



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:58 AM UTC

PDB ID : 9E7H / pdb_00009e7h
EMDB ID : EMD-47669
Title : CryoEM structure of BchN-BchB bound to Pchlde from the DPOR under turnover complex dataset
Authors : Kashyap, R.; Antony, E.
Deposited on : 2024-11-01
Resolution : 3.29 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

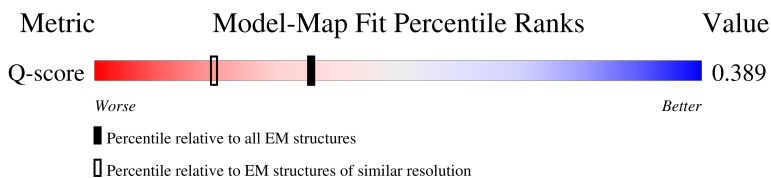
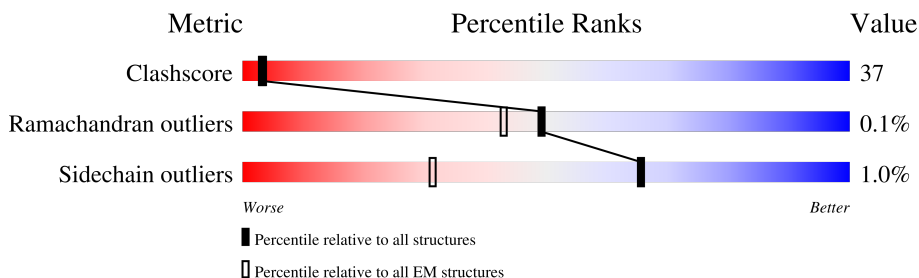
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.29 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14466 (2.79 - 3.79)

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

Mol	Chain	Length	Quality of chain
1	A	428	
1	C	428	
2	B	536	
2	D	536	

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	SF4	A	501	-	-	X	-
3	SF4	C	501	-	-	X	-
4	PMR	A	502	X	-	-	-
4	PMR	B	601	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12612 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

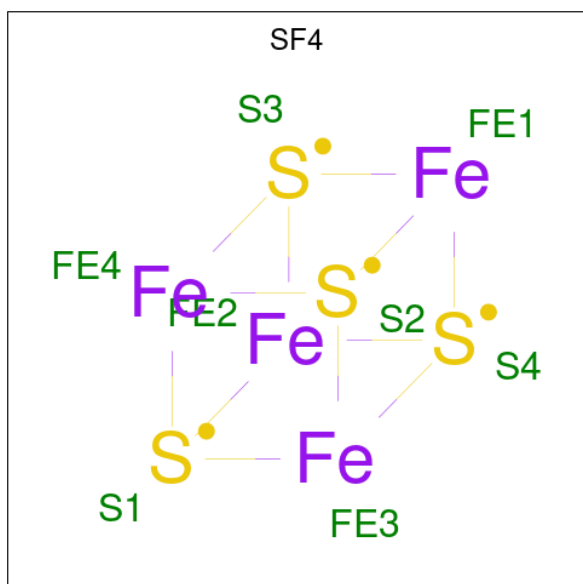
- Molecule 1 is a protein called Light-independent protochlorophyllide reductase subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	402	Total	C	N	O	S	1	0
			3063	1943	553	557	10		
1	C	389	Total	C	N	O	S	2	0
			2972	1891	535	536	10		

- Molecule 2 is a protein called Light-independent protochlorophyllide reductase subunit B.

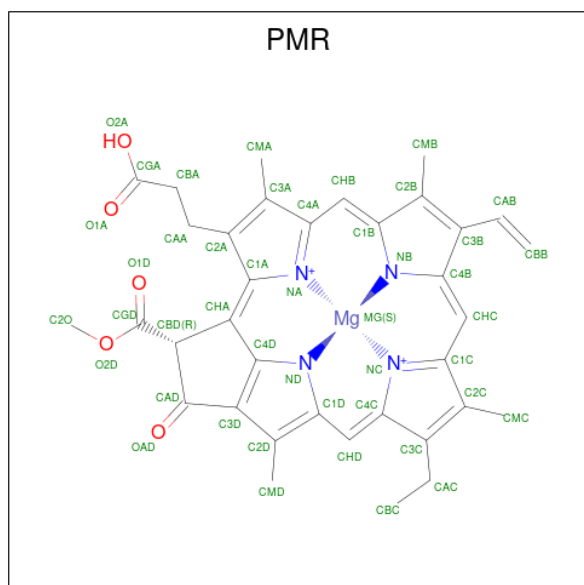
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	419	Total	C	N	O	S	1	0
			3241	2058	565	596	22		
2	D	418	Total	C	N	O	S	1	0
			3228	2046	563	598	21		

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total 8	Fe 4	S 4	0
3	C	1	Total 8	Fe 4	S 4	0

- Molecule 4 is Protochlorophyllide (CCD ID: PMR) (formula: $\text{C}_{35}\text{H}_{32}\text{MgN}_4\text{O}_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
4	B	1	Total 45	C 35	Mg 1	N 4	O 5	0

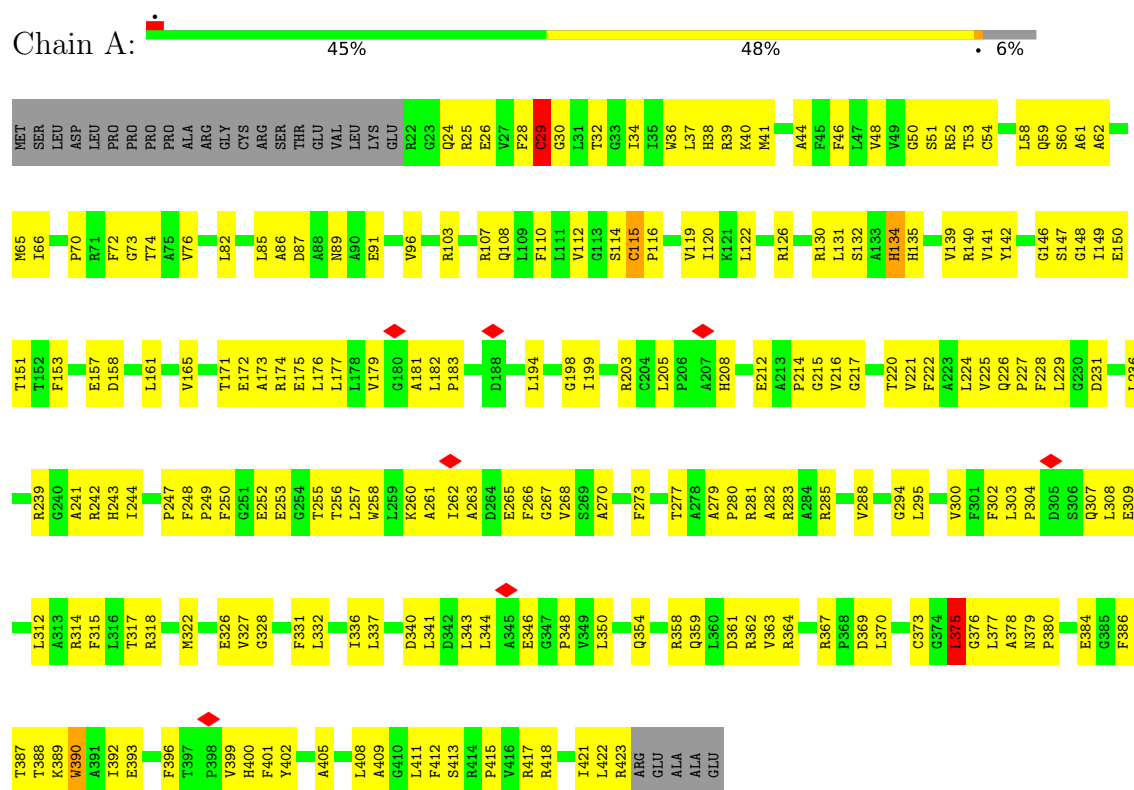
- Molecule 5 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	D	2	Total 2	Cu 2	0

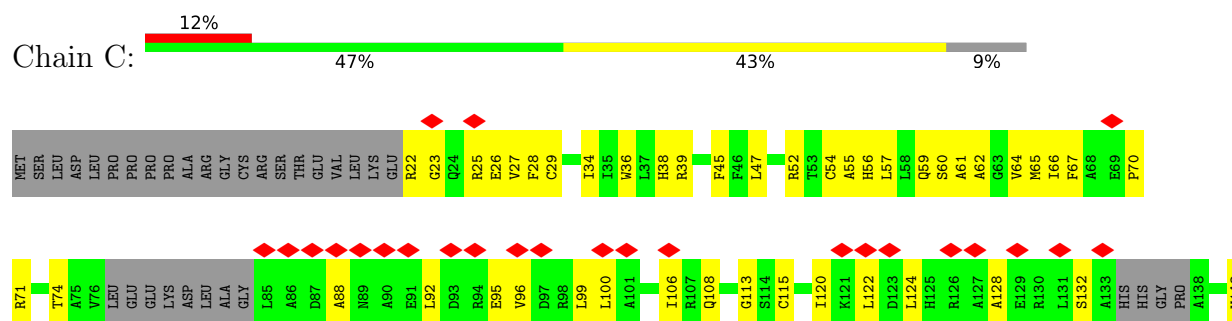
3 Residue-property plots

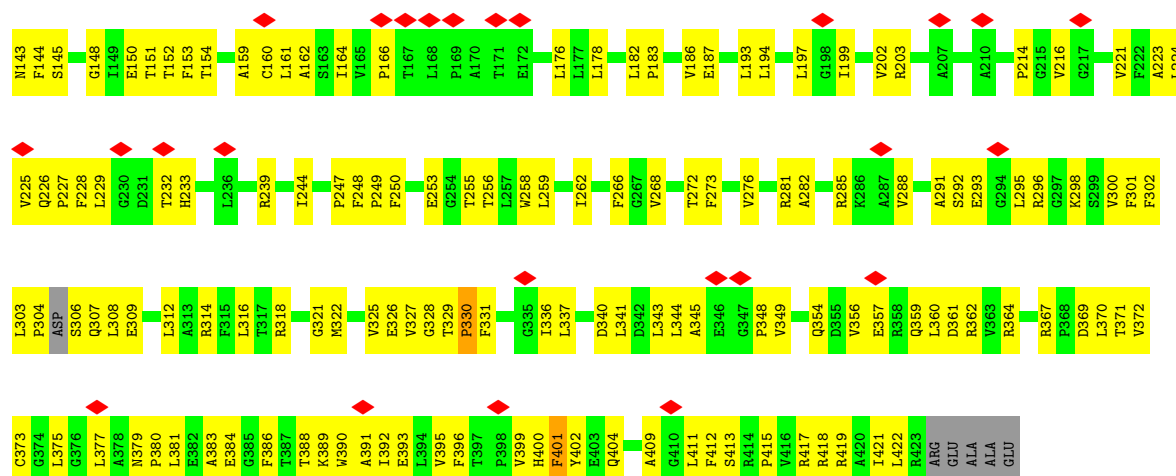
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Light-independent protochlorophyllide reductase subunit N

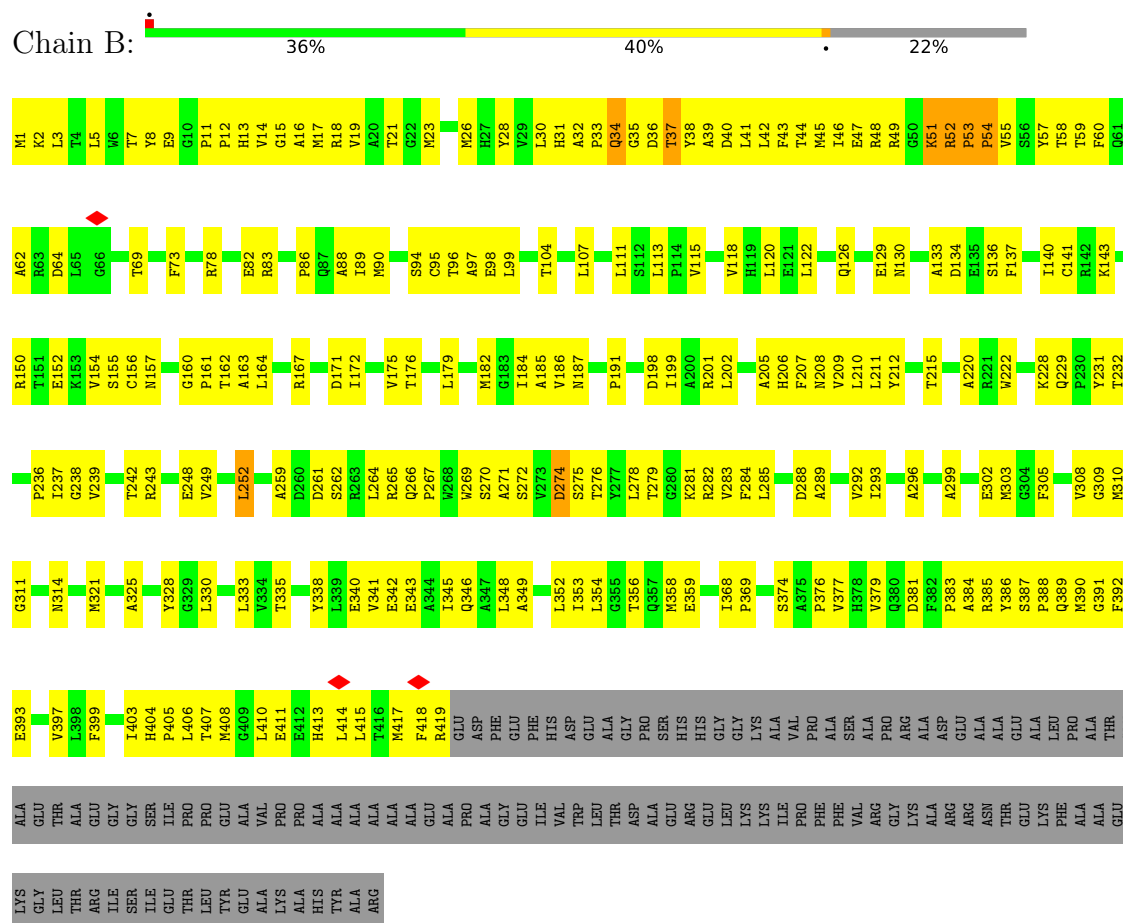


- Molecule 1: Light-independent protochlorophyllide reductase subunit N

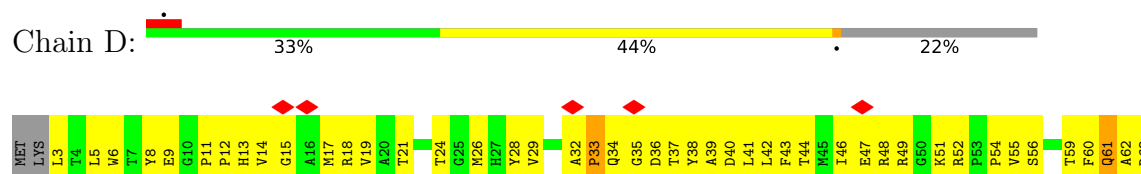




• Molecule 2: Light-independent protochlorophyllide reductase subunit B



• Molecule 2: Light-independent protochlorophyllide reductase subunit B



PHE	SER	T290	V209	A133	G66
VAL	ALA	G370	L210	D134	S67
ARG	PRO	A371	L211	E135	
GLY	ARG	V372	P213	S136	D68
LYS	ALA		E214	F137	T69
ALA	ASP	A299	T215	Q139	A70
ARG	GLU	R300	G216	I140	E71
ARG	ALA	D301	E217	C141	L72
ASN	ALA	E302	S218	R142	F73
Q370	GLU	M303		K143	Q74
Q381	ALA	G304			
D381	LEU	F305	R221	M148	D79
	PRO	E306	R222	A80	
A384	ALA	V307	A223	Y81	
R385	ALA	V308	E224	E82	
Y386	GLY		K225	R83	
S387	ALA				
P388	LYS	C312	Q229	P86	
Q389	GLY	Y313	Y231	Q87	
M390	THR	N314	T230	A88	
	ALA		T232	I89	
E393	ARG	A318	V235	M90	
G394	GLY	M321	P236	V91	
A395	GLY	R322	G238	C95	
N396	SER	A323	V239	T96	
V397	ILE	A324	T242	A97	
L398	THR	A325	V246	E98	
F399	PRO	K326		I100	
	GLU			D101	
W402	ALA	G329		D102	
	VAL	L333	V249	D103	
P405	PRO	V334	A253	T104	
M408	ALA	T335			
	ALA	D336		L107	
E412	ALA				
	ALA				
M417	ALA	L339	V258		
F418	ALA	E340		A110	
R419	GLU	F341	L264	L111	
E420	ALA	E342	R265	S112	
ASP	PRO		Q266	L113	
PHE	ALA	P350	P267	P116	
GLY	GLY	F351	W268	V117	
GLU	GLU	L352	W269	V118	
ILE	HIS	I353	S270	H119	
VAL	ASP	L354	A271	L120	
THR	GLU	G355	S272	E121	
LEU	ALA	T356	D273	L122	
THR	THR	Q357	D274	P123	
ASP	ASP	M358		S124	
ALA	ALA	E359	L278	Y125	
GLU	HIS	R360		Q126	
ARG	ARG	H361	R282	R127	
	GLY	I362	L202	K128	
LEU	LEU	A363	F284	E129	
LYS	LYS	K364	L285	M130	
LYS	LYS	R365	F286	F131	
ILE	VAL	L366	G287	G132	
VAL	ALA	G367	A289		
PRO	PRO	ALA			
PHE	PHE				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	69816	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.460	Depositor
Minimum map value	-0.689	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.0954	Depositor
Map size ($\text{\AA}$)	393.6, 393.6, 393.6	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82, 0.82, 0.82	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: SF4, CU, PMR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.23	0/3132	0.56	2/4257 (0.0%)
1	C	1.77	2/3039 (0.1%)	1.14	7/4126 (0.2%)
2	B	0.25	0/3321	0.59	3/4514 (0.1%)
2	D	0.44	4/3306 (0.1%)	0.90	9/4494 (0.2%)
All	All	0.91	6/12798 (0.0%)	0.83	21/17391 (0.1%)

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

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	330	PRO	N-CD	96.18	2.82	1.47
2	D	33	PRO	CB-CG	-11.64	0.91	1.49
2	D	191	PRO	CB-CG	-11.00	0.94	1.49
1	C	330	PRO	CG-CD	-9.35	1.19	1.50
2	D	191	PRO	CG-CD	-7.80	1.24	1.50
2	D	33	PRO	CG-CD	-7.67	1.24	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	330	PRO	N-CD-CG	-56.26	18.81	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	330	PRO	CA-N-CD	-24.93	77.10	112.00
2	D	191	PRO	CB-CG-CD	22.92	179.44	106.10
2	D	33	PRO	CB-CG-CD	18.81	166.29	106.10
2	D	33	PRO	N-CD-CG	-18.64	75.23	103.20
2	D	33	PRO	CA-CB-CG	-18.48	69.39	104.50
2	D	191	PRO	N-CD-CG	-16.97	77.74	103.20
2	D	191	PRO	CA-CB-CG	-15.80	74.48	104.50
1	C	330	PRO	CA-CB-CG	-14.78	76.43	104.50
2	B	53	PRO	N-CA-C	-14.57	92.92	110.70
2	B	54	PRO	CB-CA-C	9.71	127.57	111.56
2	D	213	PRO	N-CA-CB	8.73	112.42	103.25
2	D	33	PRO	CA-N-CD	-7.63	101.32	112.00
1	C	329	THR	C-N-CD	7.54	155.89	125.00
2	D	191	PRO	CA-N-CD	-7.05	102.13	112.00
1	C	336	ILE	N-CA-C	-6.56	106.34	112.83
1	C	330	PRO	N-CA-CB	-6.33	97.46	103.41
1	A	375	LEU	CA-CB-CG	5.96	137.15	116.30
1	C	402	TYR	CB-CA-C	-5.67	110.02	116.54
1	A	29	CYS	N-CA-C	-5.62	102.14	110.46
2	B	54	PRO	N-CA-CB	-5.02	97.98	103.25

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	375	LEU	Peptide
2	B	52	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3063	0	3075	252	0
1	C	2972	0	2994	248	0
2	B	3241	0	3210	237	0
2	D	3228	0	3189	265	0
3	A	8	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	8	0	0	12	0
4	A	45	0	31	7	0
4	B	45	0	31	12	0
5	D	2	0	0	0	0
All	All	12612	0	12530	926	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 37.

All (926) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:90:MET:HE3	2:D:120:LEU:CD1	1.36	1.53
2:B:418:PHE:CE2	1:C:39:ARG:NH1	1.91	1.38
1:C:115:CYS:SG	3:C:501:SF4:FE4	1.16	1.37
1:C:186:VAL:HG23	1:C:404:GLN:NE2	1.38	1.36
1:A:115:CYS:SG	3:A:501:SF4:FE4	1.21	1.30
1:C:393:GLU:OE2	1:C:411:LEU:HD13	1.38	1.22
1:C:54:CYS:SG	3:C:501:SF4:FE3	1.33	1.20
1:C:253:GLU:OE2	1:C:318:ARG:NH1	1.77	1.15
2:D:90:MET:HE3	2:D:120:LEU:HD11	1.24	1.11
2:D:90:MET:CE	2:D:120:LEU:HD13	1.80	1.11
2:D:90:MET:CE	2:D:120:LEU:CD1	2.29	1.11
1:C:393:GLU:OE1	1:C:411:LEU:HD22	1.51	1.09
2:D:213:PRO:HA	2:D:217:GLU:HB2	1.37	1.05
1:C:56:HIS:ND1	2:D:38:TYR:OH	1.89	1.05
2:B:45:MET:SD	2:D:274:ASP:OD1	2.16	1.03
2:D:90:MET:HE3	2:D:120:LEU:HD13	1.08	1.03
1:C:186:VAL:CG2	1:C:404:GLN:NE2	2.21	1.02
1:C:62:ALA:HB1	1:C:65:MET:HB3	1.40	0.99
1:C:66:ILE:HD12	2:D:6:TRP:CE3	1.98	0.97
1:C:115:CYS:HG	3:C:501:SF4:FE4	0.71	0.95
1:C:400:HIS:O	1:C:404:GLN:OE1	1.84	0.94
2:B:49:ARG:HH12	2:B:163:ALA:HB1	1.31	0.94
1:C:186:VAL:HG23	1:C:404:GLN:HE22	1.14	0.94
2:B:419:ARG:HD3	1:C:65:MET:HE3	1.47	0.92
2:B:41:LEU:O	2:B:45:MET:HB2	1.69	0.92
1:A:29:CYS:SG	3:A:501:SF4:FE1	1.63	0.90
2:B:90:MET:HE2	2:B:120:LEU:HD11	1.56	0.88
1:A:61:ALA:HB1	4:A:502:PMR:HBCB	1.55	0.88
1:A:171:THR:HG22	1:A:172:GLU:N	1.86	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:ILE:HD12	2:D:6:TRP:HE3	1.34	0.88
1:A:29:CYS:HG	3:A:501:SF4:FE1	0.57	0.86
1:C:186:VAL:CG2	1:C:404:GLN:CD	2.47	0.86
1:A:199:ILE:HG22	1:A:268:VAL:HG21	1.57	0.85
1:A:390[A]:TRP:CZ2	1:A:393:GLU:OE1	2.29	0.85
1:C:186:VAL:HG23	1:C:404:GLN:CD	2.01	0.85
1:C:197:LEU:HD11	1:C:273:PHE:HD2	1.39	0.85
1:A:194:LEU:HD22	1:A:199:ILE:HD11	1.59	0.84
2:B:403:ILE:HG22	2:D:380:GLN:HE22	1.43	0.83
1:C:381:LEU:HD12	1:C:386:PHE:HD2	1.43	0.83
1:A:171:THR:HG22	1:A:172:GLU:H	1.39	0.83
1:A:390[A]:TRP:CE2	1:A:393:GLU:OE1	2.31	0.83
1:C:393:GLU:OE1	1:C:411:LEU:CD2	2.25	0.83
2:B:15:GLY:HA2	2:B:18:ARG:HD3	1.61	0.83
1:A:54:CYS:SG	3:A:501:SF4:FE3	1.68	0.83
2:D:239:VAL:HG21	2:D:267:PRO:HD3	1.61	0.82
2:D:28:TYR:HB3	2:D:55:VAL:HG22	1.61	0.82
2:B:171:ASP:OD2	2:B:212:TYR:OH	1.95	0.82
2:B:210:LEU:HD13	2:B:220:ALA:CB	2.11	0.81
2:B:418:PHE:HE2	1:C:39:ARG:HH12	1.25	0.81
1:C:54:CYS:HG	3:C:501:SF4:FE3	0.98	0.81
1:C:259:LEU:HB3	1:C:273:PHE:HE2	1.46	0.81
2:D:213:PRO:CA	2:D:217:GLU:HB2	2.10	0.81
2:B:18:ARG:HG2	2:B:164:LEU:HB3	1.62	0.81
1:C:330:PRO:HG3	1:C:331:PHE:N	1.89	0.81
1:A:171:THR:CG2	1:A:172:GLU:H	1.94	0.80
2:D:29:VAL:HA	2:D:56:SER:HB2	1.62	0.80
2:D:123:PRO:HD2	2:D:127:ARG:HG3	1.61	0.80
2:B:210:LEU:HD13	2:B:220:ALA:HB2	1.62	0.80
2:B:385:ARG:NH2	2:D:387:SER:OG	2.17	0.78
1:C:56:HIS:CG	2:D:38:TYR:OH	2.37	0.78
1:C:55:ALA:HB2	1:C:74:THR:HG21	1.67	0.77
1:A:327:VAL:HG22	1:A:348:PRO:HB2	1.65	0.77
4:B:601:PMR:HMCA	1:C:61:ALA:HB1	1.67	0.77
1:C:38:HIS:ND1	1:C:71:ARG:HG2	2.00	0.77
1:C:176:LEU:HD21	1:C:262:ILE:HD12	1.67	0.76
2:D:299:ALA:HA	2:D:303:MET:HB2	1.65	0.76
1:A:317:THR:HA	1:A:322:MET:H	1.50	0.76
1:A:226:GLN:HB2	1:A:229:LEU:HD13	1.66	0.76
1:C:70:PRO:HD2	2:D:5:LEU:HD23	1.68	0.76
2:D:289:ALA:O	2:D:293:ILE:HG13	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:ASN:ND2	2:B:44:THR:O	2.18	0.76
2:B:171:ASP:OD1	2:B:389:GLN:N	2.16	0.76
2:D:73:PHE:HD2	2:D:102:ASP:OD1	1.68	0.75
1:A:171:THR:HG22	1:A:173:ALA:H	1.51	0.75
2:B:23:MET:HE1	2:B:140:ILE:HG21	1.67	0.74
2:B:208:ASN:ND2	2:B:229:GLN:OE1	2.20	0.74
2:B:283:VAL:HG12	2:B:352:LEU:HB3	1.69	0.74
2:D:73:PHE:HD2	2:D:102:ASP:CG	1.94	0.74
1:C:203:ARG:HE	1:C:214:PRO:HA	1.51	0.74
1:A:115:CYS:SG	3:A:501:SF4:S3	2.86	0.74
2:B:38:TYR:HA	2:B:41:LEU:HD13	1.67	0.73
2:B:418:PHE:CD2	1:C:39:ARG:NH1	2.56	0.73
2:D:167:ARG:HD3	2:D:387:SER:HB3	1.69	0.73
1:C:314:ARG:HD3	1:C:343:LEU:HB3	1.70	0.73
1:C:361:ASP:HA	1:C:364:ARG:HD2	1.68	0.73
1:A:222:PHE:HB3	1:A:236:LEU:HD22	1.70	0.73
1:C:56:HIS:CE1	2:D:38:TYR:OH	2.40	0.73
1:C:47:LEU:HD22	1:C:99:LEU:HD11	1.70	0.73
2:D:90:MET:CE	2:D:120:LEU:CD2	2.66	0.73
2:D:90:MET:HG2	2:D:118:VAL:HG12	1.71	0.73
1:A:176:LEU:HB3	1:A:266:PHE:HE2	1.55	0.72
2:D:14:VAL:HG13	2:D:129:GLU:HG3	1.70	0.72
2:D:266:GLN:NE2	2:D:395:ALA:O	2.21	0.72
2:B:292:VAL:HG13	2:B:321:MET:HE3	1.72	0.71
1:A:280:PRO:HB2	1:A:402:TYR:HD2	1.56	0.71
1:C:389:LYS:HB2	1:C:415:PRO:HG3	1.70	0.71
1:A:171:THR:CG2	1:A:172:GLU:N	2.51	0.71
2:D:169:ARG:NH1	2:D:170:ASP:OD1	2.24	0.71
2:B:118:VAL:HG12	2:B:143:LYS:HD2	1.72	0.71
1:A:115:CYS:SG	3:A:501:SF4:S2	2.89	0.71
1:C:381:LEU:HD12	1:C:386:PHE:CD2	2.26	0.71
2:D:73:PHE:CD2	2:D:102:ASP:OD1	2.44	0.71
2:B:47:GLU:OE1	2:B:49:ARG:NH1	2.24	0.70
2:B:171:ASP:HB3	2:B:390:MET:HB2	1.72	0.70
2:D:288:ASP:OD2	2:D:291:HIS:ND1	2.19	0.70
1:C:381:LEU:HG	1:C:386:PHE:HB2	1.73	0.70
2:B:415:LEU:HG	1:C:64:VAL:HB	1.73	0.70
2:D:35:GLY:H	2:D:37:THR:HG22	1.56	0.70
2:D:187:ASN:ND2	2:D:201:ARG:O	2.24	0.69
1:A:96:VAL:HG11	1:A:131:LEU:HD11	1.74	0.69
2:B:293:ILE:HG13	2:B:321:MET:HE2	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:LEU:HD13	1:C:99:LEU:HG	1.74	0.69
2:B:411:GLU:O	2:B:415:LEU:HB2	1.92	0.69
2:B:40:ASP:HA	2:B:53:PRO:HG2	1.74	0.69
1:A:359:GLN:O	1:A:363:VAL:HG23	1.91	0.69
1:C:115:CYS:SG	3:C:501:SF4:S3	2.90	0.69
1:C:253:GLU:HA	1:C:256:THR:HB	1.75	0.69
1:C:312:LEU:HD13	1:C:412:PHE:HZ	1.57	0.69
2:D:9:GLU:HB3	2:D:129:GLU:H	1.58	0.69
1:A:307:GLN:NE2	1:A:331:PHE:O	2.26	0.69
2:B:48:ARG:NH2	2:D:269:TRP:O	2.26	0.68
2:D:182:MET:HA	2:D:258:VAL:HB	1.74	0.68
2:D:357:GLN:NE2	2:D:381:ASP:OD2	2.27	0.68
1:C:302:PHE:HB2	1:C:327:VAL:HG12	1.76	0.68
2:B:384:ALA:O	2:D:396:ASN:ND2	2.26	0.68
1:A:370:LEU:HD11	1:A:389:LYS:HB3	1.74	0.68
1:A:295:LEU:HD22	1:A:322:MET:HE1	1.75	0.68
2:B:152:GLU:N	2:B:152:GLU:OE1	2.27	0.67
2:D:117:VAL:HG13	2:D:143:LYS:HD2	1.77	0.67
2:D:142:ARG:HG2	2:D:143:LYS:HE3	1.76	0.67
2:D:378:HIS:HD2	2:D:380:GLN:H	1.42	0.67
2:D:28:TYR:O	2:D:56:SER:N	2.27	0.67
2:D:91:VAL:HG22	2:D:119:HIS:HB2	1.76	0.67
2:D:100:ILE:HG23	2:D:101:GLN:NE2	2.09	0.67
2:B:17:MET:HE1	2:B:39:ALA:CB	2.25	0.67
1:A:222:PHE:HE1	1:A:243:HIS:HB2	1.57	0.67
1:C:259:LEU:HB3	1:C:273:PHE:CE2	2.30	0.67
1:A:65:MET:HE3	1:A:72:PHE:HZ	1.59	0.67
1:A:85:LEU:O	1:A:89:ASN:ND2	2.27	0.67
1:A:221:VAL:HG12	1:A:242:ARG:HB3	1.76	0.66
1:C:298:LYS:HD3	1:C:369:ASP:HB2	1.77	0.66
1:A:263:ALA:O	1:A:267:GLY:N	2.24	0.66
2:B:404:HIS:HA	2:D:380:GLN:HE21	1.60	0.66
1:A:26:GLU:OE1	1:A:376:GLY:N	2.29	0.66
1:A:203:ARG:HB3	1:A:214:PRO:HB3	1.78	0.66
2:D:88:ALA:HA	2:D:113:LEU:HD13	1.76	0.66
1:C:247:PRO:O	1:C:258:TRP:HB2	1.96	0.66
2:B:60:PHE:CG	2:B:69:THR:OG1	2.48	0.66
2:B:413:HIS:HA	2:B:417:MET:CE	2.26	0.66
1:C:186:VAL:HG21	1:C:404:GLN:CD	2.21	0.66
2:D:18:ARG:HG2	2:D:43:PHE:HE1	1.61	0.66
1:A:36:TRP:HE1	1:A:157:GLU:HG3	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LEU:HD11	1:A:341:LEU:HD11	1.77	0.66
1:C:27:VAL:HG11	1:C:330:PRO:HB3	1.78	0.66
2:B:182:MET:HE1	2:B:249:VAL:CG2	2.26	0.66
1:A:34:ILE:HD11	1:A:112:VAL:HG11	1.76	0.65
1:C:115:CYS:SG	3:C:501:SF4:S1	2.94	0.65
1:A:52:ARG:NH1	2:B:7:THR:OG1	2.26	0.65
2:B:13:HIS:O	2:B:17:MET:HG3	1.97	0.65
2:B:414:LEU:HB3	2:B:419:ARG:HH21	1.62	0.65
2:B:264:LEU:HD22	2:B:392:PHE:CD1	2.32	0.65
1:A:40:LYS:NZ	1:A:182:LEU:O	2.25	0.65
1:A:116:PRO:O	1:A:120:ILE:HG13	1.96	0.65
2:B:338:TYR:HB2	2:B:358:MET:HE2	1.79	0.64
1:A:253:GLU:HB3	1:A:318:ARG:HH12	1.62	0.64
1:C:52:ARG:O	1:C:56:HIS:HB3	1.98	0.64
2:B:281:LYS:HB2	2:B:305:PHE:HB3	1.79	0.64
1:C:29:CYS:SG	3:C:501:SF4:S4	2.95	0.64
1:C:128:ALA:O	1:C:132:SER:OG	2.12	0.64
1:A:277:THR:HA	1:A:280:PRO:HG2	1.80	0.63
1:C:316:LEU:HD22	1:C:322:MET:HE2	1.79	0.63
1:C:178:LEU:HD13	1:C:194:LEU:HD11	1.79	0.63
1:A:36:TRP:NE1	1:A:157:GLU:OE1	2.31	0.63
2:B:310:MET:HE2	2:B:325:ALA:HA	1.80	0.63
1:C:150:GLU:HG3	2:D:62:ALA:HB2	1.81	0.63
1:C:393:GLU:OE2	1:C:411:LEU:CD1	2.32	0.63
2:D:322:ARG:HH12	2:D:334:VAL:HG11	1.63	0.63
2:B:17:MET:HE1	2:B:39:ALA:HB1	1.81	0.63
2:D:33:PRO:HA	2:D:59:THR:HA	1.80	0.63
1:A:227:PRO:HD3	1:A:250:PHE:HE2	1.64	0.63
1:A:253:GLU:HG2	1:A:318:ARG:HH22	1.62	0.63
1:A:62:ALA:HB1	1:A:65:MET:HB3	1.80	0.63
2:B:292:VAL:HG13	2:B:321:MET:CE	2.29	0.62
1:C:255:THR:HG21	1:C:401[A]:PHE:CD1	2.34	0.62
1:C:223:ALA:HB2	1:C:262:ILE:HD11	1.80	0.62
1:A:375:LEU:HD12	1:A:378:ALA:HB2	1.81	0.62
2:B:30:LEU:HD22	2:B:32:ALA:HB2	1.82	0.62
2:D:9:GLU:HB2	2:D:128:LYS:HB3	1.80	0.62
2:B:32:ALA:HB1	2:B:36:ASP:HB2	1.80	0.62
2:B:46:ILE:HA	2:B:379:VAL:HG12	1.81	0.62
2:B:288:ASP:N	2:B:374:SER:OG	2.29	0.62
2:D:312:CYS:SG	2:D:313:TYR:N	2.73	0.62
1:A:393:GLU:OE2	1:A:411:LEU:HD11	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:PHE:HB2	2:B:64:ASP:HB2	1.82	0.62
2:B:274:ASP:HB3	4:B:601:PMR:HAA	1.80	0.62
2:B:342:GLU:O	2:B:346:GLN:HG3	2.00	0.62
2:D:184:ILE:HD12	2:D:207:PHE:HE1	1.64	0.62
2:B:16:ALA:HB1	2:B:120:LEU:HD13	1.82	0.62
2:D:14:VAL:O	2:D:18:ARG:HG3	1.98	0.62
1:C:327:VAL:HG22	1:C:348:PRO:HB2	1.82	0.61
2:B:160:GLY:O	2:B:215:THR:OG1	2.14	0.61
1:C:197:LEU:HD11	1:C:273:PHE:CD2	2.28	0.61
1:A:318:ARG:HD2	1:A:343:LEU:HD22	1.81	0.61
1:C:292:SER:HB3	1:C:409:ALA:HB1	1.82	0.61
1:A:244:ILE:HG12	1:A:262:ILE:HA	1.81	0.61
1:A:53:THR:HG23	2:B:11:PRO:HG3	1.83	0.61
1:A:302:PHE:HB3	1:A:309:GLU:HG2	1.83	0.61
1:C:360:LEU:HD12	1:C:364:ARG:NE	2.16	0.61
1:A:379:ASN:HB3	2:D:268:TRP:HH2	1.64	0.61
2:B:415:LEU:HD21	1:C:67:PHE:HB2	1.82	0.61
1:C:375:LEU:HD21	2:D:41:LEU:HD11	1.83	0.61
3:C:501:SF4:FE2	2:D:36:ASP:OD1	1.52	0.61
2:B:414:LEU:HB3	2:B:419:ARG:NH2	2.16	0.61
1:A:396:PHE:HE2	4:A:502:PMR:HACA	1.64	0.61
1:A:390[A]:TRP:NE1	1:A:393:GLU:OE1	2.33	0.60
2:B:212:TYR:CZ	2:B:390:MET:HE3	2.35	0.60
2:B:265:ARG:HB3	2:B:269:TRP:HD1	1.65	0.60
1:A:224:LEU:O	1:A:258:TRP:NE1	2.34	0.60
2:D:205:ALA:O	2:D:229:GLN:NE2	2.34	0.60
1:C:371:THR:CG2	1:C:381:LEU:HD21	2.31	0.60
2:D:90:MET:HE1	2:D:120:LEU:CD2	2.30	0.60
2:D:360:ARG:HA	2:D:370:CYS:SG	2.41	0.60
1:C:108:GLN:HA	1:C:142:TYR:HE1	1.67	0.60
1:C:393:GLU:CD	1:C:411:LEU:HD13	2.22	0.60
2:D:44:THR:HA	2:D:49:ARG:H	1.66	0.60
2:B:28:TYR:HA	2:B:90:MET:O	2.02	0.59
2:D:318:ALA:HB1	2:D:322:ARG:HH22	1.67	0.59
1:C:421:ILE:HG13	1:C:422:LEU:HD12	1.84	0.59
1:C:54:CYS:SG	3:C:501:SF4:S1	3.00	0.59
2:D:90:MET:CE	2:D:120:LEU:HD22	2.31	0.59
2:B:44:THR:CG2	2:B:53:PRO:HD3	2.32	0.59
2:B:73:PHE:CE2	2:B:104:THR:HB	2.38	0.59
1:C:227:PRO:HA	1:C:248:PHE:CE2	2.38	0.59
2:D:15:GLY:HA2	2:D:18:ARG:HE	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:100:ILE:CG2	2:D:101:GLN:NE2	2.65	0.59
1:A:110:PHE:CE1	1:A:142:TYR:HB2	2.37	0.59
2:D:96:THR:HG23	2:D:97:ALA:H	1.67	0.59
2:D:141:CYS:SG	2:D:202:LEU:HD22	2.42	0.59
1:A:379:ASN:OD1	2:D:273:VAL:HG23	2.02	0.59
2:B:39:ALA:HA	2:B:42:LEU:HD12	1.84	0.59
2:B:198:ASP:OD1	2:B:201:ARG:NH2	2.36	0.59
1:C:393:GLU:CD	1:C:411:LEU:HD22	2.27	0.59
2:B:248:GLU:O	2:B:252:LEU:HG	2.02	0.59
2:D:179:LEU:HD11	2:D:209:VAL:HG21	1.85	0.59
1:A:212:GLU:HG3	1:A:212:GLU:O	2.02	0.59
1:A:281:ARG:HG3	1:A:402:TYR:CZ	2.38	0.59
2:B:18:ARG:HH11	2:B:129:GLU:HG2	1.66	0.59
2:B:126:GLN:O	2:B:126:GLN:NE2	2.34	0.59
2:D:70:ALA:HA	2:D:102:ASP:OD2	2.02	0.58
2:D:213:PRO:HA	2:D:217:GLU:CB	2.23	0.58
1:A:51:SER:H	1:A:116:PRO:HG2	1.68	0.58
1:A:165:VAL:HG11	1:A:236:LEU:HB2	1.85	0.58
2:B:150:ARG:NH2	2:B:228:LYS:O	2.36	0.58
1:C:292:SER:HB2	1:C:295:LEU:HD12	1.85	0.58
2:B:157:ASN:ND2	2:B:187:ASN:OD1	2.35	0.58
2:B:276:THR:O	2:B:279:THR:OG1	2.22	0.58
2:D:133:ALA:HB1	2:D:162:THR:HG21	1.85	0.58
2:B:78:ARG:O	2:B:82:GLU:HG2	2.02	0.58
4:B:601:PMR:HMDDB	4:B:601:PMR:HBCB	1.85	0.58
2:B:17:MET:SD	2:B:55:VAL:HG11	2.44	0.58
2:D:157:ASN:HD21	2:D:187:ASN:HD22	1.51	0.58
1:A:247:PRO:HD2	1:A:257:LEU:HB3	1.85	0.58
1:A:327:VAL:HG11	1:A:344:LEU:HD21	1.85	0.58
1:A:225:VAL:HG13	1:A:249:PRO:HG2	1.86	0.58
2:B:266:GLN:NE2	2:B:302:GLU:OE1	2.31	0.58
1:C:325:VAL:HG22	1:C:326:GLU:H	1.68	0.58
1:A:379:ASN:HB3	2:D:268:TRP:CH2	2.38	0.58
2:B:187:ASN:O	2:B:201:ARG:NH1	2.33	0.58
1:C:296:ARG:HA	1:C:321:GLY:H	1.68	0.58
1:C:115:CYS:SG	3:C:501:SF4:S2	3.01	0.57
1:C:148:GLY:O	2:D:34:GLN:NE2	2.37	0.57
1:C:360:LEU:HD12	1:C:364:ARG:HE	1.69	0.57
2:D:90:MET:CE	2:D:120:LEU:HD11	2.14	0.57
2:D:40:ASP:OD2	2:D:52:ARG:NH2	2.31	0.57
1:A:36:TRP:HE1	1:A:157:GLU:CG	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LEU:HD22	1:A:350:LEU:HG	1.86	0.57
2:B:8:TYR:OH	2:B:359:GLU:OE2	2.20	0.57
1:C:392:ILE:HD12	1:C:392:ILE:H	1.69	0.57
2:D:378:HIS:CD2	2:D:380:GLN:H	2.23	0.57
2:B:310:MET:CE	2:B:325:ALA:HA	2.33	0.57
1:A:28:PHE:HZ	2:B:41:LEU:HD21	1.69	0.57
1:A:59:GLN:HA	1:A:66:ILE:HG21	1.86	0.57
2:B:207:PHE:HA	2:B:229:GLN:HB3	1.86	0.57
2:B:335:THR:OG1	2:B:340:GLU:OE1	2.18	0.57
2:B:419:ARG:HH12	1:C:39:ARG:NH2	2.03	0.57
1:C:166:PRO:O	1:C:239:ARG:NH1	2.38	0.57
1:C:250:PHE:CZ	1:C:308:LEU:HD22	2.39	0.57
2:B:418:PHE:HE2	1:C:39:ARG:NH1	1.77	0.57
1:A:226:GLN:HG2	1:A:400:HIS:NE2	2.20	0.57
2:B:12:PRO:HB2	2:B:122:LEU:CD1	2.35	0.57
2:B:12:PRO:HB2	2:B:122:LEU:HD13	1.87	0.57
2:B:52:ARG:O	2:B:53:PRO:C	2.48	0.57
1:A:375:LEU:HD11	1:A:390[B]:TRP:HA	1.87	0.56
2:B:53:PRO:O	2:B:55:VAL:N	2.38	0.56
1:C:360:LEU:HD22	1:C:377:LEU:HD12	1.86	0.56
2:B:155:SER:HB2	2:B:205:ALA:HA	1.87	0.56
1:C:307:GLN:CG	1:C:330:PRO:HD2	2.35	0.56
1:A:36:TRP:HB3	1:A:396:PHE:CE1	2.41	0.56
1:A:161:LEU:HD21	1:A:181:ALA:HB2	1.87	0.56
2:B:285:LEU:HG	2:B:354:LEU:HD12	1.86	0.56
1:C:224:LEU:HD11	1:C:233:HIS:HB2	1.87	0.56
1:C:227:PRO:HG2	1:C:308:LEU:CD2	2.35	0.56
1:C:359:GLN:HA	1:C:362:ARG:HD3	1.87	0.56
2:D:196:PRO:HA	2:D:199:ILE:HG22	1.86	0.56
2:D:288:ASP:OD1	2:D:288:ASP:N	2.38	0.56
1:A:114:SER:HB3	1:A:116:PRO:HD2	1.88	0.56
1:A:375:LEU:HB2	1:A:378:ALA:HB2	1.87	0.56
4:B:601:PMR:HMBB	1:C:60:SER:HB2	1.87	0.56
2:B:413:HIS:HA	2:B:417:MET:HE2	1.86	0.56
2:D:11:PRO:O	2:D:14:VAL:HG12	2.05	0.56
1:A:244:ILE:HG12	1:A:262:ILE:HG12	1.88	0.56
2:D:148:MET:N	2:D:203:GLY:HA3	2.20	0.56
1:A:44:ALA:HB2	1:A:108:GLN:HG3	1.86	0.56
2:D:68:ASP:O	2:D:72:LEU:HD23	2.06	0.56
2:D:131:PHE:HA	2:D:134:ASP:HB3	1.88	0.56
1:A:115:CYS:HG	3:A:501:SF4:FE4	0.25	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:VAL:HG21	2:B:211:LEU:HD21	1.88	0.56
1:A:199:ILE:CG2	1:A:268:VAL:HG21	2.32	0.55
2:B:94:SER:H	2:B:97:ALA:HB3	1.71	0.55
2:D:90:MET:HE1	2:D:120:LEU:HD21	1.88	0.55
1:C:371:THR:HG21	1:C:381:LEU:HD21	1.87	0.55
1:A:65:MET:HE3	1:A:72:PHE:CZ	2.39	0.55
2:B:17:MET:CE	2:B:39:ALA:HB1	2.35	0.55
2:D:59:THR:O	2:D:61[B]:GLN:NE2	2.40	0.55
2:D:355:GLY:O	2:D:372:VAL:HA	2.06	0.55
2:D:357:GLN:HA	2:D:360:ARG:HB3	1.87	0.55
2:D:207:PHE:HA	2:D:229:GLN:HB2	1.86	0.55
1:A:40:LYS:HD3	1:A:183:PRO:HA	1.88	0.55
1:A:87:ASP:O	1:A:91:GLU:HG2	2.06	0.55
2:B:49:ARG:HH12	2:B:163:ALA:CB	2.12	0.55
1:A:308:LEU:HD23	1:A:312:LEU:HD11	1.89	0.55
1:A:369:ASP:O	1:A:387:THR:HB	2.06	0.55
1:C:67:PHE:CZ	2:D:6:TRP:CZ3	2.95	0.55
2:D:360:ARG:HD2	2:D:364:LYS:HD2	1.88	0.55
2:B:413:HIS:HA	2:B:417:MET:HE1	1.89	0.55
2:B:276:THR:HG23	1:C:418:ARG:HB2	1.89	0.55
4:B:601:PMR:HBD	4:B:601:PMR:HBAA	1.88	0.55
2:D:301:ASP:OD1	2:D:302:GLU:N	2.40	0.54
1:A:303:LEU:HB2	1:A:373:CYS:HB3	1.89	0.54
2:D:211:LEU:O	2:D:390:MET:HE1	2.06	0.54
1:A:421:ILE:HG13	1:A:422:LEU:HD12	1.89	0.54
2:B:48:ARG:O	2:D:268:TRP:NE1	2.28	0.54
1:C:29:CYS:HB3	2:D:35:GLY:HA3	1.89	0.54
1:A:26:GLU:CD	1:A:377:LEU:HD13	2.33	0.54
2:B:133:ALA:HB1	2:B:162:THR:HG21	1.89	0.54
2:D:190:ALA:HB1	2:D:199:ILE:HD12	1.89	0.54
1:C:341:LEU:HD12	1:C:341:LEU:H	1.72	0.54
1:A:108:GLN:HA	1:A:140:ARG:O	2.08	0.54
1:A:242:ARG:HH22	1:A:265:GLU:HB3	1.72	0.54
2:B:179:LEU:HD11	2:B:209:VAL:HG21	1.89	0.54
2:D:137:PHE:CE2	2:D:191:PRO:HA	2.43	0.54
2:D:408:MET:O	2:D:412:GLU:HB2	2.07	0.54
1:C:360:LEU:HD11	1:C:364:ARG:NH2	2.23	0.54
1:A:260:LYS:HA	1:A:273:PHE:CZ	2.42	0.54
1:A:261:ALA:O	1:A:265:GLU:HG2	2.08	0.54
2:B:299:ALA:HA	2:B:303:MET:HB2	1.90	0.54
2:D:312:CYS:HB3	2:D:321:MET:HE2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:LEU:HA	1:A:315:PHE:CE2	2.43	0.54
2:B:17:MET:HG2	2:B:28:TYR:CE2	2.43	0.54
4:A:502:PMR:HHC	2:B:41:LEU:HD22	1.89	0.53
1:C:100:LEU:HA	1:C:106:ILE:HD11	1.89	0.53
1:A:60:SER:HB3	4:A:502:PMR:HMBB	1.90	0.53
2:B:269:TRP:HB3	2:B:399:PHE:CZ	2.44	0.53
1:C:47:LEU:HD11	2:D:3:LEU:HD21	1.90	0.53
2:D:51:LYS:HE3	2:D:54:PRO:HG3	1.90	0.53
2:B:328:TYR:HB2	2:B:330:LEU:HD13	1.90	0.53
1:C:418:ARG:HD3	1:C:419:ARG:N	2.23	0.53
1:A:62:ALA:HB3	1:A:66:ILE:HG23	1.90	0.53
1:A:390[A]:TRP:HE3	1:A:390[A]:TRP:H	1.54	0.53
1:C:306:SER:OG	1:C:309:GLU:OE2	2.24	0.53
2:B:31:HIS:CE1	2:B:69:THR:HG23	2.43	0.53
2:B:278:LEU:HB3	2:B:305:PHE:CD2	2.43	0.53
1:C:153:PHE:HE2	1:C:395:VAL:HG21	1.74	0.53
1:A:255:THR:HG21	1:A:401:PHE:HA	1.90	0.53
2:B:17:MET:HG2	2:B:28:TYR:CD2	2.44	0.53
2:D:333:LEU:HD21	2:D:340:GLU:HB3	1.89	0.53
1:A:346:GLU:OE1	1:A:346:GLU:N	2.37	0.53
2:B:45:MET:SD	2:D:274:ASP:CG	2.91	0.53
2:B:209:VAL:HA	2:B:232:THR:HG23	1.90	0.53
2:B:377:VAL:HB	2:B:381:ASP:HB2	1.89	0.53
1:C:193:LEU:O	1:C:197:LEU:HD23	2.08	0.53
1:A:96:VAL:HG11	1:A:131:LEU:CD1	2.39	0.53
1:C:249:PRO:O	1:C:400:HIS:ND1	2.33	0.53
1:C:390[A]:TRP:NE1	1:C:393:GLU:HB2	2.23	0.53
2:D:102:ASP:O	2:D:104:THR:OG1	2.25	0.53
1:A:216:VAL:HA	1:A:220:THR:HG21	1.91	0.53
2:B:49:ARG:NH1	2:B:163:ALA:HB1	2.13	0.53
4:B:601:PMR:HMAB	2:D:46:ILE:HD13	1.91	0.53
2:D:161:PRO:O	2:D:192:MET:HB2	2.09	0.53
2:D:239:VAL:HG22	2:D:264:LEU:HD11	1.91	0.53
2:D:184:ILE:HD12	2:D:207:PHE:CE1	2.43	0.52
1:A:39:ARG:NH1	2:D:418:PHE:O	2.42	0.52
1:A:373:CYS:O	1:A:375:LEU:HD22	2.09	0.52
2:B:348:LEU:HD12	2:B:348:LEU:O	2.09	0.52
1:C:144:PHE:HE1	1:C:159:ALA:HB3	1.73	0.52
2:B:419:ARG:CD	1:C:65:MET:HB2	2.40	0.52
1:C:288:VAL:HG13	1:C:409:ALA:HB2	1.91	0.52
2:D:213:PRO:CB	2:D:217:GLU:HB2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:284:PHE:HE2	2:D:286:PHE:HB2	1.74	0.52
1:A:65:MET:HG3	2:D:418:PHE:CD2	2.45	0.52
1:C:182:LEU:HD12	1:C:186:VAL:HG13	1.89	0.52
2:D:224:GLU:HB2	2:D:230:PRO:HA	1.91	0.52
1:C:28:PHE:CE1	1:C:392:ILE:HD11	2.44	0.52
2:D:8:TYR:O	2:D:376:PRO:HB3	2.09	0.52
1:A:314:ARG:HG3	1:A:315:PHE:N	2.25	0.52
1:C:367:ARG:O	1:C:367:ARG:HG3	2.10	0.52
2:D:155:SER:H	2:D:206:HIS:CD2	2.28	0.52
1:A:194:LEU:O	1:A:198:GLY:N	2.27	0.52
2:B:19:VAL:HG21	2:B:136:SER:HB2	1.91	0.52
2:B:274:ASP:OD1	2:D:48:ARG:HD3	2.10	0.52
2:B:415:LEU:HD11	2:D:361:HIS:HD2	1.75	0.52
1:A:295:LEU:HD11	1:A:412:PHE:HB3	1.90	0.52
1:C:56:HIS:HA	1:C:59:GLN:HB3	1.92	0.52
1:C:162:ALA:O	1:C:166:PRO:HD3	2.09	0.52
1:C:226:GLN:HG2	1:C:229:LEU:HG	1.91	0.52
1:C:312:LEU:HD22	1:C:412:PHE:HE2	1.75	0.52
2:D:19:VAL:HG11	2:D:136:SER:HB3	1.92	0.52
1:A:70:PRO:HD2	2:B:5:LEU:HD21	1.91	0.52
1:A:396:PHE:CE2	4:A:502:PMR:HACA	2.43	0.52
4:B:601:PMR:HMC	1:C:392:ILE:HG21	1.92	0.52
2:D:180:GLU:OE1	2:D:180:GLU:HA	2.10	0.52
1:A:107:ARG:O	1:A:140:ARG:N	2.43	0.51
2:B:17:MET:HE1	2:B:39:ALA:HB3	1.92	0.51
1:C:255:THR:HG23	1:C:281:ARG:NH1	2.25	0.51
2:D:278:LEU:HD12	2:D:305:PHE:CZ	2.45	0.51
1:A:203:ARG:HD3	1:A:215:GLY:H	1.75	0.51
2:B:156:CYS:SG	2:B:179:LEU:HD13	2.51	0.51
2:B:210:LEU:HD13	2:B:220:ALA:HB3	1.92	0.51
2:B:356:THR:HB	2:B:376:PRO:HG2	1.91	0.51
2:B:388:PRO:HD2	2:B:397:VAL:HG21	1.91	0.51
1:C:45:PHE:HD2	1:C:106:ILE:HG21	1.74	0.51
1:C:57:LEU:HD13	2:D:38:TYR:HB2	1.93	0.51
1:C:95:GLU:O	1:C:99:LEU:HD12	2.09	0.51
1:A:135:HIS:HB3	1:A:139:VAL:HB	1.91	0.51
1:C:153:PHE:CE2	1:C:306:SER:HA	2.44	0.51
2:D:171:ASP:CG	2:D:390:MET:HG3	2.35	0.51
1:A:270:ALA:HA	1:A:273:PHE:HB2	1.92	0.51
1:C:161:LEU:HD12	1:C:229:LEU:HD11	1.92	0.51
1:C:375:LEU:HD21	2:D:41:LEU:CD1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:99:LEU:HD13	2:D:124:SER:HB2	1.91	0.51
1:A:288:VAL:HG13	1:A:409:ALA:HB2	1.93	0.51
1:A:312:LEU:HA	1:A:315:PHE:CZ	2.46	0.51
2:B:259:ALA:HB1	2:B:392:PHE:HE2	1.76	0.51
2:B:262:SER:O	2:B:265:ARG:NH2	2.44	0.51
1:C:96:VAL:HA	1:C:99:LEU:HD13	1.93	0.51
2:D:288:ASP:HA	2:D:314:ASN:OD1	2.09	0.51
2:B:18:ARG:NE	2:B:164:LEU:O	2.44	0.51
2:B:48:ARG:C	2:D:268:TRP:HE1	2.16	0.51
2:B:270:SER:O	2:B:275:SER:HB2	2.11	0.51
1:A:179:VAL:HA	1:A:205:LEU:HB3	1.93	0.51
2:B:35:GLY:C	2:B:37:THR:H	2.19	0.51
2:B:95:CYS:SG	2:B:96:THR:N	2.84	0.51
1:C:302:PHE:CD1	1:C:309:GLU:HG3	2.46	0.51
1:A:114:SER:C	1:A:147:SER:HB3	2.36	0.50
4:B:601:PMR:HBB	1:C:61:ALA:HB2	1.93	0.50
2:D:46:ILE:HD13	2:D:379:VAL:HB	1.91	0.50
1:A:312:LEU:HD22	1:A:412:PHE:CE2	2.47	0.50
1:C:176:LEU:HD22	1:C:199:ILE:HG21	1.92	0.50
1:C:293:GLU:OE1	1:C:293:GLU:N	2.39	0.50
2:D:137:PHE:CZ	2:D:191:PRO:HA	2.46	0.50
1:A:304:PRO:HD3	1:A:359:GLN:HE22	1.75	0.50
2:B:419:ARG:HD2	1:C:65:MET:HA	1.92	0.50
2:D:74:GLN:HE21	2:D:107:LEU:HB2	1.75	0.50
2:D:278:LEU:HD12	2:D:305:PHE:CE1	2.47	0.50
2:B:31:HIS:HE1	2:B:69:THR:HG23	1.76	0.50
1:C:307:GLN:CG	1:C:330:PRO:CD	2.89	0.50
1:A:337:LEU:O	1:A:341:LEU:N	2.39	0.50
1:A:282:ALA:O	1:A:285:ARG:HG3	2.11	0.50
1:C:306:SER:HB3	1:C:391:ALA:HB1	1.92	0.50
2:B:137:PHE:CD1	2:B:191:PRO:HB3	2.47	0.50
2:B:236:PRO:O	2:B:391:GLY:N	2.42	0.50
2:B:264:LEU:HD22	2:B:392:PHE:HD1	1.76	0.50
1:C:380:PRO:O	1:C:384:GLU:HG3	2.11	0.50
1:A:217:GLY:O	1:A:220:THR:OG1	2.29	0.50
1:A:399:VAL:HB	1:A:408:LEU:HD22	1.93	0.50
2:B:35:GLY:C	2:B:37:THR:N	2.70	0.50
2:D:358:MET:O	2:D:362:ILE:HG13	2.12	0.50
2:D:360:ARG:HD3	2:D:370:CYS:SG	2.52	0.50
1:A:116:PRO:HD3	3:A:501:SF4:S1	2.52	0.50
1:A:248:PHE:CZ	1:A:336:ILE:HG22	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:383:PRO:HG2	2:B:387:SER:HB2	1.94	0.50
2:B:415:LEU:HD11	2:D:361:HIS:CD2	2.47	0.50
2:D:81:TYR:CD1	2:D:111:LEU:HD13	2.47	0.50
2:D:184:ILE:HD11	2:D:253:ALA:HB2	1.94	0.50
1:C:36:TRP:HB2	1:C:396:PHE:CE1	2.47	0.49
2:D:187:ASN:O	2:D:201:ARG:NH2	2.45	0.49
1:A:224:LEU:HB3	1:A:248:PHE:HE1	1.77	0.49
1:A:405:ALA:O	1:A:408:LEU:HB3	2.13	0.49
1:A:422:LEU:HD21	2:D:270:SER:O	2.12	0.49
2:D:90:MET:HE3	2:D:120:LEU:CG	2.32	0.49
1:A:179:VAL:HG13	1:A:205:LEU:HG	1.94	0.49
1:C:418:ARG:HD3	1:C:418:ARG:C	2.36	0.49
1:A:263:ALA:HB1	1:A:268:VAL:HB	1.94	0.49
1:A:375:LEU:HD11	1:A:390[A]:TRP:HA	1.94	0.49
1:A:29:CYS:SG	3:A:501:SF4:S4	3.10	0.49
1:A:30:GLY:N	1:A:146:GLY:O	2.45	0.49
1:A:158:ASP:HB2	1:A:229:LEU:HA	1.95	0.49
1:A:227:PRO:CD	1:A:250:PHE:HE2	2.24	0.49
2:B:33:PRO:HG3	2:B:60:PHE:CZ	2.48	0.49
1:C:56:HIS:CE1	2:D:42:LEU:HD21	2.47	0.49
2:D:377:VAL:HG21	2:D:381:ASP:HB2	1.94	0.49
1:C:249:PRO:HB2	1:C:401[B]:PHE:CD1	2.48	0.49
1:A:153:PHE:CZ	1:A:392:ILE:HG13	2.48	0.49
2:B:182:MET:HE1	2:B:249:VAL:HG23	1.94	0.49
1:A:384:GLU:N	1:A:384:GLU:OE1	2.46	0.49
2:B:167:ARG:O	2:B:212:TYR:OH	2.31	0.49
2:D:157:ASN:OD1	2:D:202:LEU:HG	2.12	0.49
1:A:25:ARG:N	2:B:59:THR:OG1	2.43	0.49
1:A:242:ARG:NH2	1:A:265:GLU:HB3	2.28	0.49
1:A:280:PRO:HB2	1:A:402:TYR:CD2	2.43	0.49
2:B:271:ALA:HB2	1:C:422:LEU:HB3	1.95	0.49
1:C:88:ALA:HB1	1:C:122:LEU:HD21	1.94	0.49
2:D:74:GLN:NE2	2:D:107:LEU:H	2.11	0.49
2:D:47:GLU:HB2	2:D:164:LEU:HD12	1.95	0.48
2:B:33:PRO:HG2	2:B:96:THR:HB	1.94	0.48
1:C:249:PRO:HB2	1:C:401[B]:PHE:HD1	1.76	0.48
2:D:284:PHE:CE2	2:D:286:PHE:HB2	2.48	0.48
1:A:303:LEU:HD13	1:A:359:GLN:NE2	2.28	0.48
2:B:9:GLU:OE2	2:B:130:ASN:ND2	2.46	0.48
2:B:243:ARG:HG3	2:B:243:ARG:HH11	1.78	0.48
2:D:61[A]:GLN:CD	2:D:61[A]:GLN:H	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:356:THR:HG22	2:D:376:PRO:HD2	1.95	0.48
1:A:158:ASP:OD2	1:A:231:ASP:HB2	2.13	0.48
1:A:312:LEU:HD22	1:A:412:PHE:HE2	1.77	0.48
1:C:124:LEU:HB2	1:C:143:ASN:HB2	1.94	0.48
2:D:61[A]:GLN:HB2	2:D:63:ARG:HD2	1.95	0.48
1:A:252:GLU:O	1:A:256:THR:OG1	2.18	0.48
1:A:400:HIS:HB3	1:A:401:PHE:CD1	2.48	0.48
2:D:169:ARG:NH2	2:D:384:ALA:O	2.47	0.48
1:A:222:PHE:HD2	1:A:236:LEU:CD2	2.26	0.48
1:A:216:VAL:HG11	1:A:236:LEU:HD11	1.96	0.48
1:A:370:LEU:CD1	1:A:389:LYS:HB3	2.41	0.48
2:B:21:THR:O	2:B:49:ARG:NH2	2.47	0.48
2:D:74:GLN:HE21	2:D:107:LEU:H	1.62	0.48
2:D:321:MET:HE3	2:D:321:MET:HB3	1.68	0.48
1:A:24:GLN:HB3	2:B:57:TYR:O	2.14	0.48
2:D:235:VAL:HG12	2:D:237:ILE:HG13	1.96	0.48
1:A:74:THR:HG22	1:A:74:THR:O	2.13	0.48
2:D:6:TRP:CD1	2:D:6:TRP:C	2.92	0.48
2:D:21:THR:HG22	2:D:49:ARG:HH11	1.78	0.48
2:D:322:ARG:HB3	2:D:326:LYS:NZ	2.29	0.48
2:D:371:ALA:HB2	2:D:405:PRO:HG3	1.94	0.48
1:A:85:LEU:HD23	1:A:89:ASN:ND2	2.28	0.48
2:B:340:GLU:HA	2:B:343:GLU:OE1	2.14	0.48
1:C:308:LEU:HB3	1:C:312:LEU:HG	1.95	0.48
1:C:381:LEU:HG	1:C:386:PHE:CB	2.42	0.48
2:D:222:TRP:CD1	2:D:225:LYS:HZ1	2.32	0.48
1:A:34:ILE:HA	1:A:37:LEU:HB2	1.95	0.47
1:A:255:THR:HB	1:A:402:TYR:CE1	2.49	0.47
2:B:34:GLN:HB3	2:B:59:THR:HB	1.95	0.47
1:C:38:HIS:CE1	1:C:71:ARG:H	2.33	0.47
1:C:326:GLU:HG2	1:C:349:VAL:HB	1.96	0.47
2:D:18:ARG:HB3	2:D:163:ALA:O	2.14	0.47
2:D:313:TYR:OH	2:D:376:PRO:HD3	2.13	0.47
2:B:31:HIS:NE2	2:B:69:THR:O	2.48	0.47
1:C:303:LEU:HB3	1:C:373:CYS:HA	1.94	0.47
1:A:115:CYS:SG	3:A:501:SF4:S1	3.11	0.47
1:A:358:ARG:HB2	1:A:362:ARG:HH21	1.79	0.47
1:C:162:ALA:HB2	1:C:232:THR:HA	1.96	0.47
1:A:225:VAL:HG12	1:A:400:HIS:CD2	2.50	0.47
1:A:250:PHE:HB3	1:A:315:PHE:CE2	2.50	0.47
2:B:303:MET:HE3	2:B:399:PHE:HD1	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:PRO:HA	1:A:248:PHE:CE2	2.49	0.47
1:A:373:CYS:SG	1:A:375:LEU:HB3	2.54	0.47
2:B:284:PHE:C	2:B:285:LEU:HD12	2.40	0.47
1:C:380:PRO:HA	1:C:383:ALA:HB3	1.96	0.47
2:D:38:TYR:HA	2:D:41:LEU:HD13	1.96	0.47
2:D:210:LEU:HD23	2:D:211:LEU:N	2.29	0.47
1:A:418:ARG:O	1:A:422:LEU:HB2	2.14	0.47
2:B:410:LEU:O	2:B:414:LEU:HD12	2.15	0.47
1:C:183:PRO:O	1:C:187:GLU:N	2.46	0.47
1:C:326:GLU:HA	1:C:349:VAL:H	1.80	0.47
1:C:399:VAL:HA	1:C:404:GLN:O	2.15	0.47
2:D:131:PHE:CD1	2:D:135:GLU:HG2	2.49	0.47
2:D:213:PRO:O	2:D:214:GLU:C	2.56	0.47
1:A:400:HIS:HB3	1:A:401:PHE:HD1	1.79	0.47
2:B:419:ARG:CD	1:C:65:MET:HE3	2.33	0.47
1:C:258:TRP:CE3	1:C:259:LEU:HG	2.50	0.47
2:D:95:CYS:HA	2:D:98:GLU:O	2.14	0.47
2:D:213:PRO:HB3	2:D:217:GLU:HB2	1.97	0.47
1:A:126:ARG:HH21	1:A:130:ARG:HH22	1.63	0.47
2:B:52:ARG:O	2:B:54:PRO:N	2.48	0.47
2:B:278:LEU:HB3	2:B:305:PHE:HD2	1.79	0.47
1:A:150:GLU:N	1:A:150:GLU:OE2	2.48	0.47
2:B:407:THR:OG1	2:D:380:GLN:NE2	2.48	0.47
2:D:238:GLY:O	2:D:242:THR:N	2.41	0.47
2:D:353:ILE:O	2:D:353:ILE:HG22	2.15	0.47
1:A:263:ALA:HB3	1:A:273:PHE:CZ	2.49	0.47
1:A:389:LYS:HB2	1:A:415:PRO:HG2	1.96	0.47
2:B:408:MET:O	2:B:411:GLU:HG2	2.15	0.47
1:C:74:THR:H	2:D:3:LEU:HD23	1.78	0.47
1:C:178:LEU:HD11	1:C:258:TRP:CZ2	2.50	0.47
1:A:149:ILE:O	2:B:62:ALA:N	2.44	0.46
2:B:26:MET:HE3	2:B:90:MET:HB2	1.97	0.46
2:B:311:GLY:HA3	2:B:333:LEU:HB3	1.97	0.46
1:C:153:PHE:CD2	1:C:154:THR:HG23	2.49	0.46
1:C:356:VAL:HA	1:C:359:GLN:HB3	1.96	0.46
1:A:48:VAL:HG21	1:A:58:LEU:HD11	1.98	0.46
2:B:28:TYR:CZ	2:B:120:LEU:HD12	2.50	0.46
2:B:284:PHE:HD1	2:B:353:ILE:HG13	1.79	0.46
2:D:131:PHE:HD1	2:D:135:GLU:HG2	1.81	0.46
2:B:38:TYR:O	2:B:41:LEU:N	2.47	0.46
2:B:338:TYR:CB	2:B:358:MET:HE2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:VAL:O	1:C:360:LEU:HD23	2.15	0.46
1:C:357:GLU:HB3	2:D:83:ARG:NH1	2.30	0.46
1:C:377:LEU:O	1:C:380:PRO:HD2	2.15	0.46
2:D:161:PRO:O	2:D:191:PRO:HB2	2.16	0.46
1:A:119:VAL:HG11	2:B:99:LEU:HB3	1.97	0.46
1:A:354:GLN:HB3	1:A:359:GLN:NE2	2.30	0.46
2:B:113:LEU:HD23	2:B:113:LEU:H	1.80	0.46
2:B:345:ILE:HD12	2:B:368:ILE:HD11	1.96	0.46
1:C:194:LEU:HB3	1:C:199:ILE:HD13	1.97	0.46
1:A:37:LEU:HB3	1:A:46:PHE:CZ	2.50	0.46
1:A:175:GLU:OE1	1:A:203:ARG:HD2	2.14	0.46
1:A:222:PHE:CB	1:A:236:LEU:HD22	2.44	0.46
1:A:227:PRO:HA	1:A:248:PHE:CZ	2.49	0.46
1:A:244:ILE:HG21	1:A:262:ILE:HG13	1.96	0.46
2:B:199:ILE:HA	2:B:202:LEU:HD13	1.96	0.46
2:B:272:SER:O	2:B:276:THR:OG1	2.32	0.46
2:D:163:ALA:HA	2:D:192:MET:CE	2.46	0.46
2:B:352:LEU:HD22	2:B:406:LEU:HG	1.97	0.46
1:C:199:ILE:HA	1:C:266:PHE:CE2	2.50	0.46
2:D:89:ILE:HG12	2:D:113:LEU:CD1	2.45	0.46
2:D:155:SER:HA	2:D:185:ALA:HB3	1.97	0.46
1:A:228:PHE:HB3	1:A:307:GLN:HB2	1.97	0.46
2:B:175:VAL:HG21	2:B:211:LEU:CD2	2.45	0.46
1:C:372:VAL:HB	1:C:389:LYS:HB3	1.97	0.46
1:A:312:LEU:HD13	1:A:412:PHE:HZ	1.81	0.46
2:B:387:SER:OG	2:D:385:ARG:NH2	2.41	0.46
1:C:202:VAL:HG23	1:C:203:ARG:H	1.81	0.46
2:D:70:ALA:HA	2:D:102:ASP:CG	2.40	0.46
2:D:303:MET:HE1	2:D:399:PHE:HD1	1.80	0.46
2:D:388:PRO:O	2:D:394:GLY:HA2	2.16	0.46
1:C:301:PHE:HE1	1:C:359:GLN:HE21	1.64	0.46
2:D:81:TYR:CD1	2:D:86:PRO:HD2	2.51	0.46
2:B:46:ILE:HD13	2:B:379:VAL:HG13	1.96	0.46
1:C:330:PRO:HG3	1:C:331:PHE:H	1.76	0.46
2:D:33:PRO:HD3	2:D:60:PHE:CE1	2.51	0.46
2:D:88:ALA:CA	2:D:113:LEU:HD13	2.44	0.46
2:D:246:VAL:HA	2:D:249:VAL:HG22	1.97	0.46
2:D:300:ARG:HH21	2:D:307:VAL:HB	1.81	0.46
2:D:361:HIS:HA	2:D:364:LYS:HD3	1.98	0.46
4:B:601:PMR:HBD	4:B:601:PMR:CBA	2.45	0.45
1:C:29:CYS:HB2	1:C:148:GLY:HA3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:322:ARG:NH1	2:D:334:VAL:HG11	2.30	0.45
1:A:54:CYS:SG	3:A:501:SF4:S1	3.14	0.45
1:A:302:PHE:CG	1:A:309:GLU:HB3	2.51	0.45
2:B:2:LYS:HE3	2:B:3:LEU:H	1.81	0.45
2:B:51:LYS:O	2:B:52:ARG:C	2.59	0.45
2:D:90:MET:HG2	2:D:118:VAL:CG1	2.44	0.45
1:A:73:GLY:HA2	2:B:3:LEU:HD21	1.99	0.45
1:A:326:GLU:HG3	1:A:328:GLY:H	1.81	0.45
1:C:381:LEU:CD1	1:C:386:PHE:CD2	2.98	0.45
1:A:174:ARG:HH12	1:A:242:ARG:NH2	2.15	0.45
1:A:226:GLN:HG2	1:A:400:HIS:CE1	2.52	0.45
1:C:65:MET:HG3	1:C:70:PRO:HG3	1.99	0.45
1:C:360:LEU:CD1	1:C:364:ARG:HH21	2.29	0.45
1:C:371:THR:O	1:C:371:THR:HG22	2.16	0.45
1:C:413:SER:O	1:C:417:ARG:HG2	2.16	0.45
1:A:228:PHE:HE2	1:A:308:LEU:HD12	1.82	0.45
2:B:210:LEU:CD1	2:B:220:ALA:HB2	2.40	0.45
1:C:34:ILE:HD11	1:C:144:PHE:HE2	1.82	0.45
2:D:284:PHE:HB2	2:D:350:PRO:HG2	1.99	0.45
1:A:222:PHE:HD2	1:A:236:LEU:HD23	1.81	0.45
1:A:390[B]:TRP:CE3	1:A:392:ILE:HB	2.52	0.45
2:B:212:TYR:CZ	2:B:390:MET:CE	3.00	0.45
1:C:92:LEU:O	1:C:95:GLU:HG3	2.17	0.45
1:C:186:VAL:HG21	1:C:400:HIS:O	2.16	0.45
1:C:256:THR:OG1	1:C:281:ARG:HD2	2.16	0.45
1:C:340:ASP:O	1:C:344:LEU:HB2	2.16	0.45
2:B:31:HIS:HD2	2:B:58:THR:OG1	2.00	0.45
2:B:220:ALA:HB1	2:B:231:TYR:HB2	1.99	0.45
2:D:161:PRO:HB2	2:D:172:ILE:HD11	1.99	0.45
2:D:318:ALA:HB1	2:D:322:ARG:NH2	2.30	0.45
2:B:14:VAL:O	2:B:18:ARG:HG3	2.17	0.45
1:C:186:VAL:HG21	1:C:404:GLN:OE1	2.16	0.45
1:A:86:ALA:HA	1:A:89:ASN:HD21	1.82	0.45
1:A:390[A]:TRP:HZ3	1:A:415:PRO:HG3	1.81	0.45
1:C:389:LYS:HD2	1:C:390[A]:TRP:H	1.81	0.45
2:B:86:PRO:O	2:B:115:VAL:HG11	2.17	0.45
4:B:601:PMR:CMC	1:C:392:ILE:HG21	2.47	0.45
1:C:306:SER:C	1:C:308:LEU:H	2.25	0.45
1:A:76:VAL:O	2:B:1:MET:HA	2.17	0.44
1:A:294:GLY:HA2	1:A:413:SER:HB2	2.00	0.44
1:C:227:PRO:HG2	1:C:308:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:PRO:HD2	1:C:258:TRP:HA	1.98	0.44
1:A:36:TRP:HE3	1:A:396:PHE:CE1	2.35	0.44
2:B:239:VAL:HG22	2:B:264:LEU:HD21	1.99	0.44
2:B:269:TRP:CZ3	2:D:48:ARG:HB2	2.52	0.44
1:C:312:LEU:HD22	1:C:412:PHE:CE2	2.52	0.44
1:C:377:LEU:CD2	1:C:380:PRO:HB2	2.47	0.44
2:D:32:ALA:HB1	2:D:36:ASP:HB2	2.00	0.44
2:D:138:LEU:HD13	2:D:218:SER:HB3	1.98	0.44
2:D:283:VAL:HG22	2:D:352:LEU:HB3	1.98	0.44
2:D:342:GLU:OE2	2:D:362:ILE:HG23	2.17	0.44
2:D:372:VAL:HG21	2:D:381:ASP:OD1	2.17	0.44
4:B:601:PMR:HMB	2:D:46:ILE:HG12	1.99	0.44
1:C:25:ARG:HD2	1:C:25:ARG:HA	1.79	0.44
1:C:303:LEU:HD23	1:C:304:PRO:HD2	1.99	0.44
1:A:390[B]:TRP:CD1	2:D:273:VAL:HG11	2.52	0.44
2:B:134:ASP:HB2	2:B:215:THR:HA	1.99	0.44
1:C:108:GLN:HA	1:C:142:TYR:CE1	2.49	0.44
2:D:136:SER:O	2:D:140:ILE:HG23	2.17	0.44
1:A:222:PHE:CE1	1:A:243:HIS:HB2	2.45	0.44
1:A:236:LEU:HD23	1:A:241:ALA:HB3	2.00	0.44
1:A:379:ASN:HB2	1:A:380:PRO:HD3	1.99	0.44
1:C:120:ILE:HB	1:C:122:LEU:HD23	2.00	0.44
1:C:377:LEU:HD23	1:C:380:PRO:HB2	1.99	0.44
2:D:207:PHE:HB2	2:D:230:PRO:O	2.18	0.44
2:B:309:GLY:H	2:B:330:LEU:HD23	1.82	0.44
1:C:360:LEU:CD1	1:C:364:ARG:NH2	2.80	0.44
2:D:89:ILE:HG12	2:D:113:LEU:HD11	1.99	0.44
1:A:242:ARG:HH12	1:A:265:GLU:HB3	1.82	0.44
1:A:421:ILE:O	1:A:423:ARG:NH2	2.45	0.44
1:C:197:LEU:HD13	1:C:268:VAL:HG11	1.99	0.44
1:C:248:PHE:HZ	1:C:337:LEU:HD22	1.83	0.44
2:D:90:MET:CE	2:D:120:LEU:CG	2.95	0.44
2:D:100:ILE:HG12	2:D:100:ILE:O	2.18	0.44
2:D:197:ALA:O	2:D:201:ARG:HG3	2.18	0.44
1:A:255:THR:HB	1:A:402:TYR:HE1	1.82	0.44
2:B:176:THR:HG23	2:B:186:VAL:HG21	1.99	0.44
2:B:393:GLU:OE1	2:D:386:TYR:N	2.49	0.44
2:D:74:GLN:OE1	2:D:104:THR:HB	2.18	0.44
2:D:370:CYS:O	2:D:405:PRO:HB3	2.18	0.44
1:A:66:ILE:HA	1:A:70:PRO:HG3	2.00	0.43
2:B:238:GLY:O	2:B:242:THR:OG1	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:275:SER:OG	2:D:48:ARG:NH2	2.50	0.43
1:C:74:THR:O	2:D:3:LEU:HA	2.18	0.43
1:C:304:PRO:HG3	1:C:354:GLN:OE1	2.18	0.43
1:C:360:LEU:HD11	1:C:364:ARG:HH21	1.82	0.43
2:D:208:ASN:O	2:D:231:TYR:HA	2.18	0.43
1:A:148:GLY:HA2	1:A:151:THR:O	2.19	0.43
1:A:295:LEU:CD2	1:A:322:MET:HE1	2.47	0.43
1:A:318:ARG:CD	1:A:343:LEU:HD22	2.47	0.43
1:A:367:ARG:HA	1:A:386:PHE:HE1	1.83	0.43
1:A:389:LYS:HD3	1:A:412:PHE:HA	1.99	0.43
1:C:389:LYS:HD2	1:C:390[B]:TRP:H	1.83	0.43
2:D:148:MET:H	2:D:203:GLY:HA3	1.83	0.43
2:D:266:GLN:OE1	2:D:303:MET:HE2	2.17	0.43
1:A:132:SER:OG	1:A:141:VAL:HG12	2.17	0.43
1:A:300:VAL:HB	1:A:322:MET:HE2	2.00	0.43
1:C:250:PHE:CE2	1:C:308:LEU:HD22	2.52	0.43
1:C:255:THR:HG23	1:C:281:ARG:HH11	1.83	0.43
2:D:46:ILE:O	2:D:379:VAL:HG23	2.18	0.43
2:D:184:ILE:HD11	2:D:253:ALA:CB	2.47	0.43
1:A:28:PHE:CZ	2:B:41:LEU:HD21	2.51	0.43
1:A:308:LEU:CD2	1:A:312:LEU:HD11	2.48	0.43
1:C:54:CYS:SG	3:C:501:SF4:S4	3.03	0.43
1:C:176:LEU:HD12	1:C:221:VAL:HG23	2.01	0.43
1:C:224:LEU:HD23	1:C:224:LEU:HA	1.87	0.43
1:C:248:PHE:CZ	1:C:337:LEU:HB3	2.54	0.43
1:C:291:ALA:HB3	1:C:409:ALA:HB3	1.99	0.43
1:C:381:LEU:HB3	1:C:388:THR:OG1	2.18	0.43
2:D:18:ARG:O	2:D:163:ALA:HB3	2.19	0.43
2:D:352:LEU:HD11	2:D:405:PRO:HG2	2.01	0.43
2:B:265:ARG:HB3	2:B:269:TRP:CD1	2.51	0.43
2:D:325:ALA:O	2:D:329:GLY:N	2.52	0.43
1:A:28:PHE:CE1	4:A:502:PMR:HMCB	2.54	0.43
2:B:239:VAL:O	2:B:243:ARG:HG2	2.19	0.43
2:B:341:VAL:O	2:B:345:ILE:HG23	2.17	0.43
1:C:113:GLY:H	1:C:145:SER:HA	1.83	0.43
1:A:26:GLU:CD	1:A:375:LEU:H	2.26	0.43
1:A:36:TRP:CD1	1:A:157:GLU:OE1	2.72	0.43
1:A:317:THR:HA	1:A:322:MET:N	2.27	0.43
2:B:94:SER:O	2:B:98:GLU:HG3	2.19	0.43
2:D:161:PRO:HA	2:D:168:HIS:ND1	2.33	0.43
1:A:82:LEU:HD23	1:A:82:LEU:HA	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:GLU:HA	1:A:256:THR:HB	2.00	0.43
1:A:379:ASN:ND2	2:D:272:SER:HB3	2.34	0.43
1:C:194:LEU:O	1:C:197:LEU:HB2	2.19	0.43
2:D:13:HIS:HE1	2:D:39:ALA:HB3	1.84	0.43
1:A:224:LEU:HB3	1:A:248:PHE:CE1	2.53	0.43
1:A:364:ARG:HA	1:A:386:PHE:CZ	2.54	0.43
2:B:89:ILE:HD12	2:B:89:ILE:HA	1.85	0.43
2:B:184:ILE:H	2:B:184:ILE:HD12	1.84	0.43
2:B:184:ILE:HD12	2:B:184:ILE:N	2.33	0.43
2:B:369:PRO:HB3	2:B:405:PRO:O	2.18	0.43
2:B:385:ARG:HB3	2:D:397:VAL:HA	2.00	0.43
1:C:26:GLU:O	1:C:375:LEU:HB3	2.18	0.43
1:C:227:PRO:HA	1:C:248:PHE:CD2	2.53	0.43
1:C:272:THR:O	1:C:276:VAL:HG22	2.18	0.43
2:D:356:THR:HG23	2:D:359:GLU:OE2	2.19	0.43
2:D:377:VAL:CG2	2:D:381:ASP:HB2	2.48	0.43
1:A:314:ARG:NE	1:A:340:ASP:OD1	2.52	0.43
1:A:378:ALA:HA	1:A:388:THR:HG21	2.01	0.43
1:C:160:CYS:O	1:C:164:ILE:HG13	2.19	0.43
2:D:24:THR:O	2:D:24:THR:OG1	2.36	0.43
1:A:41:MET:H	1:A:41:MET:HG2	1.67	0.42
1:A:134:HIS:CE1	1:A:135:HIS:ND1	2.87	0.42
1:C:92:LEU:HD22	1:C:122:LEU:HD12	2.01	0.42
1:C:151:THR:HG22	1:C:152:THR:N	2.35	0.42
1:C:250:PHE:CZ	1:C:308:LEU:CD2	3.01	0.42
2:D:90:MET:HB3	2:D:120:LEU:HD13	2.01	0.42
1:A:41:MET:HA	1:A:208:HIS:HA	2.01	0.42
2:B:259:ALA:HB1	2:B:392:PHE:CE2	2.54	0.42
2:B:265:ARG:O	2:B:269:TRP:HB2	2.19	0.42
2:B:386:TYR:CD2	2:D:386:TYR:HD2	2.37	0.42
1:A:34:ILE:O	1:A:38:HIS:ND1	2.48	0.42
2:B:155:SER:HA	2:B:185:ALA:O	2.19	0.42
1:C:64:VAL:HA	1:C:67:PHE:CD2	2.54	0.42
1:C:66:ILE:CD1	2:D:6:TRP:CE3	2.87	0.42
2:D:160:GLY:HA2	2:D:216:GLY:HA3	2.00	0.42
1:A:29:CYS:O	1:A:32:THR:HG22	2.19	0.42
2:B:21:THR:HG21	2:B:43:PHE:CD1	2.54	0.42
2:B:208:ASN:HD22	2:B:229:GLN:HB2	1.85	0.42
2:B:314:ASN:OD1	2:B:314:ASN:N	2.53	0.42
1:C:221:VAL:HB	1:C:244:ILE:HD11	2.01	0.42
2:D:213:PRO:HD2	2:D:290:THR:OG1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:312:CYS:HB3	2:D:321:MET:CE	2.48	0.42
1:A:153:PHE:CE2	1:A:392:ILE:HA	2.55	0.42
1:A:199:ILE:HD13	1:A:199:ILE:HG21	1.76	0.42
1:A:309:GLU:CD	1:A:309:GLU:H	2.27	0.42
1:C:52:ARG:O	1:C:56:HIS:CB	2.67	0.42
2:D:126:GLN:C	2:D:127:ARG:HG2	2.45	0.42
2:D:417:MET:O	2:D:417:MET:HG2	2.20	0.42
2:B:2:LYS:HD2	2:B:2:LYS:HA	1.86	0.42
4:B:601:PMR:CHC	1:C:390[B]:TRP:HH2	2.33	0.42
1:C:92:LEU:O	1:C:96:VAL:HG23	2.20	0.42
2:D:134:ASP:HB2	2:D:215:THR:HA	2.00	0.42
2:B:271:ALA:HB1	1:C:418:ARG:HH21	1.84	0.42
1:C:59:GLN:HA	1:C:66:ILE:HG21	2.02	0.42
1:C:389:LYS:HZ2	1:C:411:LEU:C	2.27	0.42
2:B:284:PHE:HB2	2:B:348:LEU:HD11	2.01	0.42
1:C:182:LEU:HD13	1:C:225:VAL:HG11	2.00	0.42
2:D:209:VAL:HA	2:D:232:THR:HG23	2.00	0.42
1:C:176:LEU:HB3	1:C:199:ILE:HD12	2.01	0.42
2:D:79:ASP:OD1	2:D:83:ARG:NH2	2.53	0.42
2:D:237:ILE:HD11	2:D:390:MET:HE3	2.00	0.42
1:A:122:LEU:HD12	1:A:122:LEU:HA	1.84	0.42
1:A:249:PRO:HD3	1:A:258:TRP:CD1	2.55	0.42
1:C:22:ARG:HG3	1:C:23:GLY:H	1.85	0.42
1:C:56:HIS:O	1:C:56:HIS:CD2	2.73	0.42
2:D:17:MET:HB3	2:D:43:PHE:CZ	2.55	0.42
1:A:303:LEU:HB2	1:A:373:CYS:HA	2.02	0.41
1:A:417:ARG:O	1:A:421:ILE:HG12	2.20	0.41
1:C:307:GLN:HG2	1:C:330:PRO:CD	2.50	0.41
2:D:162:THR:C	2:D:192:MET:SD	3.03	0.41
2:D:282:ARG:HB3	2:D:308:VAL:HG21	2.00	0.41
2:D:293:ILE:HG23	2:D:324:ALA:HB2	2.02	0.41
1:A:28:PHE:HA	2:B:35:GLY:HA2	2.02	0.41
1:A:248:PHE:O	1:A:314:ARG:NH2	2.52	0.41
1:A:378:ALA:HB1	2:D:273:VAL:HG21	2.02	0.41
2:B:238:GLY:C	2:B:242:THR:HG1	2.20	0.41
2:B:345:ILE:O	2:B:349:ALA:HA	2.20	0.41
1:C:38:HIS:ND1	1:C:71:ARG:NE	2.68	0.41
1:C:344:LEU:HD23	1:C:345:ALA:N	2.35	0.41
1:C:389:LYS:HD2	1:C:390[A]:TRP:CE3	2.55	0.41
2:D:43:PHE:O	2:D:49:ARG:HB2	2.21	0.41
2:D:380:GLN:OE1	2:D:380:GLN:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:393:GLU:HA	2:D:396:ASN:HB2	2.02	0.41
1:A:304:PRO:HD3	1:A:359:GLN:NE2	2.36	0.41
1:A:361:ASP:CG	2:B:83:ARG:HH12	2.28	0.41
2:B:296:ALA:HB1	2:B:328:TYR:HE2	1.84	0.41
1:C:153:PHE:CE2	1:C:154:THR:HG23	2.55	0.41
2:B:90:MET:HA	2:B:118:VAL:HG22	2.03	0.41
2:B:154:VAL:HA	2:B:206:HIS:ND1	2.35	0.41
2:B:243:ARG:NH2	2:B:261:ASP:OD2	2.53	0.41
1:C:375:LEU:HD23	1:C:375:LEU:HA	1.85	0.41
2:D:90:MET:HE2	2:D:120:LEU:HD13	1.89	0.41
1:A:103:ARG:HD3	2:D:419:ARG:HH22	1.86	0.41
1:C:66:ILE:HD12	2:D:6:TRP:CZ3	2.52	0.41
1:C:300:VAL:HA	1:C:370:LEU:O	2.21	0.41
1:C:344:LEU:HD21	1:C:348:PRO:HG2	2.02	0.41
2:D:300:ARG:NH2	2:D:307:VAL:O	2.54	0.41
2:D:363:ALA:HB1	2:D:368:ILE:O	2.21	0.41
1:A:36:TRP:HB3	1:A:396:PHE:CD1	2.54	0.41
1:A:263:ALA:HB3	1:A:273:PHE:HZ	1.85	0.41
2:B:141:CYS:HB3	2:B:222:TRP:CZ3	2.55	0.41
1:C:223:ALA:HB1	1:C:258:TRP:NE1	2.35	0.41
2:D:156:CYS:SG	2:D:179:LEU:HD13	2.61	0.41
1:A:50:GLY:O	1:A:76:VAL:HA	2.21	0.41
1:A:242:ARG:NH1	1:A:265:GLU:HB3	2.36	0.41
1:A:253:GLU:HG2	1:A:318:ARG:NH2	2.34	0.41
2:B:274:ASP:OD1	2:B:274:ASP:N	2.47	0.41
1:C:54:CYS:SG	3:C:501:SF4:S2	3.18	0.41
1:C:292:SER:O	1:C:292:SER:OG	2.27	0.41
2:D:362:ILE:O	2:D:366:LEU:N	2.54	0.41
2:D:38:TYR:CD2	2:D:38:TYR:C	2.97	0.41
1:A:308:LEU:O	1:A:312:LEU:HG	2.21	0.41
1:A:364:ARG:HA	1:A:386:PHE:HZ	1.86	0.41
1:A:390[B]:TRP:CZ2	4:A:502:PMR:H2O	2.56	0.41
2:B:30:LEU:O	2:B:57:TYR:HA	2.21	0.41
2:B:111:LEU:HD22	2:B:113:LEU:HD22	2.03	0.41
2:B:156:CYS:HB3	2:B:207:PHE:CZ	2.56	0.41
2:B:239:VAL:HG21	2:B:267:PRO:HD3	2.03	0.41
2:B:282:ARG:HB2	2:B:308:VAL:HG21	2.03	0.41
2:B:288:ASP:H	2:B:374:SER:CB	2.33	0.41
2:B:289:ALA:HB2	2:B:314:ASN:HB2	2.03	0.41
2:B:356:THR:HG22	2:B:374:SER:HB3	2.02	0.41
1:C:216:VAL:HG21	1:C:239:ARG:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:GLU:HG2	1:C:328:GLY:O	2.21	0.41
1:C:379:ASN:HB3	2:D:44:THR:OG1	2.21	0.41
2:D:26:MET:SD	2:D:90:MET:SD	3.18	0.41
2:D:303:MET:HE3	2:D:402:TRP:CE3	2.56	0.41
2:B:31:HIS:O	2:B:97:ALA:HB2	2.21	0.41
2:B:161:PRO:HB2	2:B:172:ILE:HD12	2.02	0.41
1:A:236:LEU:O	1:A:239:ARG:HB3	2.21	0.40
1:A:279:ALA:O	1:A:283:ARG:HB2	2.20	0.40
2:B:212:TYR:CE2	2:B:390:MET:CE	3.04	0.40
2:D:138:LEU:HD12	2:D:138:LEU:HA	1.86	0.40
2:D:153:LYS:HE2	2:D:153:LYS:HB2	1.86	0.40
2:D:286:PHE:HB3	2:D:359:GLU:CD	2.45	0.40
1:A:175:GLU:HG2	1:A:220:THR:HG22	2.02	0.40
1:A:177:LEU:HD23	1:A:203:ARG:HB2	2.02	0.40
1:C:154:THR:HB	1:C:228:PHE:CD1	2.55	0.40
2:D:285:LEU:HD21	2:D:354:LEU:HD12	2.03	0.40
2:D:339:LEU:HD13	2:D:339:LEU:HA	1.94	0.40
1:A:110:PHE:HA	1:A:142:TYR:O	2.22	0.40
2:B:40:ASP:O	2:B:44:THR:HG23	2.20	0.40
2:B:73:PHE:HD2	2:B:107:LEU:HD12	1.86	0.40
1:C:183:PRO:O	1:C:186:VAL:HG12	2.21	0.40
1:C:302:PHE:HB2	1:C:327:VAL:HA	2.03	0.40
2:D:201:ARG:HE	2:D:201:ARG:HB2	1.57	0.40
1:A:418:ARG:HH11	1:A:422:LEU:HD22	1.87	0.40
2:B:45:MET:CE	2:D:274:ASP:OD1	2.69	0.40
1:C:199:ILE:HA	1:C:266:PHE:CZ	2.57	0.40
1:C:282:ALA:HA	1:C:285:ARG:NH1	2.36	0.40
1:C:303:LEU:HD22	1:C:373:CYS:SG	2.61	0.40
2:D:12:PRO:HB2	2:D:122:LEU:HG	2.03	0.40
2:D:210:LEU:HD12	2:D:231:TYR:CD2	2.57	0.40
1:A:253:GLU:CB	1:A:318:ARG:HH12	2.29	0.40
2:B:88:ALA:HA	2:B:115:VAL:HB	2.02	0.40
2:B:237:ILE:HG12	2:B:389:GLN:O	2.21	0.40
2:D:283:VAL:HG22	2:D:352:LEU:CB	2.52	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	401/428 (94%)	359 (90%)	42 (10%)	0	100	100
1	C	383/428 (90%)	336 (88%)	45 (12%)	2 (0%)	24	55
2	B	418/536 (78%)	382 (91%)	36 (9%)	0	100	100
2	D	417/536 (78%)	370 (89%)	47 (11%)	0	100	100
All	All	1619/1928 (84%)	1447 (89%)	170 (10%)	2 (0%)	49	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	401[A]	PHE
1	C	401[B]	PHE

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	314/335 (94%)	309 (98%)	5 (2%)	55	72
1	C	305/335 (91%)	305 (100%)	0	100	100
2	B	335/415 (81%)	330 (98%)	5 (2%)	57	72
2	D	334/415 (80%)	329 (98%)	5 (2%)	57	72
All	All	1288/1500 (86%)	1273 (99%)	15 (1%)	65	75

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	CYS
1	A	115	CYS
1	A	134	HIS
1	A	390[A]	TRP
1	A	390[B]	TRP
2	B	34	GLN
2	B	37	THR
2	B	51	LYS
2	B	252	LEU
2	B	274	ASP
2	D	61[A]	GLN
2	D	61[B]	GLN
2	D	102	ASP
2	D	212	TYR
2	D	215	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	HIS
1	A	89	ASN
1	A	125	HIS
1	A	134	HIS
1	A	226	GLN
1	A	359	GLN
2	B	208	ASN
1	C	196	GLN
1	C	209	HIS
1	C	226	GLN
1	C	379	ASN
1	C	404	GLN
2	D	74	GLN
2	D	101	GLN
2	D	157	ASN
2	D	206	HIS
2	D	208	ASN
2	D	378	HIS
2	D	380	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	PMR	A	502	-	37,53,53	1.82	3 (8%)	36,89,89	3.29	13 (36%)
4	PMR	B	601	-	37,53,53	1.75	4 (10%)	36,89,89	3.17	12 (33%)
3	SF4	C	501	-	0,12,12	-	-	-		
3	SF4	A	501	-	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PMR	A	502	-	2/2/16/20	7/13/111/111	-
4	PMR	B	601	-	3/3/16/20	6/13/111/111	-
3	SF4	C	501	-	-	-	0/6/5/5
3	SF4	A	501	-	-	-	0/6/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	PMR	MG-NB	-6.78	1.92	2.05
4	B	601	PMR	MG-NB	-6.33	1.93	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	PMR	MG-ND	-6.18	1.93	2.05
4	B	601	PMR	MG-ND	-6.04	1.93	2.05
4	A	502	PMR	O2D-CGD	-3.27	1.25	1.33
4	B	601	PMR	O2D-CGD	-3.20	1.25	1.33
4	B	601	PMR	O2D-C2O	2.07	1.49	1.45

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	PMR	C4D-CHA-CBD	-8.63	100.27	108.97
4	A	502	PMR	C3D-C4D-CHA	8.55	121.54	108.54
4	A	502	PMR	C1A-CHA-C4D	7.52	125.91	119.15
4	A	502	PMR	C4D-CHA-CBD	-7.47	101.43	108.97
4	B	601	PMR	C3D-C4D-CHA	7.36	119.73	108.54
4	B	601	PMR	O2D-CGD-CBD	6.94	118.57	110.95
4	A	502	PMR	O2D-CGD-CBD	6.70	118.30	110.95
4	A	502	PMR	C4D-ND-C1D	6.66	110.28	105.22
4	B	601	PMR	C4D-ND-C1D	5.86	109.67	105.22
4	A	502	PMR	C2A-C1A-NA	-5.16	103.48	115.15
4	B	601	PMR	C1A-CHA-C4D	5.12	123.76	119.15
4	B	601	PMR	C2A-C1A-NA	-4.77	104.36	115.15
4	B	601	PMR	C3C-C4C-NC	-4.67	103.23	114.65
4	A	502	PMR	O1D-CGD-CBD	-3.72	119.09	124.72
4	B	601	PMR	C3D-C4D-ND	-3.61	107.15	112.94
4	B	601	PMR	O1D-CGD-CBD	-3.56	119.32	124.72
4	A	502	PMR	C3C-C4C-NC	-3.21	106.81	114.65
4	B	601	PMR	O2D-CGD-O1D	-3.01	117.98	123.85
4	A	502	PMR	C3D-C4D-ND	-2.70	108.61	112.94
4	A	502	PMR	O2D-CGD-O1D	-2.67	118.66	123.85
4	A	502	PMR	CBC-CAC-C3C	-2.55	109.22	112.87
4	B	601	PMR	C3A-C4A-NA	-2.55	103.24	110.46
4	A	502	PMR	C3A-C4A-NA	-2.54	103.27	110.46
4	B	601	PMR	CBC-CAC-C3C	-2.14	109.81	112.87
4	A	502	PMR	C4C-CHD-C1D	2.05	123.41	116.07

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	502	PMR	NB
4	A	502	PMR	NC
4	B	601	PMR	NC
4	B	601	PMR	NA

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Mol	Chain	Res	Type	Atom
4	B	601	PMR	NB

All (13) torsion outliers are listed below:

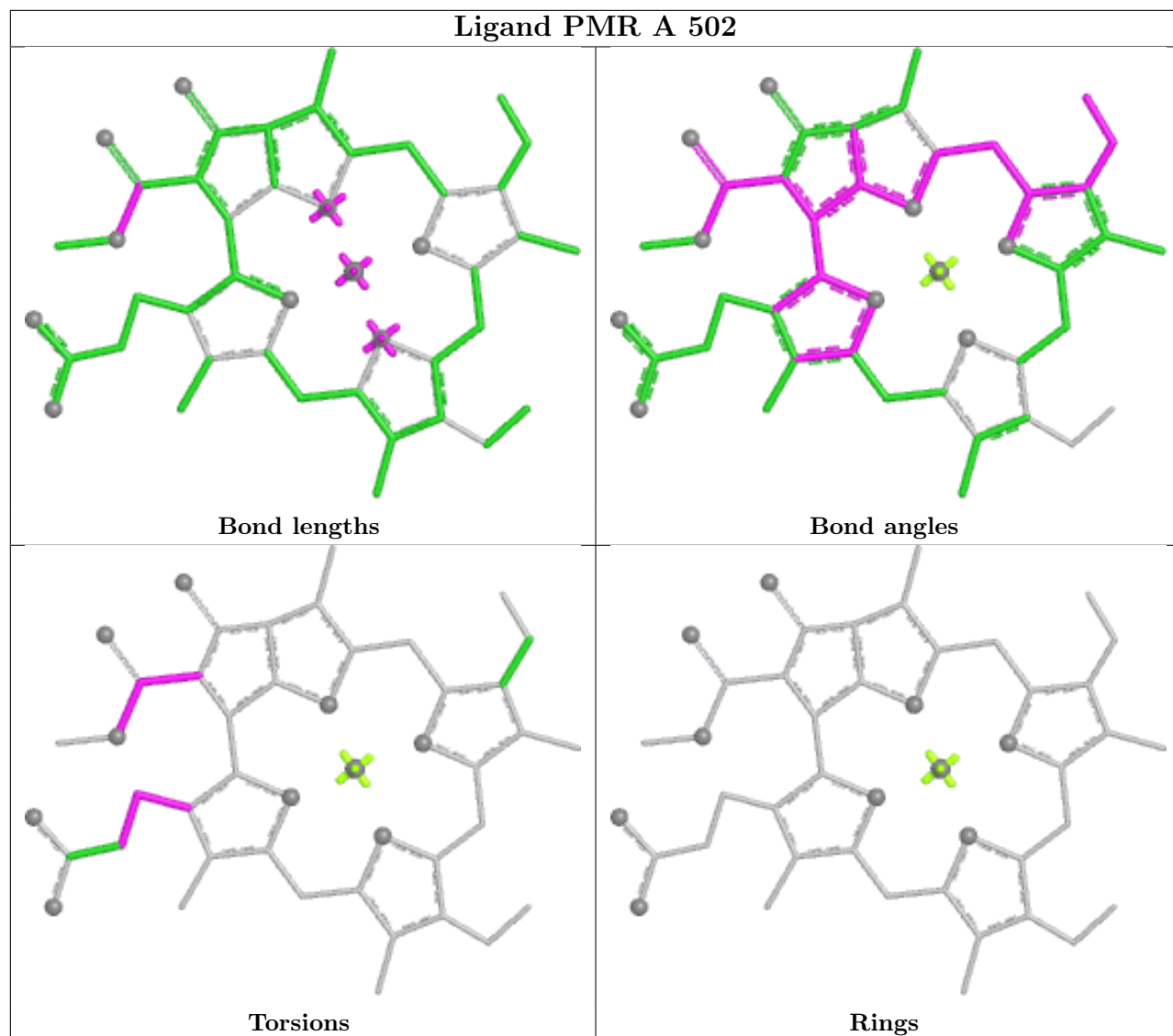
Mol	Chain	Res	Type	Atoms
4	A	502	PMR	CBD-CGD-O2D-C2O
4	A	502	PMR	C1A-C2A-CAA-CBA
4	A	502	PMR	C3A-C2A-CAA-CBA
4	B	601	PMR	CBD-CGD-O2D-C2O
4	B	601	PMR	O1D-CGD-O2D-C2O
4	A	502	PMR	O1D-CGD-O2D-C2O
4	A	502	PMR	C2A-CAA-CBA-CGA
4	B	601	PMR	C3A-C2A-CAA-CBA
4	A	502	PMR	CHA-CBD-CGD-O1D
4	A	502	PMR	CHA-CBD-CGD-O2D
4	B	601	PMR	CHA-CBD-CGD-O2D
4	B	601	PMR	C2A-CAA-CBA-CGA
4	B	601	PMR	CAA-CBA-CGA-O1A

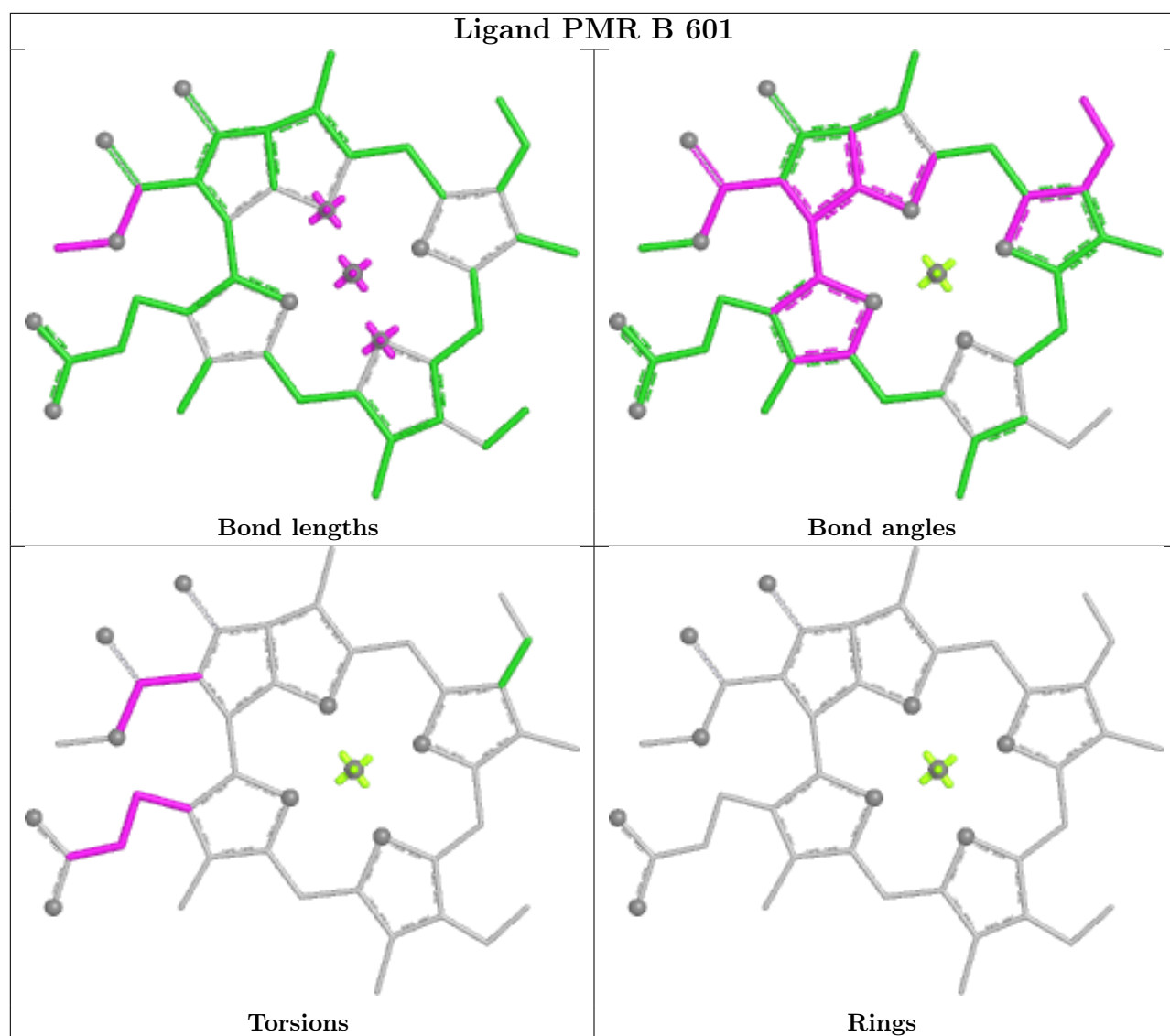
There are no ring outliers.

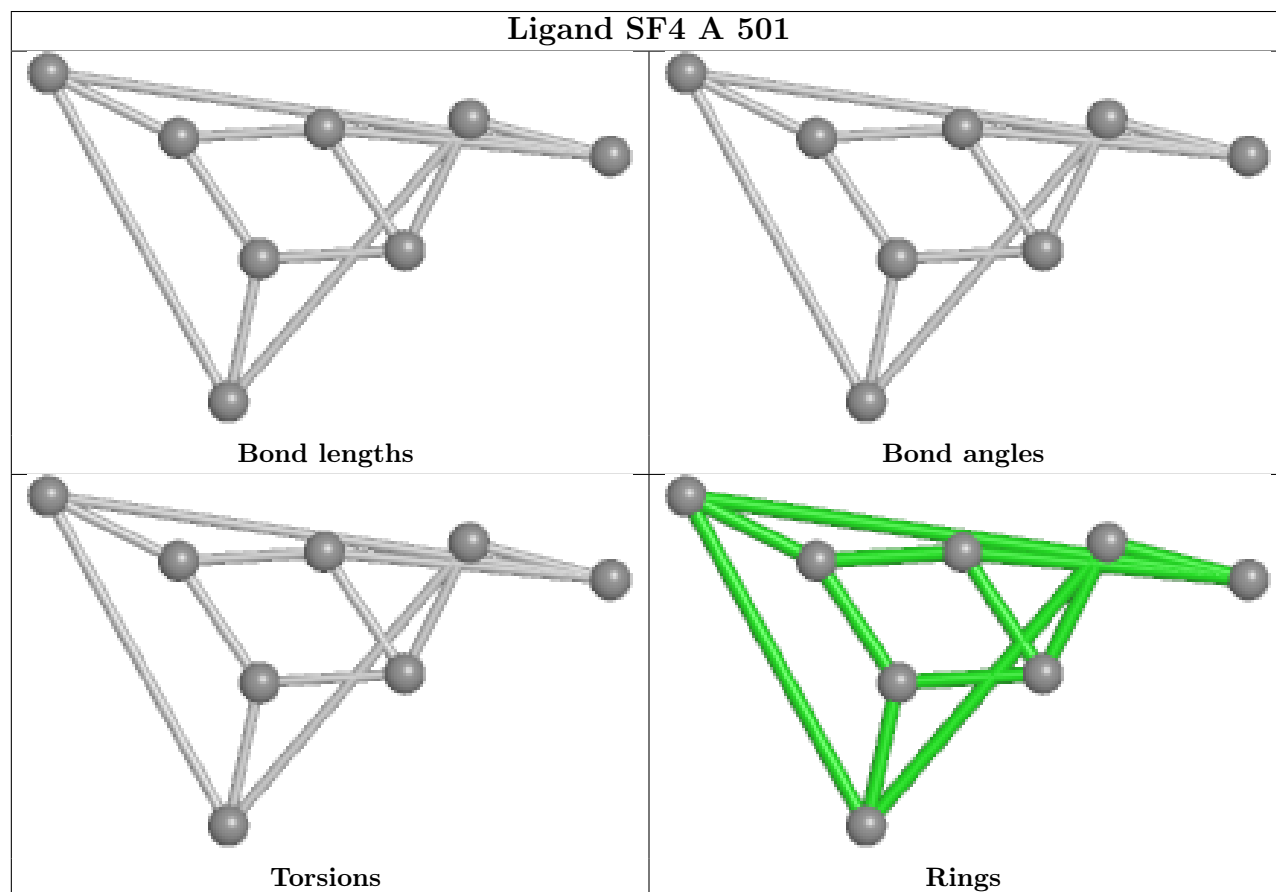
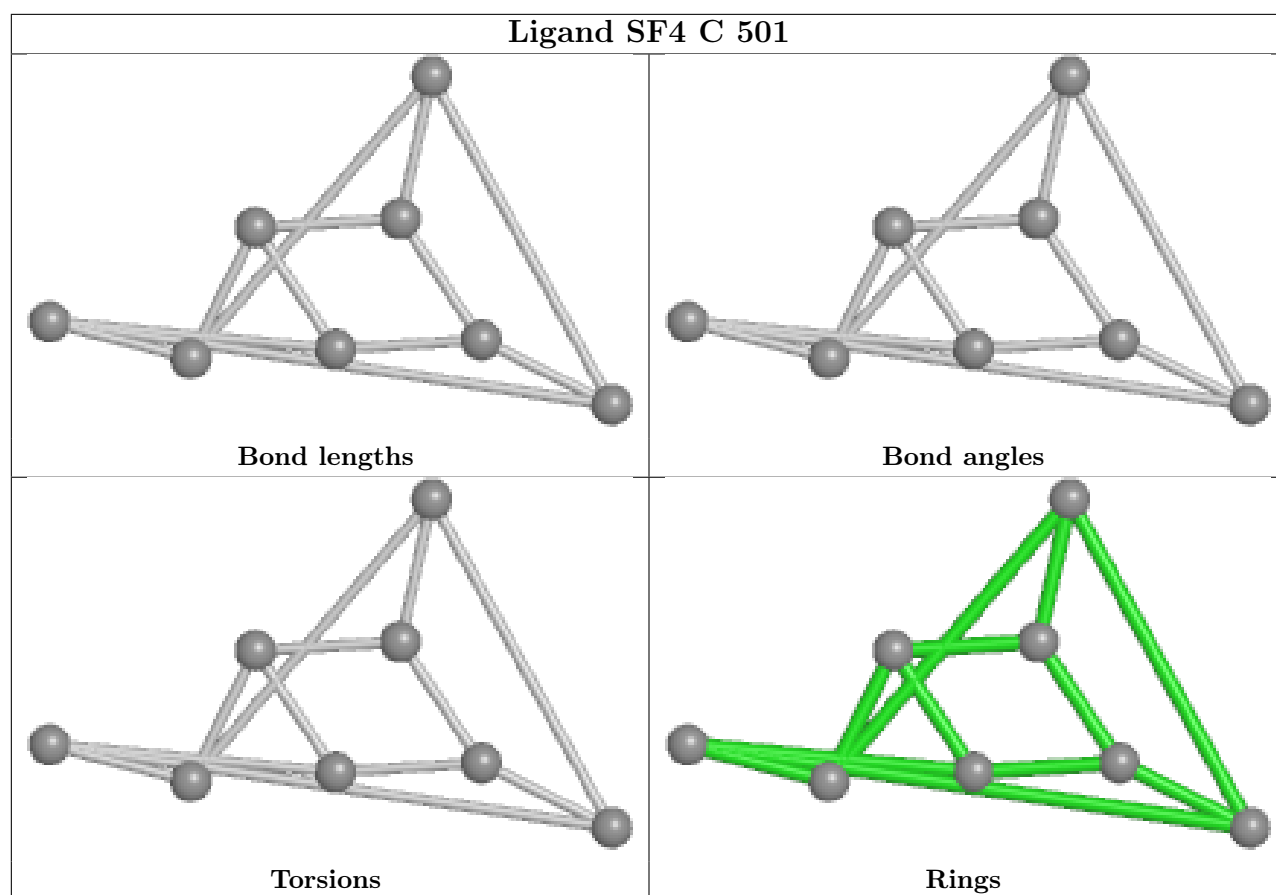
4 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	502	PMR	7	0
4	B	601	PMR	12	0
3	C	501	SF4	12	0
3	A	501	SF4	11	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

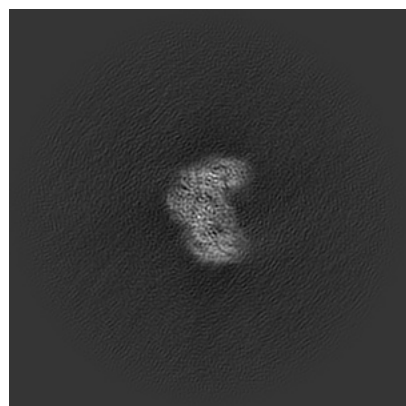
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47669. These allow visual inspection of the internal detail of the map and identification of artifacts.

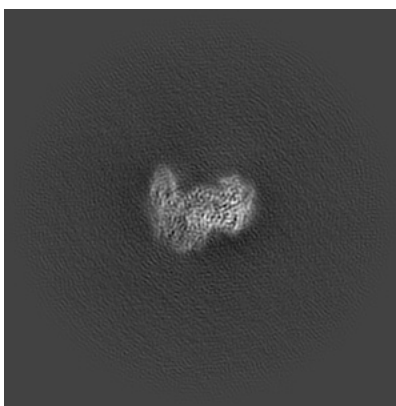
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

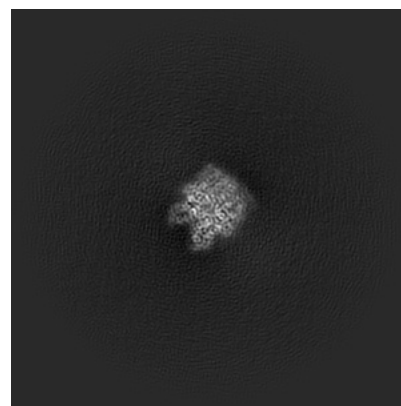
6.1.1 Primary map



X

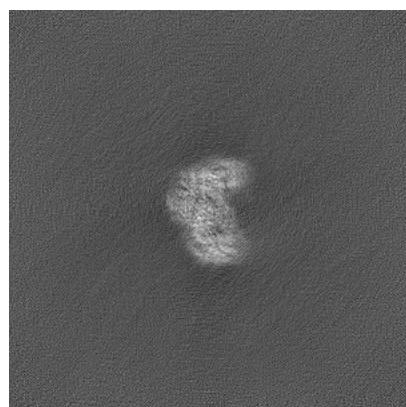


Y

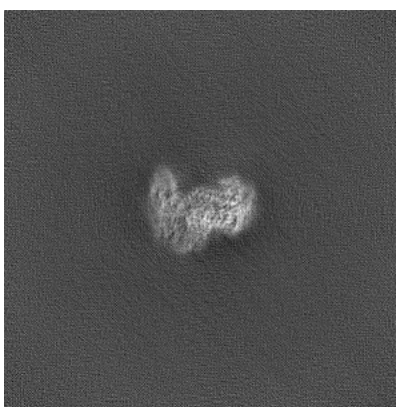


Z

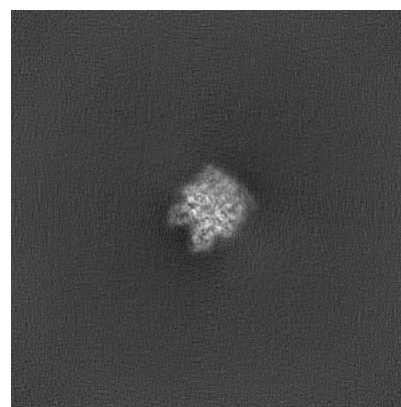
6.1.2 Raw map



X



Y

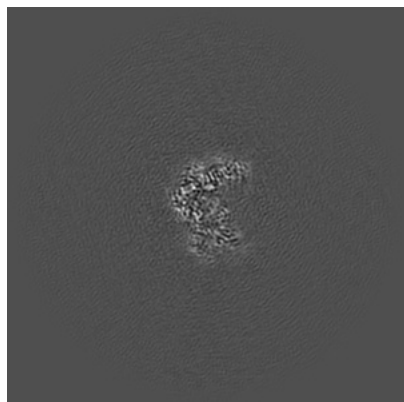


Z

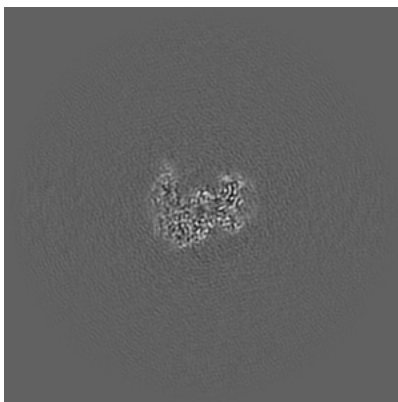
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

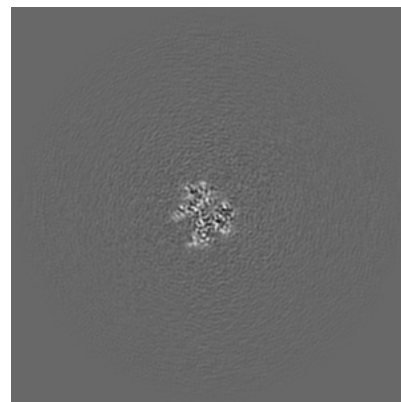
6.2.1 Primary map



X Index: 240

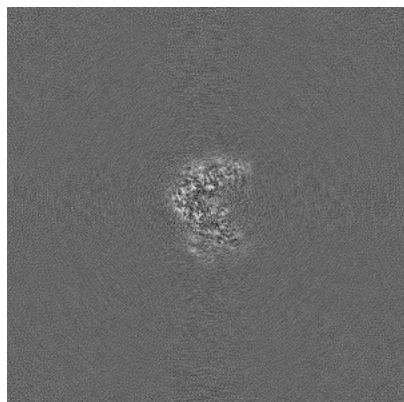


Y Index: 240

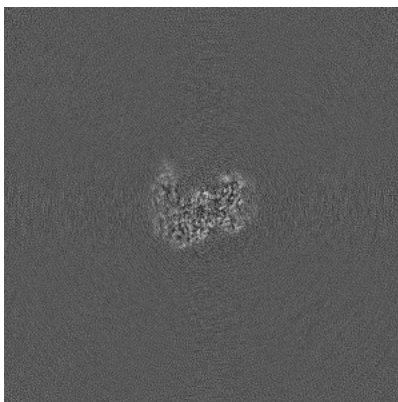


Z Index: 240

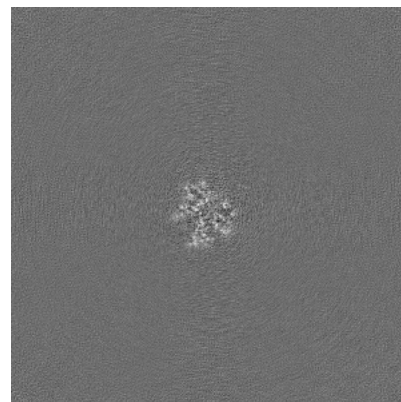
6.2.2 Raw map



X Index: 240



Y Index: 240

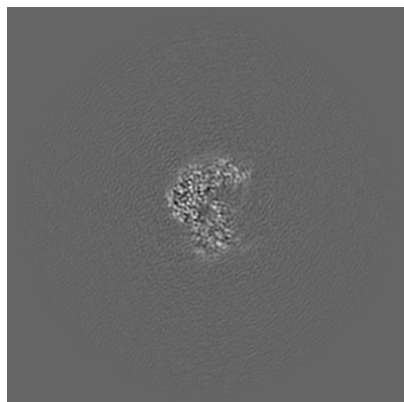


Z Index: 240

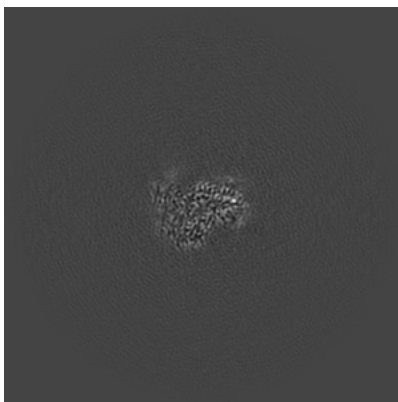
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

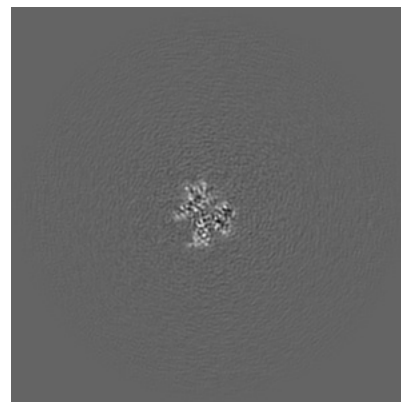
6.3.1 Primary map



X Index: 235

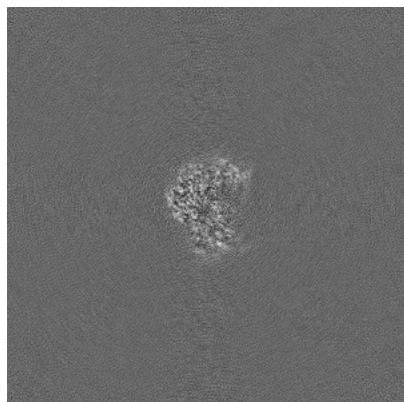


Y Index: 233

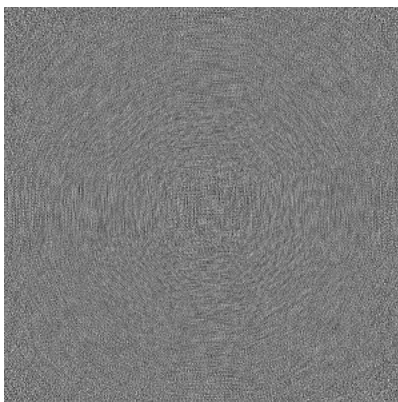


Z Index: 241

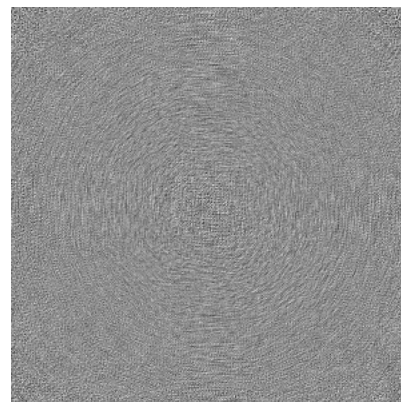
6.3.2 Raw map



X Index: 235



Y Index: 0

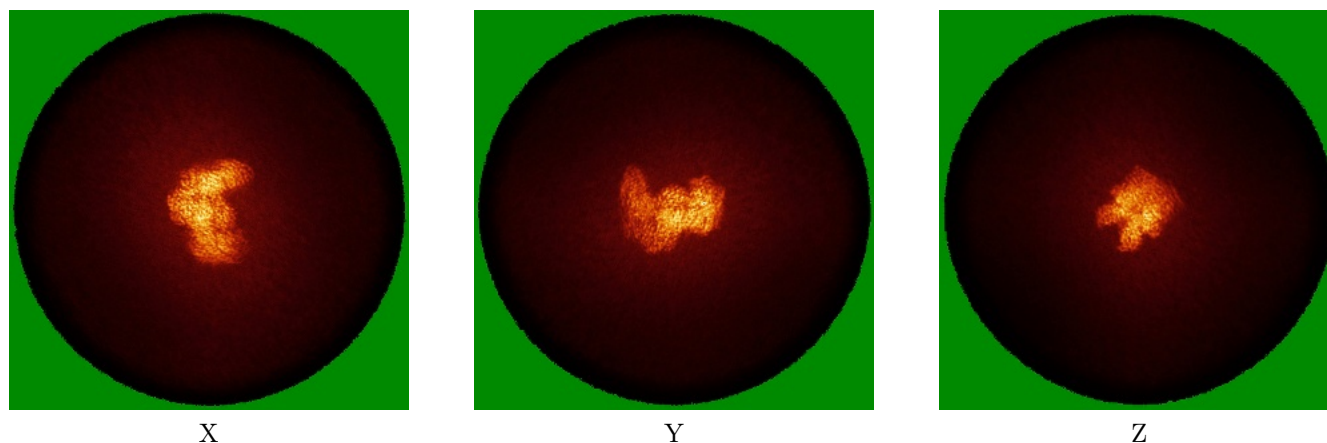


Z Index: 0

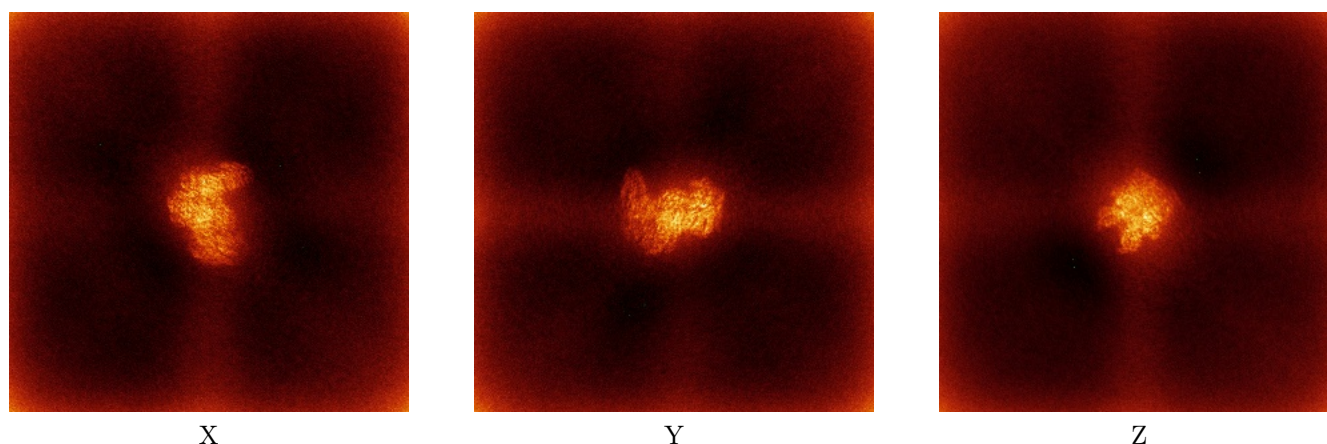
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

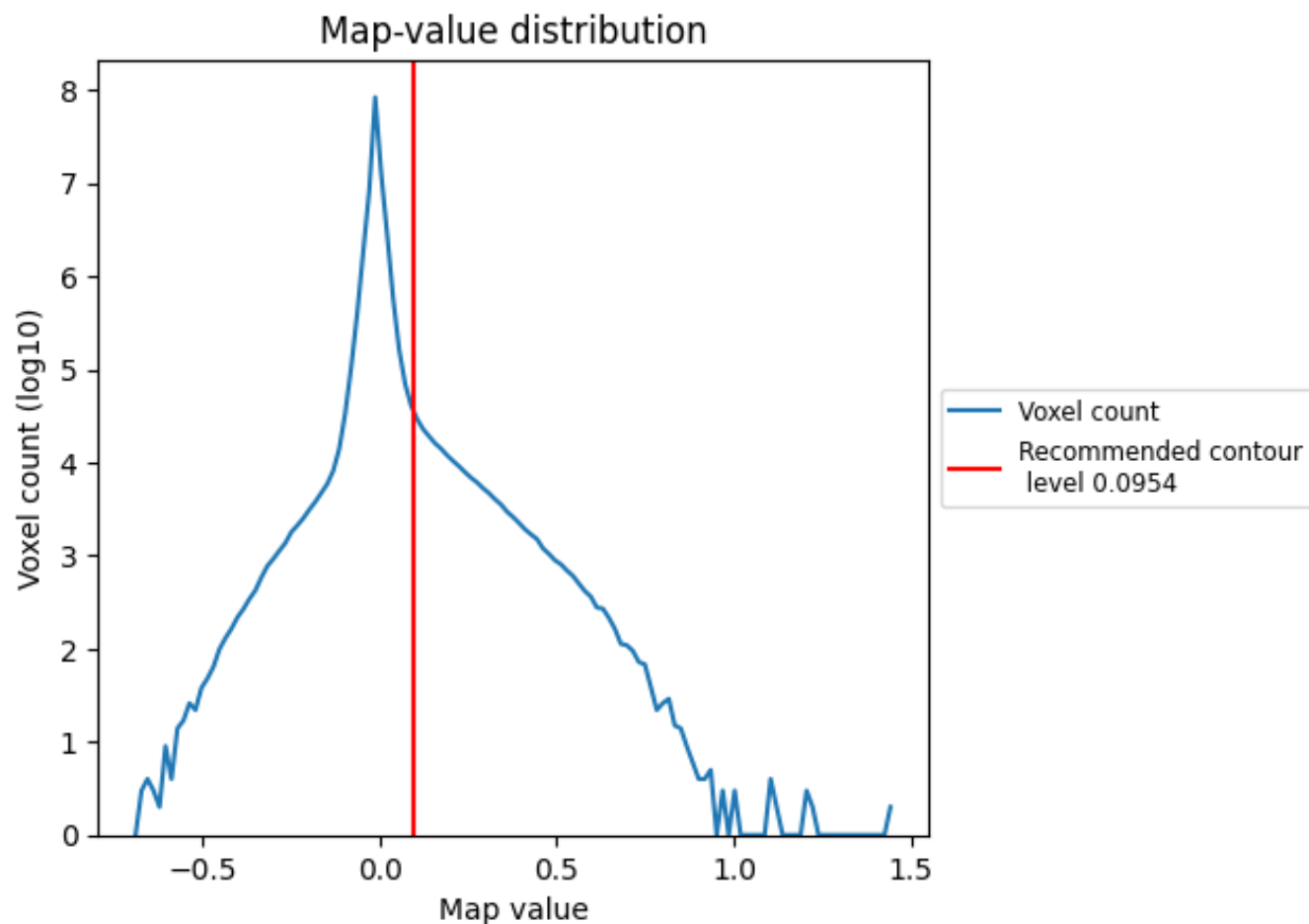
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

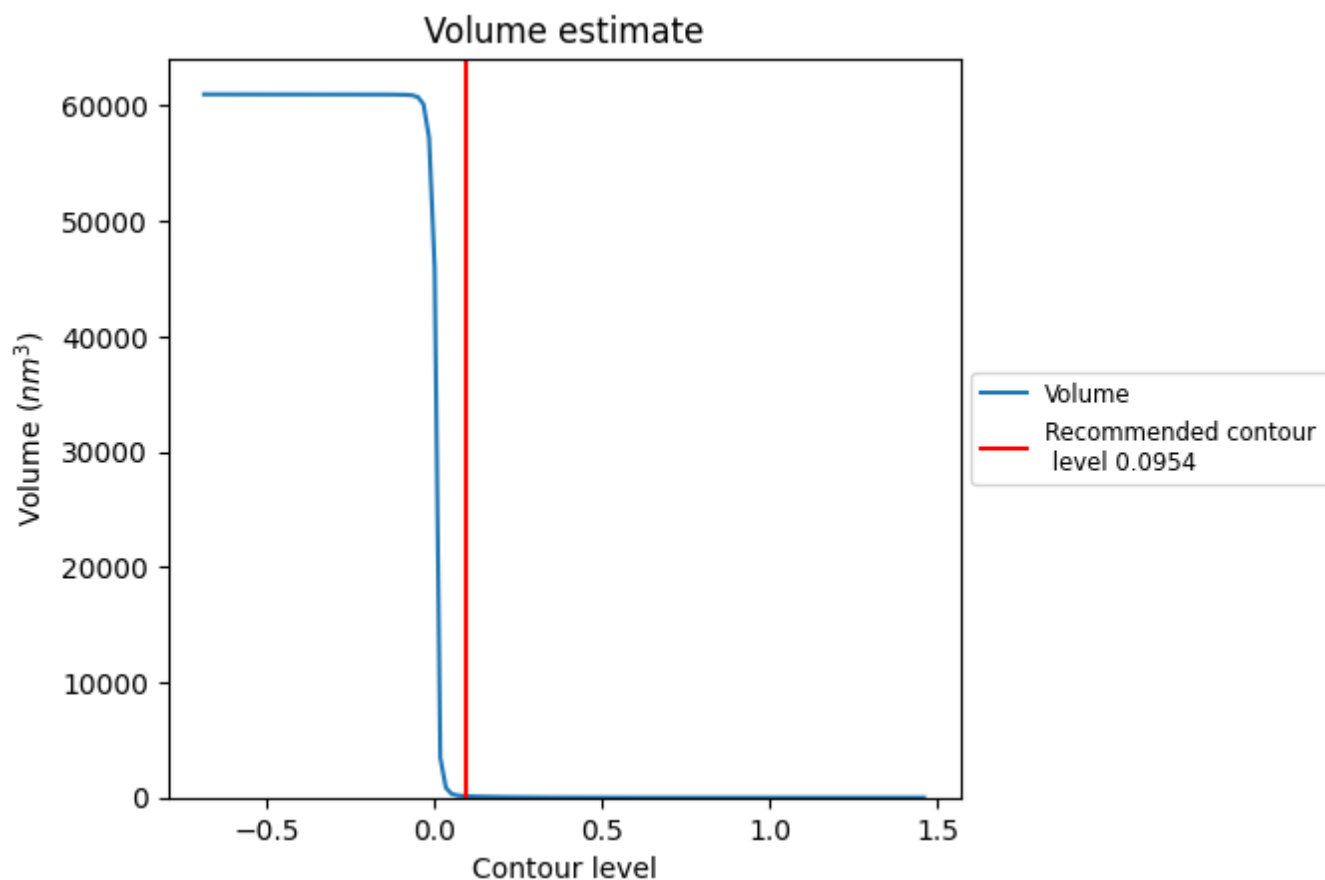
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

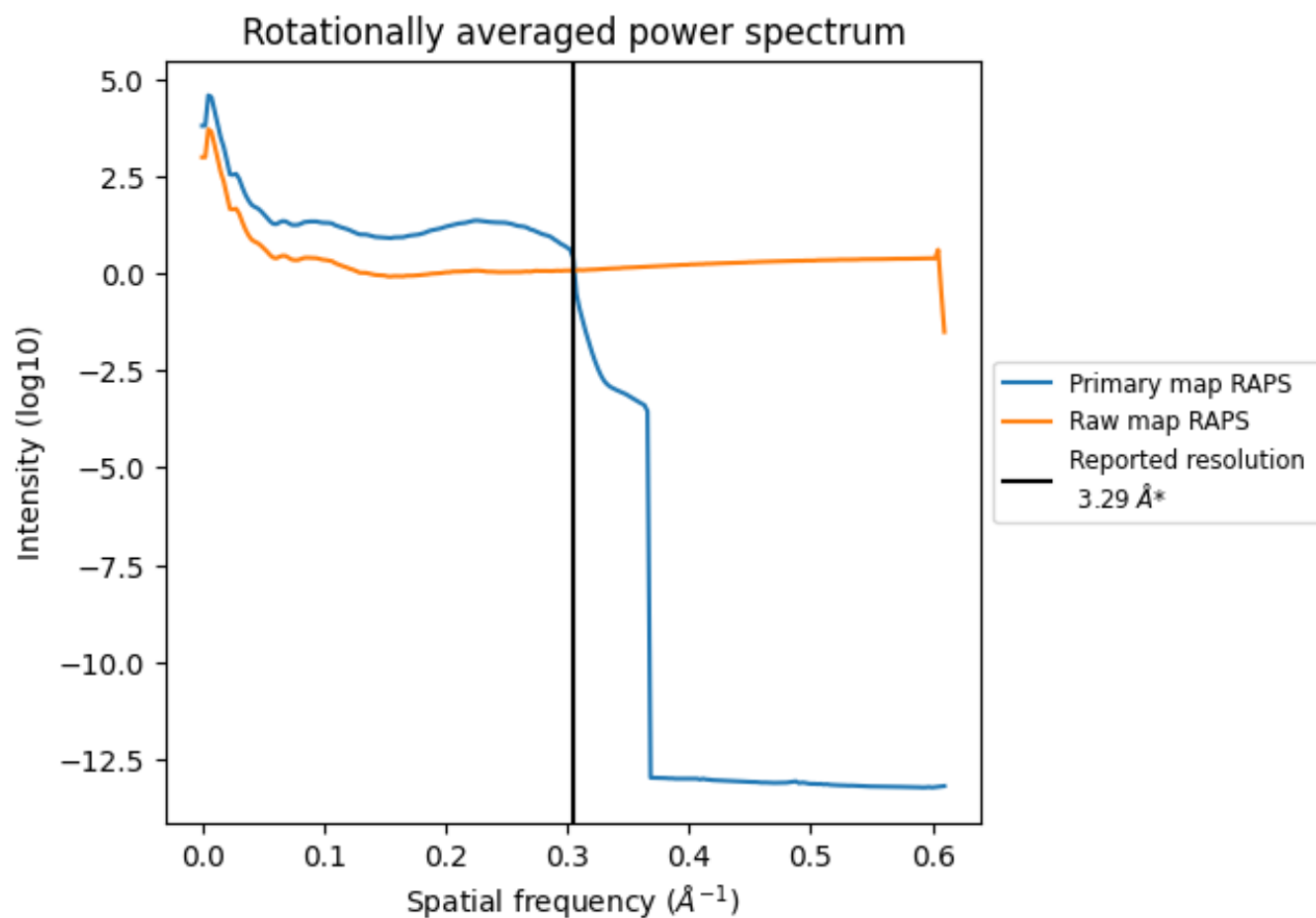
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 120 nm³; this corresponds to an approximate mass of 109 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

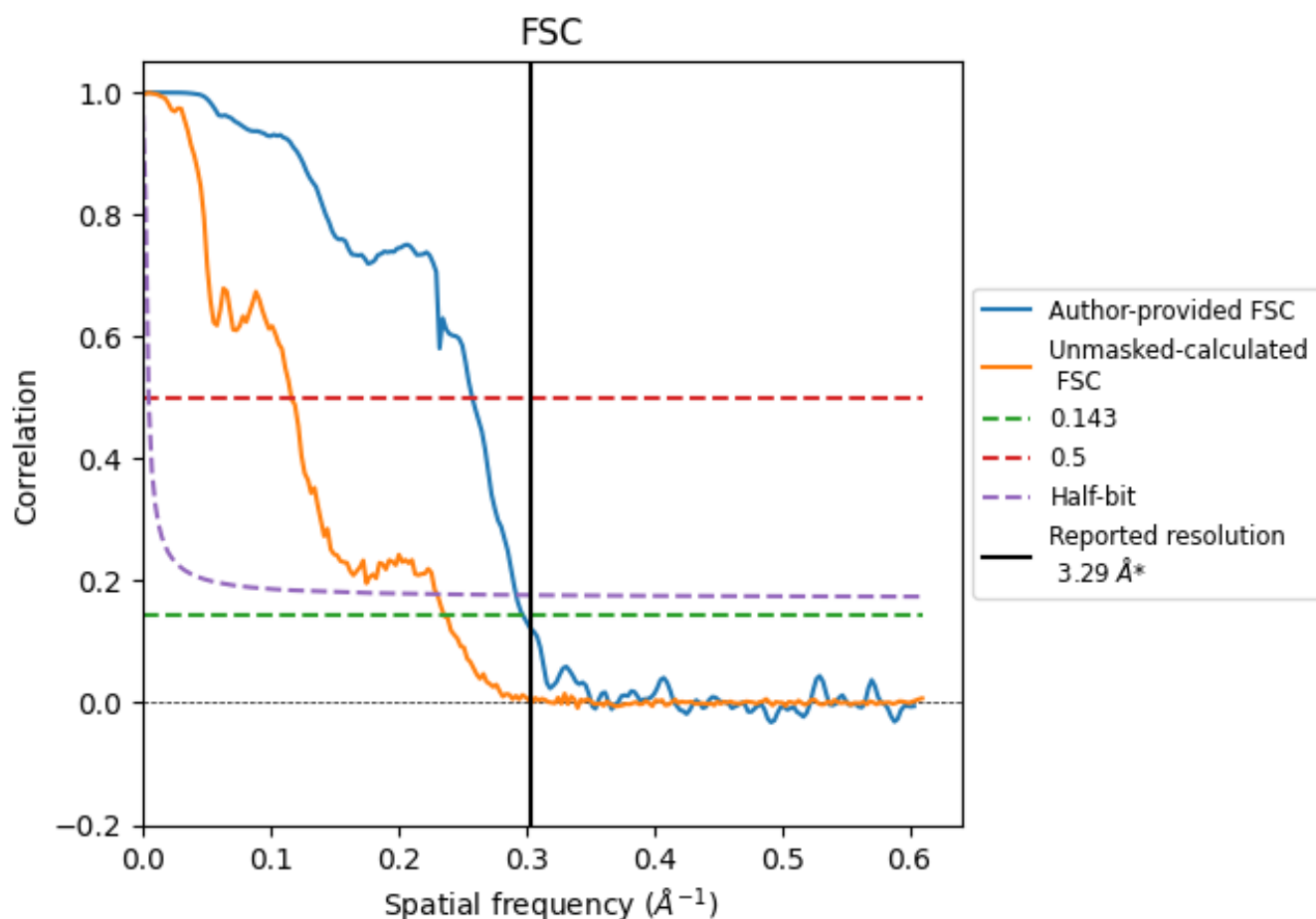


*Reported resolution corresponds to spatial frequency of 0.304 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of $0.304 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.29	-	-
Author-provided FSC curve	3.36	3.88	3.42
Unmasked-calculated*	4.24	8.58	4.34

*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 4.24 differs from the reported value 3.29 by more than 10 %

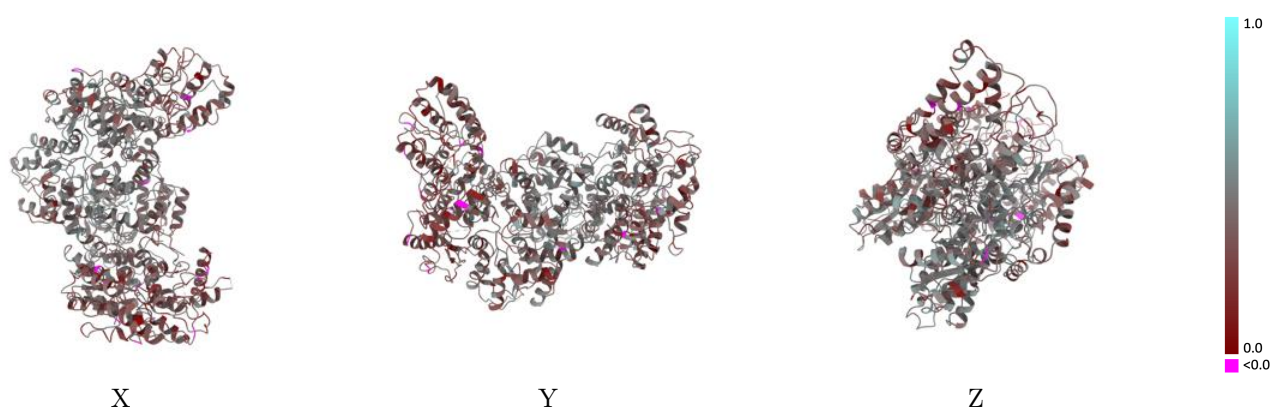
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47669 and PDB model 9E7H. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

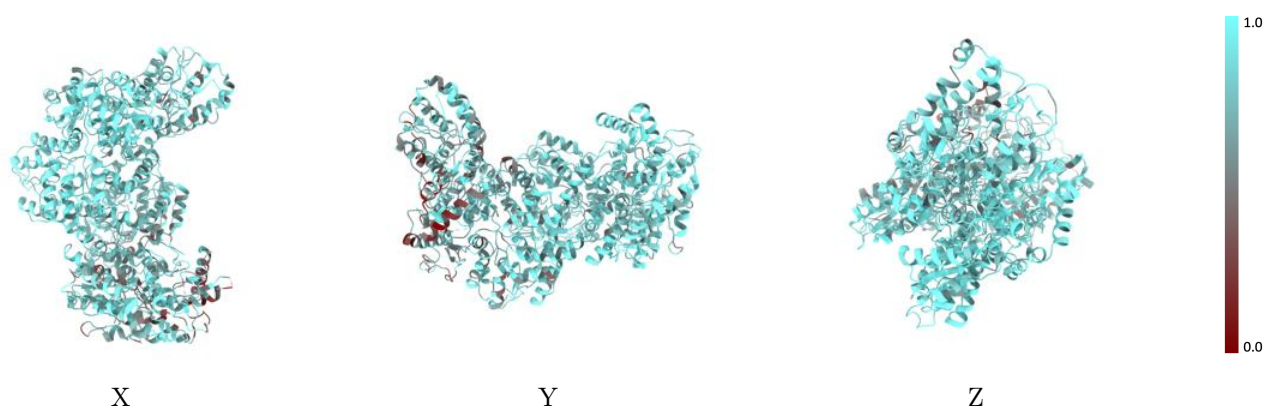
This section was not generated.

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



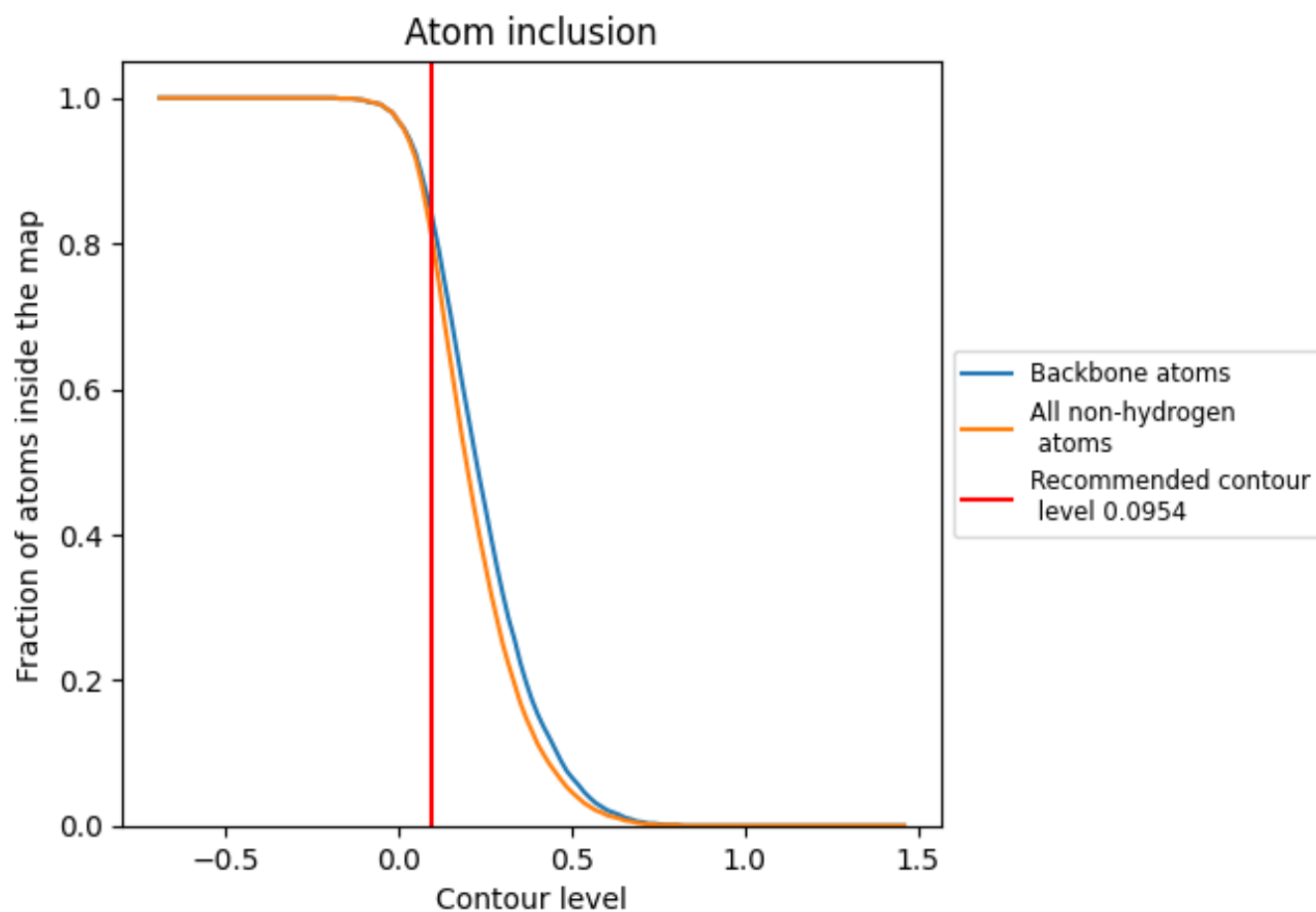
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0954).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 81% 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 (0.0954) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8120	0.3890
A	0.8490	0.3880
B	0.8930	0.4410
C	0.7030	0.3300
D	0.7930	0.3920

