Full wwPDB EM Validation Report ⓘ

Jun 3, 2024 – 12:53 PM EDT

PDB ID	:	8DME
EMDB ID	:	EMD-27534
Title	:	CYP102A1 in Open Conformation
Authors	:	Su, M.; Xu, H.
Deposited on	:	2022-07-08
Resolution	:	6.50 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:

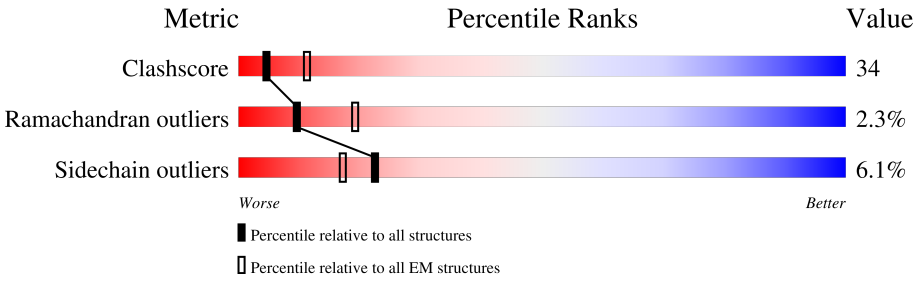
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 6.50 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1034	73% 20%
1	B	1034	74% 20%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	1C6	A	1102	-	-	X	-
3	1C6	B	1102	-	-	X	-
7	PG4	A	1109	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 16812 atoms, of which 170 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.

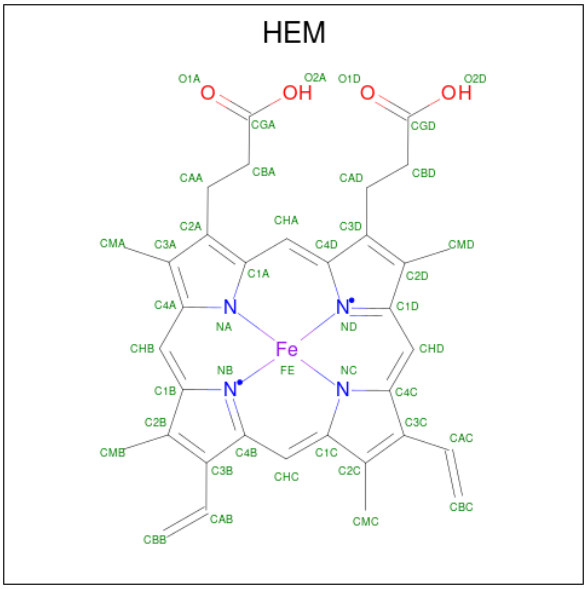
- Molecule 1 is a protein called Bifunctional cytochrome P450/NADPH–P450 reductase.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1034	Total	C	H	N	O	S	4	0
			8223	5165	87	1386	1550	35		
1	B	1034	Total	C	H	N	O	S	4	0
			8219	5165	83	1386	1550	35		

There are 26 discrepancies between the modelled and reference sequences:

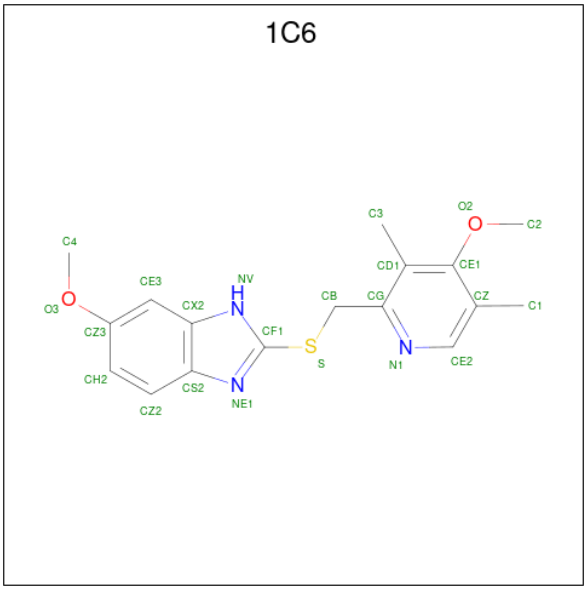
Chain	Residue	Modelled	Actual	Comment	Reference
A	82	PHE	ALA	conflict	UNP P14779
A	?	-	GLY	deletion	UNP P14779
A	?	-	GLY	deletion	UNP P14779
A	?	-	ILE	deletion	UNP P14779
A	?	-	PRO	deletion	UNP P14779
A	?	-	SER	deletion	UNP P14779
A	?	-	PRO	deletion	UNP P14779
A	?	-	SER	deletion	UNP P14779
A	?	-	THR	deletion	UNP P14779
A	?	-	GLU	deletion	UNP P14779
A	?	-	GLN	deletion	UNP P14779
A	?	-	SER	deletion	UNP P14779
A	?	-	ALA	deletion	UNP P14779
B	82	PHE	ALA	conflict	UNP P14779
B	?	-	GLY	deletion	UNP P14779
B	?	-	GLY	deletion	UNP P14779
B	?	-	ILE	deletion	UNP P14779
B	?	-	PRO	deletion	UNP P14779
B	?	-	SER	deletion	UNP P14779
B	?	-	PRO	deletion	UNP P14779
B	?	-	SER	deletion	UNP P14779
B	?	-	THR	deletion	UNP P14779
B	?	-	GLU	deletion	UNP P14779
B	?	-	GLN	deletion	UNP P14779
B	?	-	SER	deletion	UNP P14779
B	?	-	ALA	deletion	UNP P14779

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



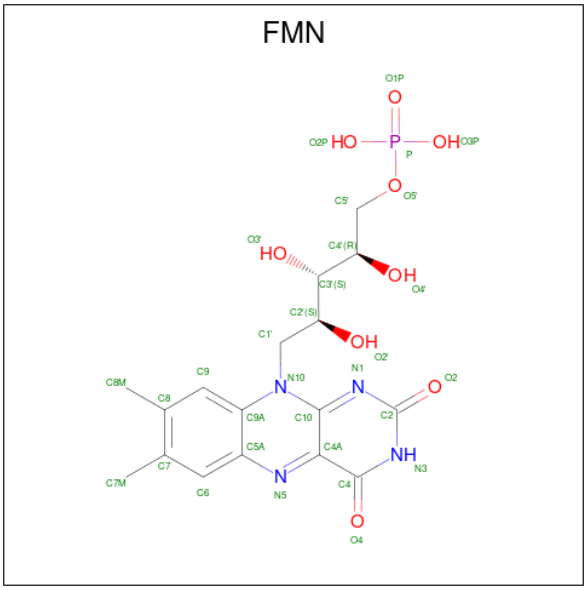
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
2	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 3 is 6-methoxy-2-{[(4-methoxy-3,5-dimethylpyridin-2-yl)methyl]sulfanyl}-1H-benzimidazole (three-letter code: 1C6) (formula: $C_{17}H_{19}N_3O_2S$).



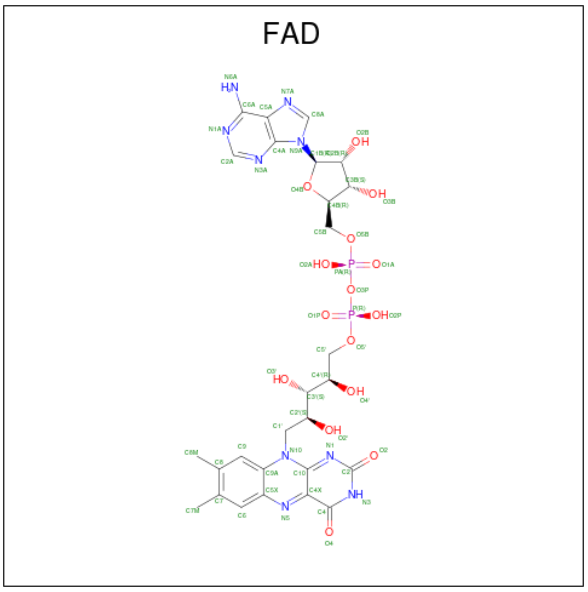
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	S	0
			23	17	3	2	1	
3	B	1	Total	C	N	O	S	0
			23	17	3	2	1	

- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



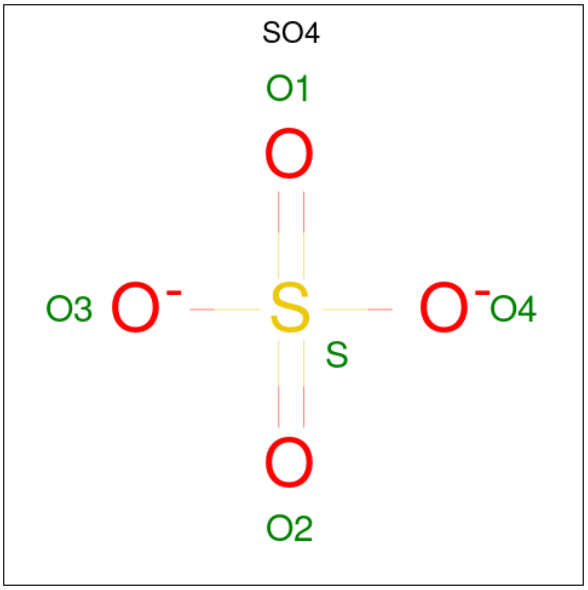
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	17	4	9	1	
4	B	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			53	27	9	15	2	
5	B	1	Total	C	N	O	P	0
			53	27	9	15	2	

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	O	S	0
			5	4	1	
6	A	1	Total	O	S	0
			5	4	1	

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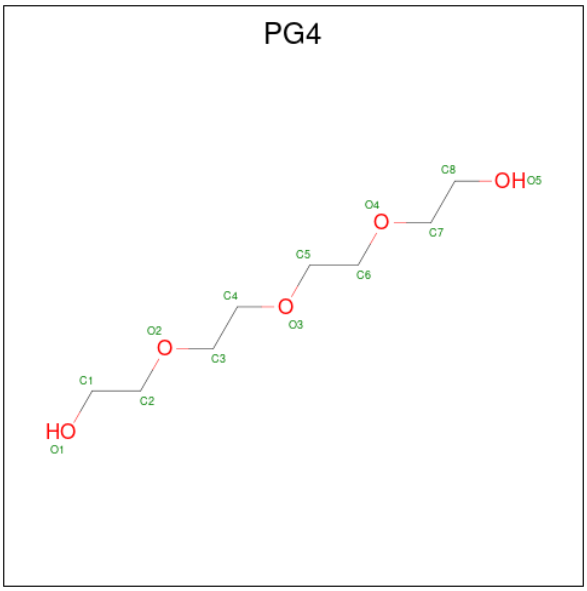
Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total O S 5 4 1	0
6	B	1	Total O S 5 4 1	0
6	B	1	Total O S 5 4 1	0
6	B	1	Total O S 5 4 1	0

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$) (labeled as "Ligand of Interest" by depositor).



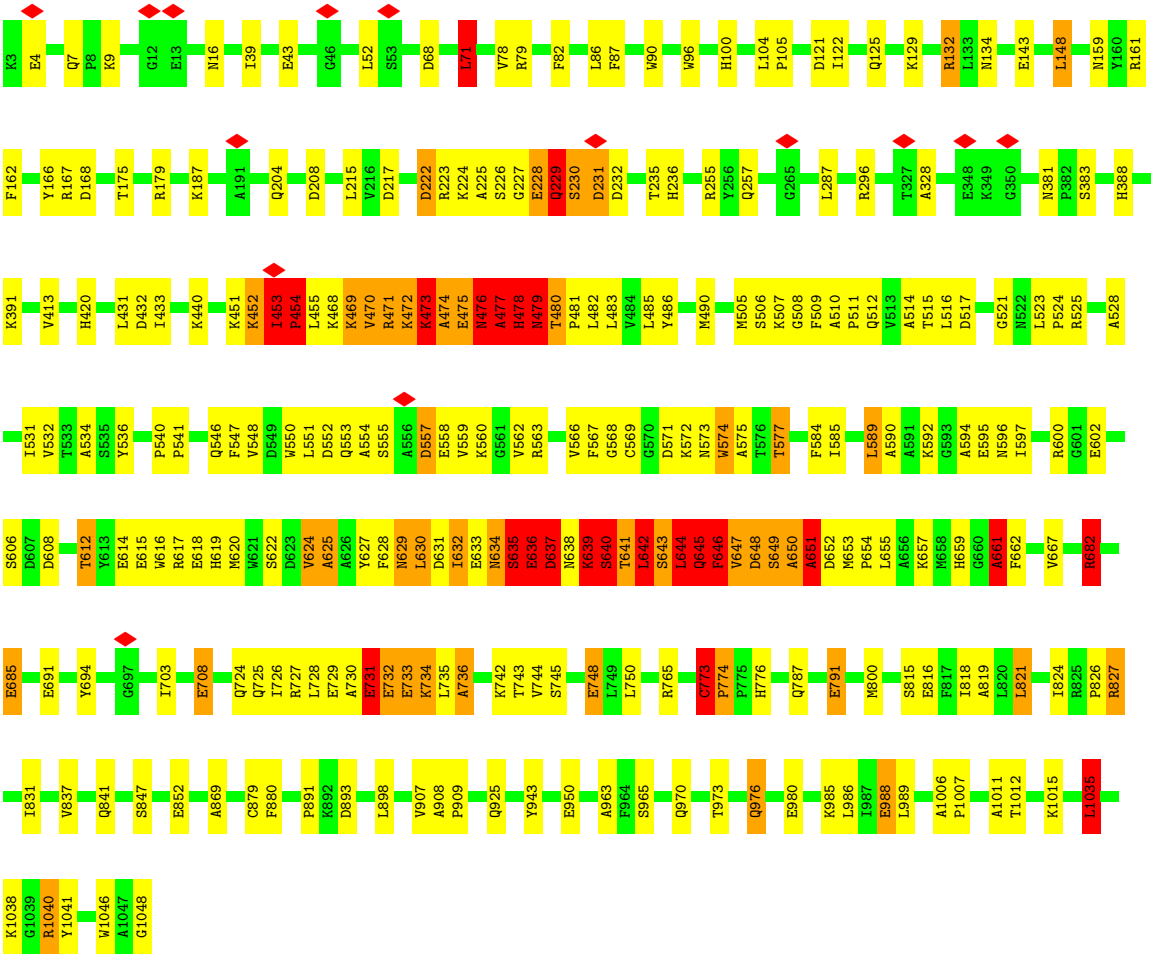
Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total C O 13 8 5	0
7	A	1	Total C O 7 4 3	0
7	B	1	Total C O 13 8 5	0
7	B	1	Total C O 7 4 3	0

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.

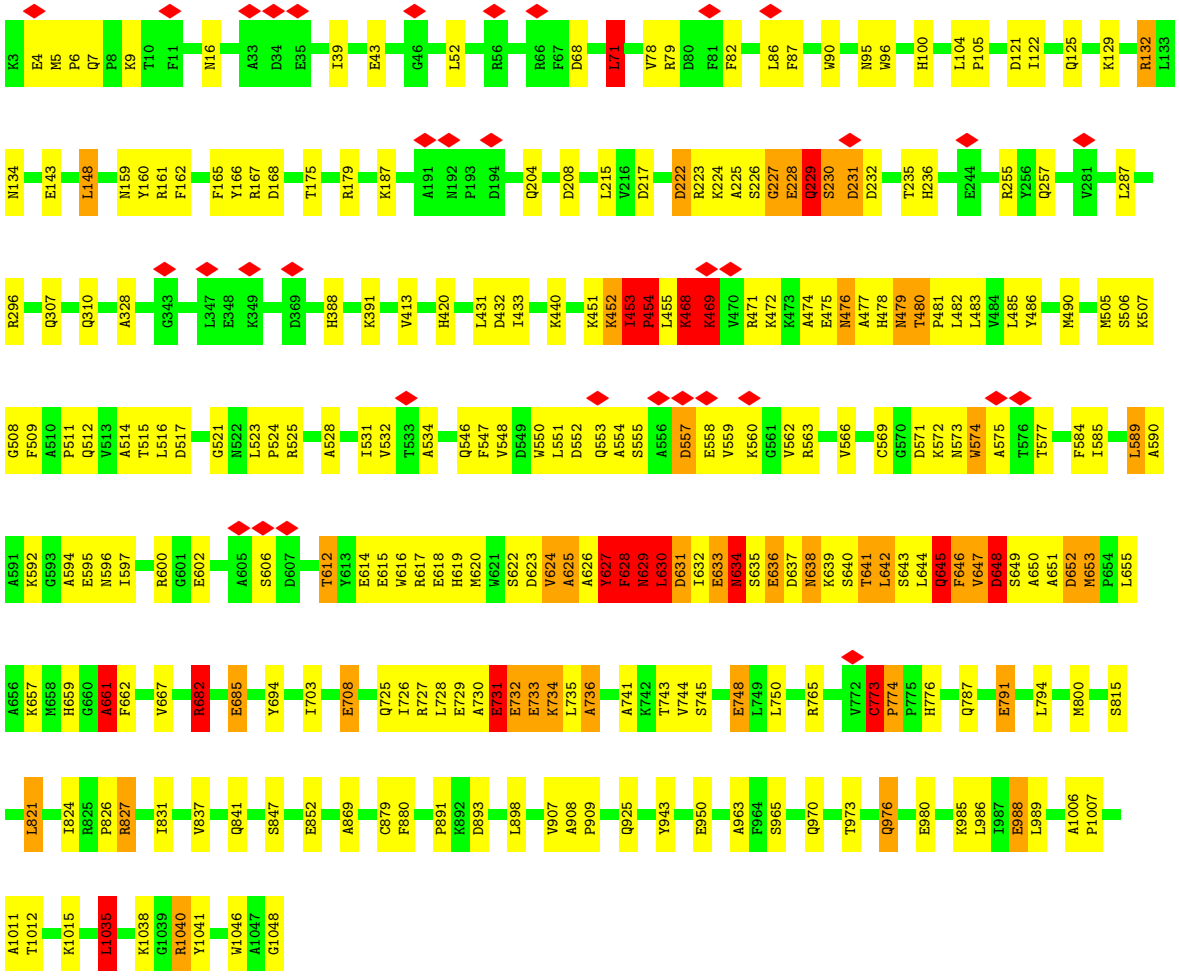
• Molecule 1: Bifunctional cytochrome P450/NADPH–P450 reductase

Chain A:



• Molecule 1: Bifunctional cytochrome P450/NADPH–P450 reductase

Chain B:


K3 E4 M5 P6 Q7 P8 K9 T10 F11 N16 A33 D34 E35 I39 E43 G46 L52 R56 R66 F67 D68 L71 V78 R79 D80 F81 F82 L86 F87 W90 N95 W96 H100 L104 P105 D121 I122 Q125 K129 R132 L133
N134 E143 L148 N159 Y160 R161 F162 F165 Y166 R167 D168 T175 R179 K187 A191 N192 P193 D194 Q204 D208 L215 V216 D217 D222 R223 K224 A225 S226 G227 E228 Q229 S230 D231 D232 T235 H236 E244 R255 Y256 Q257 V281 L287
R296 Q307 Q310 A328 G343 L347 E348 K349 D369 H388 K391 V413 H420 L431 D432 I433 K440 K451 K452 I453 P454 L455 K468 K469 V470 R471 K472 K473 A474 E475 N476 A477 H478 N479 T480 P481 L482 L483 V484 L485 Y486 M490 M505 S506 K507
G508 F509 A510 P511 Q512 V513 A514 T515 L516 D517 G521 N522 L523 P524 R525 A528 I531 V532 T533 A534 Q546 F547 V548 D549 W550 L551 D552 Q553 A554 S555 A556 D557 E558 V559 K560 G561 V562 R563 V566 C569 G570 D571 K572 N573 W574 A575 T576 T577 F584 I585 L589 A590
A591 K592 G593 A594 E595 N596 I597 R600 G601 E602 A605 S606 D607 T612 Y613 E614 E615 W616 R617 E618 H619 M620 W621 S622 D623 V624 A625 A626 Y627 F628 N629 L630 D631 I632 E633 N634 S635 E636 D637 N638 K639 S640 T641 L642 S643 L644 Q645 F646 V647 D648 S649 A650 A651 D652 M653 P654 L655
A656 K657 M658 H659 G660 A661 F662 V667 R882 E685 Y694 I703 E708 Q725 I726 R727 L728 E729 A730 E731 E732 E733 K734 L735 A736 A741 K742 T743 V744 S745 E748 L749 L750 R765 V772 C773 P774 P775 H776 Q787 E791 L794 M800 S815
L821 I824 R825 P826 R827 I831 V837 Q841 S847 E852 A869 C879 F880 P891 K892 D893 L898 V907 A908 P909 Q925 Y943 E950 A963 F964 S965 Q970 T973 Q976 E980 K985 L986 I987 E988 L989 A1006 P1007
A1011 T1012 K1015 L1035 K1038 G1039 R1040 Y1041 W1046 A1047 G1048

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	204254	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	15	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	6.944	Depositor
Minimum map value	-3.280	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.163	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	363.6, 363.6, 363.6	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.02, 2.02, 2.02	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, HEM, PG4, SO4, FMN, 1C6

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	1.38	30/8317 (0.4%)	1.27	70/11270 (0.6%)
1	B	1.33	23/8317 (0.3%)	1.19	62/11270 (0.6%)
All	All	1.36	53/16634 (0.3%)	1.23	132/22540 (0.6%)

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	5
1	B	0	6
All	All	0	11

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	478	HIS	N-CA	53.37	2.53	1.46
1	B	628	PHE	CE1-CZ	44.12	2.21	1.37
1	B	628	PHE	CD1-CE1	33.51	2.06	1.39
1	A	635	SER	C-O	30.78	1.81	1.23
1	B	628	PHE	CG-CD1	26.35	1.78	1.38
1	B	661	ALA	C-N	-20.90	0.85	1.34
1	A	661	ALA	C-N	-20.87	0.86	1.34
1	A	478	HIS	CA-CB	20.55	1.99	1.53
1	A	478	HIS	CA-C	15.28	1.92	1.52
1	B	774	PRO	N-CD	14.81	1.68	1.47
1	A	774	PRO	N-CD	14.76	1.68	1.47
1	A	478	HIS	C-O	12.22	1.46	1.23
1	A	650	ALA	N-CA	11.62	1.69	1.46
1	B	629	ASN	N-CA	-10.12	1.26	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	635	SER	N-CA	-9.91	1.26	1.46
1	A	988	GLU	CG-CD	8.92	1.65	1.51
1	B	988	GLU	CG-CD	8.90	1.65	1.51
1	B	454	PRO	CA-C	8.56	1.70	1.52
1	A	454	PRO	CA-C	8.56	1.70	1.52
1	B	454	PRO	N-CA	8.40	1.61	1.47
1	A	454	PRO	N-CA	8.34	1.61	1.47
1	B	733	GLU	N-CA	7.77	1.61	1.46
1	A	733	GLU	N-CA	7.75	1.61	1.46
1	A	636	GLU	CA-C	-7.45	1.33	1.52
1	B	748	GLU	CG-CD	7.34	1.62	1.51
1	A	748	GLU	CG-CD	7.30	1.62	1.51
1	B	469	LYS	CA-C	-7.03	1.34	1.52
1	A	477	ALA	CA-C	-6.60	1.35	1.52
1	B	629	ASN	CA-C	-6.21	1.36	1.52
1	A	454	PRO	N-CD	-6.13	1.39	1.47
1	B	454	PRO	N-CD	-6.12	1.39	1.47
1	A	637	ASP	CA-C	-6.05	1.37	1.52
1	A	143	GLU	CG-CD	6.00	1.60	1.51
1	A	636	GLU	CA-CB	5.97	1.67	1.53
1	B	143	GLU	CG-CD	5.96	1.60	1.51
1	A	1011	ALA	CA-CB	5.78	1.64	1.52
1	B	1011	ALA	CA-CB	5.76	1.64	1.52
1	B	629	ASN	C-N	-5.74	1.20	1.34
1	B	791	GLU	CG-CD	5.53	1.60	1.51
1	A	791	GLU	CG-CD	5.45	1.60	1.51
1	A	636	GLU	N-CA	-5.42	1.35	1.46
1	B	708	GLU	CG-CD	5.34	1.59	1.51
1	A	649	SER	C-N	5.31	1.46	1.34
1	A	9	LYS	CE-NZ	5.28	1.62	1.49
1	B	9	LYS	CE-NZ	5.27	1.62	1.49
1	A	708	GLU	CG-CD	5.26	1.59	1.51
1	A	646	PHE	C-N	-5.24	1.22	1.34
1	A	734	LYS	N-CA	-5.17	1.36	1.46
1	A	950	GLU	CB-CG	5.16	1.61	1.52
1	B	950	GLU	CB-CG	5.12	1.61	1.52
1	B	734	LYS	N-CA	-5.12	1.36	1.46
1	A	852	GLU	CB-CG	5.05	1.61	1.52
1	B	852	GLU	CB-CG	5.05	1.61	1.52

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	478	HIS	CB-CA-C	-44.12	22.16	110.40
1	A	736	ALA	N-CA-CB	29.32	151.15	110.10
1	B	736	ALA	N-CA-CB	29.30	151.12	110.10
1	A	453	ILE	C-N-CD	-24.46	66.78	120.60
1	B	453	ILE	C-N-CD	-24.45	66.81	120.60
1	B	628	PHE	CD1-CE1-CZ	-22.24	93.41	120.10
1	B	734	LYS	N-CA-CB	-21.80	71.36	110.60
1	A	734	LYS	N-CA-CB	-21.78	71.39	110.60
1	A	478	HIS	N-CA-CB	-20.62	73.48	110.60
1	A	661	ALA	O-C-N	-16.43	96.41	122.70
1	B	661	ALA	O-C-N	-16.41	96.44	122.70
1	A	635	SER	CA-C-O	13.94	149.38	120.10
1	B	627	TYR	O-C-N	-13.84	100.56	122.70
1	B	227	GLY	N-CA-C	-12.16	82.70	113.10
1	A	227	GLY	N-CA-C	-12.16	82.70	113.10
1	A	477	ALA	C-N-CA	12.03	151.76	121.70
1	A	635	SER	C-N-CA	-12.00	91.69	121.70
1	B	628	PHE	CD1-CG-CD2	11.40	133.12	118.30
1	B	628	PHE	CB-CG-CD1	-11.27	112.91	120.80
1	A	637	ASP	C-N-CA	-11.25	93.58	121.70
1	A	453	ILE	N-CA-C	-11.13	80.95	111.00
1	B	453	ILE	N-CA-C	-11.12	80.99	111.00
1	B	628	PHE	CB-CA-C	-10.72	88.95	110.40
1	B	628	PHE	CG-CD1-CE1	-10.30	109.47	120.80
1	B	628	PHE	CB-CG-CD2	-9.80	113.94	120.80
1	A	637	ASP	N-CA-C	-9.62	85.02	111.00
1	A	661	ALA	CA-C-N	9.41	137.90	117.20
1	B	661	ALA	CA-C-N	9.39	137.87	117.20
1	A	661	ALA	C-N-CA	9.14	144.56	121.70
1	B	661	ALA	C-N-CA	9.13	144.53	121.70
1	A	229	GLN	N-CA-C	-9.06	86.54	111.00
1	B	229	GLN	N-CA-C	-9.04	86.59	111.00
1	B	630	LEU	CA-CB-CG	-8.93	94.77	115.30
1	A	473	LYS	N-CA-C	-8.76	87.35	111.00
1	A	736	ALA	N-CA-C	-8.59	87.80	111.00
1	B	736	ALA	N-CA-C	-8.59	87.81	111.00
1	B	1040	ARG	NE-CZ-NH2	8.57	124.58	120.30
1	A	635	SER	CA-C-N	-8.50	98.51	117.20
1	A	1040	ARG	NE-CZ-NH2	8.48	124.54	120.30
1	B	641	THR	N-CA-C	8.44	133.79	111.00
1	A	682	ARG	NE-CZ-NH2	-8.25	116.17	120.30
1	B	682	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	A	646	PHE	O-C-N	-8.20	109.58	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	121	ASP	CB-CG-OD1	8.13	125.62	118.30
1	A	121	ASP	CB-CG-OD1	8.11	125.60	118.30
1	B	453	ILE	O-C-N	-8.10	105.72	121.10
1	A	453	ILE	O-C-N	-8.08	105.75	121.10
1	A	79	ARG	CG-CD-NE	7.90	128.39	111.80
1	B	79	ARG	CG-CD-NE	7.88	128.35	111.80
1	A	478	HIS	N-CA-C	-7.83	89.86	111.00
1	B	79	ARG	N-CA-CB	7.75	124.55	110.60
1	A	79	ARG	N-CA-CB	7.74	124.53	110.60
1	B	774	PRO	N-CA-CB	7.70	112.54	103.30
1	A	774	PRO	N-CA-CB	7.69	112.52	103.30
1	B	475	GLU	N-CA-C	-7.58	90.54	111.00
1	A	634	ASN	N-CA-CB	7.53	124.16	110.60
1	B	629	ASN	CA-C-N	-7.44	100.83	117.20
1	B	774	PRO	CA-N-CD	-7.42	101.12	111.50
1	A	774	PRO	CA-N-CD	-7.41	101.13	111.50
1	B	628	PHE	CG-CD2-CE2	7.27	128.80	120.80
1	B	628	PHE	CE1-CZ-CE2	7.18	132.92	120.00
1	A	477	ALA	N-CA-C	-6.95	92.22	111.00
1	A	79	ARG	CB-CA-C	-6.95	96.50	110.40
1	B	68	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	B	79	ARG	CB-CA-C	-6.92	96.56	110.40
1	A	68	ASP	CB-CG-OD2	-6.84	112.15	118.30
1	A	635	SER	O-C-N	-6.78	111.85	122.70
1	B	732	GLU	O-C-N	-6.77	111.87	122.70
1	A	732	GLU	O-C-N	-6.74	111.91	122.70
1	B	79	ARG	CA-CB-CG	6.72	128.19	113.40
1	A	478	HIS	CA-C-O	6.72	134.21	120.10
1	A	1040	ARG	NE-CZ-NH1	-6.70	116.95	120.30
1	A	79	ARG	CA-CB-CG	6.69	128.11	113.40
1	A	646	PHE	C-N-CA	-6.66	105.06	121.70
1	B	68	ASP	CB-CG-OD1	6.64	124.28	118.30
1	B	71	LEU	CB-CG-CD1	6.63	122.27	111.00
1	A	68	ASP	CB-CG-OD1	6.62	124.26	118.30
1	A	71	LEU	CB-CG-CD1	6.60	122.22	111.00
1	B	1040	ARG	NE-CZ-NH1	-6.52	117.04	120.30
1	A	636	GLU	N-CA-CB	-6.42	99.04	110.60
1	A	648	ASP	N-CA-CB	-6.40	99.08	110.60
1	B	296	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	A	296	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	B	468	LYS	C-N-CA	-6.19	106.22	121.70
1	B	645	GLN	N-CA-C	6.09	127.45	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	827	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	B	827	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	B	574	TRP	C-N-CA	5.95	136.58	121.70
1	A	574	TRP	C-N-CA	5.95	136.56	121.70
1	B	641	THR	CB-CA-C	-5.89	95.70	111.60
1	A	637	ASP	N-CA-CB	5.88	121.19	110.60
1	A	479	ASN	C-N-CA	-5.88	107.00	121.70
1	A	651	ALA	N-CA-CB	-5.83	101.93	110.10
1	A	474	ALA	N-CA-C	-5.79	95.37	111.00
1	A	765	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	B	765	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	649	SER	C-N-CA	5.71	135.97	121.70
1	A	642	LEU	CA-CB-CG	5.60	128.19	115.30
1	B	469	LYS	CB-CA-C	-5.58	99.25	110.40
1	B	648	ASP	N-CA-C	-5.57	95.97	111.00
1	B	476	ASN	N-CA-CB	-5.56	100.59	110.60
1	A	635	SER	N-CA-C	-5.54	96.04	111.00
1	A	893	ASP	CB-CG-OD2	-5.54	113.32	118.30
1	A	650	ALA	C-N-CA	-5.54	107.86	121.70
1	B	893	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	A	773	CYS	C-N-CD	5.53	140.01	128.40
1	A	640	SER	N-CA-C	-5.51	96.12	111.00
1	B	773	CYS	C-N-CD	5.51	139.97	128.40
1	B	432	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	A	432	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	A	296	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	A	634	ASN	N-CA-C	-5.40	96.41	111.00
1	B	296	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	A	454	PRO	N-CA-C	5.39	126.11	112.10
1	B	454	PRO	N-CA-C	5.38	126.09	112.10
1	A	1035	LEU	CA-CB-CG	5.28	127.44	115.30
1	B	1035	LEU	CA-CB-CG	5.26	127.40	115.30
1	B	629	ASN	N-CA-C	5.26	125.20	111.00
1	A	79	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	B	733	GLU	C-N-CA	-5.22	108.64	121.70
1	A	733	GLU	C-N-CA	-5.21	108.67	121.70
1	B	79	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	A	132	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	476	ASN	CA-C-N	-5.14	105.90	117.20
1	B	629	ASN	N-CA-CB	-5.08	101.45	110.60
1	B	96	TRP	CA-CB-CG	-5.07	104.06	113.70
1	B	132	ARG	NE-CZ-NH1	5.06	122.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	96	TRP	CA-CB-CG	-5.05	104.09	113.70
1	A	647	VAL	C-N-CA	-5.05	109.08	121.70
1	B	652	ASP	N-CA-C	-5.03	97.43	111.00
1	B	634	ASN	N-CA-CB	5.01	119.61	110.60
1	A	651	ALA	CB-CA-C	-5.00	102.60	110.10

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	224	LYS	Mainchain
1	A	476	ASN	Mainchain
1	A	477	ALA	Peptide
1	A	646	PHE	Mainchain
1	A	661	ALA	Mainchain
1	B	224	LYS	Mainchain
1	B	468	LYS	Mainchain
1	B	627	TYR	Mainchain,Peptide
1	B	629	ASN	Mainchain
1	B	661	ALA	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	8136	87	7887	681	0
1	B	8136	83	7889	712	0
2	A	43	0	30	1	0
2	B	43	0	30	1	0
3	A	23	0	19	11	0
3	B	23	0	19	11	0
4	A	31	0	19	1	0
4	B	31	0	19	1	0
5	A	53	0	31	5	0
5	B	53	0	31	4	0
6	A	15	0	0	0	0
6	B	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	20	0	27	8	0
7	B	20	0	27	7	0
All	All	16642	170	16028	1125	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 34.

All (1125) 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:B:628:PHE:CG	1:B:628:PHE:CD1	1.78	1.59
1:A:650:ALA:N	1:A:650:ALA:CA	1.69	1.56
1:A:646:PHE:CD1	1:B:727:ARG:CG	1.74	1.53
1:B:1046:TRP:CD1	1:B:1048:GLY:C	1.83	1.52
1:A:1046:TRP:CD1	1:A:1048:GLY:C	1.83	1.52
1:B:624:VAL:HA	1:B:628:PHE:CZ	1.45	1.52
1:A:478:HIS:CA	1:A:479:ASN:HA	1.39	1.51
1:A:727:ARG:C	1:B:645:GLN:HG2	1.25	1.48
1:A:161:ARG:H	1:B:134:ASN:ND2	1.12	1.47
1:A:161:ARG:N	1:B:134:ASN:HD21	1.06	1.46
1:B:774:PRO:N	1:B:774:PRO:CD	1.68	1.45
1:B:1046:TRP:HD1	1:B:1048:GLY:C	1.18	1.43
1:B:478:HIS:C	1:B:479:ASN:CB	1.86	1.43
1:B:478:HIS:C	1:B:479:ASN:HB3	1.07	1.42
1:B:628:PHE:CD1	1:B:628:PHE:CE1	2.06	1.42
1:B:627:TYR:HB3	1:B:628:PHE:CZ	1.53	1.40
1:A:644:LEU:CD2	1:B:815:SER:HB2	1.28	1.39
1:A:1046:TRP:HD1	1:A:1048:GLY:C	1.18	1.39
1:A:478:HIS:CA	1:A:478:HIS:CB	1.99	1.38
1:A:134:ASN:HD21	1:B:161:ARG:N	1.15	1.38
1:A:478:HIS:CA	1:A:478:HIS:C	1.92	1.37
1:A:731:GLU:OE1	1:B:641:THR:CG2	1.72	1.36
1:A:132:ARG:O	1:B:161:ARG:CD	1.73	1.36
1:A:1048:GLY:O	5:A:1104:FAD:H1'2	1.22	1.35
1:A:774:PRO:CD	1:A:774:PRO:N	1.68	1.34
1:B:627:TYR:CB	1:B:628:PHE:CE1	2.11	1.33
1:A:646:PHE:CE1	1:B:727:ARG:HG3	1.64	1.32
1:B:1048:GLY:O	5:B:1104:FAD:H1'2	1.23	1.32
1:A:661:ALA:O	1:A:662:PHE:N	1.58	1.32
1:A:727:ARG:HG2	1:B:645:GLN:CG	1.60	1.31
1:B:624:VAL:C	1:B:628:PHE:CE1	2.03	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:ILE:HG22	1:B:648:ASP:CB	1.60	1.29
1:B:628:PHE:CZ	1:B:628:PHE:CE1	2.21	1.29
1:A:727:ARG:O	1:B:645:GLN:HG2	1.21	1.29
1:B:661:ALA:O	1:B:662:PHE:N	1.58	1.29
1:A:732:GLU:OE1	1:B:640:SER:HB3	1.28	1.27
1:B:476:ASN:HA	1:B:505:MET:O	1.35	1.27
1:A:125:GLN:HG2	1:B:132:ARG:NH1	1.49	1.26
1:A:726:ILE:CA	1:B:648:ASP:HA	1.56	1.26
1:B:624:VAL:O	1:B:628:PHE:CD1	1.88	1.26
1:A:646:PHE:CE1	1:B:727:ARG:CG	2.17	1.26
1:A:727:ARG:CG	1:B:645:GLN:HG3	1.65	1.25
1:A:134:ASN:ND2	1:B:161:ARG:N	1.86	1.24
1:A:726:ILE:CG2	1:B:648:ASP:HB3	1.66	1.24
1:A:726:ILE:HA	1:B:648:ASP:CA	1.65	1.24
1:A:134:ASN:ND2	1:B:161:ARG:H	1.36	1.24
1:A:478:HIS:CA	1:A:479:ASN:CA	2.15	1.24
1:A:731:GLU:OE1	1:B:641:THR:HG22	1.29	1.23
1:B:478:HIS:O	1:B:479:ASN:HB3	1.09	1.23
1:B:627:TYR:C	1:B:628:PHE:CD1	2.13	1.23
1:B:627:TYR:N	1:B:628:PHE:CE1	2.06	1.22
1:A:478:HIS:C	1:A:480:THR:H	1.43	1.22
1:A:132:ARG:NH1	1:B:125:GLN:HG2	1.53	1.21
1:A:732:GLU:OE1	1:B:640:SER:CB	1.86	1.21
1:A:644:LEU:HD21	1:B:815:SER:CB	1.69	1.21
1:A:726:ILE:CG2	1:B:647:VAL:O	1.86	1.21
1:B:472:LYS:CD	1:B:474:ALA:HB2	1.68	1.21
1:A:478:HIS:HB2	1:A:478:HIS:O	1.03	1.20
1:A:727:ARG:O	1:B:645:GLN:CG	1.90	1.20
1:B:477:ALA:H	1:B:505:MET:HA	1.06	1.19
1:A:635:SER:O	1:A:635:SER:C	1.81	1.19
1:A:478:HIS:C	1:A:478:HIS:CG	2.16	1.18
1:A:478:HIS:CB	1:A:480:THR:H	1.57	1.17
1:A:726:ILE:HG22	1:B:648:ASP:CA	1.72	1.17
1:A:815:SER:O	1:B:642:LEU:HD11	1.41	1.17
1:B:472:LYS:HD3	1:B:474:ALA:CB	1.74	1.17
1:B:627:TYR:N	1:B:628:PHE:CD1	2.13	1.16
1:B:624:VAL:CA	1:B:628:PHE:CZ	2.28	1.16
1:B:627:TYR:CB	1:B:628:PHE:CZ	2.27	1.16
1:B:627:TYR:HB3	1:B:628:PHE:CE1	1.74	1.15
1:A:727:ARG:C	1:B:645:GLN:CG	2.15	1.15
1:B:627:TYR:CA	1:B:628:PHE:CD1	2.28	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:TYR:CE2	1:B:129:LYS:HB2	1.81	1.14
1:B:452:LYS:HE2	1:B:455:LEU:H	0.99	1.14
1:A:132:ARG:O	1:B:161:ARG:HD2	0.98	1.14
1:B:477:ALA:H	1:B:505:MET:CA	1.60	1.13
1:A:478:HIS:N	1:A:631:ASP:OD2	1.81	1.13
1:B:476:ASN:CB	1:B:505:MET:HB3	1.78	1.13
1:A:125:GLN:CG	1:B:132:ARG:NH1	2.12	1.13
1:A:644:LEU:CD2	1:B:815:SER:CB	2.20	1.13
1:A:732:GLU:OE1	1:B:640:SER:CA	1.96	1.12
1:A:647:VAL:HB	1:A:648:ASP:OD2	1.49	1.12
1:A:125:GLN:CG	1:B:132:ARG:CZ	2.28	1.12
1:A:644:LEU:N	1:B:729:GLU:O	1.83	1.11
1:A:726:ILE:HA	1:B:648:ASP:HA	1.13	1.10
1:B:628:PHE:CD1	1:B:628:PHE:N	2.17	1.10
1:A:452:LYS:HE2	1:A:455:LEU:H	0.99	1.10
1:A:661:ALA:C	1:A:662:PHE:CA	2.19	1.10
1:B:661:ALA:C	1:B:662:PHE:CA	2.19	1.09
1:A:635:SER:O	1:A:636:GLU:CA	2.01	1.09
1:B:477:ALA:CB	1:B:505:MET:HG2	1.82	1.09
1:A:726:ILE:HG22	1:B:647:VAL:O	1.47	1.09
1:B:477:ALA:N	1:B:505:MET:HA	1.67	1.09
1:B:478:HIS:CD2	1:B:632:ILE:HG22	1.86	1.09
1:A:478:HIS:HA	1:A:508:GLY:O	1.54	1.08
1:A:728:LEU:HD22	1:B:644:LEU:HD12	1.15	1.07
1:A:166:TYR:CZ	1:B:129:LYS:HA	1.88	1.07
1:B:477:ALA:HB2	1:B:505:MET:HG2	1.08	1.07
1:A:730:ALA:O	1:B:641:THR:HG21	1.52	1.07
1:A:132:ARG:C	1:B:161:ARG:HD2	1.74	1.06
1:A:644:LEU:CD2	1:B:728:LEU:HD22	1.84	1.06
1:B:624:VAL:O	1:B:628:PHE:CE1	2.08	1.06
1:A:730:ALA:HA	1:B:642:LEU:O	1.53	1.05
1:B:623:ASP:O	1:B:628:PHE:CE1	2.10	1.05
1:B:624:VAL:CA	1:B:628:PHE:CE1	2.39	1.05
1:A:635:SER:O	1:A:636:GLU:HA	1.53	1.05
1:A:644:LEU:HD23	1:B:728:LEU:CD2	1.87	1.04
1:A:132:ARG:NH1	1:B:125:GLN:CG	2.19	1.04
1:A:78:VAL:CG1	1:A:82:PHE:CD2	2.40	1.04
1:A:230:SER:H	1:B:471:ARG:NH2	1.32	1.04
1:B:478:HIS:O	1:B:632:ILE:HG21	1.57	1.04
1:A:478:HIS:C	1:A:480:THR:HG22	1.78	1.03
1:A:646:PHE:CD1	1:B:727:ARG:HG2	1.59	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:VAL:CG1	1:B:82:PHE:CD2	2.40	1.03
1:A:727:ARG:O	1:B:645:GLN:N	1.90	1.03
1:B:476:ASN:HB3	1:B:505:MET:CB	1.87	1.03
1:B:1048:GLY:O	5:B:1104:FAD:C1'	2.07	1.03
1:A:166:TYR:CE2	1:B:129:LYS:CB	2.42	1.02
1:A:728:LEU:HD23	1:B:644:LEU:HA	1.41	1.02
1:A:773:CYS:SG	1:A:776:HIS:CG	2.52	1.02
1:A:1048:GLY:O	5:A:1104:FAD:C1'	2.07	1.02
1:B:623:ASP:O	1:B:628:PHE:HE1	1.39	1.02
1:B:773:CYS:SG	1:B:776:HIS:CG	2.52	1.02
1:A:726:ILE:CG2	1:B:648:ASP:CB	2.31	1.02
1:B:477:ALA:HB2	1:B:505:MET:CG	1.89	1.02
1:A:230:SER:N	1:B:471:ARG:NH2	1.83	1.01
1:A:728:LEU:CD2	1:B:644:LEU:HA	1.89	1.01
1:A:815:SER:O	1:B:644:LEU:CD1	2.07	1.01
1:A:168[B]:ASP:OD1	1:B:167:ARG:HA	1.60	1.01
1:A:646:PHE:CD1	1:B:727:ARG:HG3	1.63	1.01
1:B:661:ALA:CA	1:B:662:PHE:N	2.23	1.01
1:B:625:ALA:HB2	1:B:630:LEU:HD22	1.38	1.01
1:A:478:HIS:HB3	1:A:480:THR:H	1.21	1.01
1:A:644:LEU:HD21	1:B:815:SER:HB2	1.04	1.01
1:A:726:ILE:HG23	1:B:648:ASP:HB3	1.43	1.01
1:A:727:ARG:O	1:B:645:GLN:CA	2.09	1.01
1:B:627:TYR:C	1:B:628:PHE:CG	2.30	1.00
1:A:661:ALA:CA	1:A:662:PHE:N	2.23	1.00
1:A:731:GLU:OE1	1:B:641:THR:HG21	1.57	1.00
1:A:134:ASN:CG	1:B:161:ARG:H	1.63	1.00
1:A:451:LYS:O	1:A:454:PRO:N	1.94	1.00
1:A:507:LYS:HA	1:A:632:ILE:HB	1.02	1.00
1:A:730:ALA:HB1	1:B:641:THR:HG23	1.42	0.99
1:B:451:LYS:O	1:B:454:PRO:N	1.94	0.99
1:A:478:HIS:C	1:A:478:HIS:HB3	1.38	0.99
1:A:478:HIS:HB3	1:A:480:THR:N	1.76	0.99
1:A:478:HIS:HA	1:A:479:ASN:HA	1.00	0.99
1:A:644:LEU:HD23	1:B:728:LEU:HD22	0.99	0.99
1:B:627:TYR:HB2	1:B:628:PHE:CE1	1.97	0.98
1:A:735:LEU:HD12	1:A:736:ALA:N	1.79	0.98
1:A:815:SER:O	1:B:642:LEU:CD1	2.11	0.98
1:A:980:GLU:CB	1:A:980:GLU:OE2	2.12	0.98
1:B:980:GLU:OE2	1:B:980:GLU:CB	2.12	0.98
1:A:478:HIS:CG	1:A:478:HIS:N	2.32	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:ILE:CG2	1:B:648:ASP:CA	2.42	0.97
1:A:166:TYR:HE2	1:B:129:LYS:HB2	1.14	0.97
1:B:478:HIS:NE2	1:B:632:ILE:O	1.96	0.97
1:A:129:LYS:HA	1:B:166:TYR:OH	1.65	0.96
1:A:217:ASP:OD1	1:A:255:ARG:NH1	1.98	0.96
1:B:735:LEU:HD12	1:B:736:ALA:N	1.79	0.96
1:B:476:ASN:HB3	1:B:505:MET:HB3	0.97	0.96
1:B:452:LYS:O	1:B:454:PRO:N	1.99	0.95
1:A:728:LEU:HA	1:B:645:GLN:H	1.31	0.95
1:A:452:LYS:O	1:A:454:PRO:N	1.99	0.95
1:B:477:ALA:HB1	1:B:511:PRO:HD2	1.45	0.95
1:A:727:ARG:O	1:B:645:GLN:CB	2.14	0.95
1:B:472:LYS:HE3	1:B:506:SER:HB3	1.46	0.95
1:B:627:TYR:CA	1:B:628:PHE:CE1	2.49	0.95
1:B:472:LYS:NZ	1:B:474:ALA:HA	1.82	0.95
1:A:161:ARG:HD2	1:B:132:ARG:O	1.67	0.95
1:B:217:ASP:OD1	1:B:255:ARG:NH1	1.98	0.95
1:A:729:GLU:CB	1:B:645:GLN:OE1	2.14	0.94
1:A:452:LYS:C	1:A:454:PRO:N	2.16	0.94
1:B:625:ALA:O	1:B:628:PHE:CD1	2.20	0.94
1:A:125:GLN:CD	1:B:132:ARG:CZ	2.35	0.94
1:A:478:HIS:N	1:A:631:ASP:CG	2.20	0.94
1:A:726:ILE:HG21	1:B:647:VAL:O	1.67	0.94
1:A:125:GLN:CD	1:B:132:ARG:NH1	2.21	0.94
1:B:478:HIS:O	1:B:479:ASN:CB	2.03	0.94
3:B:1102:1C6:H3	3:B:1102:1C6:H8	1.50	0.93
3:A:1102:1C6:H8	3:A:1102:1C6:H3	1.50	0.93
1:A:452:LYS:HE2	1:A:455:LEU:N	1.82	0.93
1:A:728:LEU:CD2	1:B:644:LEU:HD12	1.99	0.93
1:B:625:ALA:O	1:B:628:PHE:HD1	1.49	0.93
1:A:633:GLU:HA	1:A:634:ASN:CG	1.89	0.92
1:B:655:LEU:HD22	1:B:824:ILE:O	1.69	0.92
1:A:132:ARG:HD3	1:B:125:GLN:OE1	1.70	0.92
1:A:452:LYS:HB3	1:A:455:LEU:HG	1.51	0.92
1:A:646:PHE:CE1	1:B:727:ARG:HG2	1.94	0.92
1:A:726:ILE:HG22	1:B:647:VAL:C	1.90	0.91
1:B:624:VAL:HA	1:B:628:PHE:HZ	1.34	0.91
1:A:507:LYS:HA	1:A:632:ILE:CB	1.97	0.91
1:A:655:LEU:HD22	1:A:824:ILE:O	1.69	0.91
1:A:728:LEU:HD22	1:B:644:LEU:CD1	2.00	0.91
1:B:452:LYS:HE2	1:B:455:LEU:N	1.82	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:LYS:HB3	1:B:455:LEU:HG	1.51	0.91
1:B:452:LYS:C	1:B:454:PRO:N	2.16	0.91
1:B:590:ALA:HA	1:B:594:ALA:HB2	1.53	0.91
1:A:634:ASN:O	1:A:635:SER:CB	2.18	0.91
1:A:724:GLN:CD	1:B:648:ASP:OD2	2.09	0.91
1:A:507:LYS:NZ	1:A:634:ASN:HD21	1.70	0.90
1:A:661:ALA:C	1:A:662:PHE:N	0.86	0.90
1:A:507:LYS:HZ2	1:A:634:ASN:HD21	1.19	0.90
1:B:661:ALA:C	1:B:662:PHE:N	0.86	0.90
1:B:477:ALA:C	1:B:509:PHE:O	2.10	0.90
1:B:659:HIS:HB3	1:B:880:PHE:CD1	2.07	0.90
1:A:646:PHE:HE1	1:B:727:ARG:HG3	1.37	0.90
1:A:659:HIS:HB3	1:A:880:PHE:CD1	2.07	0.90
1:A:452:LYS:HE3	1:A:468:LYS:HG2	1.53	0.90
1:A:648:ASP:H	1:B:726:ILE:HG22	1.37	0.90
1:B:477:ALA:HA	1:B:509:PHE:O	1.72	0.90
1:B:472:LYS:HG2	1:B:474:ALA:N	1.87	0.89
1:B:734:LYS:O	1:B:736:ALA:O	1.91	0.89
1:A:452:LYS:O	1:A:453:ILE:C	2.10	0.89
1:B:452:LYS:O	1:B:453:ILE:C	2.10	0.89
1:B:597:ILE:HG21	1:B:628:PHE:HZ	1.38	0.89
1:B:477:ALA:N	1:B:505:MET:CA	2.29	0.89
1:A:125:GLN:HG2	1:B:132:ARG:HH12	1.16	0.89
1:A:478:HIS:N	1:A:631:ASP:OD1	2.06	0.89
1:B:78:VAL:CG1	1:B:82:PHE:HD2	1.85	0.88
1:A:734:LYS:O	1:A:736:ALA:O	1.91	0.88
1:B:508:GLY:HA3	1:B:632:ILE:HB	1.56	0.88
1:A:642:LEU:HA	1:B:732:GLU:OE2	1.71	0.88
1:A:728:LEU:N	1:B:645:GLN:HG2	1.68	0.88
1:A:478:HIS:CA	1:A:631:ASP:CG	2.41	0.88
1:A:816:GLU:HA	1:B:642:LEU:CD1	2.04	0.87
1:A:590:ALA:HA	1:A:594:ALA:HB2	1.53	0.87
1:B:452:LYS:HE3	1:B:468:LYS:HG2	1.53	0.87
1:B:648:ASP:O	1:B:649:SER:OG	1.90	0.87
1:A:78:VAL:CG1	1:A:82:PHE:HD2	1.85	0.87
1:A:773:CYS:SG	1:A:776:HIS:ND1	2.48	0.87
1:A:642:LEU:CA	1:B:732:GLU:OE2	2.23	0.86
1:A:726:ILE:CA	1:B:648:ASP:CA	2.36	0.86
1:B:773:CYS:SG	1:B:776:HIS:ND1	2.48	0.86
1:A:815:SER:O	1:B:644:LEU:HD11	1.73	0.85
1:A:478:HIS:C	1:A:480:THR:N	2.29	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:PHE:CE2	1:B:728:LEU:CB	1.96	0.85
1:A:478:HIS:CB	1:A:478:HIS:C	0.75	0.85
1:A:132:ARG:HH12	1:B:125:GLN:HG2	1.34	0.85
1:A:730:ALA:CA	1:B:642:LEU:O	2.24	0.84
1:A:815:SER:O	1:B:644:LEU:HD13	1.77	0.84
1:B:7:GLN:HE21	1:B:16:ASN:HD21	1.25	0.84
1:A:168[B]:ASP:OD1	1:B:167:ARG:CA	2.25	0.84
1:B:627:TYR:HB3	1:B:628:PHE:CE2	2.11	0.84
1:A:819:ALA:HB3	1:B:642:LEU:HD12	1.60	0.84
1:B:624:VAL:HA	1:B:628:PHE:CE1	2.10	0.83
1:A:125:GLN:HG3	1:B:132:ARG:NH2	1.94	0.83
1:A:646:PHE:CE2	1:B:728:LEU:HB2	2.13	0.83
1:B:646:PHE:C	1:B:648:ASP:H	1.79	0.83
1:A:659:HIS:HB3	1:A:880:PHE:CE1	2.13	0.83
1:A:724:GLN:HG3	1:B:648:ASP:HB3	1.60	0.83
1:B:627:TYR:HB3	1:B:628:PHE:CD1	2.14	0.83
1:B:976:GLN:HE21	1:B:976:GLN:H	1.27	0.83
1:A:228:GLU:O	1:B:471:ARG:NH1	2.00	0.83
1:B:507:LYS:HA	1:B:634:ASN:HB2	1.61	0.83
1:B:659:HIS:HB3	1:B:880:PHE:CE1	2.13	0.83
1:B:477:ALA:CB	1:B:511:PRO:HD2	2.07	0.83
1:B:661:ALA:HA	1:B:879:CYS:O	1.79	0.83
1:A:129:LYS:HG3	1:B:166:TYR:CE2	2.14	0.82
1:A:507:LYS:CA	1:A:632:ILE:HB	1.98	0.82
1:A:730:ALA:C	1:B:641:THR:HG21	2.00	0.82
1:A:168[B]:ASP:OD1	1:B:167:ARG:CB	2.27	0.82
1:A:517:ASP:HB2	1:A:546:GLN:HB2	1.61	0.82
1:B:517:ASP:HB2	1:B:546:GLN:HB2	1.61	0.82
1:A:7:GLN:HE21	1:A:16:ASN:HD21	1.25	0.82
1:A:661:ALA:HA	1:A:879:CYS:O	1.79	0.82
1:A:815:SER:C	1:B:642:LEU:HD11	2.00	0.82
1:B:478:HIS:C	1:B:479:ASN:HB2	1.98	0.82
1:A:651:ALA:O	1:A:653:MET:SD	2.38	0.81
1:A:724:GLN:HE21	1:B:648:ASP:HB2	1.46	0.81
1:B:627:TYR:CB	1:B:628:PHE:CD1	2.64	0.81
1:A:78:VAL:HG12	1:A:82:PHE:HD2	1.45	0.81
1:A:726:ILE:HG22	1:B:648:ASP:HB3	1.30	0.81
1:A:508:GLY:HA3	1:A:631:ASP:CB	2.11	0.81
1:B:628:PHE:CD1	1:B:629:ASN:N	2.48	0.81
1:A:478:HIS:CB	1:A:480:THR:N	2.36	0.81
1:A:125:GLN:OE1	1:B:132:ARG:NE	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:734:LYS:HG2	1:A:736:ALA:O	1.82	0.80
1:A:819:ALA:CB	1:B:642:LEU:HD12	2.12	0.80
1:A:451:LYS:C	1:A:453:ILE:N	2.29	0.80
1:A:976:GLN:H	1:A:976:GLN:HE21	1.27	0.80
1:B:451:LYS:C	1:B:453:ILE:N	2.29	0.80
1:A:633:GLU:N	1:A:635:SER:HB2	1.97	0.80
1:A:661:ALA:O	1:A:662:PHE:CA	2.28	0.80
1:A:816:GLU:HA	1:B:642:LEU:HD13	1.62	0.80
1:A:643:SER:C	1:B:729:GLU:O	2.20	0.79
1:A:726:ILE:HG22	1:B:648:ASP:N	1.96	0.79
1:B:629:ASN:HB3	1:B:630:LEU:HD12	1.63	0.79
1:A:129:LYS:HB2	1:B:166:TYR:CE2	2.17	0.79
1:A:644:LEU:CD2	1:B:728:LEU:CD2	2.54	0.79
1:B:78:VAL:HG12	1:B:82:PHE:HD2	1.45	0.79
1:B:472:LYS:HZ3	1:B:474:ALA:HA	1.45	0.79
1:B:730:ALA:HB1	1:B:732:GLU:HG2	1.64	0.79
1:B:734:LYS:HG2	1:B:736:ALA:O	1.81	0.79
1:B:661:ALA:O	1:B:662:PHE:CA	2.28	0.79
1:A:168[B]:ASP:OD1	1:B:167:ARG:CG	2.32	0.78
1:B:477:ALA:CA	1:B:509:PHE:O	2.31	0.78
1:A:125:GLN:HG2	1:B:132:ARG:CZ	2.02	0.78
1:A:125:GLN:CG	1:B:132:ARG:NH2	2.47	0.78
1:A:646:PHE:O	1:B:726:ILE:HB	1.84	0.78
1:A:132:ARG:CZ	1:B:125:GLN:CG	2.62	0.78
1:A:161:ARG:N	1:B:134:ASN:ND2	1.90	0.78
1:A:168[B]:ASP:OD1	1:B:167:ARG:HG2	1.82	0.78
1:A:166:TYR:CZ	1:B:129:LYS:CA	2.67	0.78
1:A:16:ASN:HD22	1:A:43:GLU:H	1.31	0.78
1:A:472:LYS:HE3	1:A:474:ALA:HB2	1.64	0.78
1:A:508:GLY:HA3	1:A:631:ASP:HB3	1.65	0.77
1:B:472:LYS:HD3	1:B:474:ALA:HB2	0.83	0.77
1:A:166:TYR:OH	1:B:129:LYS:HA	1.83	0.77
1:B:627:TYR:HB3	1:B:628:PHE:CG	2.19	0.77
1:A:161:ARG:CD	1:B:132:ARG:O	2.32	0.77
1:A:625:ALA:HB1	1:A:630:LEU:HD12	1.65	0.77
1:A:634:ASN:O	1:A:635:SER:HB2	1.83	0.77
1:A:161:ARG:HD2	1:B:132:ARG:C	2.04	0.77
1:A:730:ALA:HB1	1:A:732:GLU:HG2	1.64	0.77
1:A:129:LYS:CG	1:B:166:TYR:CE2	2.67	0.77
1:A:478:HIS:HA	1:A:479:ASN:CA	1.96	0.77
1:A:507:LYS:HG2	1:A:632:ILE:HG22	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:627:TYR:HD1	1:B:628:PHE:CD2	2.03	0.77
1:A:732:GLU:OE1	1:B:640:SER:HA	1.85	0.76
1:B:478:HIS:N	1:B:509:PHE:O	2.18	0.76
1:A:129:LYS:HB2	1:B:166:TYR:HE2	1.50	0.76
1:B:659:HIS:CB	1:B:880:PHE:CE1	2.69	0.76
1:A:744:VAL:HG23	1:A:748:GLU:HG3	1.67	0.76
1:B:744:VAL:HG23	1:B:748:GLU:HG3	1.67	0.75
1:A:132:ARG:O	1:B:161:ARG:HD3	1.85	0.75
1:A:223:ARG:HA	1:A:226:SER:CB	2.15	0.75
1:B:16:ASN:HD22	1:B:43:GLU:H	1.31	0.75
1:B:78:VAL:HG12	1:B:82:PHE:CD2	2.20	0.75
1:B:223:ARG:HA	1:B:226:SER:CB	2.15	0.75
1:A:1046:TRP:NE1	1:A:1048:GLY:C	2.39	0.75
1:A:451:LYS:O	1:A:453:ILE:N	2.20	0.75
1:B:451:LYS:O	1:B:453:ILE:N	2.20	0.75
1:A:646:PHE:C	1:B:727:ARG:H	1.82	0.75
1:B:1046:TRP:NE1	1:B:1048:GLY:C	2.39	0.75
1:A:637:ASP:OD2	1:A:639:LYS:HD2	1.86	0.74
1:A:659:HIS:CB	1:A:880:PHE:CE1	2.69	0.74
1:A:644:LEU:HD21	1:B:815:SER:HB3	1.69	0.74
1:B:627:TYR:H	1:B:628:PHE:HE1	1.27	0.74
1:A:78:VAL:HG12	1:A:82:PHE:CD2	2.20	0.74
1:A:726:ILE:CG2	1:B:647:VAL:C	2.50	0.74
1:B:628:PHE:CG	1:B:629:ASN:N	2.30	0.74
1:A:642:LEU:C	1:B:732:GLU:OE2	2.26	0.74
1:B:624:VAL:O	1:B:628:PHE:CG	2.40	0.74
1:B:452:LYS:HB3	1:B:455:LEU:CG	2.18	0.74
1:B:635:SER:HB2	1:B:639:LYS:HD3	1.69	0.74
1:A:388:HIS:HA	1:A:391:LYS:HD3	1.69	0.73
1:B:1046:TRP:HD1	1:B:1048:GLY:CA	2.01	0.73
1:A:1046:TRP:HD1	1:A:1048:GLY:CA	2.01	0.73
1:B:78:VAL:HG11	1:B:82:PHE:CD2	2.23	0.73
1:B:476:ASN:CA	1:B:505:MET:O	2.27	0.73
1:B:628:PHE:CD1	1:B:628:PHE:CB	2.69	0.73
1:B:632:ILE:O	1:B:633:GLU:HB2	1.89	0.73
1:A:86:LEU:H	1:A:257:GLN:HE22	1.37	0.73
1:A:728:LEU:HA	1:B:645:GLN:N	2.03	0.73
1:B:162:PHE:CE1	1:B:215:LEU:HD21	2.24	0.73
1:B:628:PHE:CD1	1:B:628:PHE:CA	2.72	0.73
1:A:162:PHE:CE1	1:A:215:LEU:HD21	2.24	0.73
1:B:86:LEU:H	1:B:257:GLN:HE22	1.37	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:728:LEU:HD22	1:B:644:LEU:HA	1.70	0.73
1:A:726:ILE:HA	1:B:648:ASP:N	2.03	0.73
1:B:627:TYR:CD1	1:B:628:PHE:CD2	2.77	0.73
1:A:452:LYS:HB3	1:A:455:LEU:CG	2.18	0.72
1:A:78:VAL:HG11	1:A:82:PHE:CD2	2.23	0.72
1:A:125:GLN:OE1	1:B:132:ARG:HD3	1.90	0.72
1:A:129:LYS:HA	1:B:166:TYR:CZ	2.24	0.72
1:A:129:LYS:CB	1:B:166:TYR:CE2	2.72	0.72
1:A:478:HIS:CA	1:A:478:HIS:N	2.53	0.72
1:A:682:ARG:HD2	1:A:869:ALA:HA	1.71	0.72
1:A:728:LEU:HB3	1:B:644:LEU:H	1.54	0.72
1:A:732:GLU:OE2	1:B:642:LEU:N	2.22	0.72
1:B:641:THR:O	1:B:642:LEU:HB3	1.87	0.72
1:B:730:ALA:O	1:B:731:GLU:HB3	1.89	0.72
1:B:388:HIS:HA	1:B:391:LYS:HD3	1.69	0.72
1:B:477:ALA:H	1:B:505:MET:C	1.93	0.72
1:B:477:ALA:CA	1:B:505:MET:HA	2.19	0.72
1:A:728:LEU:N	1:B:645:GLN:CG	2.49	0.72
1:A:166:TYR:HA	1:B:165:PHE:O	1.90	0.72
1:A:732:GLU:OE1	1:B:640:SER:C	2.27	0.72
1:B:479:ASN:N	1:B:632:ILE:HG13	2.05	0.72
1:B:682:ARG:HD2	1:B:869:ALA:HA	1.71	0.72
1:A:129:LYS:CA	1:B:166:TYR:OH	2.37	0.71
1:B:637:ASP:HB3	1:B:639:LYS:HG3	1.70	0.71
1:A:724:GLN:HG3	1:B:648:ASP:CB	2.19	0.71
1:A:478:HIS:O	1:A:480:THR:HG22	1.89	0.71
1:A:479:ASN:HA	1:A:508:GLY:O	1.90	0.71
1:A:726:ILE:CB	1:B:648:ASP:HA	2.20	0.71
1:A:641:THR:CG2	1:B:732:GLU:OE1	2.39	0.71
1:B:550:TRP:O	1:B:554:ALA:HB3	1.91	0.71
1:B:963:ALA:HB1	1:B:973:THR:HG22	1.72	0.71
1:B:472:LYS:HZ2	1:B:474:ALA:HA	1.55	0.71
1:A:229:GLN:O	1:A:230:SER:C	2.29	0.71
1:A:724:GLN:CG	1:B:648:ASP:OD2	2.38	0.71
1:A:730:ALA:O	1:A:731:GLU:HB3	1.89	0.71
1:B:478:HIS:C	1:B:508:GLY:O	2.28	0.71
1:A:7:GLN:HE21	1:A:16:ASN:ND2	1.89	0.70
1:B:548:VAL:HG13	1:B:584:PHE:CE2	2.26	0.70
1:B:162:PHE:HE1	1:B:215:LEU:HD21	1.57	0.70
1:A:166:TYR:CD2	1:B:129:LYS:HG3	2.26	0.70
1:A:125:GLN:HG3	1:B:132:ARG:CZ	2.18	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:HIS:CA	1:A:480:THR:N	2.55	0.70
1:A:963:ALA:HB1	1:A:973:THR:HG22	1.72	0.70
1:A:548:VAL:HG13	1:A:584:PHE:CE2	2.26	0.70
1:B:451:LYS:C	1:B:453:ILE:H	1.94	0.70
1:A:1035:LEU:HD13	1:A:1041:TYR:HB2	1.74	0.70
1:B:468:LYS:O	1:B:469:LYS:HB2	1.92	0.70
1:A:506:SER:HB3	1:A:637:ASP:CB	2.22	0.70
1:A:550:TRP:O	1:A:554:ALA:HB3	1.91	0.70
1:A:134:ASN:HD21	1:B:161:ARG:CA	2.04	0.70
1:A:730:ALA:CB	1:B:641:THR:HG23	2.21	0.70
1:B:7:GLN:HE21	1:B:16:ASN:ND2	1.89	0.70
1:A:125:GLN:OE1	1:B:132:ARG:CD	2.40	0.69
1:A:161:ARG:NH1	1:B:132:ARG:HG2	2.05	0.69
1:A:641:THR:HG22	1:B:732:GLU:OE1	1.92	0.69
1:A:726:ILE:CG2	1:B:648:ASP:HA	2.14	0.69
1:B:1035:LEU:HD13	1:B:1041:TYR:HB2	1.74	0.69
1:A:478:HIS:CA	1:A:480:THR:H	2.04	0.69
1:A:633:GLU:HB2	1:A:634:ASN:HB2	1.73	0.69
1:A:479:ASN:O	1:A:480:THR:C	2.28	0.69
1:B:773:CYS:HB3	1:B:776:HIS:HB2	1.73	0.69
1:A:667:VAL:HG22	1:A:685:GLU:HB3	1.73	0.69
1:A:773:CYS:HB3	1:A:776:HIS:HB2	1.73	0.69
1:B:229:GLN:O	1:B:230:SER:C	2.29	0.69
1:B:528:ALA:HA	1:B:563:ARG:O	1.93	0.69
1:B:773:CYS:SG	1:B:776:HIS:CE1	2.86	0.69
1:B:635:SER:HB3	1:B:637:ASP:O	1.92	0.68
1:A:478:HIS:HB2	1:A:480:THR:HG22	1.75	0.68
1:A:773:CYS:SG	1:A:776:HIS:CE1	2.86	0.68
1:A:1015:LYS:HD3	7:A:1109:PG4:H81	1.73	0.68
1:B:482:LEU:O	1:B:511:PRO:HA	1.92	0.68
1:A:482:LEU:O	1:A:511:PRO:HA	1.92	0.68
1:A:523:LEU:HD23	1:A:562:VAL:HG11	1.74	0.68
1:B:667:VAL:HG22	1:B:685:GLU:HB3	1.74	0.68
1:A:641:THR:O	1:A:642:LEU:HD13	1.94	0.68
1:A:731:GLU:CD	1:B:641:THR:CG2	2.62	0.68
1:A:451:LYS:C	1:A:453:ILE:H	1.94	0.68
1:B:655:LEU:HD11	1:B:826:PRO:HD3	1.76	0.68
1:A:528:ALA:HA	1:A:563:ARG:O	1.93	0.68
1:A:161:ARG:CA	1:B:134:ASN:HD21	2.02	0.68
1:B:229:GLN:HG2	1:B:230:SER:H	1.59	0.68
1:B:523:LEU:HD23	1:B:562:VAL:HG11	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168[A]:ASP:HB2	1:B:167:ARG:HA	1.76	0.68
1:B:452:LYS:HB2	1:B:454:PRO:HA	1.76	0.68
1:A:162:PHE:HE1	1:A:215:LEU:HD21	1.56	0.67
1:A:633:GLU:CB	1:A:634:ASN:HB2	2.09	0.67
1:A:742:LYS:O	1:B:646:PHE:CZ	2.47	0.67
1:B:485:LEU:HD22	1:B:515:THR:O	1.95	0.67
1:A:639:LYS:O	1:A:641:THR:N	2.27	0.67
1:A:645:GLN:OE1	1:B:728:LEU:C	2.21	0.67
1:A:633:GLU:C	1:A:634:ASN:OD1	2.31	0.67
1:A:223:ARG:HD3	1:A:228:GLU:HB3	1.76	0.67
1:A:485:LEU:HD22	1:A:515:THR:O	1.95	0.67
1:B:627:TYR:HB3	1:B:628:PHE:CD2	2.30	0.67
1:B:659:HIS:CG	1:B:880:PHE:CZ	2.83	0.67
1:A:179:ARG:NH1	1:A:204:GLN:OE1	2.28	0.67
1:A:222:ASP:O	1:A:226:SER:N	2.28	0.67
1:A:729:GLU:CB	1:B:645:GLN:CD	2.62	0.67
1:B:472:LYS:C	1:B:474:ALA:H	1.98	0.67
1:B:1046:TRP:CD1	1:B:1048:GLY:O	2.46	0.67
1:A:125:GLN:OE1	1:B:132:ARG:CZ	2.42	0.66
1:A:452:LYS:HB2	1:A:454:PRO:HA	1.76	0.66
1:B:642:LEU:HD21	1:B:644:LEU:HB2	1.76	0.66
1:A:452:LYS:O	1:A:454:PRO:CA	2.43	0.66
1:A:638:ASN:O	1:A:640:SER:N	2.27	0.66
1:A:645:GLN:O	1:B:727:ARG:O	2.06	0.66
1:B:222:ASP:O	1:B:226:SER:N	2.28	0.66
1:B:1015:LYS:HD3	7:B:1109:PG4:H81	1.76	0.66
1:A:452:LYS:HD3	1:A:468:LYS:NZ	2.10	0.66
1:A:479:ASN:HB2	1:A:510:ALA:HB2	1.76	0.66
1:A:470:VAL:O	1:A:471:ARG:HB3	1.95	0.66
1:A:635:SER:O	1:A:636:GLU:CB	2.42	0.66
1:B:223:ARG:HD3	1:B:228:GLU:HB3	1.76	0.66
1:B:661:ALA:CA	1:B:879:CYS:O	2.44	0.66
1:A:655:LEU:HD11	1:A:826:PRO:HD3	1.76	0.66
1:B:452:LYS:HD3	1:B:468:LYS:NZ	2.11	0.66
1:B:478:HIS:O	1:B:632:ILE:CG2	2.38	0.66
1:B:635:SER:CB	1:B:639:LYS:HD3	2.25	0.66
1:A:229:GLN:HG2	1:A:230:SER:H	1.58	0.65
1:A:659:HIS:CG	1:A:880:PHE:CZ	2.83	0.65
1:B:452:LYS:O	1:B:454:PRO:CA	2.43	0.65
1:A:166:TYR:OH	1:B:129:LYS:CA	2.44	0.65
1:A:661:ALA:CA	1:A:879:CYS:O	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1015:LYS:CD	7:A:1109:PG4:H81	2.26	0.65
1:B:508:GLY:CA	1:B:632:ILE:HB	2.26	0.65
1:A:478:HIS:CB	1:A:631:ASP:OD1	2.45	0.65
1:A:478:HIS:CG	1:A:631:ASP:OD1	2.50	0.65
1:A:166:TYR:CE2	1:B:129:LYS:CG	2.79	0.65
1:A:645:GLN:H	1:B:728:LEU:HA	1.62	0.65
1:A:728:LEU:CA	1:B:645:GLN:H	2.08	0.65
1:A:132:ARG:CZ	1:B:125:GLN:HG3	2.25	0.65
1:A:478:HIS:CA	1:A:631:ASP:OD1	2.44	0.65
1:A:633:GLU:H	1:A:635:SER:HB2	1.60	0.65
1:A:1046:TRP:CD1	1:A:1048:GLY:O	2.46	0.65
1:A:175:THR:HG22	1:A:179:ARG:HH21	1.62	0.64
1:A:478:HIS:ND1	1:A:631:ASP:OD1	2.30	0.64
1:A:471:ARG:HG2	1:A:472:LYS:H	1.62	0.64
1:B:628:PHE:CD1	1:B:628:PHE:C	2.71	0.64
1:B:175:THR:HG22	1:B:179:ARG:HH21	1.62	0.64
1:B:179:ARG:NH1	1:B:204:GLN:OE1	2.28	0.64
1:B:625:ALA:HA	1:B:630:LEU:HB2	1.79	0.64
1:A:726:ILE:CB	1:B:648:ASP:CA	2.76	0.64
1:A:470:VAL:HG13	1:A:471:ARG:H	1.62	0.64
1:A:734:LYS:O	1:A:734:LYS:HG2	1.97	0.64
1:B:452:LYS:HD2	1:B:455:LEU:HG	1.80	0.64
1:B:628:PHE:N	1:B:628:PHE:HD1	1.87	0.64
1:B:633:GLU:O	1:B:634:ASN:HB2	1.98	0.64
1:A:452:LYS:HD2	1:A:455:LEU:HG	1.80	0.64
1:B:597:ILE:HG21	1:B:628:PHE:CZ	2.26	0.64
1:A:452:LYS:O	1:A:453:ILE:O	2.17	0.63
1:A:659:HIS:ND1	1:A:880:PHE:CZ	2.67	0.63
1:A:731:GLU:CD	1:B:641:THR:HG22	2.14	0.63
1:B:100:HIS:CE1	1:B:104:LEU:HD11	2.33	0.63
1:B:652:ASP:O	1:B:653:MET:C	2.35	0.63
1:B:734:LYS:O	1:B:734:LYS:HG2	1.97	0.63
1:A:608:ASP:OD1	1:B:794:LEU:HD12	1.99	0.63
1:B:563:ARG:HG2	1:B:595:GLU:CB	2.28	0.63
1:A:452:LYS:CE	1:A:468:LYS:H	2.11	0.63
1:A:729:GLU:O	1:B:642:LEU:O	2.04	0.63
1:B:452:LYS:CE	1:B:468:LYS:H	2.11	0.63
1:A:132:ARG:CD	1:B:125:GLN:OE1	2.45	0.63
1:B:646:PHE:HB2	1:B:648:ASP:H	1.62	0.63
1:B:659:HIS:ND1	1:B:880:PHE:CZ	2.67	0.63
1:B:773:CYS:SG	1:B:776:HIS:CD2	2.92	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:HIS:CE1	1:A:104:LEU:HD11	2.33	0.63
1:A:773:CYS:SG	1:A:776:HIS:CD2	2.92	0.63
1:B:1015:LYS:CD	7:B:1109:PG4:H81	2.29	0.62
1:A:229:GLN:C	1:A:231:ASP:N	2.52	0.62
1:A:563:ARG:HG2	1:A:595:GLU:CB	2.28	0.62
1:A:641:THR:HB	1:B:732:GLU:OE1	1.98	0.62
1:B:631:ASP:O	1:B:632:ILE:HD13	1.98	0.62
1:A:161:ARG:O	1:B:134:ASN:OD1	2.16	0.62
1:A:634:ASN:O	1:A:635:SER:OG	2.17	0.62
1:A:724:GLN:NE2	1:B:648:ASP:HB2	2.15	0.62
1:A:1035:LEU:HD22	1:A:1040:ARG:HB2	1.81	0.62
1:B:735:LEU:HD12	1:B:735:LEU:C	2.20	0.62
1:A:132:ARG:HG2	1:B:161:ARG:NH1	2.15	0.62
1:A:632:ILE:HG23	1:A:636:GLU:H	1.63	0.62
1:B:477:ALA:HB1	1:B:511:PRO:CD	2.26	0.62
1:B:595:GLU:OE2	1:B:627:TYR:OH	2.18	0.62
1:A:628:PHE:CB	1:A:629:ASN:HD22	2.13	0.62
1:B:507:LYS:HG2	1:B:634:ASN:CB	2.29	0.62
1:A:161:ARG:HD2	1:B:132:ARG:HA	1.82	0.62
1:A:223:ARG:C	1:A:226:SER:H	2.03	0.62
1:A:659:HIS:CG	1:A:880:PHE:CE1	2.88	0.62
1:B:476:ASN:HA	1:B:505:MET:C	2.18	0.62
1:B:477:ALA:CB	1:B:511:PRO:CD	2.76	0.62
1:B:516:LEU:HD21	1:B:531:ILE:HG23	1.82	0.62
1:B:452:LYS:O	1:B:453:ILE:O	2.17	0.61
1:B:472:LYS:CG	1:B:474:ALA:HB2	2.29	0.61
1:B:571:ASP:OD1	1:B:573:ASN:HB2	2.00	0.61
1:A:563:ARG:HG2	1:A:595:GLU:HB3	1.83	0.61
1:A:571:ASP:OD1	1:A:573:ASN:HB2	2.00	0.61
1:A:728:LEU:HD22	1:B:644:LEU:CA	2.30	0.61
1:B:508:GLY:HA3	1:B:632:ILE:CB	2.30	0.61
1:B:627:TYR:CD1	1:B:628:PHE:CE2	2.88	0.61
1:B:1035:LEU:HD22	1:B:1040:ARG:HB2	1.81	0.61
1:A:166:TYR:CE2	1:B:129:LYS:CA	2.82	0.61
1:A:482:LEU:HB2	1:A:509:PHE:CD2	2.35	0.61
1:A:161:ARG:HD2	1:B:132:ARG:CA	2.30	0.61
1:A:452:LYS:HD3	1:A:468:LYS:HZ2	1.65	0.61
1:A:659:HIS:CB	1:A:880:PHE:CD1	2.83	0.61
1:B:624:VAL:O	1:B:629:ASN:HB2	2.00	0.61
1:A:732:GLU:CD	1:B:641:THR:N	2.54	0.61
1:B:78:VAL:HG11	1:B:82:PHE:CE2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:625:ALA:C	1:B:628:PHE:CD1	2.72	0.61
1:A:735:LEU:HD12	1:A:735:LEU:C	2.20	0.61
1:B:229:GLN:C	1:B:231:ASP:N	2.52	0.61
1:B:659:HIS:CG	1:B:880:PHE:CE1	2.88	0.61
1:A:134:ASN:OD1	1:B:161:ARG:O	2.19	0.61
1:A:475:GLU:CD	1:A:632:ILE:HG13	2.21	0.61
1:B:482:LEU:HB2	1:B:509:PHE:CD2	2.35	0.61
1:B:1012:THR:HA	7:B:1109:PG4:H82	1.82	0.61
1:A:516:LEU:HD21	1:A:531:ILE:HG23	1.82	0.61
1:A:629:ASN:CG	1:A:630:LEU:N	2.51	0.61
1:A:734:LYS:CG	1:A:736:ALA:O	2.49	0.60
1:B:223:ARG:C	1:B:226:SER:H	2.03	0.60
1:A:452:LYS:HB2	1:A:454:PRO:CA	2.31	0.60
1:A:166:TYR:CE2	1:B:129:LYS:HA	2.36	0.60
1:A:644:LEU:HG	1:B:815:SER:C	2.21	0.60
1:B:455:LEU:O	1:B:469:LYS:N	2.34	0.60
1:A:648:ASP:N	1:B:726:ILE:HG22	2.15	0.60
1:B:638:ASN:H	1:B:638:ASN:ND2	1.99	0.60
1:B:229:GLN:O	1:B:231:ASP:N	2.35	0.60
1:A:478:HIS:CA	1:A:631:ASP:OD2	2.49	0.60
1:A:635:SER:O	1:A:636:GLU:HB3	2.00	0.60
1:A:451:LYS:O	1:A:452:LYS:C	2.40	0.60
1:B:787:GLN:HE21	1:B:791:GLU:CD	2.04	0.60
1:A:787:GLN:HE21	1:A:791:GLU:CD	2.04	0.60
1:A:1012:THR:HA	7:A:1109:PG4:H82	1.82	0.60
1:B:87[A]:PHE:HZ	3:B:1102:1C6:CE2	2.15	0.60
1:B:625:ALA:HA	1:B:630:LEU:HD13	1.82	0.60
1:A:478:HIS:CA	1:A:479:ASN:N	2.64	0.60
1:A:229:GLN:O	1:A:231:ASP:N	2.35	0.60
1:B:452:LYS:HB2	1:B:454:PRO:CA	2.31	0.60
1:B:659:HIS:HB3	1:B:880:PHE:CG	2.37	0.60
1:A:161:ARG:CD	1:B:132:ARG:HA	2.32	0.59
1:A:729:GLU:CB	1:B:645:GLN:NE2	2.64	0.59
1:B:635:SER:O	1:B:636:GLU:C	2.38	0.59
1:B:646:PHE:O	1:B:647:VAL:HB	2.02	0.59
1:A:653:MET:SD	1:A:653:MET:N	2.75	0.59
1:B:624:VAL:C	1:B:628:PHE:CZ	2.75	0.59
1:B:624:VAL:O	1:B:628:PHE:CZ	2.55	0.59
1:A:78:VAL:HG11	1:A:82:PHE:CE2	2.36	0.59
1:A:730:ALA:HB2	1:B:642:LEU:C	2.23	0.59
1:A:506:SER:HA	1:A:637:ASP:OD2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:732:GLU:OE2	1:B:641:THR:N	2.35	0.59
1:B:563:ARG:HG2	1:B:595:GLU:HB3	1.83	0.59
1:B:616:TRP:O	1:B:620:MET:HB2	2.02	0.59
1:B:734:LYS:CG	1:B:736:ALA:O	2.49	0.59
1:A:87[A]:PHE:HZ	3:A:1102:1C6:CE2	2.15	0.59
1:A:478:HIS:C	1:A:478:HIS:HB2	0.56	0.59
1:A:644:LEU:HD22	1:A:645:GLN:N	2.17	0.59
1:A:647:VAL:CB	1:A:648:ASP:OD2	2.38	0.59
1:B:627:TYR:CG	1:B:628:PHE:CZ	2.90	0.59
1:A:628:PHE:HB3	1:A:629:ASN:HD22	1.68	0.59
1:A:659:HIS:HB3	1:A:880:PHE:CG	2.37	0.59
1:A:166:TYR:CE2	1:B:129:LYS:HG3	2.38	0.59
1:A:479:ASN:N	1:A:479:ASN:OD1	2.35	0.59
1:A:730:ALA:HB1	1:B:641:THR:CG2	2.26	0.59
1:B:478:HIS:CD2	1:B:632:ILE:CG2	2.75	0.59
1:A:452:LYS:CB	1:A:455:LEU:HG	2.29	0.59
1:A:659:HIS:NE2	1:A:826:PRO:HG3	2.18	0.59
1:B:659:HIS:CB	1:B:880:PHE:CD1	2.83	0.59
1:A:87[A]:PHE:CZ	3:A:1102:1C6:CE2	2.86	0.59
1:A:616:TRP:O	1:A:620:MET:HB2	2.02	0.59
1:B:659:HIS:NE2	1:B:826:PRO:HG3	2.18	0.59
1:A:478:HIS:C	1:A:631:ASP:OD1	2.42	0.58
1:A:633:GLU:H	1:A:635:SER:CB	2.15	0.58
1:A:472:LYS:CE	1:A:474:ALA:HB2	2.33	0.58
1:B:477:ALA:N	1:B:505:MET:CB	2.67	0.58
1:A:230:SER:O	1:A:232:ASP:N	2.36	0.58
1:B:478:HIS:CE1	1:B:632:ILE:O	2.56	0.58
1:B:478:HIS:CE1	1:B:633:GLU:HB2	2.39	0.58
1:A:383:SER:OG	1:B:574:TRP:CH2	2.56	0.58
1:A:471:ARG:HE	1:A:472:LYS:C	2.07	0.58
1:A:632:ILE:HD13	1:A:637:ASP:N	2.18	0.58
1:A:476:ASN:HD21	1:A:479:ASN:CG	2.06	0.58
1:A:646:PHE:HZ	1:B:741:ALA:H	1.52	0.58
1:A:507:LYS:O	1:A:631:ASP:HB2	2.04	0.57
1:A:608:ASP:OD1	1:B:794:LEU:CD1	2.51	0.57
1:A:641:THR:CB	1:B:732:GLU:OE1	2.52	0.57
1:B:230:SER:O	1:B:232:ASP:N	2.36	0.57
1:B:650:ALA:O	1:B:651:ALA:C	2.41	0.57
1:A:383:SER:OG	1:B:574:TRP:CZ3	2.47	0.57
1:B:223:ARG:HG3	1:B:228:GLU:OE2	2.03	0.57
1:A:223:ARG:O	1:A:226:SER:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:ARG:O	1:B:226:SER:N	2.37	0.57
1:B:452:LYS:CD	1:B:455:LEU:HG	2.35	0.57
1:B:507:LYS:HA	1:B:633:GLU:O	2.04	0.57
1:B:597:ILE:HD13	1:B:628:PHE:CE2	2.40	0.57
1:B:655:LEU:HD23	1:B:703:ILE:HG23	1.87	0.57
1:A:655:LEU:HD23	1:A:703:ILE:HG23	1.87	0.57
1:A:223:ARG:HG3	1:A:228:GLU:OE2	2.03	0.57
1:A:523:LEU:HD11	1:A:547:PHE:HE1	1.69	0.57
1:A:381:ASN:OD1	1:B:573:ASN:CG	2.43	0.57
1:B:87[A]:PHE:CZ	3:B:1102:1C6:CE2	2.87	0.57
1:A:479:ASN:HB3	1:A:508:GLY:O	2.04	0.56
1:A:507:LYS:NZ	1:A:634:ASN:ND2	2.48	0.56
1:A:485:LEU:HA	1:A:514:ALA:O	2.06	0.56
1:A:508:GLY:HA3	1:A:631:ASP:HB2	1.87	0.56
1:A:646:PHE:O	1:B:727:ARG:N	2.31	0.56
1:B:624:VAL:HG22	1:B:628:PHE:CZ	2.41	0.56
1:B:646:PHE:C	1:B:648:ASP:N	2.48	0.56
1:A:134:ASN:HD21	1:B:160:TYR:C	1.99	0.56
1:A:647:VAL:O	1:A:649:SER:N	2.37	0.56
1:A:648:ASP:H	1:B:726:ILE:CG2	2.16	0.56
1:B:476:ASN:CA	1:B:505:MET:HB3	2.34	0.56
1:B:652:ASP:HB3	1:B:657:LYS:HE3	1.87	0.56
1:B:451:LYS:O	1:B:452:LYS:C	2.40	0.56
1:B:485:LEU:HA	1:B:514:ALA:O	2.05	0.56
1:A:651:ALA:O	1:A:652:ASP:C	2.40	0.56
1:A:728:LEU:HA	1:B:644:LEU:CA	2.35	0.56
1:A:815:SER:C	1:B:644:LEU:HD11	2.04	0.56
1:A:891:PRO:CD	1:A:898:LEU:HD21	2.36	0.56
1:A:452:LYS:CD	1:A:455:LEU:HG	2.35	0.56
1:A:1015:LYS:HB3	7:A:1109:PG4:H81	1.88	0.56
3:A:1102:1C6:H3	3:A:1102:1C6:C2	2.31	0.56
1:B:78:VAL:CG1	1:B:82:PHE:CE2	2.89	0.56
1:B:452:LYS:CB	1:B:455:LEU:HG	2.29	0.56
1:B:787:GLN:NE2	1:B:791:GLU:OE1	2.38	0.56
1:A:166:TYR:OH	1:B:129:LYS:N	2.39	0.55
1:A:162:PHE:HE1	1:A:215:LEU:CD2	2.19	0.55
1:A:645:GLN:OE1	1:B:728:LEU:O	2.24	0.55
1:B:523:LEU:HD11	1:B:547:PHE:HE1	1.69	0.55
1:B:627:TYR:HB2	1:B:628:PHE:CZ	2.37	0.55
1:A:632:ILE:HD12	1:A:637:ASP:CA	2.36	0.55
1:A:633:GLU:HA	1:A:634:ASN:OD1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:ALA:HA	1:A:880:PHE:HB3	1.89	0.55
1:A:477:ALA:C	1:A:631:ASP:OD2	2.43	0.55
1:B:635:SER:C	1:B:637:ASP:N	2.52	0.55
1:B:891:PRO:CD	1:B:898:LEU:HD21	2.36	0.55
1:A:161:ARG:CB	1:B:132:ARG:O	2.55	0.55
1:B:478:HIS:HD2	1:B:632:ILE:HG22	1.65	0.55
1:B:634:ASN:O	1:B:635:SER:C	2.45	0.55
1:A:452:LYS:HE2	1:A:468:LYS:H	1.72	0.55
1:B:472:LYS:HG2	1:B:474:ALA:CA	2.36	0.55
1:B:627:TYR:CB	1:B:628:PHE:CG	2.90	0.55
1:A:650:ALA:N	1:A:650:ALA:CB	2.64	0.55
1:B:472:LYS:C	1:B:474:ALA:N	2.61	0.55
1:A:475:GLU:O	1:A:476:ASN:C	2.43	0.54
1:A:727:ARG:O	1:B:646:PHE:N	2.40	0.54
1:A:976:GLN:H	1:A:976:GLN:NE2	2.01	0.54
1:B:71:LEU:HD22	1:B:90:TRP:CE2	2.42	0.54
1:B:223:ARG:HD3	1:B:226:SER:CB	2.38	0.54
1:A:223:ARG:HD3	1:A:226:SER:CB	2.38	0.54
1:A:632:ILE:CD1	1:A:637:ASP:N	2.70	0.54
1:B:623:ASP:C	1:B:628:PHE:CE1	2.79	0.54
1:A:472:LYS:HG3	1:A:474:ALA:HB2	1.87	0.54
1:A:625:ALA:CB	1:A:630:LEU:HD12	2.38	0.54
1:A:727:ARG:HG2	1:B:645:GLN:HG3	0.71	0.54
1:A:132:ARG:NH1	1:B:125:GLN:CD	2.61	0.54
1:B:78:VAL:HG13	1:B:82:PHE:CD2	2.38	0.54
1:B:641:THR:HG23	1:B:642:LEU:N	2.22	0.54
1:A:632:ILE:HD12	1:A:637:ASP:CB	2.38	0.54
1:B:452:LYS:HD3	1:B:468:LYS:HZ2	1.70	0.54
1:B:468:LYS:O	1:B:469:LYS:CB	2.50	0.54
1:A:71:LEU:HD22	1:A:90:TRP:CE2	2.42	0.54
1:A:787:GLN:NE2	1:A:791:GLU:OE1	2.38	0.54
1:B:506:SER:O	1:B:634:ASN:ND2	2.41	0.54
1:B:625:ALA:CA	1:B:630:LEU:HB2	2.37	0.54
1:B:162:PHE:HE1	1:B:215:LEU:CD2	2.19	0.54
1:A:742:LYS:O	1:B:646:PHE:CE2	2.61	0.54
1:A:633:GLU:CA	1:A:634:ASN:OD1	2.56	0.53
1:A:650:ALA:O	1:A:652:ASP:N	2.41	0.53
1:B:651:ALA:C	1:B:653:MET:H	2.09	0.53
1:A:635:SER:HB3	1:A:636:GLU:OE2	2.07	0.53
1:A:78:VAL:HG13	1:A:82:PHE:CD2	2.37	0.53
1:A:166:TYR:CD2	1:B:129:LYS:CG	2.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:744:VAL:CG2	1:A:748:GLU:HG3	2.39	0.53
1:B:452:LYS:HE2	1:B:468:LYS:H	1.72	0.53
1:A:482:LEU:HB2	1:A:509:PHE:HD2	1.73	0.53
1:A:476:ASN:ND2	1:A:479:ASN:OD1	2.41	0.53
1:A:383:SER:CB	1:B:574:TRP:CH2	2.91	0.53
1:B:482:LEU:HB2	1:B:509:PHE:HD2	1.73	0.53
1:B:626:ALA:C	1:B:628:PHE:CD1	2.81	0.53
1:A:381:ASN:ND2	1:B:573:ASN:OD1	2.42	0.53
1:B:661:ALA:HA	1:B:880:PHE:HB3	1.89	0.53
1:B:551:LEU:HD11	1:B:589:LEU:HD13	1.90	0.53
1:A:431:LEU:HD21	1:A:433:ILE:HD11	1.91	0.53
1:B:431:LEU:HD21	1:B:433:ILE:HD11	1.91	0.53
1:A:644:LEU:C	1:A:645:GLN:HG3	2.29	0.52
1:A:726:ILE:CB	1:B:648:ASP:N	2.72	0.52
1:B:625:ALA:CB	1:B:630:LEU:HB2	2.38	0.52
1:A:661:ALA:O	1:A:662:PHE:HA	2.09	0.52
1:B:585:ILE:O	1:B:589:LEU:HB2	2.09	0.52
1:A:818:ILE:HG22	1:B:644:LEU:HD11	1.91	0.52
1:A:636:GLU:HB3	1:A:638:ASN:OD1	2.10	0.52
1:A:642:LEU:N	1:A:642:LEU:HD22	2.25	0.52
1:A:726:ILE:HA	1:B:646:PHE:HB2	1.90	0.52
1:B:479:ASN:HA	1:B:508:GLY:O	2.10	0.52
1:A:551:LEU:HD11	1:A:589:LEU:HD13	1.90	0.52
1:B:420:HIS:CE1	1:B:453:ILE:HG21	2.45	0.52
1:A:420:HIS:CE1	1:A:453:ILE:HG21	2.45	0.52
1:A:585:ILE:O	1:A:589:LEU:HB2	2.09	0.52
1:A:659:HIS:HB3	1:A:880:PHE:CZ	2.45	0.52
1:B:1015:LYS:HB3	7:B:1109:PG4:H81	1.92	0.52
1:A:563:ARG:HG2	1:A:595:GLU:CG	2.41	0.52
1:B:1006:ALA:HB3	1:B:1007:PRO:HD3	1.92	0.52
1:B:1012:THR:HA	7:B:1109:PG4:H61	1.92	0.52
1:A:452:LYS:CE	1:A:468:LYS:HG2	2.35	0.51
1:A:733:GLU:CD	1:A:734:LYS:N	2.64	0.51
1:B:452:LYS:CE	1:B:468:LYS:HG2	2.35	0.51
1:B:642:LEU:HD11	1:B:644:LEU:HD22	1.92	0.51
1:B:659:HIS:HB3	1:B:880:PHE:CZ	2.45	0.51
1:A:452:LYS:O	1:A:454:PRO:C	2.49	0.51
1:A:478:HIS:CB	1:A:478:HIS:N	2.73	0.51
1:A:624:VAL:O	1:A:627:TYR:HB3	2.11	0.51
1:A:1006:ALA:HB3	1:A:1007:PRO:HD3	1.92	0.51
1:A:724:GLN:NE2	1:B:648:ASP:CG	2.64	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:GLU:CD	1:B:641:THR:HG21	2.28	0.51
1:B:618:GLU:OE1	1:B:618:GLU:HA	2.11	0.51
1:B:655:LEU:CD2	1:B:824:ILE:O	2.52	0.51
1:B:976:GLN:H	1:B:976:GLN:NE2	2.01	0.51
1:B:452:LYS:O	1:B:454:PRO:C	2.49	0.51
1:B:624:VAL:HG22	1:B:628:PHE:CE2	2.44	0.51
1:A:728:LEU:CD2	1:B:644:LEU:CA	2.75	0.51
1:B:563:ARG:HG2	1:B:595:GLU:CG	2.41	0.51
1:B:571:ASP:HB3	1:B:574:TRP:HE3	1.76	0.51
1:B:661:ALA:O	1:B:662:PHE:HA	2.09	0.51
1:A:618:GLU:HA	1:A:618:GLU:OE1	2.11	0.51
1:A:635:SER:C	1:A:636:GLU:HG3	2.31	0.51
1:B:452:LYS:NZ	1:B:454:PRO:HA	2.26	0.51
1:A:78:VAL:CG1	1:A:82:PHE:CE2	2.89	0.51
1:A:727:ARG:HB3	1:B:646:PHE:H	1.62	0.51
1:A:730:ALA:HB2	1:B:642:LEU:CA	2.41	0.51
1:A:179:ARG:NH1	1:A:208:ASP:OD1	2.44	0.51
1:A:471:ARG:HG2	1:A:472:LYS:N	2.24	0.51
1:A:629:ASN:C	1:A:630:LEU:HD13	2.32	0.51
1:A:735:LEU:CD1	1:A:736:ALA:N	2.64	0.50
1:B:87[A]:PHE:CE2	3:B:1102:1C6:H11	2.46	0.50
1:B:733:GLU:CD	1:B:734:LYS:N	2.64	0.50
3:B:1102:1C6:H3	3:B:1102:1C6:C2	2.31	0.50
1:A:632:ILE:CD1	1:A:637:ASP:CA	2.90	0.50
1:A:1012:THR:HA	7:A:1109:PG4:H61	1.93	0.50
1:B:87[A]:PHE:CE2	3:B:1102:1C6:C1	2.94	0.50
1:B:179:ARG:NH1	1:B:208:ASP:OD1	2.44	0.50
1:A:381:ASN:CG	1:B:573:ASN:OD1	2.50	0.50
1:A:87[A]:PHE:CE2	3:A:1102:1C6:C1	2.94	0.50
1:A:452:LYS:NZ	1:A:454:PRO:HA	2.26	0.50
1:A:1015:LYS:HB3	7:A:1109:PG4:C8	2.42	0.50
1:B:744:VAL:CG2	1:B:748:GLU:HG3	2.39	0.50
1:A:87[A]:PHE:CE2	3:A:1102:1C6:H11	2.47	0.50
1:A:571:ASP:HB3	1:A:574:TRP:HE3	1.76	0.50
1:A:647:VAL:O	1:A:648:ASP:HB2	2.11	0.50
1:A:653:MET:O	1:A:654:PRO:C	2.48	0.50
1:A:104:LEU:N	1:A:105:PRO:CD	2.75	0.49
1:A:161:ARG:CD	1:B:132:ARG:CA	2.89	0.49
1:A:597:ILE:HG22	1:A:597:ILE:O	2.11	0.49
1:B:230:SER:O	1:B:235:THR:OG1	2.30	0.49
1:B:597:ILE:HG22	1:B:597:ILE:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:724:GLN:NE2	1:B:648:ASP:CB	2.74	0.49
1:B:477:ALA:N	1:B:505:MET:O	2.45	0.49
1:B:735:LEU:CD1	1:B:736:ALA:N	2.64	0.49
1:A:230:SER:O	1:A:235:THR:OG1	2.30	0.49
1:B:641:THR:HG23	1:B:642:LEU:H	1.76	0.49
1:A:476:ASN:O	1:A:477:ALA:HB3	2.12	0.49
1:A:632:ILE:HG22	1:A:632:ILE:O	2.12	0.49
1:A:732:GLU:CD	1:B:640:SER:C	2.71	0.49
3:A:1102:1C6:H8	3:A:1102:1C6:C3	2.34	0.49
1:B:232:ASP:O	1:B:236:HIS:HD2	1.96	0.49
1:B:646:PHE:HB2	1:B:648:ASP:N	2.27	0.49
1:B:725:GLN:OE1	1:B:743:THR:HG22	2.13	0.49
1:A:728:LEU:HA	1:B:644:LEU:N	2.28	0.49
1:B:642:LEU:HG	1:B:643:SER:N	2.28	0.49
1:A:134:ASN:ND2	1:B:161:ARG:CB	2.75	0.49
1:A:819:ALA:HB2	1:B:642:LEU:HD12	1.91	0.49
1:B:104:LEU:N	1:B:105:PRO:CD	2.75	0.49
1:A:134:ASN:OD1	1:B:161:ARG:N	2.43	0.49
1:A:725:GLN:OE1	1:A:743:THR:HG22	2.13	0.49
1:B:477:ALA:HA	1:B:505:MET:HA	1.95	0.49
1:A:632:ILE:HG23	1:A:636:GLU:N	2.28	0.49
1:B:87[A]:PHE:HE2	3:B:1102:1C6:C1	2.26	0.49
1:B:638:ASN:HB2	1:B:640:SER:OG	2.13	0.49
1:A:168[B]:ASP:HB2	1:B:168[B]:ASP:HB2	1.95	0.48
1:A:232:ASP:O	1:A:236:HIS:HD2	1.96	0.48
1:A:728:LEU:CB	1:B:644:LEU:H	2.24	0.48
1:A:727:ARG:CG	1:B:645:GLN:CG	2.52	0.48
1:B:87[A]:PHE:CE2	3:B:1102:1C6:CZ	2.97	0.48
1:A:129:LYS:HG3	1:B:166:TYR:CD2	2.48	0.48
1:A:483:LEU:HD12	1:A:512:GLN:O	2.14	0.48
1:B:452:LYS:HE3	1:B:468:LYS:CG	2.37	0.48
1:B:625:ALA:O	1:B:629:ASN:O	2.31	0.48
1:A:486:TYR:HA	1:A:532:VAL:O	2.13	0.48
1:A:506:SER:HA	1:A:637:ASP:CG	2.34	0.48
1:A:571:ASP:HB3	1:A:574:TRP:CE3	2.48	0.48
1:A:655:LEU:CD2	1:A:824:ILE:O	2.52	0.48
1:A:523:LEU:HD11	1:A:547:PHE:CE1	2.48	0.48
1:A:470:VAL:HG22	1:A:471:ARG:N	2.27	0.48
1:A:641:THR:C	1:A:642:LEU:HD22	2.34	0.48
1:B:571:ASP:HB3	1:B:574:TRP:CE3	2.48	0.48
1:B:735:LEU:HD12	1:B:736:ALA:CA	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:GLU:CD	1:A:637:ASP:H	2.16	0.48
1:B:505:MET:HG3	1:B:511:PRO:HG2	1.96	0.48
1:B:547:PHE:O	1:B:550:TRP:HE3	1.96	0.48
1:A:87[A]:PHE:HE2	3:A:1102:1C6:C1	2.27	0.48
1:A:452:LYS:HB2	1:A:452:LYS:HZ3	1.78	0.48
1:A:471:ARG:HH21	1:A:473:LYS:N	2.12	0.48
1:A:547:PHE:O	1:A:550:TRP:HE3	1.96	0.48
1:A:614:GLU:HA	1:A:617:ARG:NH2	2.29	0.48
1:A:644:LEU:C	1:A:645:GLN:CG	2.82	0.48
1:B:635:SER:OG	1:B:637:ASP:HB3	2.13	0.48
1:A:383:SER:HB3	1:B:574:TRP:CZ2	2.49	0.47
1:B:478:HIS:C	1:B:479:ASN:CA	2.77	0.47
1:B:614:GLU:HA	1:B:617:ARG:NH2	2.29	0.47
1:B:637:ASP:CG	1:B:639:LYS:H	2.17	0.47
1:A:87[A]:PHE:CE2	3:A:1102:1C6:CZ	2.97	0.47
1:B:486:TYR:HA	1:B:532:VAL:O	2.13	0.47
1:A:125:GLN:NE2	1:B:132:ARG:NH1	2.62	0.47
1:A:161:ARG:H	1:B:134:ASN:CG	2.00	0.47
1:B:642:LEU:HG	1:B:643:SER:H	1.78	0.47
2:B:1101:HEM:CMB	2:B:1101:HEM:HBB2	2.44	0.47
1:A:597:ILE:HG12	1:A:627:TYR:CE1	2.48	0.47
1:B:523:LEU:HD11	1:B:547:PHE:CE1	2.48	0.47
1:B:534:ALA:HA	1:B:569:CYS:O	2.15	0.47
1:A:383:SER:HA	1:B:574:TRP:CH2	2.50	0.47
1:A:627:TYR:HD2	1:A:628:PHE:CG	2.33	0.47
1:A:650:ALA:O	1:A:651:ALA:C	2.51	0.47
1:B:1038:LYS:HE3	7:B:1108:PG4:H11	1.97	0.47
1:A:129:LYS:HA	1:B:166:TYR:HH	1.74	0.47
1:A:478:HIS:CA	1:A:479:ASN:C	2.79	0.47
1:A:506:SER:O	1:A:632:ILE:HD12	2.14	0.47
1:A:815:SER:HA	1:B:644:LEU:HD11	1.48	0.47
1:B:559:VAL:HG22	1:B:592:LYS:O	2.15	0.47
3:B:1102:1C6:H8	3:B:1102:1C6:C3	2.34	0.47
1:A:506:SER:HB3	1:A:637:ASP:HB2	1.97	0.47
1:A:624:VAL:O	1:A:628:PHE:HD1	1.98	0.47
1:A:647:VAL:HB	1:A:648:ASP:CG	2.29	0.47
1:B:452:LYS:HD3	1:B:468:LYS:HZ3	1.80	0.47
1:B:483:LEU:HD12	1:B:512:GLN:O	2.14	0.47
1:B:508:GLY:HA3	1:B:632:ILE:C	2.35	0.47
1:B:452:LYS:HE3	1:B:468:LYS:H	1.80	0.47
1:B:637:ASP:C	1:B:639:LYS:N	2.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:LYS:HZ2	1:A:473:LYS:C	2.18	0.47
1:A:726:ILE:CB	1:B:647:VAL:C	2.82	0.47
1:B:589:LEU:HD12	1:B:589:LEU:HA	1.82	0.47
1:B:637:ASP:O	1:B:639:LYS:NZ	2.36	0.47
1:B:638:ASN:O	1:B:639:LYS:C	2.51	0.47
1:A:726:ILE:HB	1:B:647:VAL:C	2.35	0.46
1:A:534:ALA:HA	1:A:569:CYS:O	2.15	0.46
1:A:559:VAL:HG22	1:A:592:LYS:O	2.15	0.46
1:A:505:MET:HG3	1:A:511:PRO:HG2	1.96	0.46
1:A:517:ASP:HA	1:A:547:PHE:HB2	1.96	0.46
1:B:39:ILE:HD12	1:B:52:LEU:CD2	2.46	0.46
1:B:479:ASN:N	1:B:479:ASN:OD1	2.48	0.46
1:A:827:ARG:HD2	5:A:1104:FAD:O1P	2.15	0.46
2:A:1101:HEM:CMB	2:A:1101:HEM:HBB2	2.44	0.46
1:B:557:ASP:OD1	1:B:557:ASP:N	2.48	0.46
1:A:223:ARG:CD	1:A:228:GLU:HB3	2.44	0.46
1:A:452:LYS:C	1:A:453:ILE:HG12	2.36	0.46
1:A:735:LEU:O	1:A:736:ALA:C	2.54	0.46
1:B:452:LYS:HB2	1:B:452:LYS:HZ3	1.80	0.46
1:A:735:LEU:HD12	1:A:736:ALA:CA	2.44	0.46
1:B:517:ASP:HA	1:B:547:PHE:HB2	1.96	0.46
1:B:625:ALA:CA	1:B:630:LEU:HD13	2.45	0.46
1:A:132:ARG:HA	1:B:161:ARG:NE	2.31	0.46
1:B:745:SER:OG	1:B:748:GLU:HG2	2.16	0.46
1:A:167:ARG:HG2	1:B:168[B]:ASP:OD1	2.16	0.46
1:A:452:LYS:HE3	1:A:468:LYS:H	1.80	0.46
1:A:472:LYS:HG3	1:A:474:ALA:CB	2.46	0.46
1:A:645:GLN:C	1:A:646:PHE:CD2	2.88	0.46
1:A:39:ILE:HD12	1:A:52:LEU:CD2	2.46	0.45
1:A:730:ALA:C	1:B:641:THR:CG2	2.77	0.45
1:B:87[A]:PHE:CZ	3:B:1102:1C6:CZ	2.99	0.45
1:B:452:LYS:C	1:B:453:ILE:HG12	2.36	0.45
1:A:383:SER:OG	1:B:573:ASN:HB3	2.15	0.45
1:A:726:ILE:CG2	1:B:648:ASP:N	2.67	0.45
1:B:735:LEU:O	1:B:736:ALA:C	2.54	0.45
1:B:1015:LYS:HB3	7:B:1109:PG4:C8	2.46	0.45
1:A:87[A]:PHE:CZ	3:A:1102:1C6:CZ	3.00	0.45
1:B:148:LEU:HD21	1:B:413:VAL:HG21	1.98	0.45
1:B:479:ASN:N	1:B:632:ILE:CG1	2.78	0.45
1:B:655:LEU:HD21	1:B:826:PRO:HD3	1.98	0.45
1:A:1015:LYS:CG	7:A:1109:PG4:H81	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:LEU:HD23	1:B:524:PRO:CG	2.47	0.45
1:B:629:ASN:CB	1:B:630:LEU:HD12	2.42	0.45
1:B:632:ILE:O	1:B:633:GLU:CB	2.62	0.45
1:B:827:ARG:HD2	5:B:1104:FAD:O1P	2.16	0.45
1:B:455:LEU:O	1:B:468:LYS:C	2.54	0.45
1:B:490:MET:HE3	4:B:1103:FMN:HM83	1.98	0.45
1:A:745:SER:OG	1:A:748:GLU:HG2	2.16	0.45
1:A:455:LEU:O	1:A:468:LYS:C	2.54	0.45
1:A:557:ASP:OD1	1:A:557:ASP:N	2.48	0.45
1:A:636:GLU:CB	1:A:638:ASN:OD1	2.65	0.45
1:A:644:LEU:CA	1:B:729:GLU:O	2.62	0.45
1:B:517:ASP:CB	1:B:546:GLN:HB2	2.41	0.45
1:A:655:LEU:HD21	1:A:826:PRO:HD3	1.99	0.45
1:A:1038:LYS:HE3	7:A:1108:PG4:H11	1.97	0.45
1:B:639:LYS:HE2	1:B:639:LYS:HB2	1.63	0.45
1:A:629:ASN:OD1	1:A:630:LEU:N	2.50	0.44
1:A:148:LEU:HD21	1:A:413:VAL:HG21	1.98	0.44
1:A:644:LEU:HG	1:B:815:SER:O	2.17	0.44
1:B:480:THR:HG21	1:B:629:ASN:ND2	2.33	0.44
1:B:480:THR:HA	1:B:481:PRO:HD3	1.70	0.44
1:B:625:ALA:HB1	1:B:630:LEU:HB2	1.99	0.44
1:A:627:TYR:HB3	1:A:628:PHE:H	1.49	0.44
1:A:724:GLN:CG	1:B:648:ASP:CB	2.94	0.44
1:A:726:ILE:HG22	1:B:648:ASP:CG	2.31	0.44
1:A:567:PHE:HD1	1:A:616:TRP:CD2	2.35	0.44
1:B:226:SER:O	1:B:227:GLY:C	2.53	0.44
1:B:521:GLY:HA2	1:B:550:TRP:CZ2	2.53	0.44
1:A:521:GLY:HA2	1:A:550:TRP:CZ2	2.53	0.44
1:A:602:GLU:O	1:A:612:THR:HG21	2.18	0.44
1:A:615:GLU:O	1:A:619:HIS:ND1	2.51	0.44
1:A:633:GLU:N	1:A:633:GLU:CD	2.71	0.44
1:A:732:GLU:CD	1:B:640:SER:HB3	2.23	0.44
1:B:472:LYS:CD	1:B:474:ALA:CB	2.58	0.44
1:B:631:ASP:C	1:B:632:ILE:HG12	2.36	0.44
1:A:222:ASP:O	1:A:225:ALA:HB3	2.18	0.44
1:A:590:ALA:CA	1:A:594:ALA:HB2	2.37	0.44
1:A:732:GLU:OE1	1:B:641:THR:N	2.51	0.44
1:B:122:ILE:HG22	1:B:148:LEU:HD12	1.99	0.44
1:B:222:ASP:O	1:B:225:ALA:HB3	2.18	0.44
1:B:472:LYS:CE	1:B:634:ASN:HD21	2.30	0.44
1:B:479:ASN:CA	1:B:632:ILE:HG13	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ARG:CA	1:B:161:ARG:CD	2.96	0.44
1:A:134:ASN:HD21	1:B:161:ARG:CB	2.31	0.44
1:A:451:LYS:O	1:A:454:PRO:CD	2.65	0.44
1:A:644:LEU:HD22	1:A:644:LEU:C	2.38	0.44
1:A:730:ALA:CB	1:B:642:LEU:O	2.66	0.44
1:B:651:ALA:CB	1:B:653:MET:HG3	2.48	0.44
1:A:473:LYS:HZ3	1:A:476:ASN:H	1.65	0.44
1:A:490:MET:HE3	1:A:536:TYR:HE2	1.83	0.44
1:B:628:PHE:HB2	1:B:629:ASN:ND2	2.33	0.44
1:A:129:LYS:CA	1:B:166:TYR:CZ	2.99	0.43
1:A:470:VAL:HG13	1:A:471:ARG:N	2.30	0.43
1:A:483:LEU:HD23	1:A:524:PRO:HG3	2.00	0.43
1:B:223:ARG:CD	1:B:228:GLU:HB3	2.44	0.43
1:B:476:ASN:OD1	1:B:506:SER:N	2.51	0.43
1:A:732:GLU:OE2	1:B:640:SER:C	2.56	0.43
1:B:615:GLU:O	1:B:619:HIS:ND1	2.51	0.43
1:B:642:LEU:HD11	1:B:644:LEU:HD13	2.00	0.43
1:B:651:ALA:C	1:B:653:MET:N	2.71	0.43
1:B:730:ALA:O	1:B:731:GLU:CB	2.62	0.43
1:A:122:ILE:HG22	1:A:148:LEU:HD12	1.99	0.43
1:A:125:GLN:HG2	1:B:132:ARG:NH2	2.25	0.43
1:A:452:LYS:HE3	1:A:468:LYS:CG	2.37	0.43
1:A:483:LEU:HD23	1:A:524:PRO:CG	2.47	0.43
1:A:486:TYR:O	1:A:516:LEU:N	2.50	0.43
1:B:5:MET:HA	1:B:6:PRO:HD3	1.88	0.43
1:A:470:VAL:O	1:A:471:ARG:NH1	2.51	0.43
1:A:478:HIS:N	1:A:478:HIS:CD2	2.83	0.43
1:B:472:LYS:CE	1:B:634:ASN:ND2	2.81	0.43
1:B:602:GLU:O	1:B:612:THR:HG21	2.18	0.43
1:B:685:GLU:HG2	1:B:841:GLN:OE1	2.19	0.43
1:A:228:GLU:H	1:A:228:GLU:HG2	1.75	0.43
1:A:473:LYS:HA	1:A:473:LYS:HD2	1.77	0.43
1:A:963:ALA:CB	1:A:973:THR:HG22	2.45	0.43
1:B:637:ASP:O	1:B:639:LYS:HG3	2.19	0.43
1:B:646:PHE:O	1:B:648:ASP:O	2.37	0.43
1:B:624:VAL:HG12	1:B:630:LEU:HD13	2.00	0.43
1:A:472:LYS:HZ3	1:A:473:LYS:H	1.67	0.43
1:A:646:PHE:CE1	1:B:741:ALA:N	2.84	0.43
1:A:724:GLN:CD	1:B:648:ASP:CG	2.76	0.43
1:B:624:VAL:C	1:B:628:PHE:CD1	2.79	0.43
1:B:636:GLU:N	1:B:636:GLU:CD	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:LYS:HB3	1:A:469:LYS:HE3	1.24	0.43
1:A:555:SER:HB3	1:A:592:LYS:HE3	2.00	0.43
1:A:827:ARG:HG2	5:A:1104:FAD:H3'	2.01	0.43
1:B:624:VAL:CG2	1:B:628:PHE:CZ	3.01	0.43
1:B:95:ASN:HD22	1:B:95:ASN:HA	1.68	0.43
1:A:908:ALA:HB3	1:A:909:PRO:HD3	2.01	0.42
1:B:225:ALA:O	1:B:226:SER:C	2.56	0.42
1:A:647:VAL:C	1:A:648:ASP:CG	2.73	0.42
1:B:328:ALA:HB1	3:B:1102:1C6:N1	2.34	0.42
1:B:563:ARG:HD3	1:B:627:TYR:OH	2.19	0.42
1:A:506:SER:HB3	1:A:637:ASP:HB3	2.01	0.42
1:A:628:PHE:HB2	1:A:629:ASN:H	1.26	0.42
1:B:627:TYR:CG	1:B:628:PHE:CE2	3.07	0.42
1:A:455:LEU:HD12	1:A:468:LYS:N	2.35	0.42
1:A:685:GLU:HG2	1:A:841:GLN:OE1	2.19	0.42
1:B:597:ILE:HD13	1:B:628:PHE:HE2	1.84	0.42
1:B:637:ASP:CB	1:B:639:LYS:HG3	2.44	0.42
1:A:475:GLU:OE2	1:A:508:GLY:N	2.53	0.42
1:A:630:LEU:N	1:A:630:LEU:HD22	2.35	0.42
1:B:452:LYS:O	1:B:453:ILE:HG12	2.20	0.42
1:B:508:GLY:HA3	1:B:632:ILE:CA	2.49	0.42
1:B:637:ASP:HB3	1:B:639:LYS:CG	2.44	0.42
1:A:480:THR:HA	1:A:481:PRO:HD3	1.70	0.42
1:A:726:ILE:CA	1:B:648:ASP:N	2.74	0.42
1:A:637:ASP:HB3	1:A:639:LYS:HD2	2.02	0.42
1:B:602:GLU:O	1:B:612:THR:CG2	2.68	0.42
1:B:800:MET:HE1	1:B:821:LEU:HD13	2.02	0.42
1:A:452:LYS:O	1:A:453:ILE:HG12	2.20	0.42
1:B:483:LEU:HD23	1:B:524:PRO:HG3	2.00	0.42
1:B:555:SER:HB3	1:B:592:LYS:HE3	2.00	0.42
1:B:563:ARG:HA	1:B:595:GLU:CB	2.50	0.42
1:A:168[A]:ASP:OD2	1:B:167:ARG:HG2	2.20	0.42
1:A:452:LYS:HZ3	1:A:454:PRO:HA	1.84	0.42
1:A:472:LYS:NZ	1:A:473:LYS:H	2.17	0.42
1:A:602:GLU:O	1:A:612:THR:CG2	2.68	0.42
1:B:908:ALA:HB3	1:B:909:PRO:HD3	2.01	0.42
1:B:970:GLN:OE1	1:B:970:GLN:HA	2.20	0.42
1:A:548:VAL:HG13	1:A:584:PHE:HE2	1.78	0.42
1:A:635:SER:CA	1:A:636:GLU:HG3	2.50	0.42
1:A:815:SER:O	1:B:642:LEU:HD12	2.09	0.42
1:B:451:LYS:O	1:B:454:PRO:CD	2.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:486:TYR:O	1:B:516:LEU:N	2.50	0.42
1:B:907:VAL:O	1:B:907:VAL:HG22	2.20	0.42
1:A:517:ASP:CB	1:A:546:GLN:HB2	2.41	0.41
1:A:566:VAL:O	1:A:600:ARG:HA	2.20	0.41
1:A:567:PHE:CD2	1:A:568:GLY:N	2.88	0.41
1:B:455:LEU:HD12	1:B:468:LYS:N	2.35	0.41
1:B:476:ASN:CB	1:B:505:MET:CB	2.69	0.41
1:B:625:ALA:HA	1:B:630:LEU:CB	2.49	0.41
1:B:734:LYS:C	1:B:736:ALA:O	2.57	0.41
1:A:624:VAL:HG13	1:A:628:PHE:CE1	2.55	0.41
1:B:485:LEU:HB3	1:B:516:LEU:HD23	2.02	0.41
1:B:733:GLU:OE2	1:B:734:LYS:N	2.54	0.41
1:A:225:ALA:O	1:A:226:SER:C	2.56	0.41
1:A:641:THR:HG22	1:A:642:LEU:H	1.85	0.41
1:A:727:ARG:HG2	1:B:645:GLN:CB	2.38	0.41
1:A:731:GLU:OE1	1:A:732:GLU:HB3	2.20	0.41
1:A:732:GLU:OE2	1:B:641:THR:CA	2.68	0.41
1:B:731:GLU:O	1:B:731:GLU:HG2	2.16	0.41
1:B:827:ARG:HG2	5:B:1104:FAD:H3'	2.02	0.41
1:A:381:ASN:OD1	1:B:573:ASN:OD1	2.38	0.41
1:A:478:HIS:HA	1:A:508:GLY:C	2.33	0.41
1:A:509:PHE:C	1:A:511:PRO:HD3	2.41	0.41
1:A:970:GLN:HA	1:A:970:GLN:OE1	2.20	0.41
1:B:735:LEU:C	1:B:735:LEU:CD1	2.88	0.41
1:A:563:ARG:HA	1:A:595:GLU:CB	2.50	0.41
1:A:728:LEU:HD22	1:B:644:LEU:CG	2.50	0.41
1:A:907:VAL:HG22	1:A:907:VAL:O	2.20	0.41
1:B:566:VAL:O	1:B:600:ARG:HA	2.20	0.41
1:A:577:THR:HB	4:A:1103:FMN:O4	2.21	0.41
1:A:733:GLU:OE2	1:A:734:LYS:N	2.54	0.41
1:A:1046:TRP:HD1	1:A:1048:GLY:N	2.18	0.41
1:B:694:TYR:CE2	1:B:831:ILE:HG21	2.56	0.41
1:A:132:ARG:HB3	1:B:161:ARG:HD3	2.03	0.41
1:A:328:ALA:HB1	3:A:1102:1C6:N1	2.36	0.41
1:A:1048:GLY:C	5:A:1104:FAD:C1'	2.84	0.41
1:B:476:ASN:C	1:B:505:MET:HB3	2.41	0.41
1:B:509:PHE:C	1:B:511:PRO:HD3	2.41	0.41
1:B:624:VAL:CB	1:B:628:PHE:CZ	3.02	0.41
1:A:479:ASN:CA	1:A:508:GLY:O	2.65	0.41
1:B:477:ALA:N	1:B:505:MET:HB3	2.36	0.41
1:B:731:GLU:OE1	1:B:732:GLU:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:GLU:CD	1:A:691:GLU:H	2.24	0.41
1:A:730:ALA:O	1:A:731:GLU:CB	2.62	0.41
1:B:1046:TRP:HD1	1:B:1048:GLY:N	2.18	0.41
1:A:129:LYS:CB	1:B:166:TYR:CZ	3.03	0.40
1:A:134:ASN:CG	1:B:161:ARG:HB2	2.41	0.40
1:A:388:HIS:HD2	1:A:391:LYS:NZ	2.19	0.40
1:A:476:ASN:ND2	1:A:477:ALA:H	2.19	0.40
1:A:647:VAL:H	1:A:647:VAL:HG22	1.66	0.40
1:A:472:LYS:HD2	1:A:472:LYS:HA	1.26	0.40
1:B:548:VAL:HG13	1:B:584:PHE:HE2	1.78	0.40
1:A:540:PRO:HA	1:A:541:PRO:HD3	1.94	0.40
1:A:633:GLU:H	1:A:633:GLU:CD	2.25	0.40
1:B:507:LYS:HG2	1:B:634:ASN:OD1	2.21	0.40
1:A:485:LEU:HB3	1:A:516:LEU:HD23	2.02	0.40
1:A:646:PHE:HA	1:B:727:ARG:HB3	1.84	0.40
1:A:652:ASP:HB3	1:A:657:LYS:HE3	2.03	0.40
1:A:731:GLU:O	1:A:731:GLU:HG2	2.16	0.40
1:A:818:ILE:CG2	1:B:644:LEU:HD11	2.50	0.40
1:B:624:VAL:HG13	1:B:629:ASN:OD1	2.22	0.40
1:A:134:ASN:ND2	1:B:161:ARG:HG3	2.37	0.40
1:A:628:PHE:HB2	1:A:629:ASN:HD22	1.82	0.40
1:A:646:PHE:HE2	1:B:728:LEU:HB3	1.77	0.40
1:A:694:TYR:CE2	1:A:831:ILE:HG21	2.56	0.40
1:A:735:LEU:C	1:A:735:LEU:CD1	2.88	0.40
1:A:800:MET:HE1	1:A:821:LEU:HD13	2.03	0.40
1:B:307:GLN:O	1:B:310[A]:GLN:HB2	2.22	0.40
1:B:507:LYS:HG2	1:B:634:ASN:CG	2.41	0.40
1:B:508:GLY:C	1:B:632:ILE:HB	2.41	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	1032/1034 (100%)	945 (92%)	63 (6%)	24 (2%)	6	34
1	B	1032/1034 (100%)	951 (92%)	58 (6%)	23 (2%)	6	35
All	All	2064/2068 (100%)	1896 (92%)	121 (6%)	47 (2%)	9	34

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	ASP
1	A	452	LYS
1	A	454	PRO
1	A	470	VAL
1	A	558	GLU
1	A	575	ALA
1	A	635	SER
1	A	639	LYS
1	A	731	GLU
1	B	231	ASP
1	B	452	LYS
1	B	454	PRO
1	B	558	GLU
1	B	575	ALA
1	B	628	PHE
1	B	630	LEU
1	B	633	GLU
1	B	634	ASN
1	B	647	VAL
1	B	648	ASP
1	B	731	GLU
1	A	230	SER
1	A	596	ASN
1	A	636	GLU
1	B	230	SER
1	B	468	LYS
1	B	596	ASN
1	B	627	TYR
1	A	476	ASN
1	A	552	ASP
1	A	629	ASN
1	B	552	ASP
1	A	625	ALA
1	A	640	SER
1	A	643	SER

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Mol	Chain	Res	Type
1	A	644	LEU
1	A	645	GLN
1	B	469	LYS
1	B	625	ALA
1	A	637	ASP
1	A	651	ALA
1	B	645	GLN
1	B	653	MET
1	A	773	CYS
1	B	773	CYS
1	A	453	ILE
1	B	453	ILE

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	853/879 (97%)	798 (94%)	55 (6%)	17	42
1	B	853/879 (97%)	804 (94%)	49 (6%)	20	45
All	All	1706/1758 (97%)	1602 (94%)	104 (6%)	22	44

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	71	LEU
1	A	148	LEU
1	A	159	ASN
1	A	187	LYS
1	A	222	ASP
1	A	228	GLU
1	A	229	GLN
1	A	287	LEU
1	A	440	LYS
1	A	453	ILE

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Mol	Chain	Res	Type
1	A	469	LYS
1	A	471	ARG
1	A	472	LYS
1	A	473	LYS
1	A	475	GLU
1	A	478	HIS
1	A	479	ASN
1	A	480	THR
1	A	525	ARG
1	A	553	GLN
1	A	557	ASP
1	A	560	LYS
1	A	572	LYS
1	A	577	THR
1	A	589	LEU
1	A	606	SER
1	A	612	THR
1	A	622	SER
1	A	624	VAL
1	A	630	LEU
1	A	632	ILE
1	A	636	GLU
1	A	639	LYS
1	A	641	THR
1	A	642	LEU
1	A	644	LEU
1	A	645	GLN
1	A	682	ARG
1	A	685	GLU
1	A	708	GLU
1	A	731	GLU
1	A	750	LEU
1	A	821	LEU
1	A	837	VAL
1	A	847	SER
1	A	925	GLN
1	A	943	TYR
1	A	965	SER
1	A	976	GLN
1	A	985	LYS
1	A	986	LEU
1	A	988	GLU

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Mol	Chain	Res	Type
1	A	989	LEU
1	A	1035	LEU
1	B	4	GLU
1	B	71	LEU
1	B	148	LEU
1	B	159	ASN
1	B	187	LYS
1	B	222	ASP
1	B	228	GLU
1	B	229	GLN
1	B	287	LEU
1	B	440	LYS
1	B	453	ILE
1	B	479	ASN
1	B	480	THR
1	B	525	ARG
1	B	553	GLN
1	B	557	ASP
1	B	560	LYS
1	B	572	LYS
1	B	577	THR
1	B	589	LEU
1	B	606	SER
1	B	612	THR
1	B	622	SER
1	B	624	VAL
1	B	628	PHE
1	B	631	ASP
1	B	634	ASN
1	B	636	GLU
1	B	638	ASN
1	B	642	LEU
1	B	645	GLN
1	B	646	PHE
1	B	682	ARG
1	B	685	GLU
1	B	708	GLU
1	B	731	GLU
1	B	750	LEU
1	B	821	LEU
1	B	837	VAL
1	B	847	SER

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Mol	Chain	Res	Type
1	B	925	GLN
1	B	943	TYR
1	B	965	SER
1	B	976	GLN
1	B	985	LYS
1	B	986	LEU
1	B	988	GLU
1	B	989	LEU
1	B	1035	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	95	ASN
1	A	100	HIS
1	A	134	ASN
1	A	159	ASN
1	A	201	ASN
1	A	236	HIS
1	A	253	ASN
1	A	257	GLN
1	A	283	ASN
1	A	388	HIS
1	A	403	GLN
1	A	476	ASN
1	A	519	HIS
1	A	546	GLN
1	A	573	ASN
1	A	629	ASN
1	A	634	ASN
1	A	665	ASN
1	A	724	GLN
1	A	787	GLN
1	A	923	GLN
1	A	976	GLN
1	A	992	GLN
1	B	16	ASN
1	B	95	ASN
1	B	100	HIS
1	B	128	GLN
1	B	134	ASN

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Mol	Chain	Res	Type
1	B	159	ASN
1	B	163	ASN
1	B	201	ASN
1	B	236	HIS
1	B	253	ASN
1	B	257	GLN
1	B	283	ASN
1	B	388	HIS
1	B	403	GLN
1	B	479	ASN
1	B	519	HIS
1	B	546	GLN
1	B	665	ASN
1	B	787	GLN
1	B	923	GLN
1	B	976	GLN
1	B	992	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	1C6	A	1102	-	23,25,25	3.25	7 (30%)	28,35,35	2.46	11 (39%)
3	1C6	B	1102	-	23,25,25	3.26	7 (30%)	28,35,35	2.45	10 (35%)
6	SO4	B	1107	-	4,4,4	0.30	0	6,6,6	0.32	0
6	SO4	B	1105	-	4,4,4	0.40	0	6,6,6	1.15	1 (16%)
4	FMN	B	1103	-	33,33,33	1.36	4 (12%)	48,50,50	1.89	13 (27%)
5	FAD	A	1104	-	53,58,58	1.47	6 (11%)	68,89,89	1.52	14 (20%)
7	PG4	B	1108	-	12,12,12	0.78	0	11,11,11	1.05	0
2	HEM	A	1101	1	41,50,50	1.87	7 (17%)	45,82,82	2.11	13 (28%)
2	HEM	B	1101	1	41,50,50	1.88	6 (14%)	45,82,82	2.11	13 (28%)
6	SO4	A	1107	-	4,4,4	0.32	0	6,6,6	0.38	0
7	PG4	B	1109	-	6,6,12	1.47	1 (16%)	5,5,11	1.57	1 (20%)
7	PG4	A	1108	-	12,12,12	0.78	0	11,11,11	1.05	0
6	SO4	A	1105	-	4,4,4	0.47	0	6,6,6	1.22	1 (16%)
6	SO4	B	1106	-	4,4,4	0.16	0	6,6,6	1.20	1 (16%)
4	FMN	A	1103	-	33,33,33	1.36	4 (12%)	48,50,50	1.89	13 (27%)
6	SO4	A	1106	-	4,4,4	0.29	0	6,6,6	0.84	0
7	PG4	A	1109	-	6,6,12	1.47	1 (16%)	5,5,11	1.57	1 (20%)
5	FAD	B	1104	-	53,58,58	1.47	6 (11%)	68,89,89	1.52	14 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1C6	A	1102	-	-	6/7/9/9	0/3/3/3
3	1C6	B	1102	-	-	6/7/9/9	0/3/3/3
4	FMN	B	1103	-	-	5/18/18/18	0/3/3/3
5	FAD	A	1104	-	-	0/30/50/50	0/6/6/6
7	PG4	B	1108	-	-	8/10/10/10	-
2	HEM	A	1101	1	-	2/12/54/54	-
2	HEM	B	1101	1	-	2/12/54/54	-
7	PG4	B	1109	-	-	3/4/4/10	-
7	PG4	A	1108	-	-	8/10/10/10	-
4	FMN	A	1103	-	-	5/18/18/18	0/3/3/3
7	PG4	A	1109	-	-	3/4/4/10	-
5	FAD	B	1104	-	-	0/30/50/50	0/6/6/6

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1102	1C6	CD1-CG	10.98	1.50	1.39
3	A	1102	1C6	CD1-CG	10.95	1.50	1.39
2	A	1101	HEM	C3D-C2D	6.72	1.51	1.36
2	B	1101	HEM	C3D-C2D	6.71	1.51	1.36
3	A	1102	1C6	CE1-CD1	6.45	1.50	1.39
3	B	1102	1C6	CE1-CD1	6.43	1.50	1.39
2	A	1101	HEM	C3C-C2C	-5.32	1.33	1.40
2	B	1101	HEM	C3C-C2C	-5.29	1.33	1.40
3	B	1102	1C6	CE1-CZ	5.14	1.49	1.40
3	A	1102	1C6	CE1-CZ	5.06	1.49	1.40
3	B	1102	1C6	CB-S	-4.88	1.71	1.82
3	A	1102	1C6	CB-S	-4.86	1.71	1.82
5	B	1104	FAD	C4X-N5	4.59	1.39	1.30
5	A	1104	FAD	C4X-N5	4.57	1.39	1.30
4	A	1103	FMN	P-O5'	-4.26	1.46	1.60
4	B	1103	FMN	P-O5'	-4.24	1.46	1.60
5	B	1104	FAD	C2A-N3A	3.61	1.37	1.32
5	A	1104	FAD	C2A-N3A	3.59	1.37	1.32
4	B	1103	FMN	C5A-N5	-3.11	1.33	1.39
4	A	1103	FMN	C5A-N5	-3.10	1.33	1.39
5	B	1104	FAD	C1'-C2'	3.05	1.57	1.52
5	A	1104	FAD	C1'-C2'	3.03	1.56	1.52
5	B	1104	FAD	C8M-C8	2.86	1.56	1.51
5	A	1104	FAD	C8M-C8	2.86	1.56	1.51
4	A	1103	FMN	O5'-C5'	2.55	1.54	1.44
4	B	1103	FMN	O5'-C5'	2.54	1.54	1.44
2	A	1101	HEM	O1A-CGA	2.53	1.30	1.22
2	B	1101	HEM	O1A-CGA	2.53	1.30	1.22
3	A	1102	1C6	CF1-S	-2.37	1.71	1.75
5	A	1104	FAD	C10-N1	2.37	1.38	1.33
5	B	1104	FAD	C10-N1	2.34	1.38	1.33
2	B	1101	HEM	C4D-ND	-2.28	1.36	1.40
3	B	1102	1C6	CF1-S	-2.26	1.71	1.75
3	B	1102	1C6	CZ2-CS2	-2.25	1.38	1.41
3	A	1102	1C6	CZ2-CS2	-2.24	1.38	1.41
5	A	1104	FAD	C5A-N7A	-2.24	1.31	1.39
2	A	1101	HEM	C4D-ND	-2.23	1.36	1.40
4	B	1103	FMN	C10-N10	2.22	1.42	1.37
4	A	1103	FMN	C10-N10	2.21	1.42	1.37
5	B	1104	FAD	C5A-N7A	-2.21	1.31	1.39
2	B	1101	HEM	CMD-C2D	2.11	1.55	1.50
3	A	1102	1C6	CE3-CZ3	2.07	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	HEM	CMD-C2D	2.07	1.55	1.50
7	B	1109	PG4	C7-C8	2.06	1.60	1.49
7	A	1109	PG4	C7-C8	2.05	1.60	1.49
2	B	1101	HEM	C1A-CHA	-2.04	1.35	1.41
2	A	1101	HEM	C1A-CHA	-2.04	1.35	1.41
2	A	1101	HEM	CBD-CAD	2.03	1.58	1.52
3	B	1102	1C6	CE3-CZ3	2.02	1.40	1.37

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1101	HEM	C4D-ND-C1D	6.21	111.49	105.07
2	B	1101	HEM	C4D-ND-C1D	6.19	111.47	105.07
3	B	1102	1C6	CE2-N1-CG	5.68	124.92	117.75
3	A	1102	1C6	CE2-N1-CG	5.68	124.91	117.75
4	B	1103	FMN	O4'-C4'-C3'	-5.30	96.21	109.10
4	A	1103	FMN	O4'-C4'-C3'	-5.29	96.24	109.10
3	A	1102	1C6	CD1-CG-N1	-5.08	118.98	123.95
3	B	1102	1C6	CD1-CG-N1	-5.03	119.03	123.95
2	B	1101	HEM	C4C-CHD-C1D	4.69	128.75	122.56
2	A	1101	HEM	C4C-CHD-C1D	4.69	128.75	122.56
3	B	1102	1C6	CZ-CE1-CD1	-4.54	117.71	121.53
3	A	1102	1C6	CZ-CE1-CD1	-4.52	117.72	121.53
3	B	1102	1C6	O2-CE1-CD1	4.49	125.13	118.83
3	A	1102	1C6	CB-CG-CD1	4.46	124.49	120.29
3	A	1102	1C6	O2-CE1-CD1	4.46	125.09	118.83
3	B	1102	1C6	CB-CG-CD1	4.34	124.38	120.29
4	B	1103	FMN	C4-N3-C2	-4.15	117.97	125.64
4	A	1103	FMN	C4-N3-C2	-4.12	118.04	125.64
2	A	1101	HEM	CHA-C4D-ND	4.05	129.39	124.38
2	B	1101	HEM	CHA-C4D-ND	4.02	129.35	124.38
2	B	1101	HEM	CBA-CAA-C2A	-3.88	106.00	112.62
2	A	1101	HEM	CBA-CAA-C2A	-3.87	106.02	112.62
2	A	1101	HEM	CMA-C3A-C4A	-3.73	122.73	128.46
2	B	1101	HEM	CMA-C3A-C4A	-3.70	122.78	128.46
4	A	1103	FMN	C5A-N5-C4A	3.51	123.91	118.07
4	B	1103	FMN	C5A-N5-C4A	3.48	123.85	118.07
2	A	1101	HEM	CBD-CAD-C3D	-3.30	103.45	112.63
2	B	1101	HEM	CBD-CAD-C3D	-3.29	103.47	112.63
4	A	1103	FMN	O5'-C5'-C4'	-3.29	100.59	109.36
4	B	1103	FMN	O5'-C5'-C4'	-3.28	100.61	109.36
5	A	1104	FAD	P-O3P-PA	-3.24	121.71	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1104	FAD	P-O3P-PA	-3.24	121.72	132.83
4	B	1103	FMN	C4'-C3'-C2'	-3.18	106.75	113.36
3	A	1102	1C6	CZ-CE2-N1	-3.17	121.87	125.11
4	A	1103	FMN	C4'-C3'-C2'	-3.15	106.81	113.36
3	B	1102	1C6	CZ-CE2-N1	-3.13	121.91	125.11
2	B	1101	HEM	C4B-C3B-C2B	3.09	109.57	107.11
4	A	1103	FMN	C4-C4A-N5	3.04	122.56	118.23
5	A	1104	FAD	N3A-C2A-N1A	-3.04	123.92	128.68
4	B	1103	FMN	C4-C4A-N5	3.04	122.56	118.23
5	B	1104	FAD	N3A-C2A-N1A	-3.03	123.94	128.68
5	A	1104	FAD	C4X-C4-N3	3.02	120.87	113.19
5	B	1104	FAD	C4X-C4-N3	3.02	120.87	113.19
2	A	1101	HEM	C4B-C3B-C2B	3.01	109.50	107.11
3	B	1102	1C6	CB-S-CF1	-3.00	99.12	102.42
3	A	1102	1C6	CB-S-CF1	-2.97	99.16	102.42
5	A	1104	FAD	C4-N3-C2	-2.92	120.25	125.64
5	A	1104	FAD	C4A-C5A-N7A	-2.91	106.37	109.40
5	B	1104	FAD	C4-N3-C2	-2.90	120.29	125.64
5	B	1104	FAD	C9A-C5X-N5	-2.89	119.29	122.43
5	B	1104	FAD	C4A-C5A-N7A	-2.88	106.40	109.40
5	A	1104	FAD	C9A-C5X-N5	-2.85	119.33	122.43
4	B	1103	FMN	C4A-C4-N3	2.83	120.38	113.19
4	A	1103	FMN	C4A-C4-N3	2.82	120.35	113.19
5	A	1104	FAD	O4B-C1B-C2B	-2.79	102.85	106.93
5	B	1104	FAD	O4B-C1B-C2B	-2.79	102.85	106.93
5	B	1104	FAD	C5X-C9A-N10	2.72	120.76	117.95
6	B	1106	SO4	O4-S-O3	2.70	120.60	109.06
2	B	1101	HEM	O1A-CGA-CBA	-2.70	114.41	123.08
2	A	1101	HEM	O1A-CGA-CBA	-2.69	114.42	123.08
4	B	1103	FMN	O2P-P-O5'	2.69	113.90	106.73
5	A	1104	FAD	C5X-C9A-N10	2.69	120.73	117.95
4	A	1103	FMN	O2P-P-O5'	2.69	113.88	106.73
4	A	1103	FMN	O3P-P-O5'	2.66	113.82	106.73
4	B	1103	FMN	O3P-P-O5'	2.64	113.75	106.73
3	B	1102	1C6	C4-O3-CZ3	2.59	123.14	117.51
3	A	1102	1C6	C4-O3-CZ3	2.58	123.11	117.51
5	A	1104	FAD	O3B-C3B-C4B	-2.52	103.77	111.05
3	A	1102	1C6	CE3-CX2-NV	2.51	138.01	130.83
3	B	1102	1C6	CE3-CX2-NV	2.50	137.97	130.83
5	B	1104	FAD	O3B-C3B-C4B	-2.49	103.85	111.05
4	A	1103	FMN	C9A-C5A-N5	-2.47	119.74	122.43
5	B	1104	FAD	O2'-C2'-C3'	-2.46	103.12	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1105	SO4	O3-S-O2	2.45	122.11	109.31
5	A	1104	FAD	O2'-C2'-C3'	-2.45	103.14	109.10
2	B	1101	HEM	C4B-CHC-C1C	2.44	125.78	122.56
4	B	1103	FMN	C9A-C5A-N5	-2.44	119.78	122.43
6	B	1105	SO4	O4-S-O1	2.43	121.98	109.31
2	A	1101	HEM	C4B-CHC-C1C	2.43	125.76	122.56
4	B	1103	FMN	C10-C4A-N5	-2.41	119.74	124.86
4	A	1103	FMN	C10-C4A-N5	-2.39	119.78	124.86
2	A	1101	HEM	CMA-C3A-C2A	2.35	129.37	124.94
2	B	1101	HEM	CMA-C3A-C2A	2.34	129.36	124.94
4	A	1103	FMN	O5'-P-O1P	2.34	113.04	106.47
4	B	1103	FMN	O5'-P-O1P	2.34	113.04	106.47
3	A	1102	1C6	CE2-CZ-CE1	2.32	119.08	116.27
2	B	1101	HEM	C1B-NB-C4B	2.32	107.47	105.07
2	A	1101	HEM	C1B-NB-C4B	2.31	107.46	105.07
3	B	1102	1C6	CE2-CZ-CE1	2.28	119.03	116.27
5	A	1104	FAD	C9A-C9-C8	2.23	123.79	119.30
5	B	1104	FAD	C9A-C9-C8	2.19	123.72	119.30
5	A	1104	FAD	O4-C4-C4X	-2.18	120.82	126.60
5	B	1104	FAD	O4-C4-C4X	-2.18	120.83	126.60
2	B	1101	HEM	C1D-C2D-C3D	-2.17	104.67	106.96
2	A	1101	HEM	CBB-CAB-C3B	-2.17	116.83	127.62
2	A	1101	HEM	C1D-C2D-C3D	-2.17	104.68	106.96
2	B	1101	HEM	CBB-CAB-C3B	-2.17	116.84	127.62
5	A	1104	FAD	C1'-C2'-C3'	2.16	115.83	109.79
5	B	1104	FAD	C1'-C2'-C3'	2.16	115.83	109.79
4	A	1103	FMN	C6-C5A-N5	2.16	122.28	118.51
5	A	1104	FAD	C7M-C7-C8	-2.14	116.34	120.74
4	B	1103	FMN	C6-C5A-N5	2.13	122.23	118.51
5	B	1104	FAD	C7M-C7-C8	-2.13	116.38	120.74
3	A	1102	1C6	C3-CD1-CG	-2.03	120.92	122.69
7	A	1109	PG4	O4-C6-C5	2.01	118.90	110.07
7	B	1109	PG4	O4-C6-C5	2.01	118.88	110.07

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1108	PG4	O1-C1-C2-O2
7	A	1109	PG4	O3-C5-C6-O4
7	B	1108	PG4	O1-C1-C2-O2
7	B	1109	PG4	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
3	A	1102	1C6	CD1-CE1-O2-C2
3	B	1102	1C6	CD1-CE1-O2-C2
7	A	1108	PG4	O4-C7-C8-O5
7	B	1108	PG4	O4-C7-C8-O5
3	A	1102	1C6	CH2-CZ3-O3-C4
4	A	1103	FMN	O3'-C3'-C4'-C5'
3	B	1102	1C6	CH2-CZ3-O3-C4
3	A	1102	1C6	CE3-CZ3-O3-C4
3	B	1102	1C6	CE3-CZ3-O3-C4
7	A	1109	PG4	O4-C7-C8-O5
7	B	1109	PG4	O4-C7-C8-O5
4	B	1103	FMN	O3'-C3'-C4'-C5'
7	A	1109	PG4	C8-C7-O4-C6
7	B	1109	PG4	C8-C7-O4-C6
3	A	1102	1C6	S-CB-CG-N1
3	B	1102	1C6	S-CB-CG-N1
4	A	1103	FMN	C2'-C3'-C4'-C5'
4	B	1103	FMN	C2'-C3'-C4'-C5'
7	B	1108	PG4	C6-C5-O3-C4
7	A	1108	PG4	C6-C5-O3-C4
7	A	1108	PG4	C5-C6-O4-C7
7	B	1108	PG4	C5-C6-O4-C7
7	A	1108	PG4	C8-C7-O4-C6
7	B	1108	PG4	C8-C7-O4-C6
7	A	1108	PG4	C3-C4-O3-C5
7	B	1108	PG4	C3-C4-O3-C5
4	A	1103	FMN	C1'-C2'-C3'-O3'
4	B	1103	FMN	C1'-C2'-C3'-O3'
3	A	1102	1C6	CZ-CE1-O2-C2
3	B	1102	1C6	CZ-CE1-O2-C2
7	A	1108	PG4	C4-C3-O2-C2
7	B	1108	PG4	C4-C3-O2-C2
4	A	1103	FMN	O3'-C3'-C4'-O4'
4	B	1103	FMN	O3'-C3'-C4'-O4'
4	A	1103	FMN	O2'-C2'-C3'-O3'
4	B	1103	FMN	O2'-C2'-C3'-O3'
3	A	1102	1C6	S-CB-CG-CD1
3	B	1102	1C6	S-CB-CG-CD1
2	A	1101	HEM	CAD-CBD-CGD-O2D
2	B	1101	HEM	CAD-CBD-CGD-O2D
2	A	1101	HEM	CAD-CBD-CGD-O1D
2	B	1101	HEM	CAD-CBD-CGD-O1D

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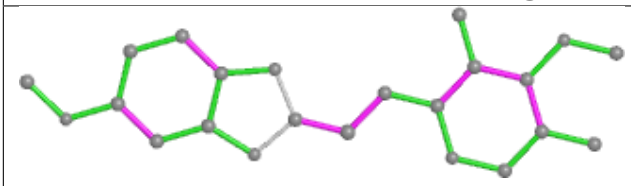
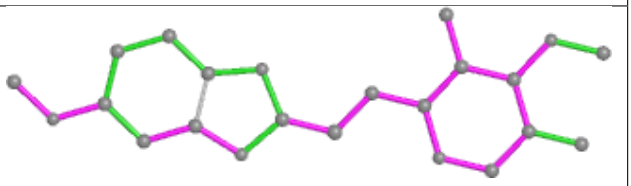
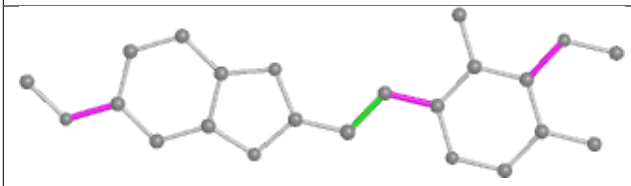
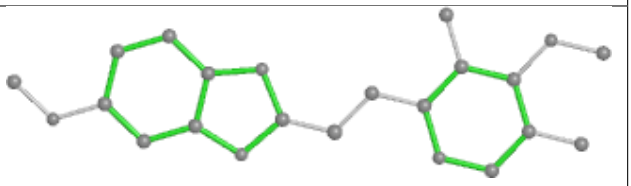
Mol	Chain	Res	Type	Atoms
7	A	1108	PG4	O3-C5-C6-O4
7	B	1108	PG4	O3-C5-C6-O4

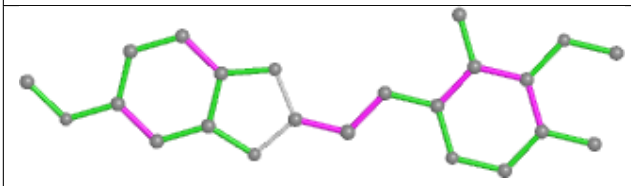
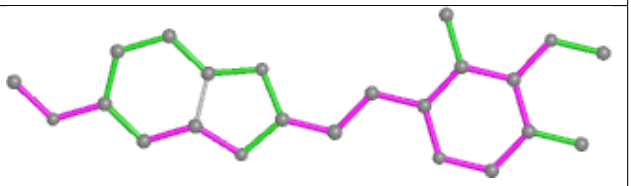
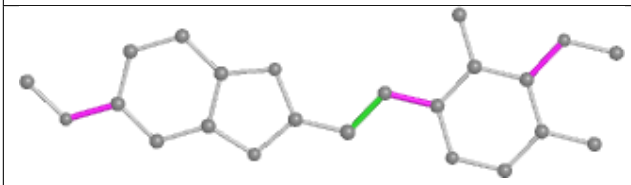
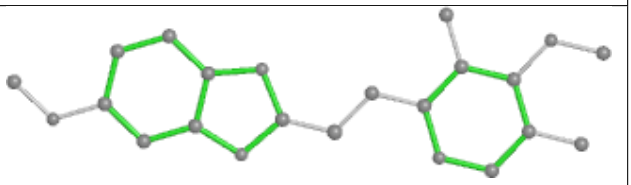
There are no ring outliers.

12 monomers are involved in 50 short contacts:

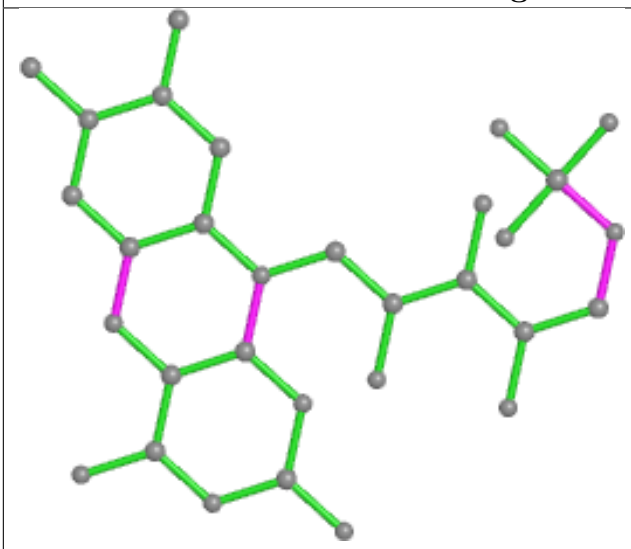
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1102	1C6	11	0
3	B	1102	1C6	11	0
4	B	1103	FMN	1	0
5	A	1104	FAD	5	0
7	B	1108	PG4	1	0
2	A	1101	HEM	1	0
2	B	1101	HEM	1	0
7	B	1109	PG4	6	0
7	A	1108	PG4	1	0
4	A	1103	FMN	1	0
7	A	1109	PG4	7	0
5	B	1104	FAD	4	0

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 1C6 A 1102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand 1C6 B 1102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand FMN B 1103



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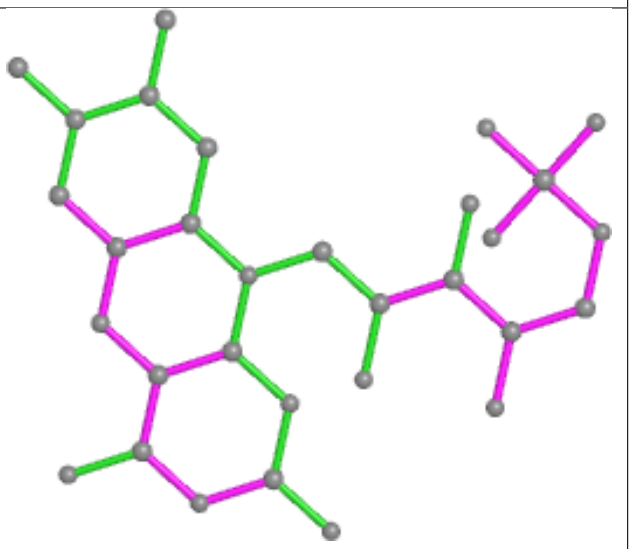
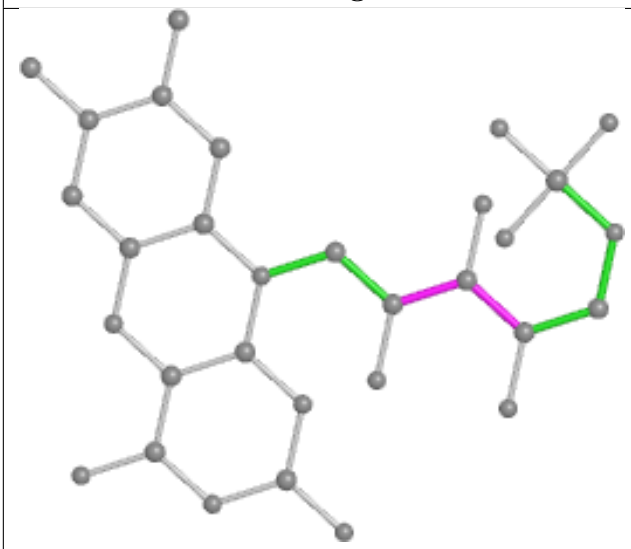
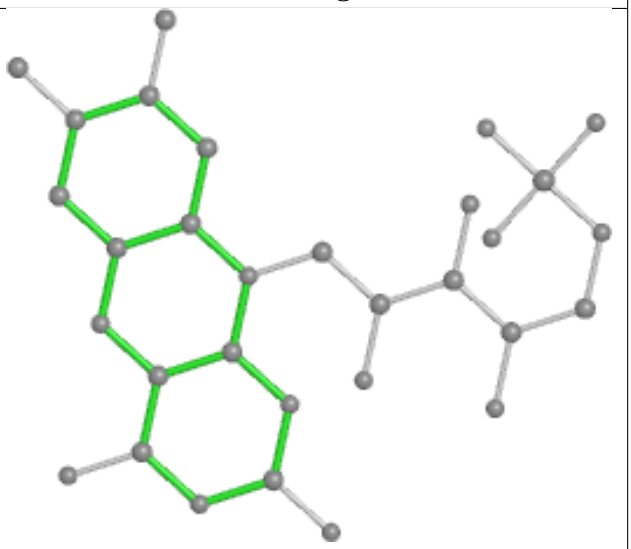


Bond angles

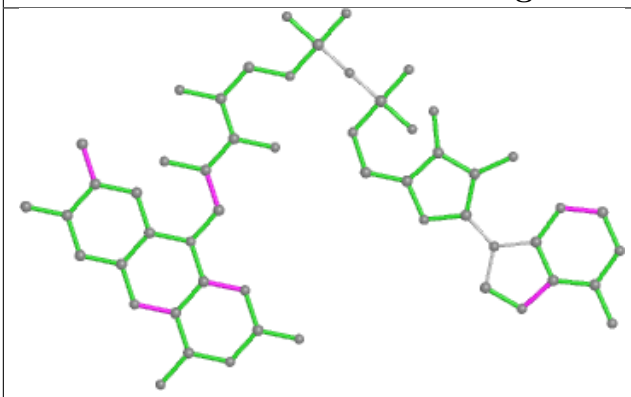


Torsions



Rings

Ligand FAD A 1104



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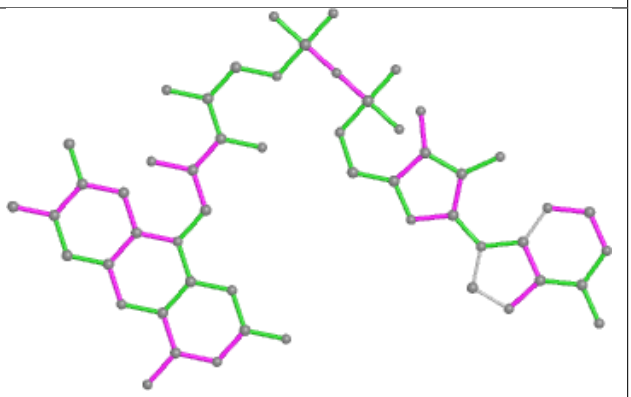

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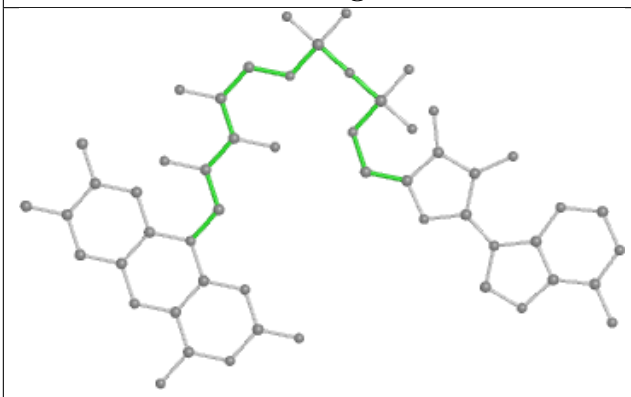

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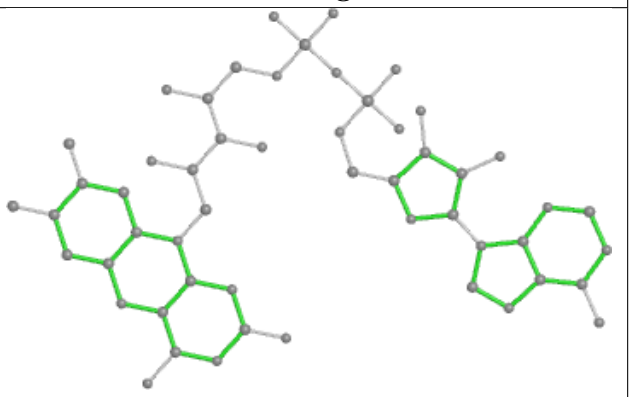
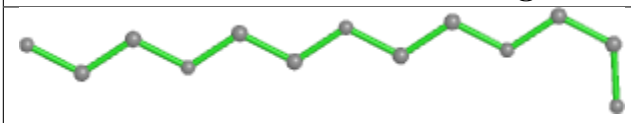
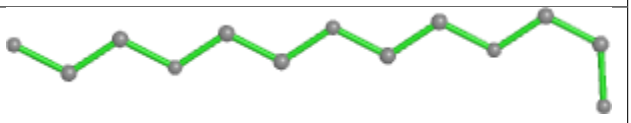


Rings

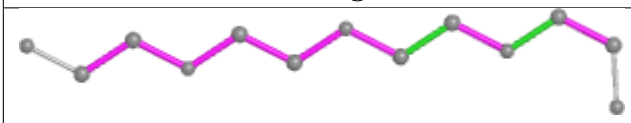
Ligand PG4 B 1108



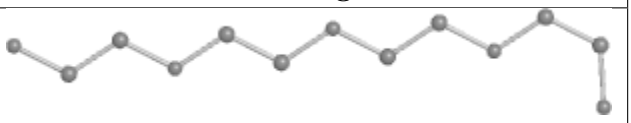
Bond lengths



Bond angles

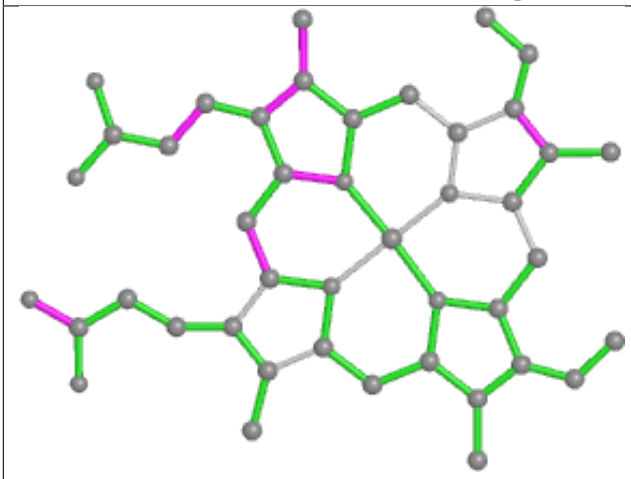


Torsions



Rings

Ligand HEM A 1101



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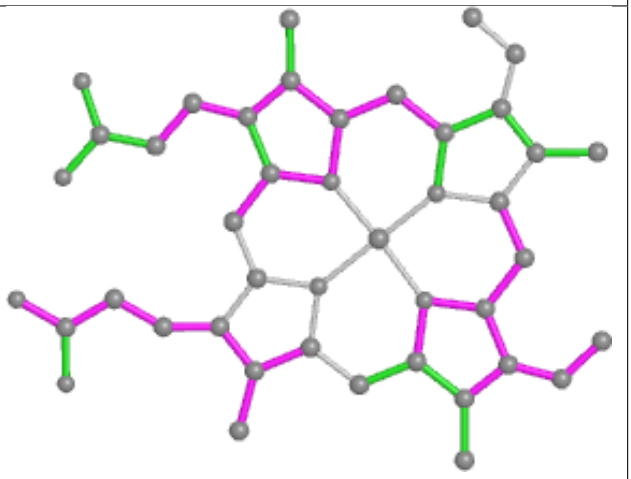

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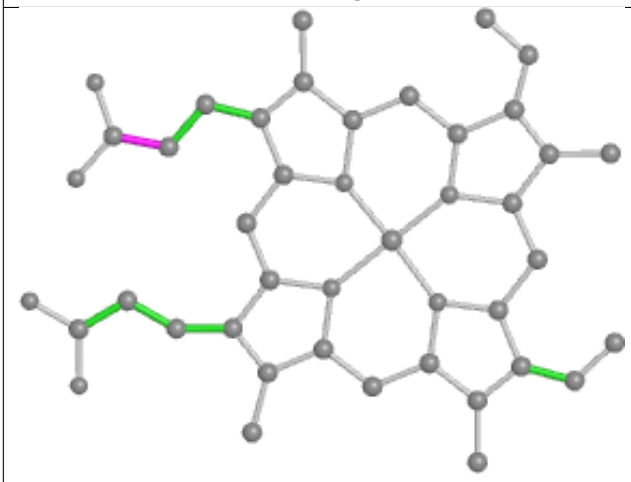

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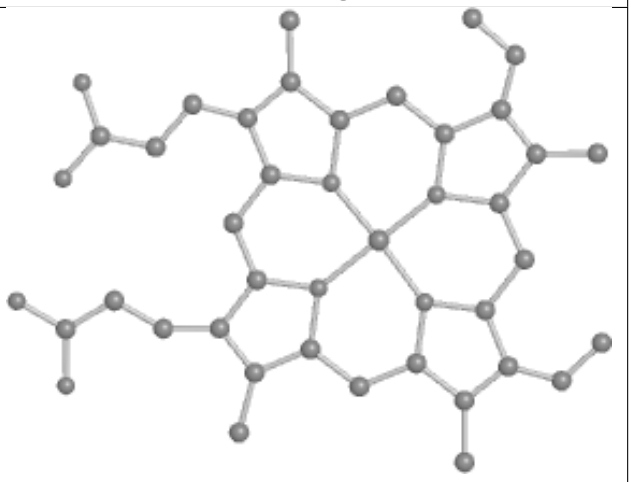
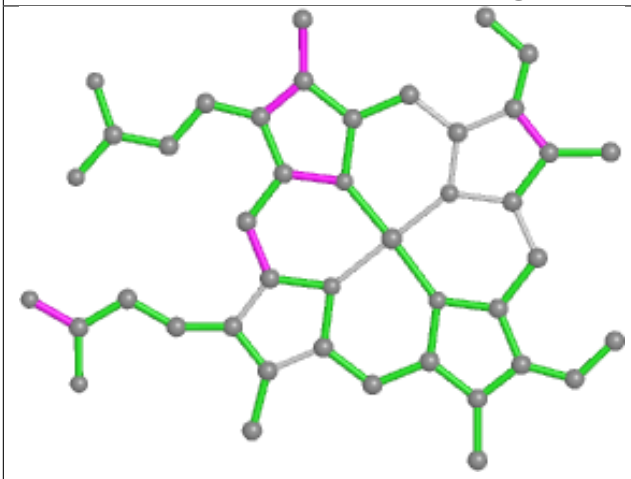


Rings

Ligand HEM B 1101



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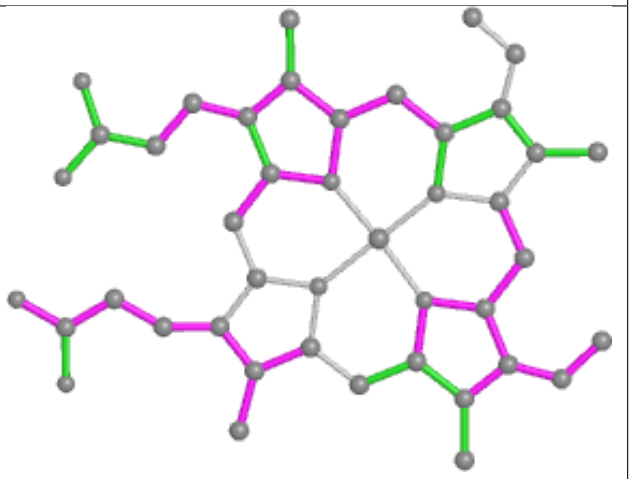

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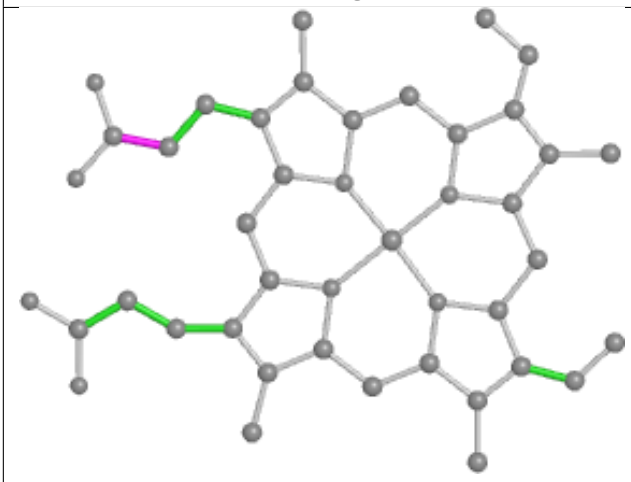

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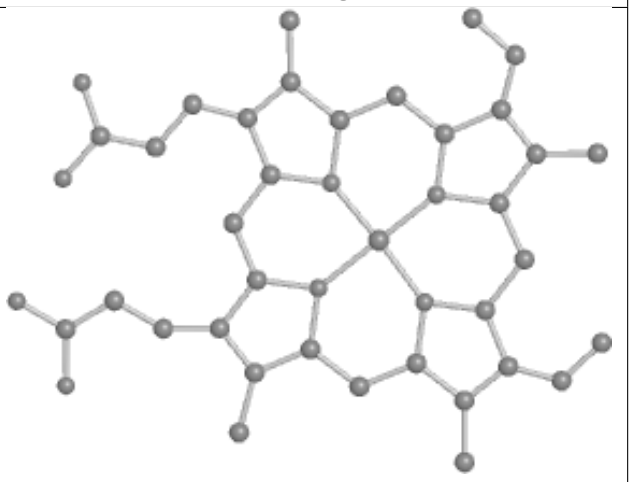
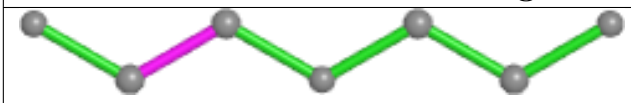


Rings

Ligand PG4 B 1109



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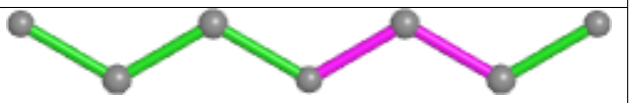

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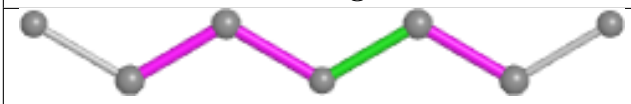
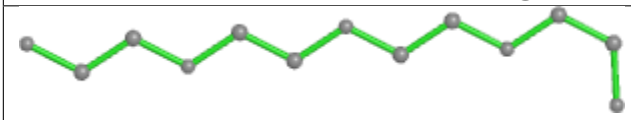


Torsions

Rings

Ligand PG4 A 1108



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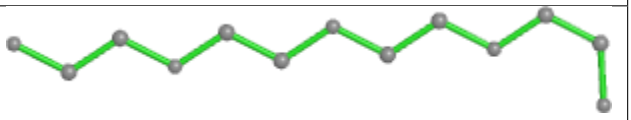
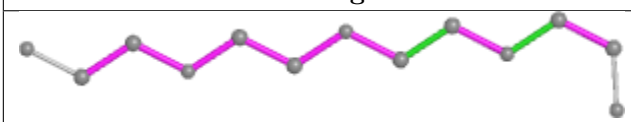


Bond angles



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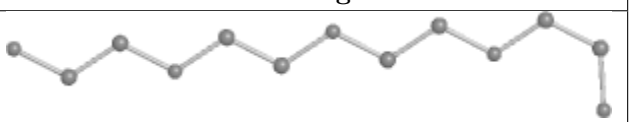
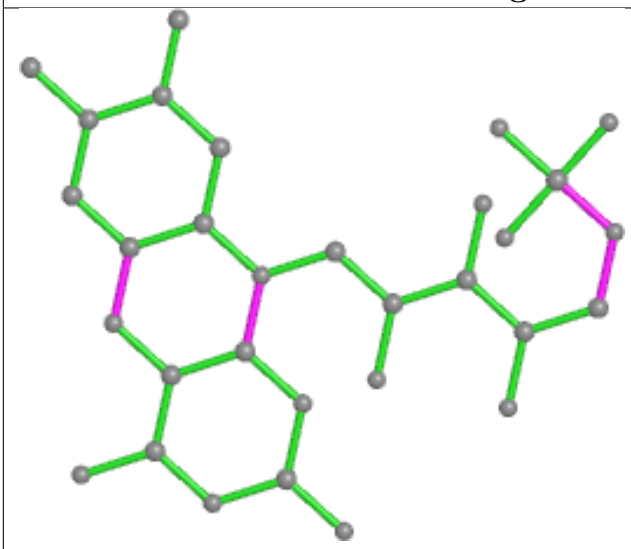


Rings

Ligand FMN A 1103



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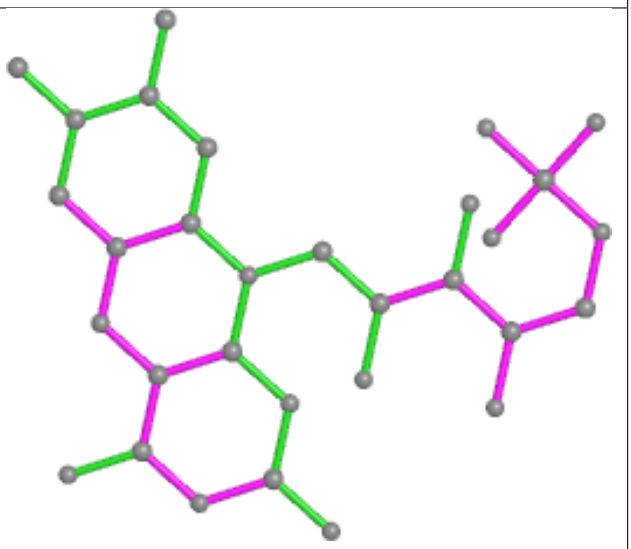
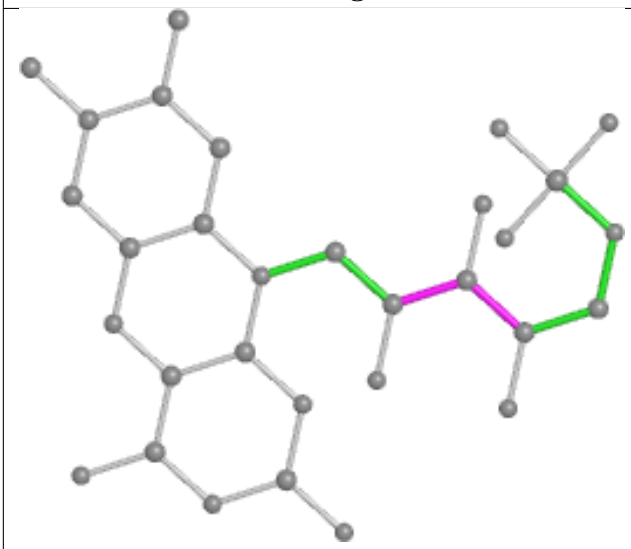


Bond angles



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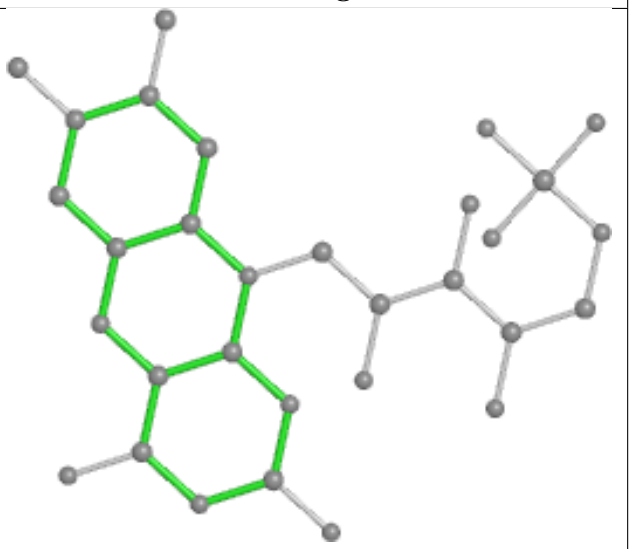
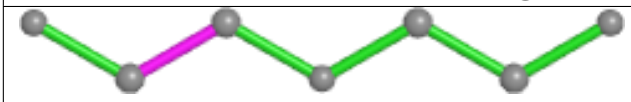
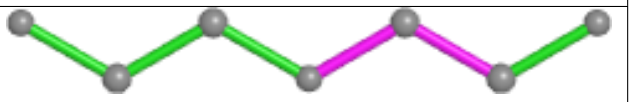


Rings

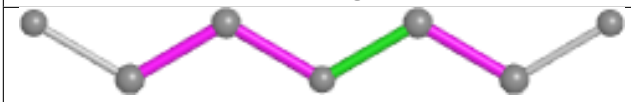
Ligand PG4 A 1109



Bond lengths



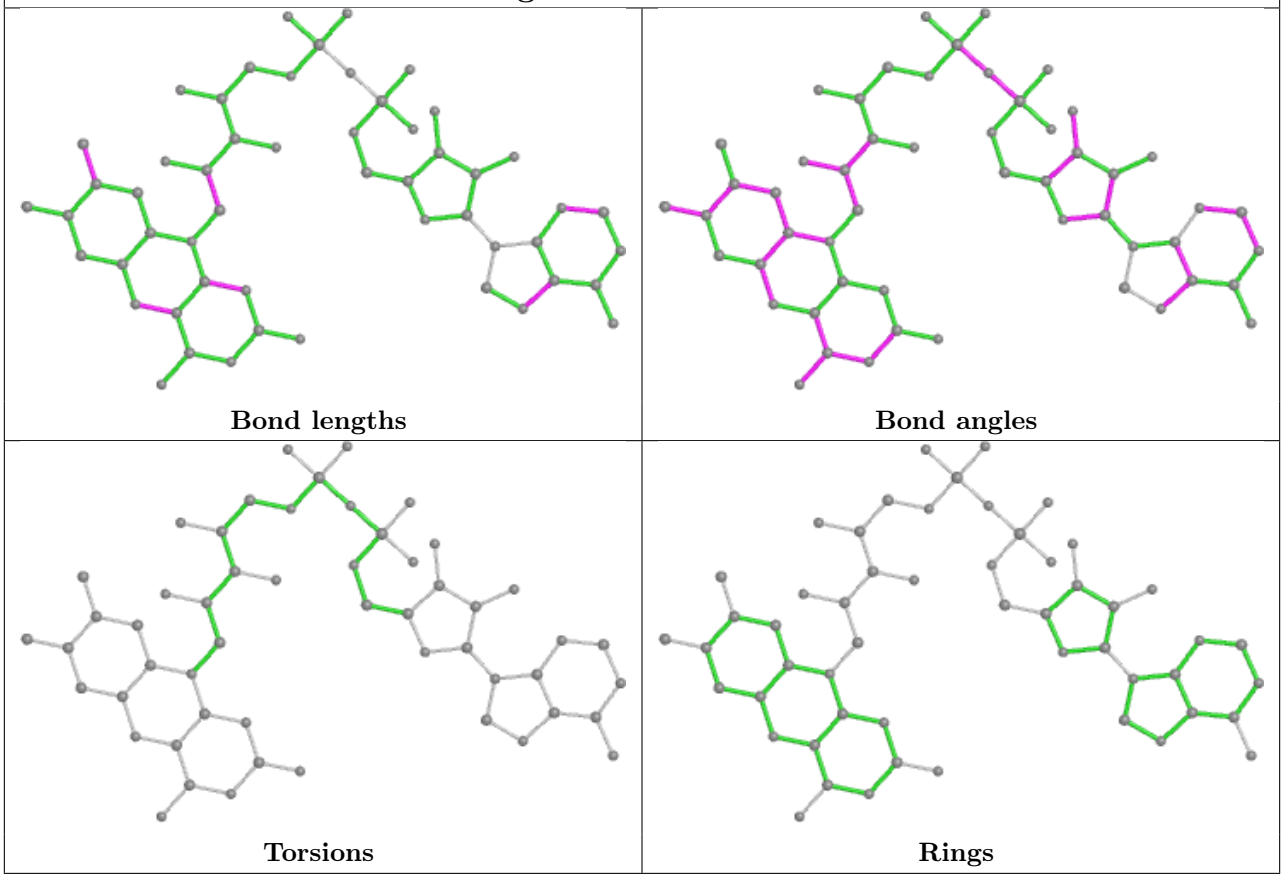
Bond angles



Torsions

Rings

Ligand FAD B 1104



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	3
1	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	470:VAL	C	471:ARG	N	6.27
1	B	478:HIS	C	479:ASN	N	3.78
1	A	478:HIS	C	479:ASN	N	3.54
1	A	633:GLU	C	634:ASN	N	2.43
1	A	661:ALA	C	662:PHE	N	0.86

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	661:ALA	C	662:PHE	N	0.86

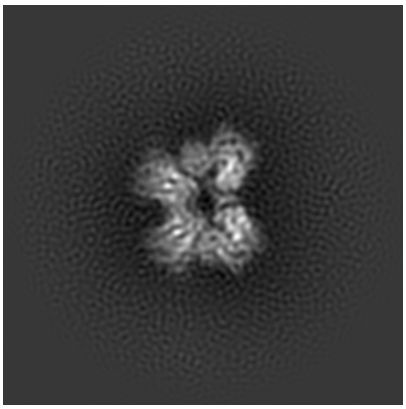
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-27534. These allow visual inspection of the internal detail of the map and identification of artifacts.

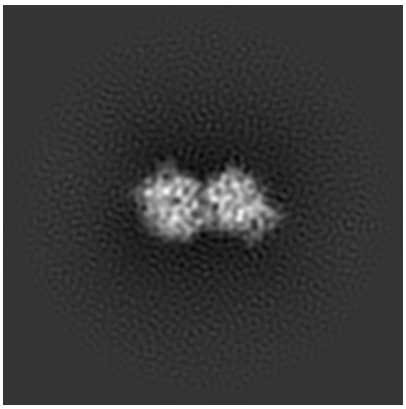
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

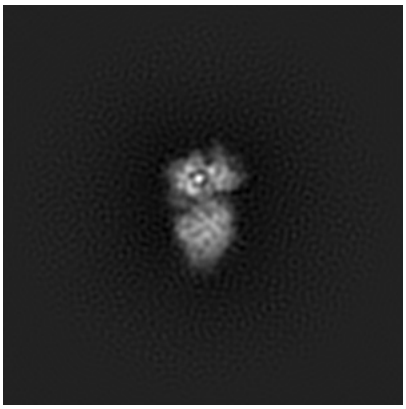
6.1.1 Primary map



X

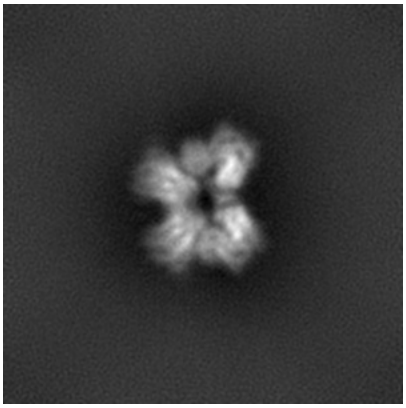


Y

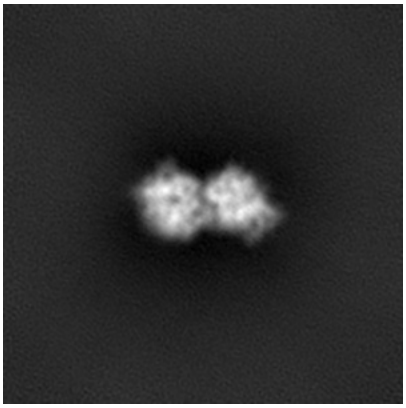


Z

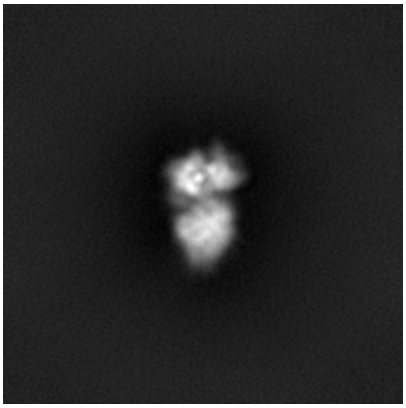
6.1.2 Raw map



X



Y

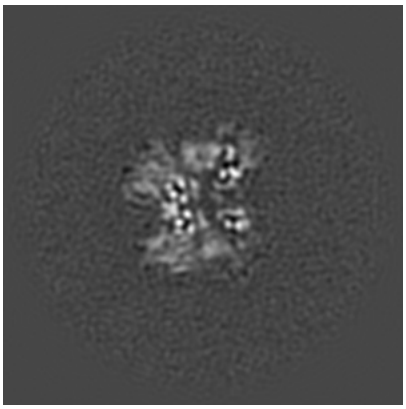


Z

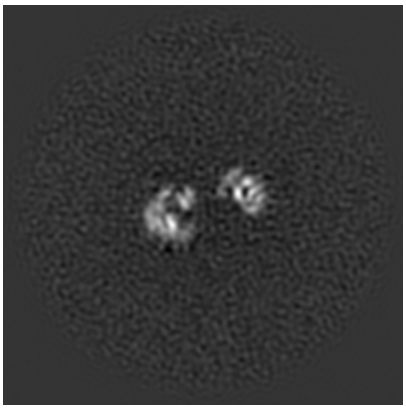
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

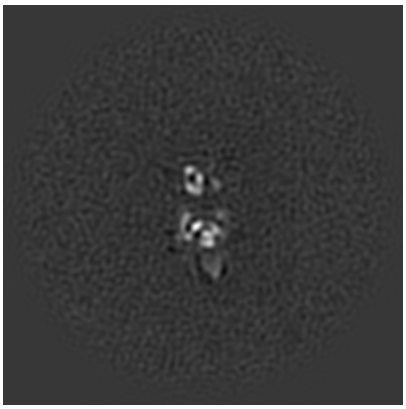
6.2.1 Primary map



X Index: 90

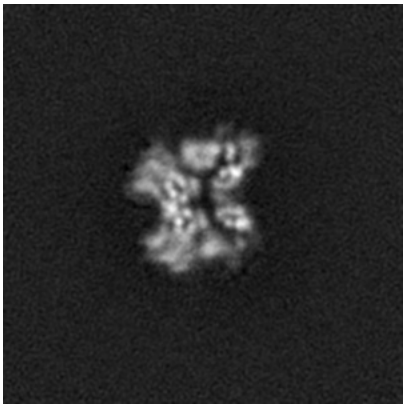


Y Index: 90

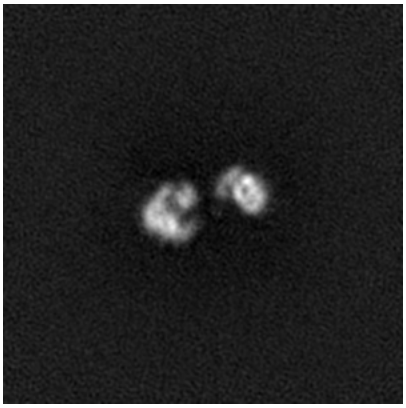


Z Index: 90

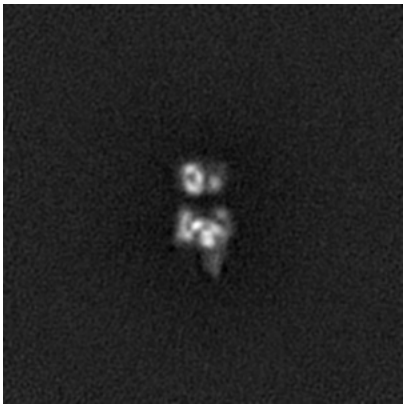
6.2.2 Raw map



X Index: 90



Y Index: 90

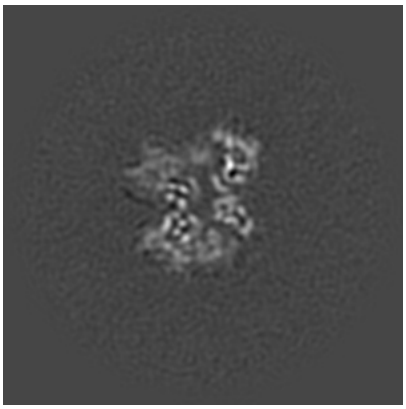


Z Index: 90

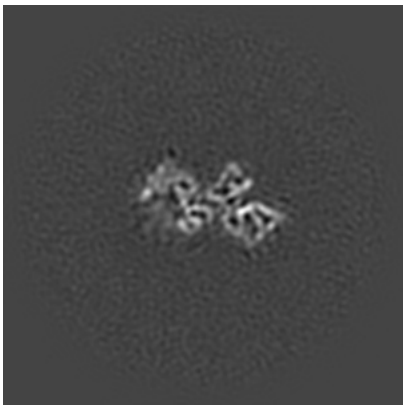
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

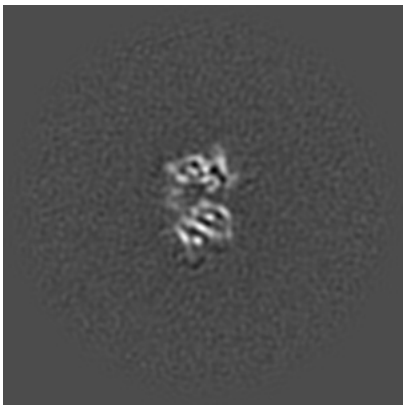
6.3.1 Primary map



X Index: 87

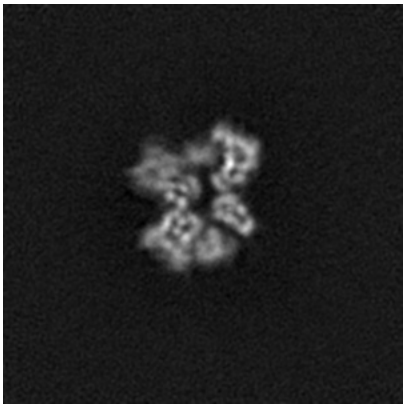


Y Index: 101

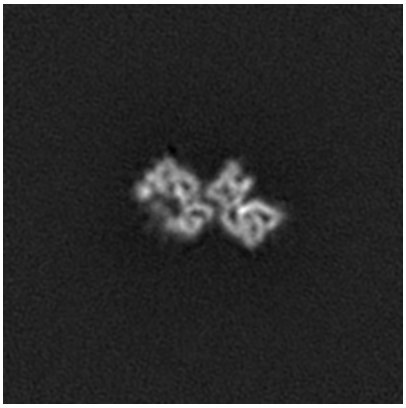


Z Index: 81

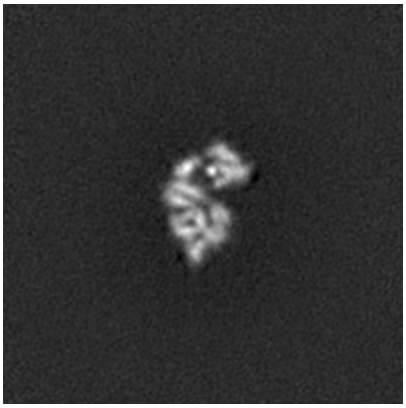
6.3.2 Raw map



X Index: 87



Y Index: 102

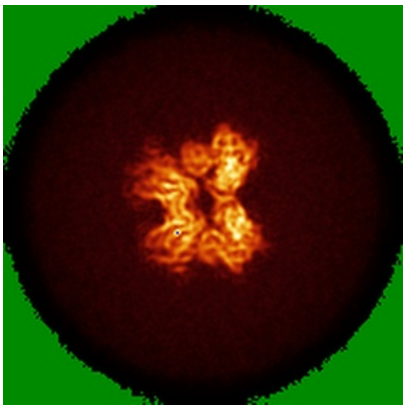


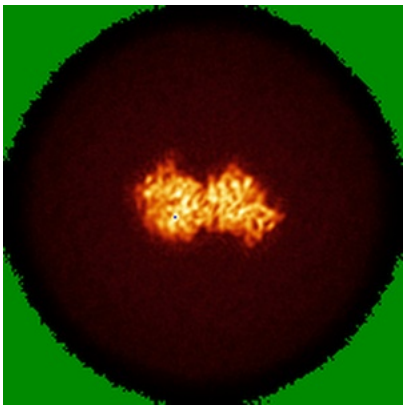
Z Index: 76

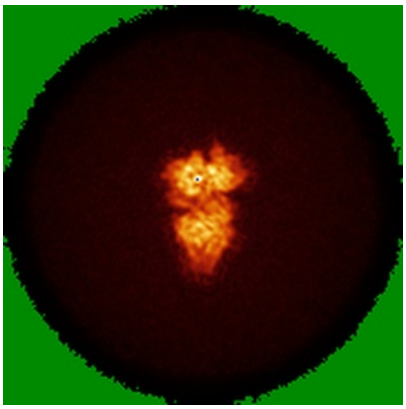
The images above show the largest variance slices of the map in three orthogonal directions.

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

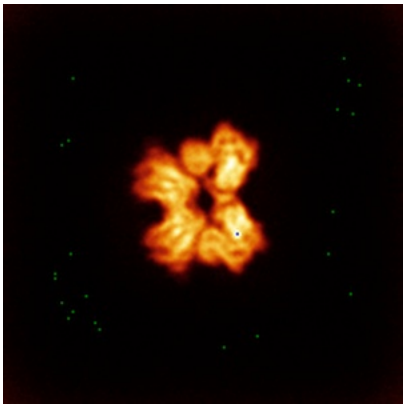
6.4.1 Primary map

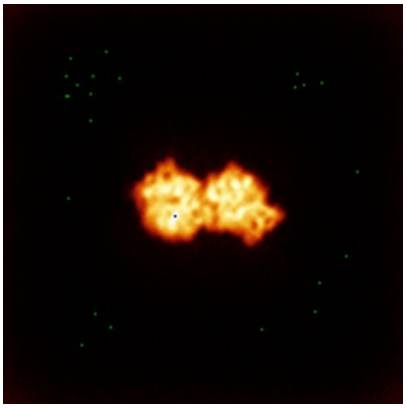

X

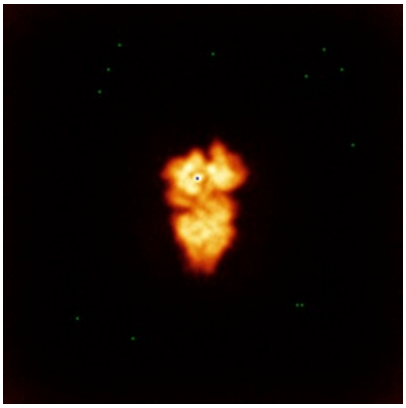

Y


Z

6.4.2 Raw map


X

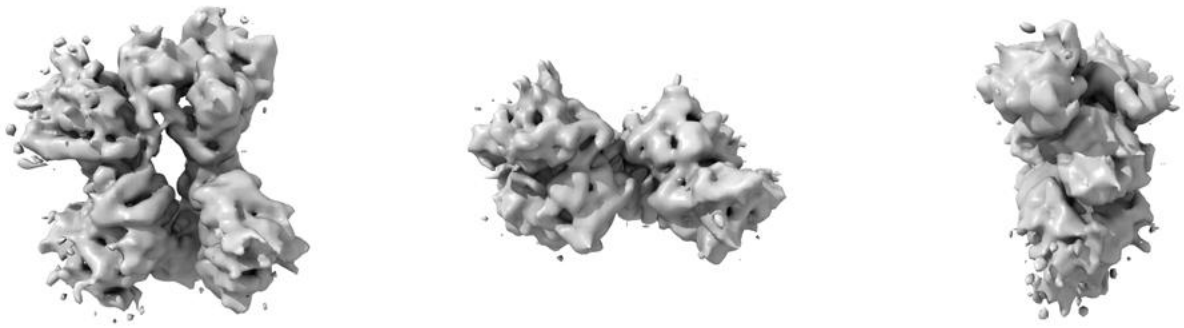

Y


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)

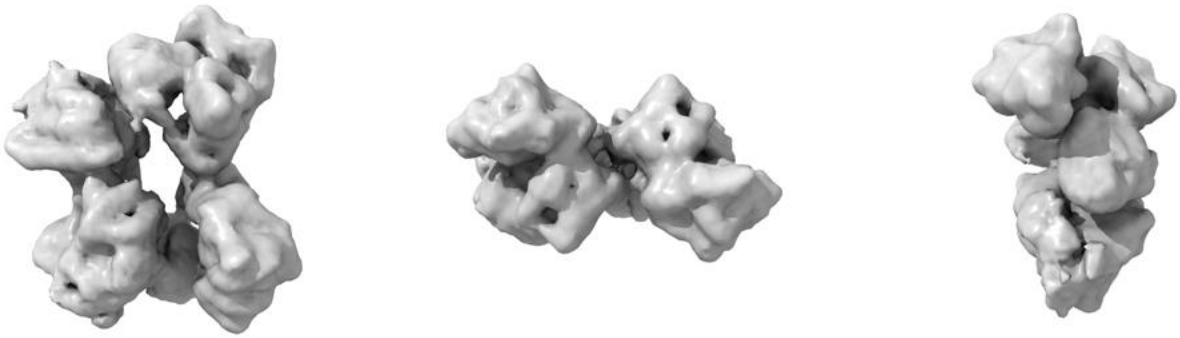
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.8. 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.

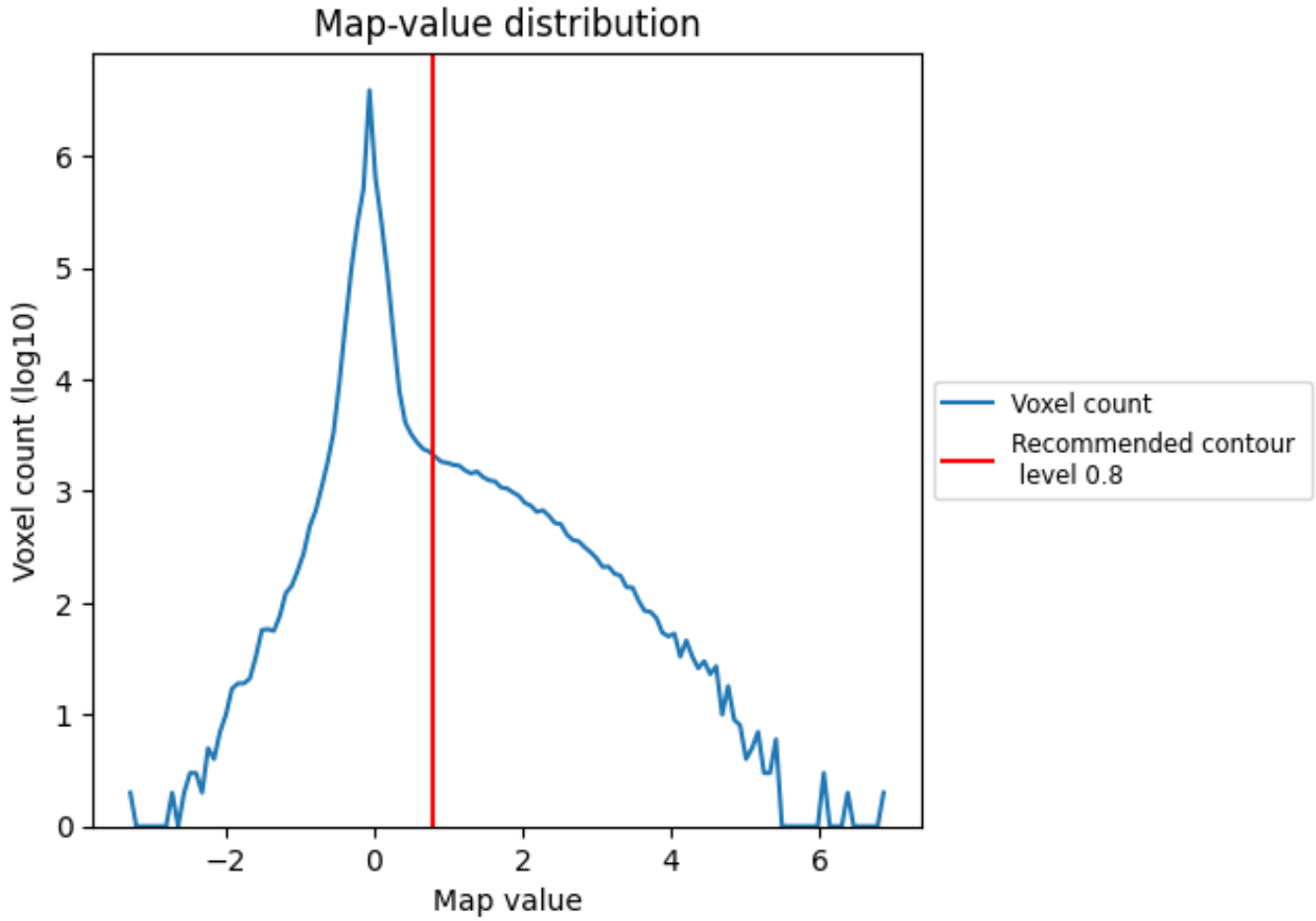
6.6 Mask visualisation (i)

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

7 Map analysis

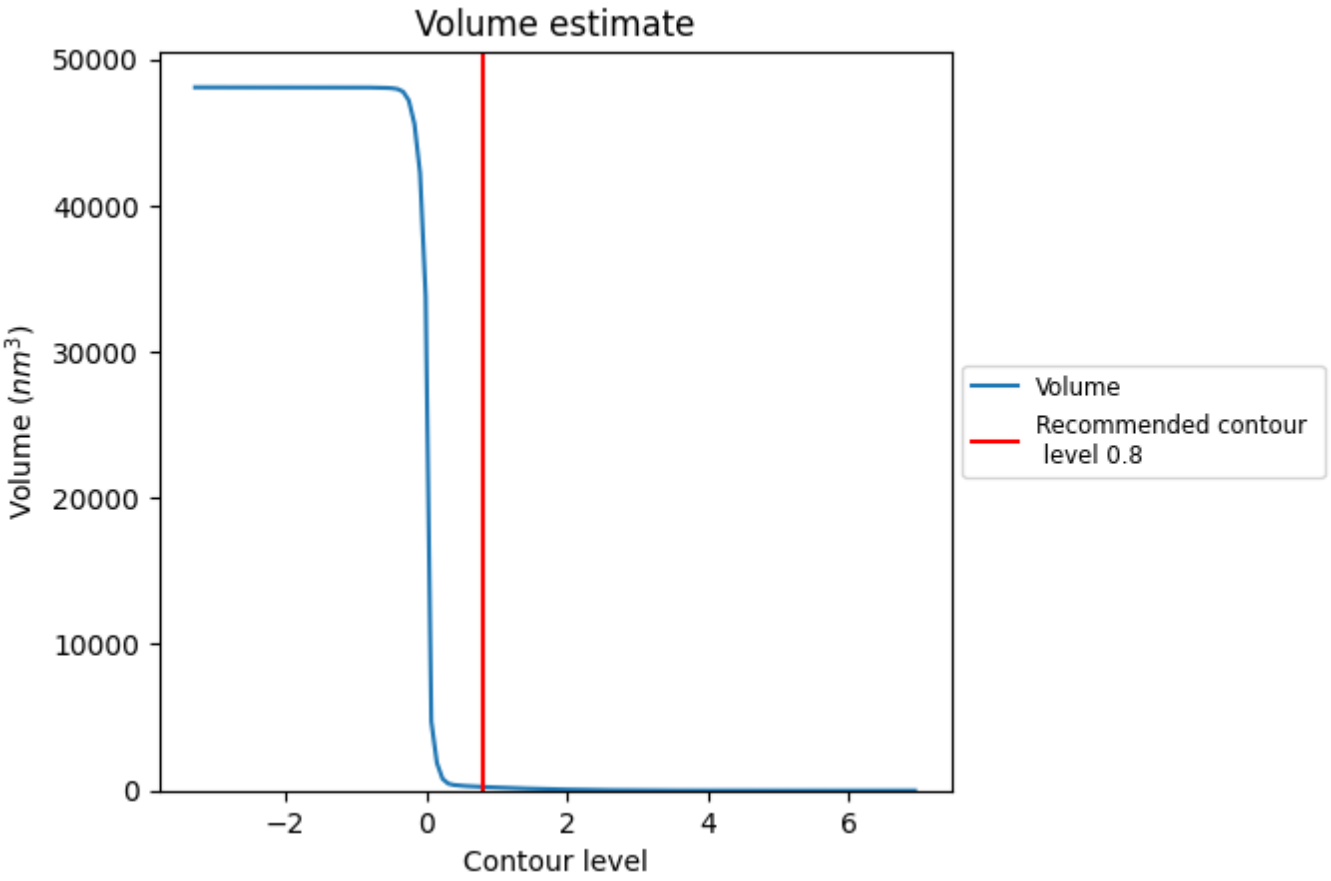
This section contains the results of statistical analysis of the map.

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.

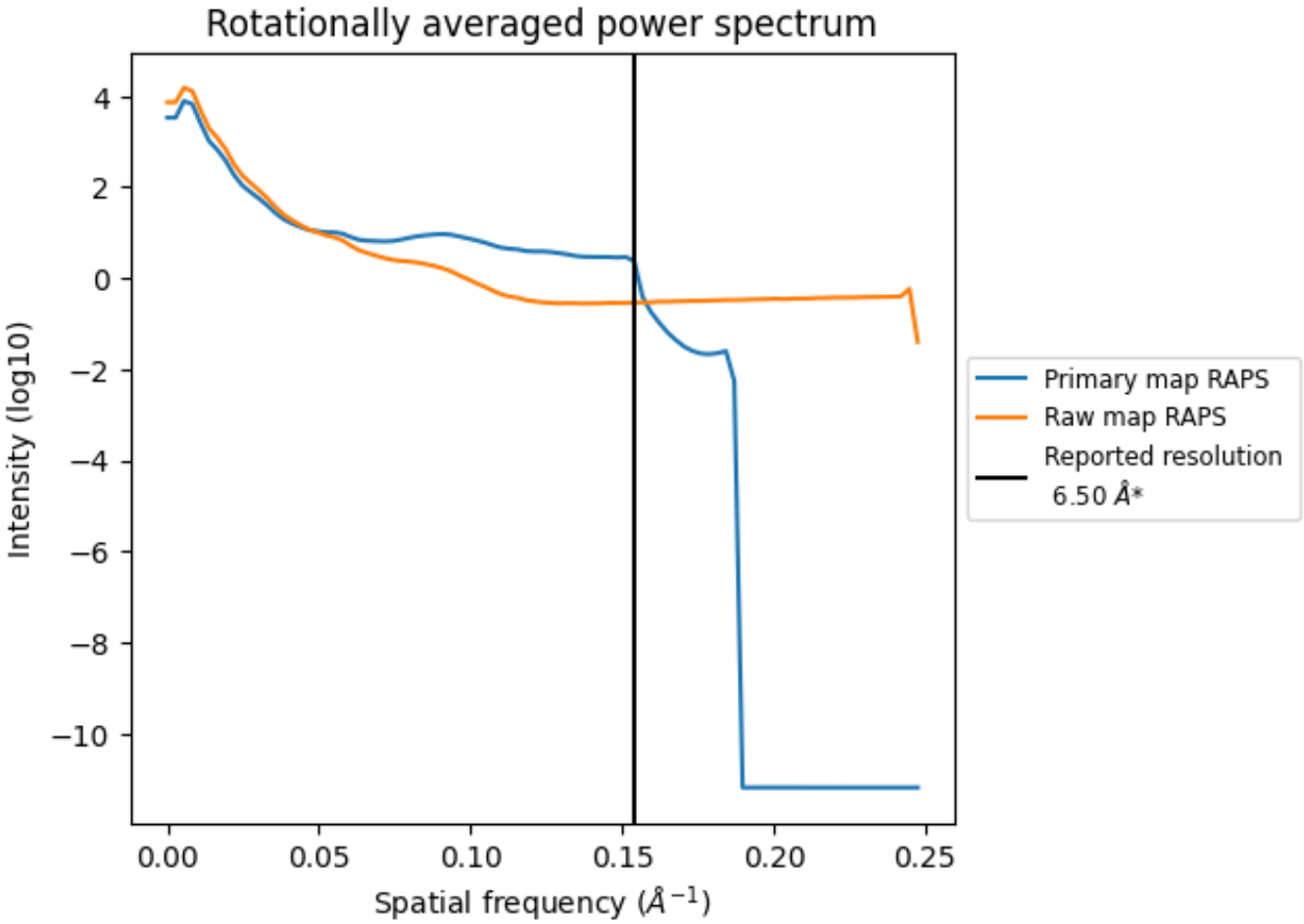
7.2 Volume estimate



The volume at the recommended contour level is 250 nm^3; this corresponds to an approximate mass of 226 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)

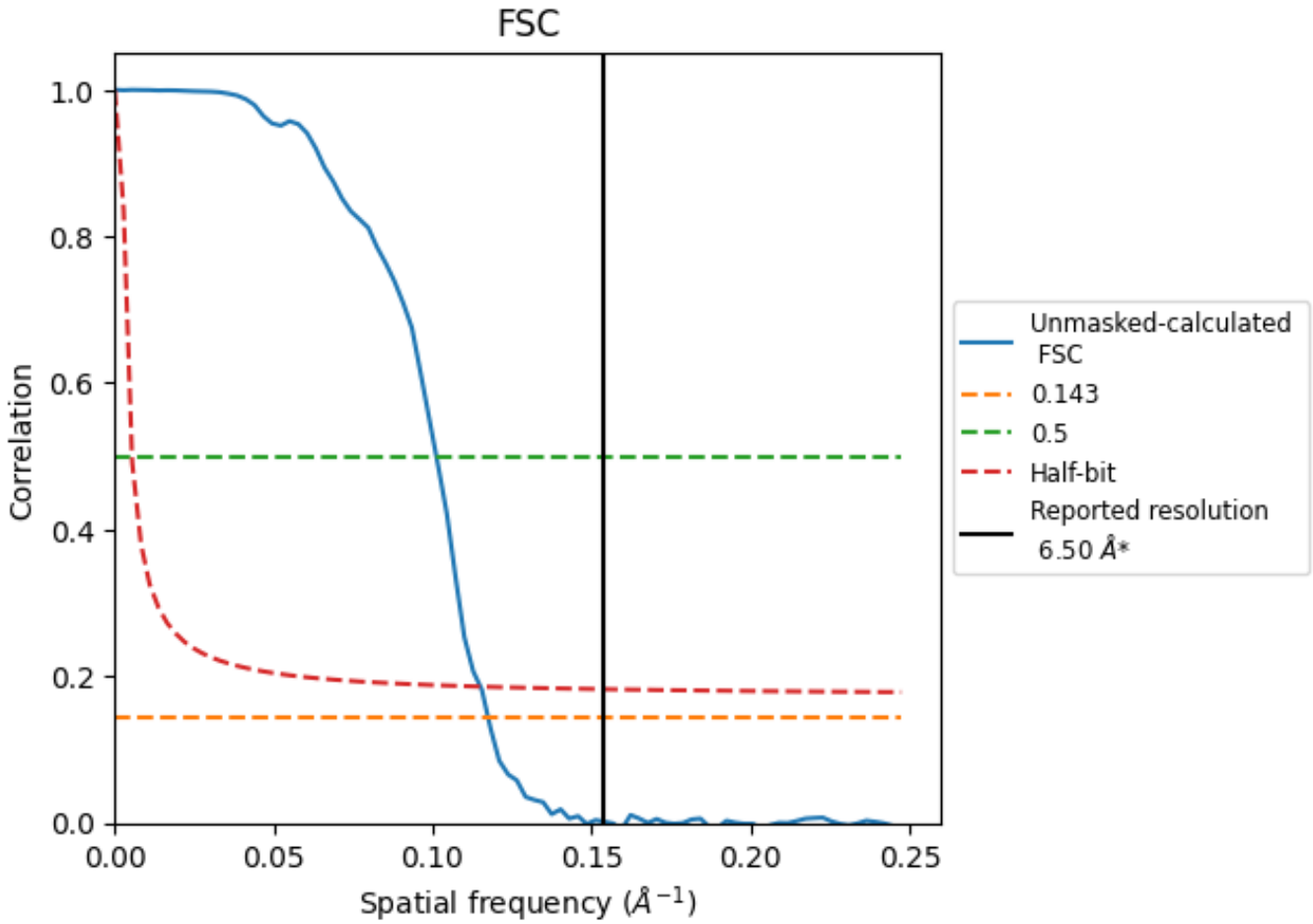


*Reported resolution corresponds to spatial frequency of 0.154 Å^{-1}

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 0.154 Å^{-1}

8.2 Resolution estimates (i)

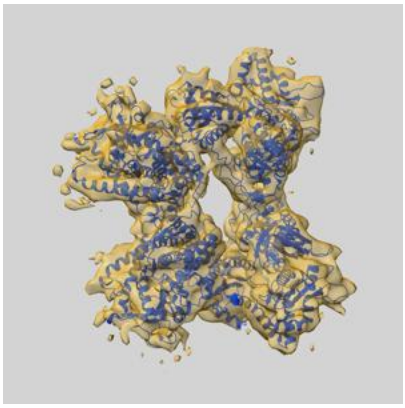
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.51	9.88	8.69

*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 8.51 differs from the reported value 6.5 by more than 10 %

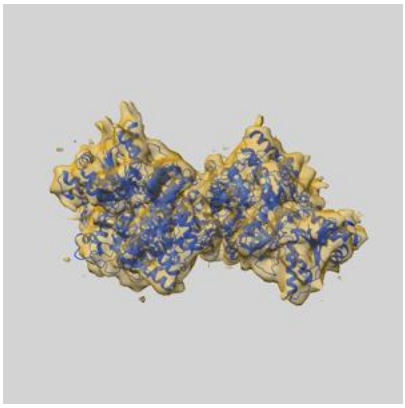
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-27534 and PDB model 8DME. Per-residue inclusion information can be found in section 3 on page 8.

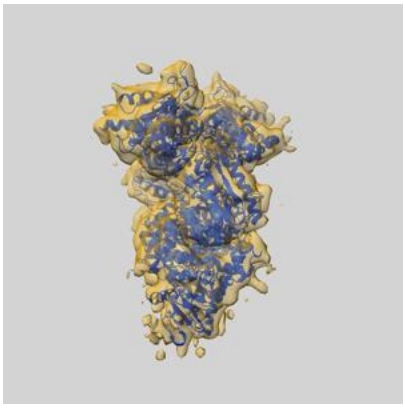
9.1 Map-model overlay



X



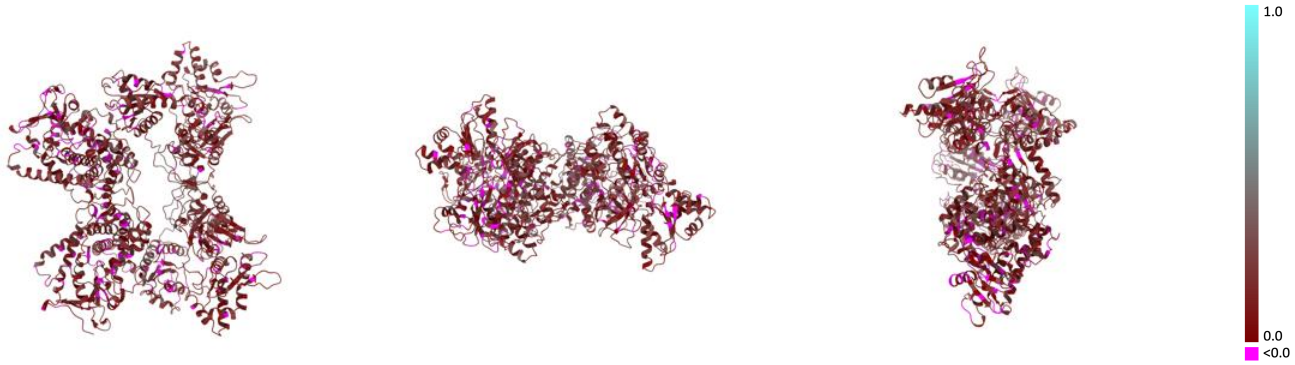
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.8 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.

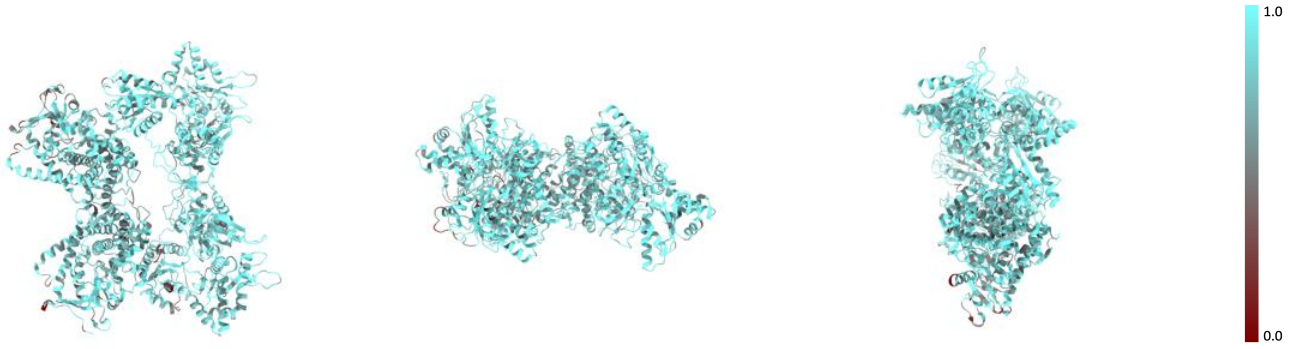
9.2 Q-score mapped to coordinate model



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.

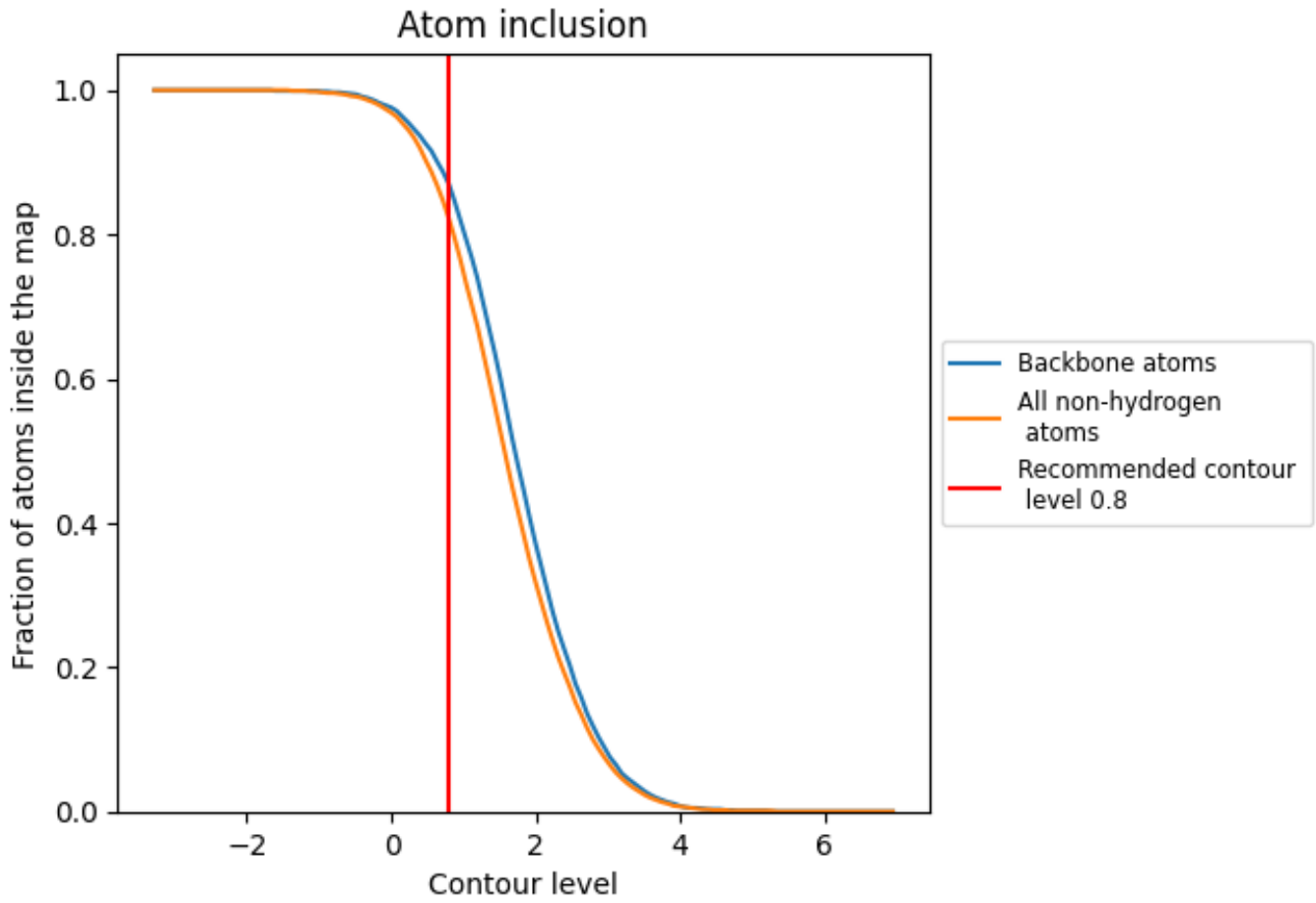
9.3 Atom inclusion mapped to coordinate model



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 (0.8).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 82% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8210	0.1470
A	0.8330	0.1490
B	0.8180	0.1440