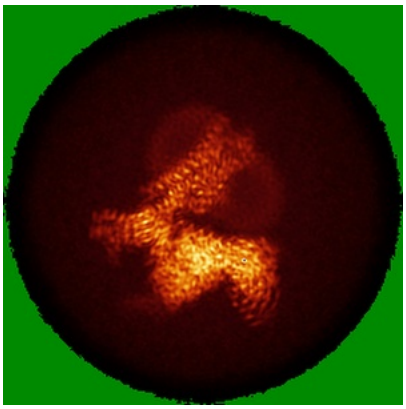


Z Index: 88

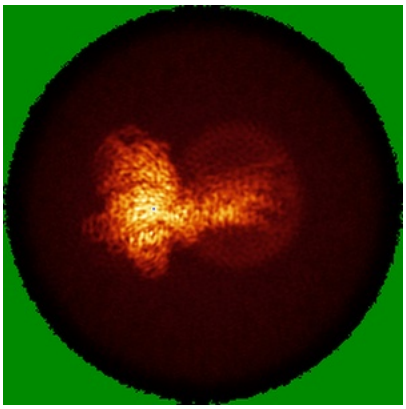
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

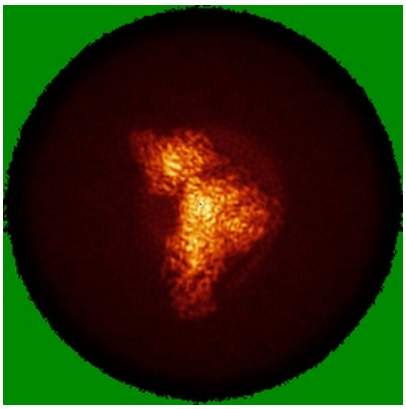
6.4.1 Primary map



X

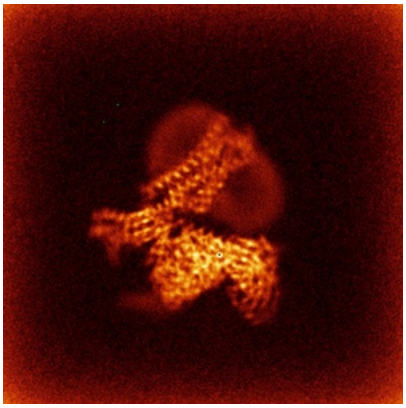


Y

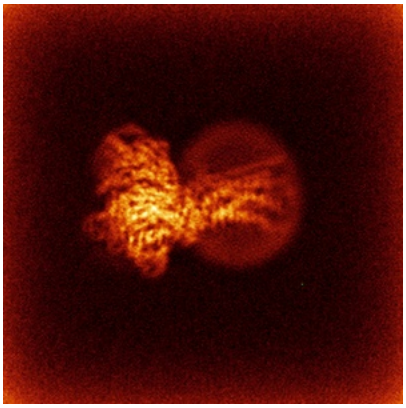


Z

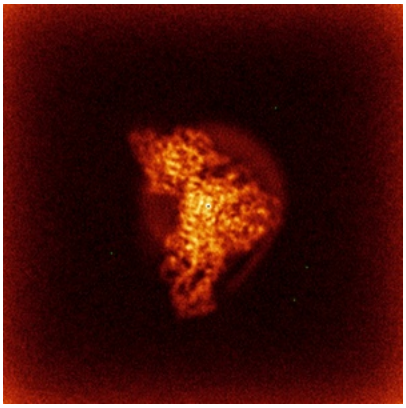
6.4.2 Raw map



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.

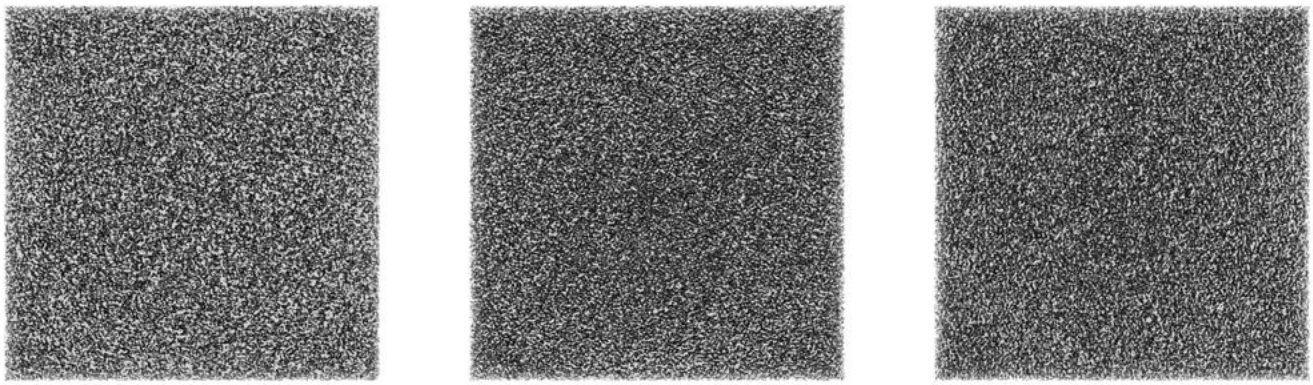
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

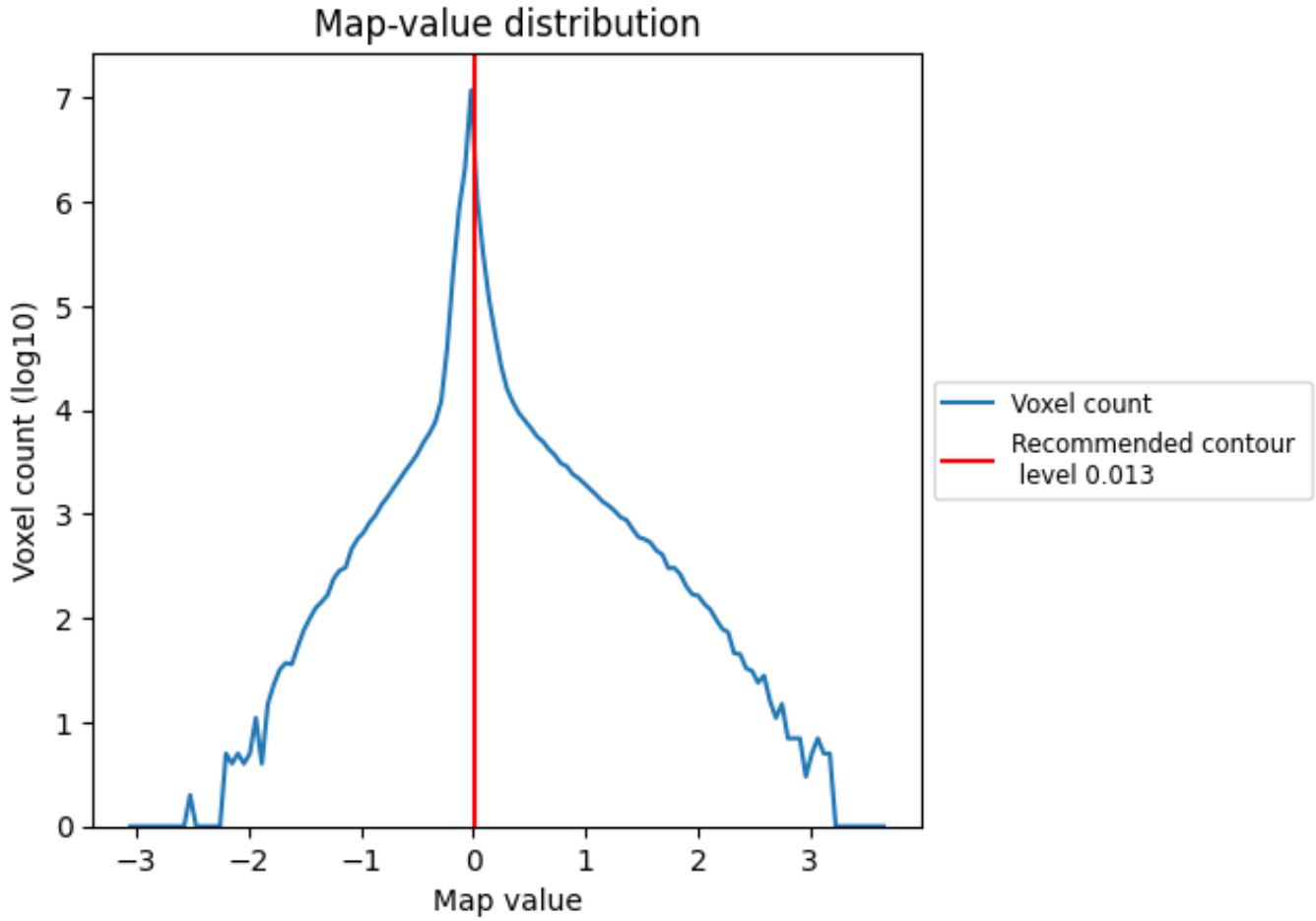
6.6 Mask visualisation (i)

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

7 Map analysis

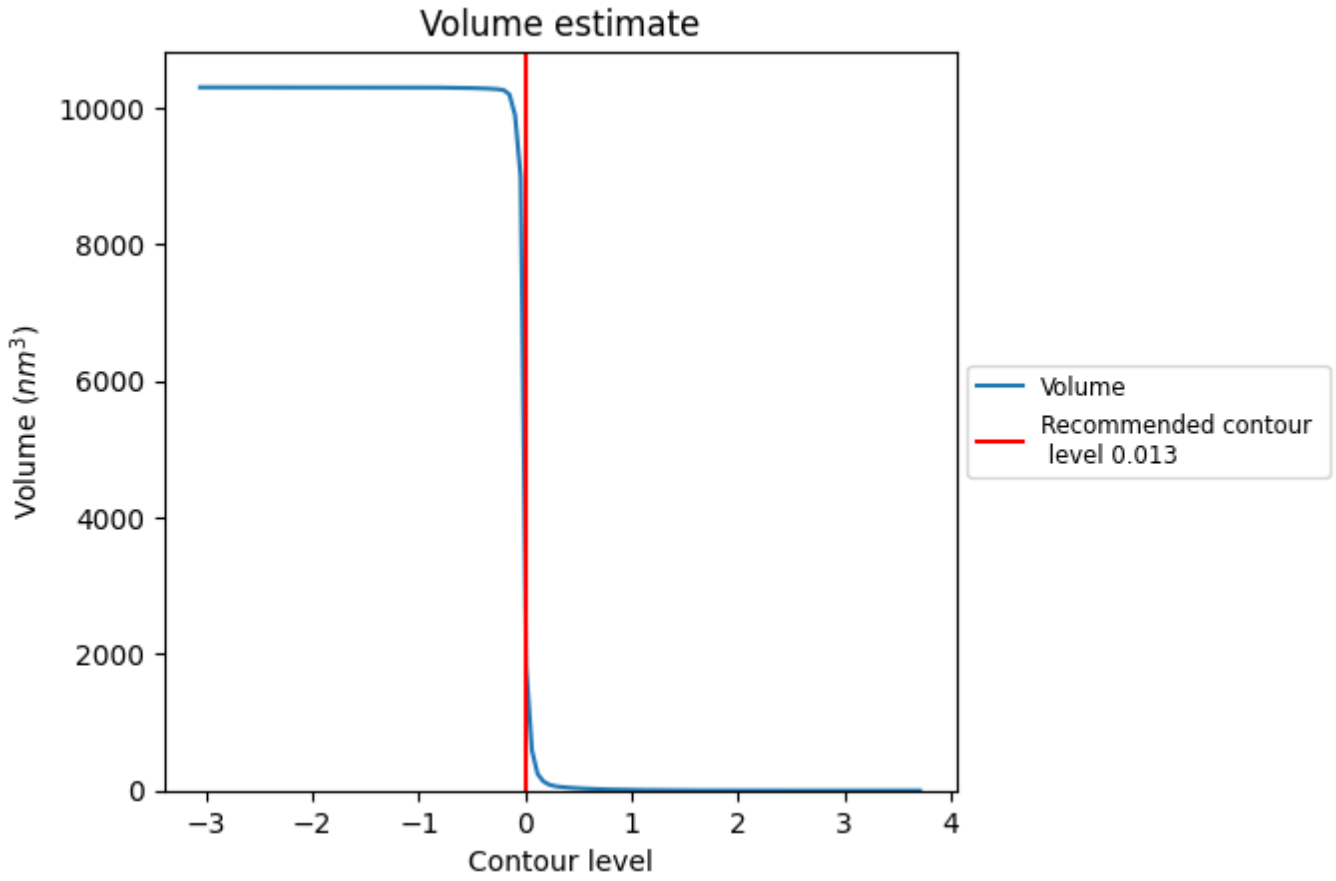
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

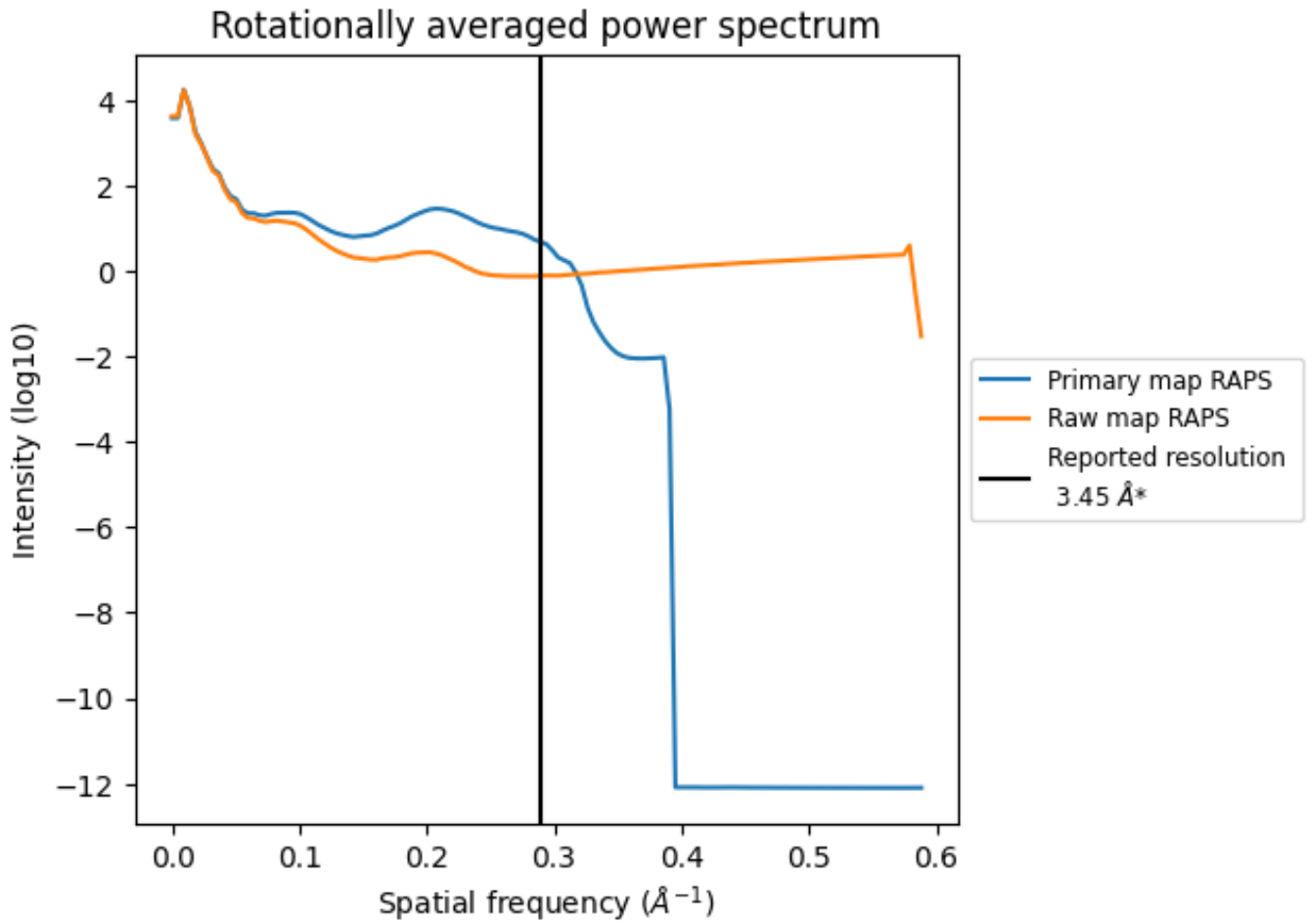
7.2 Volume estimate



The volume at the recommended contour level is 1715 nm^3; this corresponds to an approximate mass of 1549 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 (i)

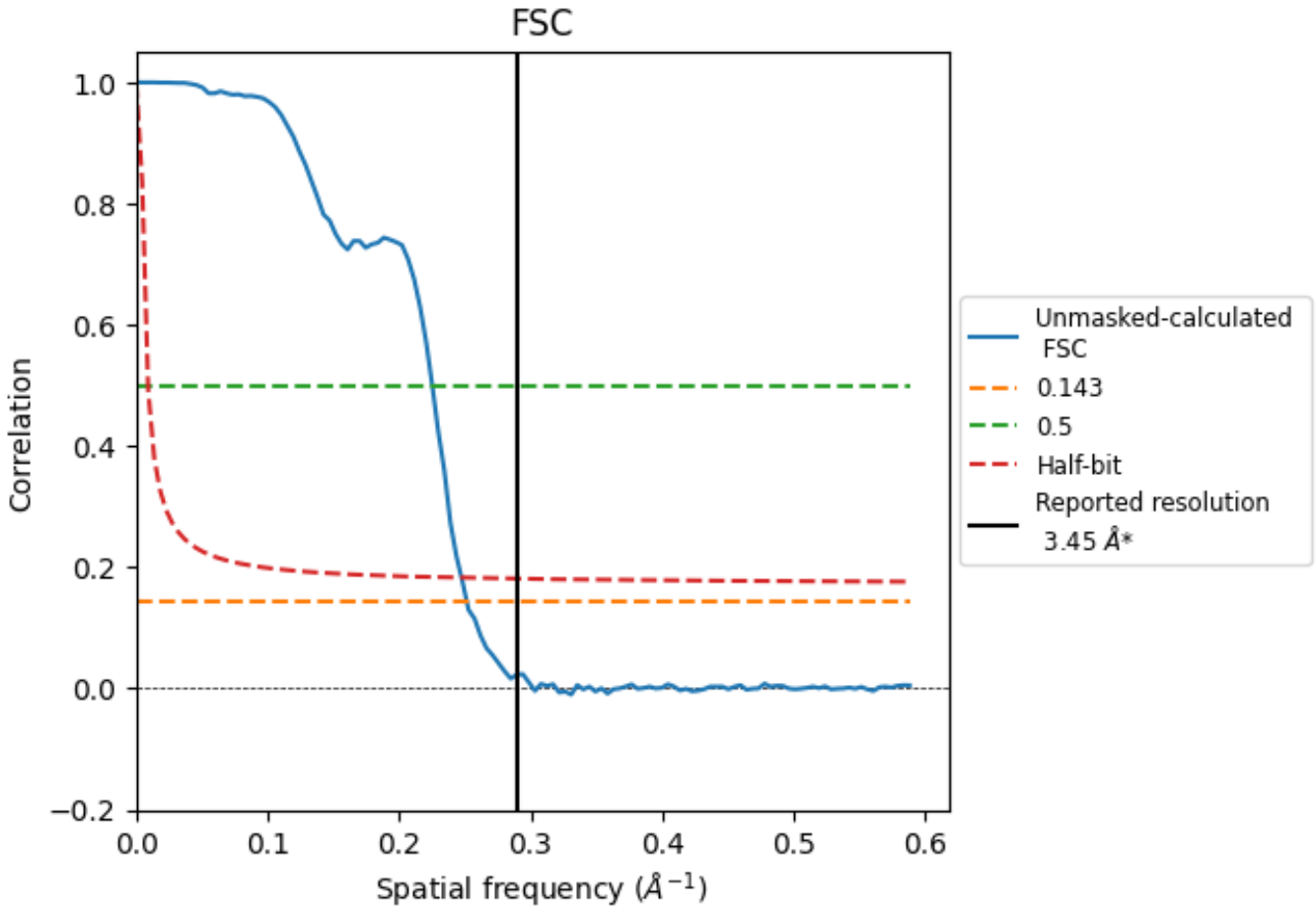


*Reported resolution corresponds to spatial frequency of 0.290 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.290 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.45	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.98	4.44	4.04

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.98 differs from the reported value 3.45 by more than 10 %

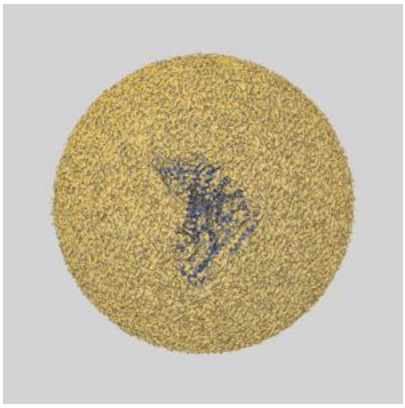
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38909 and PDB model 8Y45. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay

X

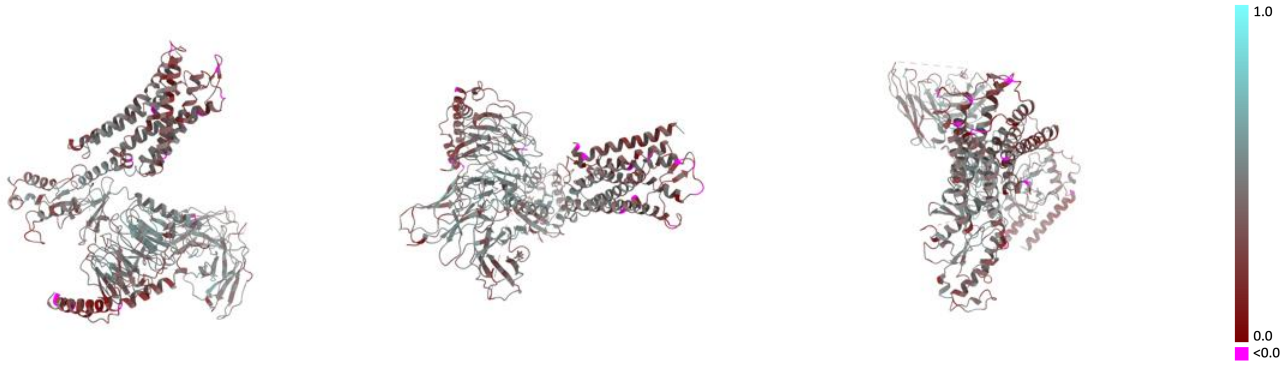
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.013 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.

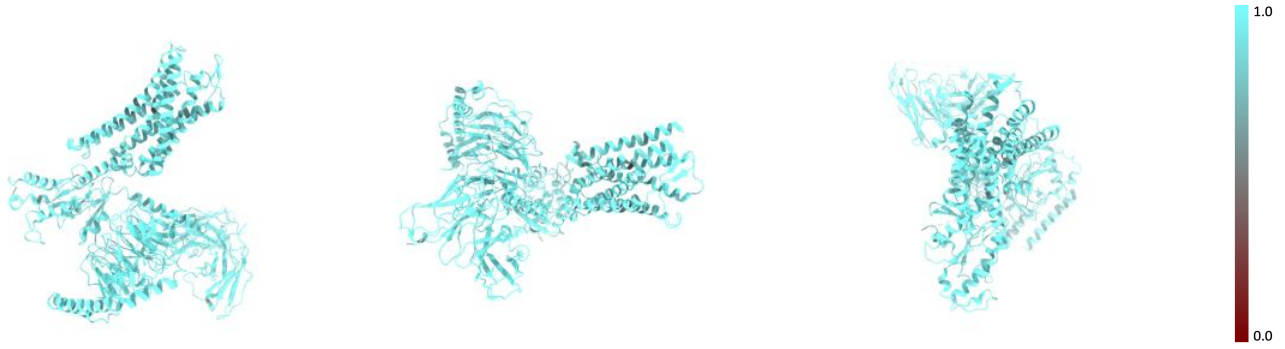
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

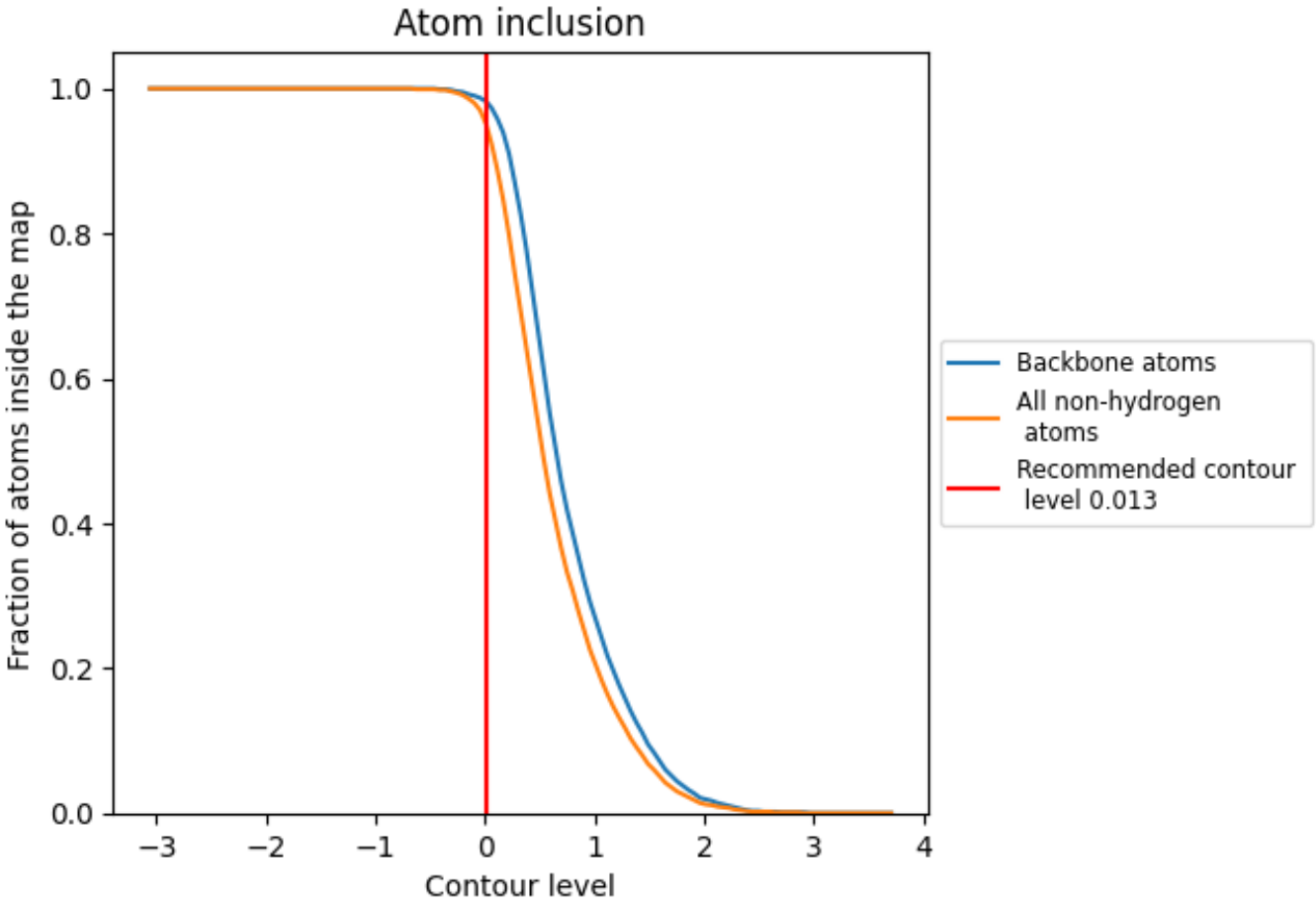
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.013).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 95% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9500	0.4070
A	0.9370	0.3520
B	0.9600	0.4430
C	0.9120	0.2650
D	0.9490	0.4180
S	0.9640	0.4480