



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 09:28 AM UTC

PDB ID : 5LD2 / pdb_00005ld2
EMDB ID : EMD-4038
Title : Cryo-EM structure of RecBCD+DNA complex revealing activated nuclease domain
Authors : Wilkinson, M.; Chaban, Y.; Wigley, D.B.
Deposited on : 2016-06-23
Resolution : 3.83 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 EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

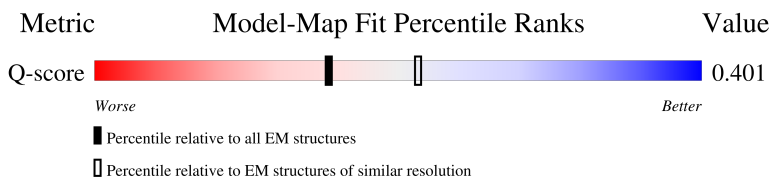
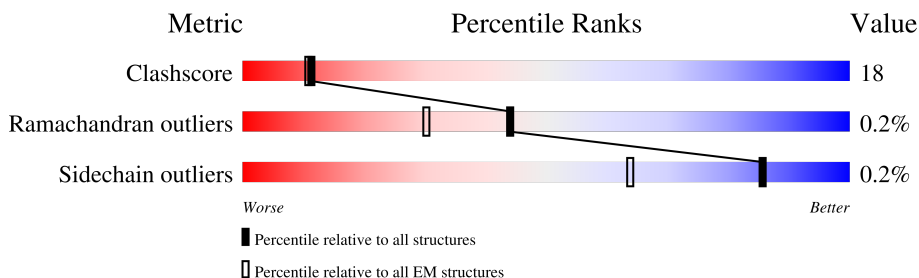
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.83 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	9087 (3.33 - 4.33)

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	B	1181	
2	C	1122	
3	D	609	
4	X	70	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23981 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 RecBCD enzyme subunit RecB, RecBCD enzyme subunit RecB, RecBCD enzyme subunit RecB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1151	Total	C	N	O	S	0	0
			9164	5781	1628	1717	38		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP P08394
B	1080	ALA	ASP	engineered mutation	UNP P08394

- Molecule 2 is a protein called RecBCD enzyme subunit RecC.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1121	Total	C	N	O	S	0	0
			9078	5783	1568	1684	43		

- Molecule 3 is a protein called RecBCD enzyme subunit RecD.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	605	Total	C	N	O	S	0	0
			4672	2916	862	874	20		

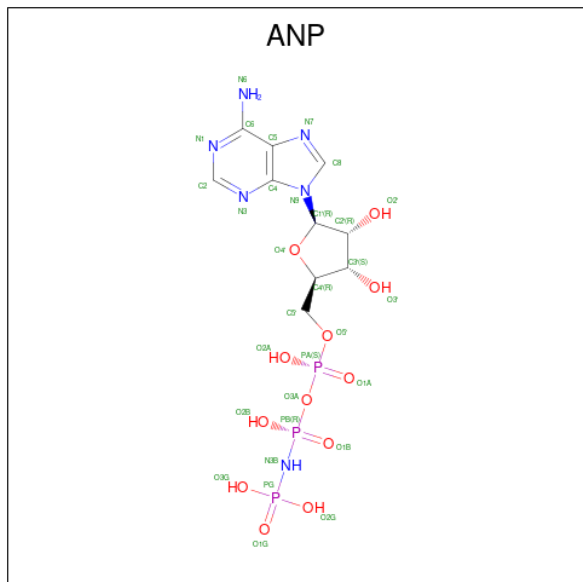
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	initiating methionine	UNP P04993
D	1	GLY	-	expression tag	UNP P04993

- Molecule 4 is a DNA chain called Fork-Hairpin DNA (70-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	51	Total	C	N	O	P	0	0
			1035	501	165	319	50		

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	P	0
			31	10	6	12	3	

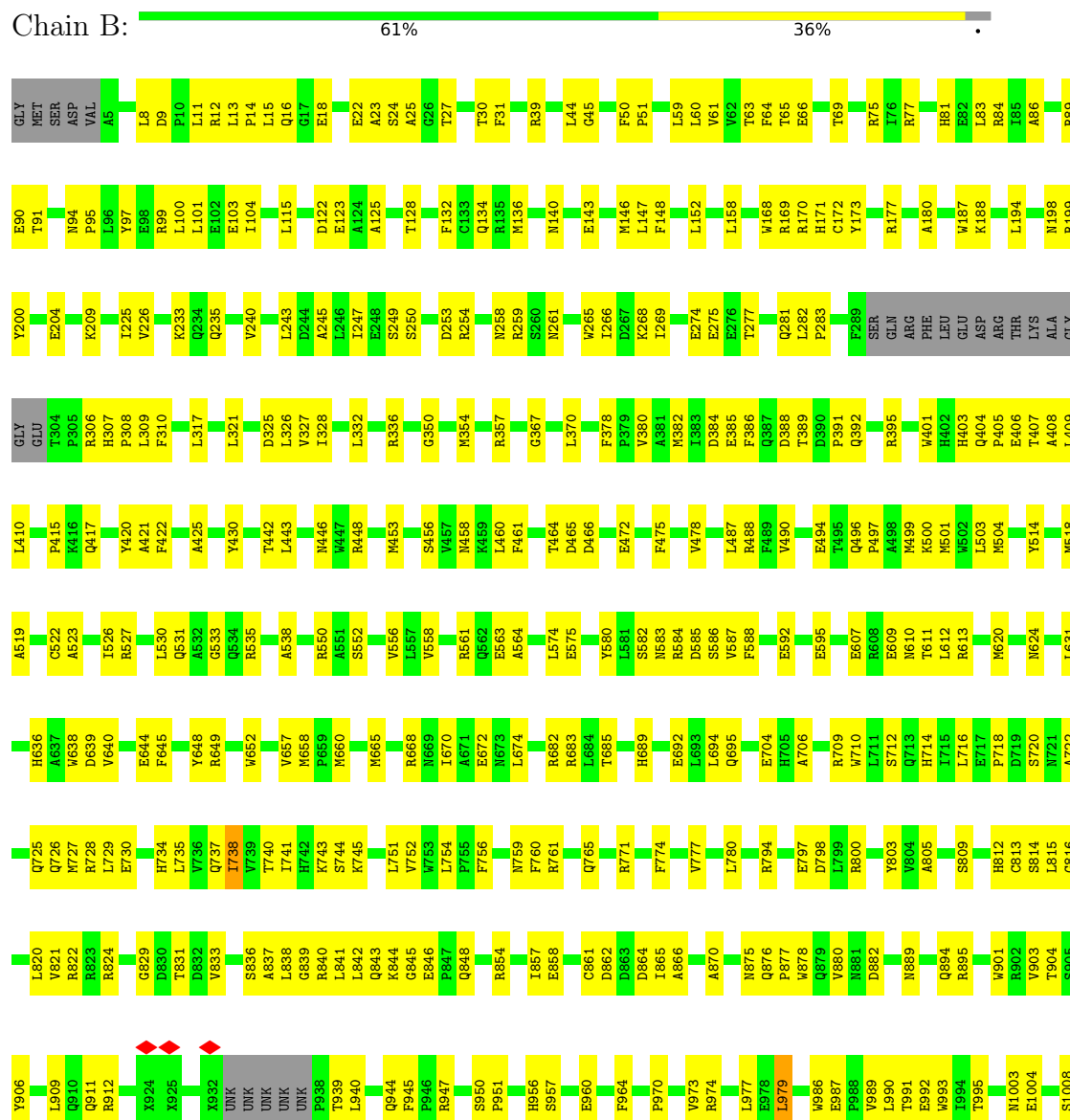
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

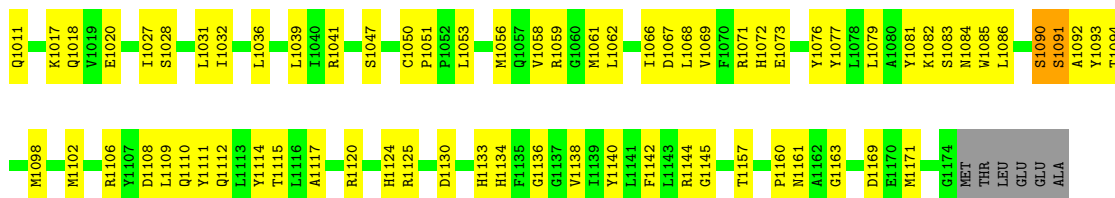
Mol	Chain	Residues	Atoms		AltConf
6	B	1	Total	Mg	0
			1	1	

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.

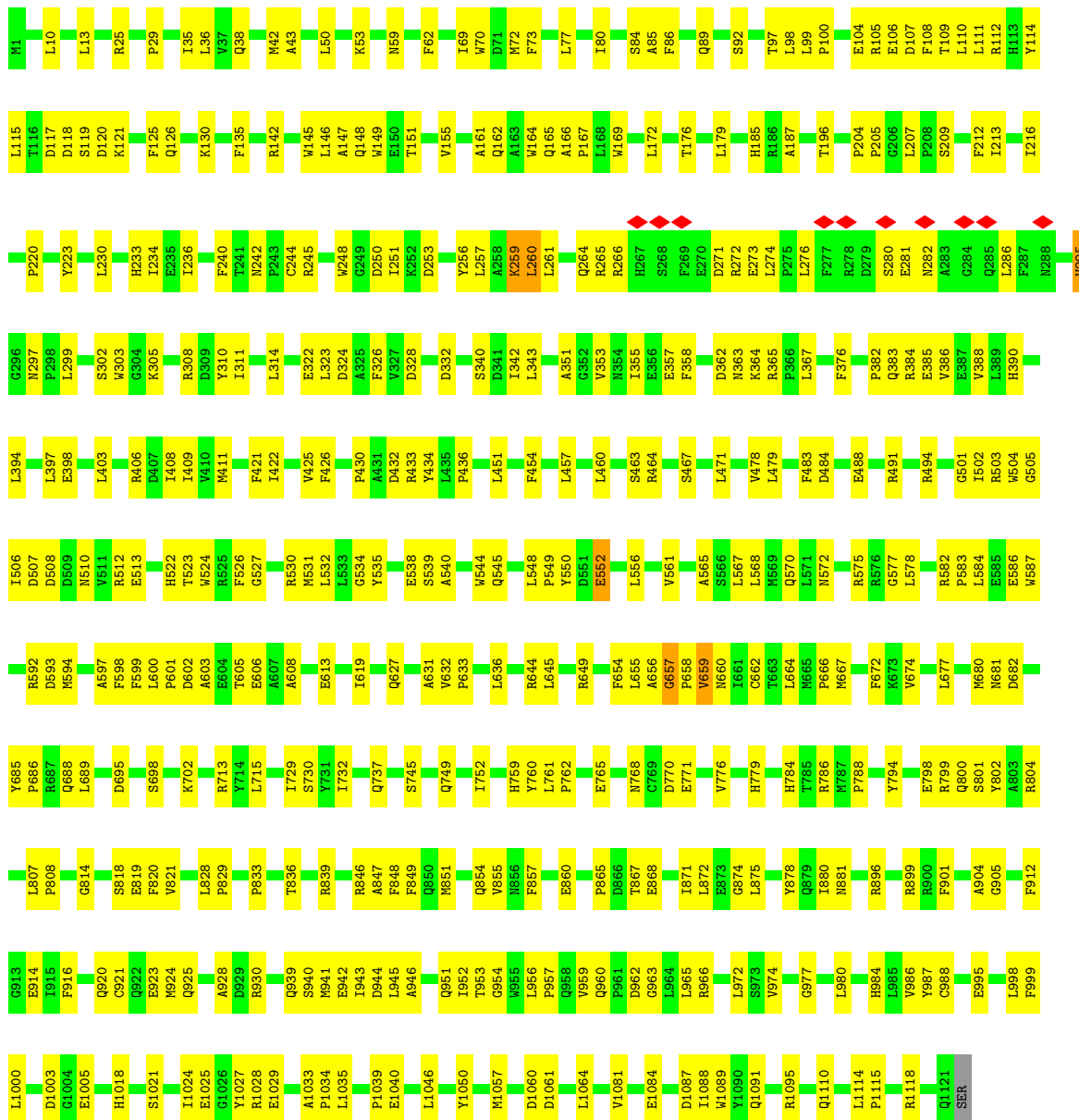
- Molecule 1: RecBCD enzyme subunit RecB, RecBCD enzyme subunit RecB, RecBCD enzyme subunit RecB





• Molecule 2: RecBCD enzyme subunit RecC

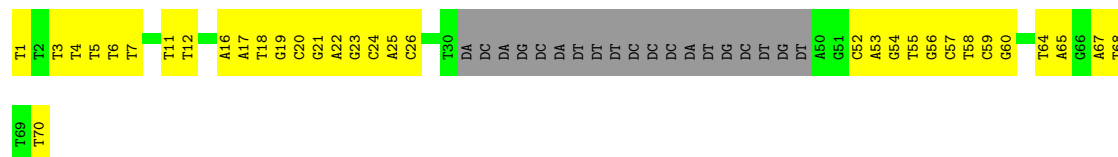
Chain C: 64% 36%



• Molecule 3: RecBCD enzyme subunit RecD

Chain D: 65% 34%

- Molecule 4: Fork-Hairpin DNA (70-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	74656	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 ($e^-/\text{\AA}^2$)	1.2	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3800	Depositor
Magnification	37313	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.145	Depositor
Minimum map value	-0.059	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	241.20001, 241.20001, 241.20001	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.34, 1.34, 1.34	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: ANP, MG

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	B	0.43	0/9262	0.68	7/12563 (0.1%)
2	C	0.51	2/9305 (0.0%)	0.62	7/12644 (0.1%)
3	D	0.38	1/4752 (0.0%)	0.54	3/6437 (0.0%)
4	X	0.40	0/1153	0.57	0/1776
All	All	0.45	3/24472 (0.0%)	0.63	17/33420 (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	B	0	1
2	C	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	259	LYS	C-N	13.98	1.54	1.33
2	C	260	LEU	C-N	10.42	1.49	1.33
3	D	359	TYR	C-N	9.91	1.46	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	738	ILE	N-CA-C	-11.23	91.35	107.75
1	B	738	ILE	N-CA-CB	8.13	122.21	111.64
2	C	688	GLN	N-CA-C	6.76	119.44	108.41
1	B	737	GLN	N-CA-C	-6.63	94.56	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	854	GLN	N-CA-C	6.26	120.87	113.23
2	C	657	GLY	CA-C-N	-6.04	113.72	119.76
2	C	657	GLY	C-N-CA	-6.04	113.72	119.76
2	C	552	GLU	CA-C-N	-6.02	114.49	122.85
2	C	552	GLU	C-N-CA	-6.02	114.49	122.85
1	B	846	GLU	CA-C-N	-5.63	114.17	119.85
1	B	846	GLU	C-N-CA	-5.63	114.17	119.85
3	D	473	HIS	N-CA-C	5.55	117.33	111.28
3	D	532	THR	CB-CA-C	5.47	118.65	109.89
3	D	532	THR	N-CA-C	-5.22	102.13	109.96
1	B	829	GLY	N-CA-C	-5.17	107.39	114.64
2	C	689	LEU	N-CA-C	-5.11	99.97	108.34
1	B	752	VAL	CB-CA-C	-5.04	102.98	110.33

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	720	SER	Peptide
2	C	259	LYS	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	B	9164	0	8943	346	0
2	C	9078	0	8877	330	0
3	D	4672	0	4703	173	0
4	X	1035	0	588	44	0
5	B	31	0	13	1	0
6	B	1	0	0	0	0
All	All	23981	0	23124	847	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 18.

All (847) 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:C:251:ILE:HG22	2:C:286:LEU:HD22	1.28	1.08
2:C:251:ILE:CG2	2:C:286:LEU:HD22	1.85	1.06
1:B:460:LEU:HD23	1:B:841:LEU:HD13	1.41	1.02
2:C:941:MET:HE1	2:C:987:TYR:HD1	1.23	1.00
2:C:245:ARG:HH21	2:C:266:ARG:HH22	1.00	0.98
1:B:911:GLN:HG3	1:B:912:ARG:H	1.29	0.95
2:C:941:MET:HE3	2:C:956:LEU:HD12	1.52	0.91
1:B:460:LEU:CD2	1:B:841:LEU:HD13	2.01	0.90
3:D:24:ALA:O	3:D:28:ALA:HB3	1.71	0.90
2:C:654:PHE:HD2	2:C:655:LEU:HG	1.37	0.89
3:D:17:ARG:HH12	3:D:47:GLY:HA3	1.36	0.89
2:C:681:ASN:HD21	2:C:732:ILE:HB	1.38	0.89
2:C:503:ARG:HE	2:C:865:PRO:HG2	1.36	0.88
1:B:235:GLN:HB3	1:B:309:LEU:HD22	1.56	0.88
1:B:1066:ILE:HG21	1:B:1069:VAL:HG23	1.54	0.87
1:B:522:CYS:O	1:B:526:ILE:HG13	1.74	0.87
2:C:530:ARG:HH22	2:C:548:LEU:HB3	1.40	0.87
2:C:577:GLY:O	2:C:582:ARG:NH2	2.10	0.85
2:C:245:ARG:NH2	2:C:266:ARG:HH22	1.75	0.84
2:C:654:PHE:CD2	2:C:655:LEU:HG	2.12	0.84
3:D:425:ARG:NH2	3:D:503:ASP:O	2.10	0.83
1:B:464:THR:CG2	1:B:844:LYS:HA	2.08	0.83
2:C:539:SER:HA	2:C:549:PRO:HG2	1.59	0.83
2:C:245:ARG:HH21	2:C:266:ARG:NH2	1.76	0.83
2:C:592:ARG:NH2	2:C:613:GLU:OE2	2.12	0.83
3:D:67:LEU:O	3:D:71:CYS:HB3	1.78	0.82
2:C:548:LEU:HD12	2:C:549:PRO:HD2	1.60	0.82
1:B:249:SER:HB2	4:X:26:DC:H4'	1.62	0.81
2:C:508:ASP:OD2	2:C:512:ARG:NH1	2.13	0.81
1:B:226:VAL:HG13	1:B:269:ILE:HG21	1.62	0.81
1:B:30:THR:HG22	1:B:75:ARG:HH22	1.45	0.80
1:B:889:ASN:O	2:C:800:GLN:NE2	2.15	0.80
1:B:940:LEU:HG	1:B:989:VAL:HG22	1.63	0.78
2:C:478:VAL:HG21	2:C:605:THR:HG21	1.66	0.78
2:C:941:MET:CE	2:C:987:TYR:HD1	1.96	0.78
1:B:527:ARG:NH1	1:B:876:GLN:O	2.17	0.77
2:C:941:MET:HE1	2:C:987:TYR:CD1	2.15	0.77
1:B:771:ARG:O	1:B:774:PHE:CE1	2.37	0.77
2:C:250:ASP:OD1	2:C:308:ARG:NH2	2.18	0.76
3:D:584:ARG:HD2	3:D:584:ARG:N	1.98	0.76
1:B:18:GLU:HG2	1:B:409:LEU:HD23	1.67	0.76
1:B:911:GLN:HG3	1:B:912:ARG:N	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:478:GLU:HG3	3:D:502:LEU:HA	1.68	0.76
1:B:148:PHE:CD2	2:C:130:LYS:HG3	2.20	0.76
3:D:240:LEU:HD11	3:D:282:LEU:HD12	1.68	0.76
1:B:652:TRP:HE1	1:B:704:GLU:HB3	1.51	0.75
1:B:169:ARG:HH21	2:C:868:GLU:HG2	1.51	0.75
2:C:941:MET:CE	2:C:956:LEU:HD12	2.16	0.75
2:C:584:LEU:O	2:C:587:TRP:N	2.18	0.75
2:C:556:LEU:HG	3:D:305:GLU:HG2	1.69	0.74
2:C:1018:HIS:O	2:C:1021:SER:OG	2.04	0.74
1:B:461:PHE:CE1	1:B:841:LEU:HD11	2.23	0.74
2:C:248:TRP:O	2:C:308:ARG:NH1	2.21	0.74
1:B:148:PHE:HD2	2:C:130:LYS:HG3	1.51	0.73
2:C:230:LEU:HD22	2:C:236:ILE:HD11	1.69	0.73
2:C:261:LEU:HD21	2:C:281:GLU:OE2	1.88	0.73
1:B:307:HIS:HB2	1:B:308:PRO:HD2	1.71	0.72
1:B:261:ASN:O	1:B:265:TRP:N	2.19	0.72
3:D:188:LEU:HD11	3:D:265:VAL:HG11	1.72	0.72
1:B:13:LEU:HD12	1:B:14:PRO:HD2	1.72	0.72
1:B:609:GLU:HG3	1:B:610:ASN:N	2.04	0.72
2:C:666:PRO:HA	2:C:715:LEU:HD21	1.72	0.71
1:B:233:LYS:NZ	1:B:268:LYS:O	2.21	0.71
1:B:122:ASP:OD1	1:B:123:GLU:N	2.24	0.71
3:D:187:ALA:O	3:D:191:MET:HB2	1.91	0.71
1:B:461:PHE:HE1	1:B:841:LEU:HD11	1.54	0.71
3:D:438:TYR:HA	3:D:548:HIS:O	1.90	0.71
1:B:973:VAL:HG13	1:B:990:LEU:HD23	1.71	0.70
3:D:67:LEU:O	3:D:71:CYS:CB	2.39	0.70
3:D:265:VAL:HG12	3:D:291:ARG:HB2	1.71	0.70
1:B:527:ARG:NH2	1:B:875:ASN:H	1.89	0.70
1:B:194:LEU:O	1:B:198:ASN:HB2	1.92	0.70
3:D:137:LEU:HD21	3:D:162:LEU:HD13	1.73	0.70
2:C:974:VAL:O	2:C:977:GLY:N	2.25	0.69
1:B:448:ARG:HH21	5:B:1501:ANP:HNB1	1.39	0.69
2:C:941:MET:HG2	2:C:959:VAL:HG21	1.75	0.69
1:B:563:GLU:HG3	1:B:756:PHE:HD2	1.56	0.69
1:B:526:ILE:O	1:B:530:LEU:HG	1.93	0.69
4:X:18:DT:H2"	4:X:19:DG:C8	2.27	0.69
1:B:382:MET:HG2	1:B:410:LEU:HD12	1.74	0.69
2:C:506:ILE:HG22	2:C:510:ASN:HD22	1.58	0.69
1:B:728:ARG:O	2:C:786:ARG:NH2	2.25	0.69
2:C:357:GLU:OE2	2:C:363:ASN:ND2	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:37:LEU:HD23	3:D:67:LEU:HD21	1.75	0.69
1:B:101:LEU:HD23	1:B:104:ILE:HD12	1.75	0.68
1:B:460:LEU:CD2	1:B:841:LEU:CD1	2.72	0.68
1:B:761:ARG:HH12	4:X:68:DT:P	2.16	0.68
2:C:145:TRP:O	2:C:148:GLN:N	2.27	0.68
1:B:380:VAL:HG23	1:B:408:ALA:HB3	1.74	0.68
3:D:523:GLN:HG3	3:D:524:PRO:CD	2.23	0.68
1:B:8:LEU:HD23	1:B:443:LEU:HD21	1.76	0.67
2:C:513:GLU:OE1	2:C:575:ARG:NH1	2.16	0.67
2:C:244:CYS:HB3	2:C:248:TRP:CD1	2.28	0.67
1:B:388:ASP:OD2	1:B:745:LYS:NZ	2.28	0.67
2:C:952:ILE:HD11	2:C:1024:ILE:HD11	1.76	0.67
2:C:376:PHE:CE2	2:C:752:ILE:HG22	2.30	0.67
1:B:761:ARG:NH1	4:X:67:DA:O3'	2.27	0.66
1:B:624:ASN:OD1	2:C:818:SER:OG	2.14	0.66
3:D:474:SER:O	3:D:475:ARG:HB3	1.96	0.66
2:C:530:ARG:NH2	2:C:548:LEU:HB3	2.11	0.66
3:D:178:THR:HG21	3:D:215:SER:HB3	1.78	0.66
3:D:165:ARG:NH2	3:D:287:PRO:O	2.27	0.66
1:B:1108:ASP:HA	1:B:1111:TYR:CE2	2.31	0.66
3:D:17:ARG:NH1	3:D:47:GLY:HA3	2.10	0.66
2:C:38:GLN:HB2	2:C:216:ILE:HG12	1.77	0.66
2:C:273:GLU:HG3	2:C:274:LEU:H	1.61	0.66
1:B:1091:SER:O	1:B:1094:THR:HG23	1.96	0.65
3:D:200:ARG:HE	3:D:243:LEU:HD13	1.60	0.65
1:B:386:PHE:O	1:B:389:THR:OG1	2.12	0.65
1:B:499:MET:HE3	1:B:815:LEU:HD21	1.77	0.65
1:B:563:GLU:HG3	1:B:756:PHE:CD2	2.31	0.65
1:B:947:ARG:HE	1:B:1086:LEU:HA	1.61	0.65
1:B:639:ASP:C	1:B:639:ASP:OD2	2.40	0.65
1:B:759:ASN:OD1	1:B:760:PHE:N	2.29	0.65
1:B:940:LEU:N	1:B:940:LEU:HD12	2.12	0.65
3:D:62:GLU:HG2	3:D:67:LEU:HB2	1.77	0.65
1:B:964:PHE:HD2	1:B:1017:LYS:HZ3	1.42	0.65
1:B:1125:ARG:NH1	2:C:29:PRO:O	2.30	0.65
3:D:523:GLN:HG3	3:D:524:PRO:HD2	1.77	0.65
2:C:846:ARG:HG3	2:C:1089:TRP:CE2	2.32	0.64
2:C:398:GLU:OE1	2:C:802:TYR:OH	2.10	0.64
2:C:460:LEU:O	2:C:463:SER:N	2.30	0.64
3:D:483:MET:O	3:D:530:HIS:HA	1.97	0.64
1:B:639:ASP:OD2	1:B:639:ASP:O	2.16	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:155:VAL:H	2:C:162:GLN:HE22	1.44	0.64
1:B:143:GLU:CD	1:B:143:GLU:H	2.06	0.64
2:C:578:LEU:HD11	2:C:594:MET:HE1	1.80	0.64
2:C:930:ARG:HH22	2:C:1003:ASP:HA	1.61	0.64
1:B:461:PHE:CE1	1:B:841:LEU:CD1	2.81	0.64
1:B:461:PHE:HE1	1:B:841:LEU:CD1	2.10	0.64
1:B:464:THR:HG22	1:B:844:LYS:HB3	1.80	0.63
2:C:302:SER:O	2:C:713:ARG:NH1	2.30	0.63
3:D:33:PRO:HB2	3:D:70:THR:HG23	1.79	0.63
2:C:69:ILE:HG13	2:C:223:TYR:HD1	1.63	0.63
1:B:66:GLU:O	1:B:69:THR:OG1	2.17	0.63
1:B:992:GLU:O	1:B:995:THR:OG1	2.15	0.63
3:D:583:GLU:O	3:D:587:SER:CB	2.46	0.63
1:B:169:ARG:HA	1:B:173:TYR:CD2	2.34	0.63
1:B:658:MET:H	1:B:695:GLN:HE21	1.46	0.63
1:B:833:VAL:HG12	1:B:839:GLY:HA3	1.79	0.63
4:X:11:DT:H2"	4:X:12:DT:H5"	1.80	0.63
1:B:461:PHE:HE2	1:B:803:TYR:HD1	1.47	0.63
1:B:682:ARG:HH12	1:B:726:GLN:HB3	1.62	0.63
3:D:329:LEU:HD23	3:D:332:LEU:HD12	1.81	0.63
2:C:35:ILE:HG12	2:C:212:PHE:HB2	1.79	0.63
1:B:612:LEU:HD22	1:B:638:TRP:CH2	2.34	0.62
2:C:593:ASP:O	2:C:597:ALA:HB2	1.99	0.62
1:B:527:ARG:HH22	1:B:875:ASN:H	1.45	0.62
1:B:992:GLU:HG3	1:B:993:TRP:H	1.64	0.62
3:D:65:HIS:ND1	3:D:70:THR:OG1	2.30	0.62
2:C:600:LEU:HD12	2:C:601:PRO:HD2	1.81	0.62
1:B:939:THR:O	1:B:944:GLN:NE2	2.32	0.62
2:C:602:ASP:OD1	2:C:603:ALA:N	2.30	0.62
3:D:256:HIS:CD2	3:D:258:GLY:H	2.16	0.62
3:D:477:TYR:CZ	3:D:480:ARG:HB3	2.35	0.62
2:C:507:ASP:OD2	2:C:572:ASN:ND2	2.33	0.62
3:D:82:GLU:O	3:D:86:LEU:HB3	1.98	0.62
3:D:24:ALA:O	3:D:28:ALA:CB	2.45	0.62
3:D:485:ALA:HB3	3:D:529:GLU:CB	2.30	0.62
1:B:200:TYR:O	1:B:336:ARG:NH2	2.33	0.62
2:C:572:ASN:O	2:C:575:ARG:HG2	2.00	0.62
4:X:20:DC:H2"	4:X:21:DG:C8	2.34	0.62
1:B:503:LEU:CD2	1:B:854:ARG:HG3	2.30	0.62
1:B:243:LEU:HD12	1:B:245:ALA:H	1.65	0.61
3:D:112:MET:O	3:D:116:GLU:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:119:SER:HB3	2:C:121:LYS:H	1.64	0.61
2:C:161:ALA:HB1	2:C:164:TRP:HE1	1.65	0.61
2:C:257:LEU:HD13	2:C:281:GLU:OE1	1.99	0.61
1:B:63:THR:HG22	1:B:64:PHE:H	1.66	0.61
1:B:552:SER:HB3	1:B:734:HIS:HB3	1.83	0.61
1:B:824:ARG:HB2	4:X:18:DT:H5'	1.83	0.61
3:D:57:ARG:NH2	3:D:597:ARG:HE	1.99	0.61
2:C:828:LEU:HD12	2:C:829:PRO:HD2	1.83	0.60
2:C:451:LEU:HD22	2:C:645:LEU:HD13	1.81	0.60
1:B:1071:ARG:HB3	1:B:1076:TYR:CD1	2.36	0.60
1:B:1084:ASN:O	1:B:1144:ARG:NH1	2.35	0.60
1:B:1112:GLN:O	1:B:1115:THR:OG1	2.18	0.60
2:C:257:LEU:HD13	2:C:281:GLU:CD	2.26	0.60
2:C:980:LEU:HD22	2:C:998:LEU:HB2	1.84	0.60
1:B:527:ARG:HD3	1:B:574:LEU:HD13	1.83	0.60
1:B:30:THR:HG22	1:B:75:ARG:NH2	2.14	0.60
2:C:77:LEU:HD21	2:C:196:THR:HG21	1.83	0.60
2:C:105:ARG:HD3	2:C:108:PHE:HE2	1.65	0.60
1:B:812:HIS:HE2	1:B:814:SER:HG	1.48	0.60
1:B:1068:LEU:HD23	1:B:1079:LEU:HD23	1.82	0.60
2:C:768:ASN:HD22	2:C:771:GLU:HG3	1.66	0.60
2:C:695:ASP:OD2	2:C:698:SER:N	2.29	0.60
2:C:1025:GLU:OE2	2:C:1028:ARG:NH1	2.35	0.60
3:D:72:VAL:HG22	3:D:79:GLN:HB3	1.83	0.60
3:D:425:ARG:HH22	3:D:504:ARG:HA	1.66	0.60
4:X:70:DT:H5''	4:X:70:DT:H6	1.67	0.60
2:C:38:GLN:HG2	2:C:667:MET:HG3	1.84	0.59
2:C:504:TRP:CG	2:C:505:GLY:H	2.19	0.59
2:C:972:LEU:HA	2:C:1000:LEU:HD22	1.84	0.59
1:B:199:ARG:HH11	1:B:765:GLN:HE22	1.48	0.59
3:D:78:LEU:HD13	3:D:83:GLU:HG3	1.84	0.59
3:D:477:TYR:CE1	3:D:480:ARG:HB3	2.37	0.59
1:B:727:MET:HA	2:C:737:GLN:HG3	1.84	0.59
1:B:957:SER:HA	1:B:960:GLU:CD	2.27	0.59
2:C:488:GLU:HA	2:C:491:ARG:NH1	2.17	0.59
1:B:822:ARG:O	1:B:824:ARG:NH1	2.36	0.59
3:D:269:ASP:OD1	3:D:270:GLU:N	2.36	0.59
1:B:580:TYR:CZ	1:B:582:SER:HB2	2.38	0.59
1:B:611:THR:HG22	1:B:611:THR:O	2.01	0.59
2:C:945:LEU:O	2:C:951:GLN:HA	2.03	0.59
4:X:59:DC:H2''	4:X:60:DG:C8	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:682:ARG:O	1:B:685:THR:OG1	2.21	0.59
1:B:143:GLU:HB3	1:B:370:LEU:HB2	1.85	0.59
1:B:169:ARG:NE	2:C:868:GLU:OE2	2.36	0.59
3:D:78:LEU:HD12	3:D:84:CYS:HA	1.85	0.59
1:B:250:SER:O	4:X:58:DT:H5"	2.02	0.59
1:B:903:VAL:HG22	1:B:1061:MET:HB2	1.85	0.59
2:C:658:PRO:O	2:C:659:VAL:C	2.45	0.59
2:C:1029:GLU:HA	2:C:1029:GLU:OE2	2.03	0.59
3:D:583:GLU:O	3:D:587:SER:OG	2.17	0.59
2:C:548:LEU:HD23	2:C:904:ALA:HB2	1.85	0.58
2:C:605:THR:O	2:C:608:ALA:N	2.36	0.58
1:B:1051:PRO:O	1:B:1106:ARG:NH1	2.36	0.58
2:C:924:MET:O	2:C:928:ALA:HB2	2.03	0.58
3:D:485:ALA:HB3	3:D:529:GLU:HB2	1.84	0.58
2:C:457:LEU:HD13	2:C:598:PHE:HD2	1.69	0.58
2:C:999:PHE:C	2:C:1000:LEU:HD12	2.28	0.58
3:D:484:ILE:HG13	3:D:493:LEU:HD13	1.86	0.58
1:B:519:ALA:HB2	1:B:756:PHE:HZ	1.68	0.58
3:D:255:HIS:HA	3:D:259:ASN:HB2	1.85	0.58
1:B:652:TRP:HZ3	1:B:657:VAL:HG13	1.68	0.57
2:C:364:LYS:HB2	2:C:760:TYR:HD2	1.69	0.57
3:D:52:CYS:HA	3:D:108:TYR:HB3	1.86	0.57
1:B:306:ARG:HG3	1:B:307:HIS:ND1	2.20	0.57
2:C:105:ARG:HD3	2:C:108:PHE:CE2	2.39	0.57
3:D:511:TRP:CZ3	3:D:519:ILE:HD12	2.40	0.57
1:B:761:ARG:O	1:B:794:ARG:NE	2.31	0.57
4:X:55:DT:H2"	4:X:56:DG:C8	2.39	0.57
1:B:199:ARG:NH1	1:B:765:GLN:HE22	2.03	0.57
1:B:1083:SER:O	1:B:1085:TRP:HE3	1.87	0.57
2:C:761:LEU:HG	2:C:776:VAL:HG22	1.86	0.57
3:D:57:ARG:HH21	3:D:597:ARG:HE	1.50	0.57
2:C:340:SER:O	2:C:343:LEU:N	2.38	0.57
2:C:436:PRO:O	2:C:659:VAL:HG12	2.04	0.57
1:B:672:GLU:HG2	2:C:814:GLY:HA3	1.87	0.57
2:C:1081:VAL:HG22	4:X:12:DT:H2"	1.85	0.57
2:C:504:TRP:CD1	2:C:505:GLY:H	2.23	0.57
2:C:874:GLY:HA2	4:X:11:DT:O2	2.04	0.57
3:D:210:ALA:O	3:D:213:THR:OG1	2.19	0.57
1:B:464:THR:HG22	1:B:844:LYS:CB	2.35	0.56
2:C:532:LEU:O	2:C:535:TYR:N	2.35	0.56
2:C:939:GLN:N	2:C:939:GLN:OE1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:PRO:HB3	1:B:430:TYR:CE2	2.40	0.56
3:D:487:ASN:OD1	3:D:495:ASN:N	2.34	0.56
1:B:1133:HIS:HD2	1:B:1134:HIS:CE1	2.23	0.56
2:C:1024:ILE:O	2:C:1027:TYR:N	2.38	0.56
3:D:170:SER:OG	3:D:314:CYS:SG	2.61	0.56
1:B:861:CYS:SG	1:B:866:ALA:HA	2.45	0.56
2:C:299:LEU:HD22	2:C:303:TRP:CH2	2.40	0.56
1:B:729:LEU:HD12	1:B:730:GLU:HG2	1.88	0.56
3:D:321:PHE:O	3:D:349:ARG:NH2	2.39	0.56
2:C:386:VAL:HG12	2:C:425:VAL:HG21	1.88	0.56
4:X:57:DC:H2'	4:X:58:DT:H71	1.87	0.56
1:B:11:LEU:HD13	1:B:99:ARG:HH12	1.72	0.56
1:B:585:ASP:OD1	1:B:586:SER:N	2.38	0.56
3:D:223:LEU:HG	3:D:224:PRO:HD2	1.88	0.56
3:D:583:GLU:O	3:D:587:SER:HB2	2.05	0.56
2:C:148:GLN:O	2:C:151:THR:OG1	2.18	0.55
4:X:20:DC:H2''	4:X:21:DG:H8	1.71	0.55
1:B:388:ASP:OD2	1:B:420:TYR:HD2	1.88	0.55
2:C:36:LEU:HD12	2:C:213:ILE:HG12	1.88	0.55
2:C:251:ILE:HG21	2:C:286:LEU:HB3	1.88	0.55
1:B:209:LYS:HE3	1:B:777:VAL:HG11	1.87	0.55
1:B:225:ILE:HG23	1:B:321:LEU:HD22	1.88	0.55
1:B:797:GLU:HA	1:B:800:ARG:HE	1.71	0.55
2:C:502:ILE:CG1	2:C:527:GLY:HA3	2.35	0.55
2:C:530:ARG:HG2	2:C:550:TYR:HB2	1.88	0.55
2:C:943:ILE:O	2:C:953:THR:HA	2.07	0.55
1:B:384:ASP:OD1	1:B:385:GLU:N	2.36	0.55
1:B:649:ARG:O	1:B:652:TRP:HB3	2.07	0.55
1:B:665:MET:HG2	1:B:670:ILE:HD11	1.87	0.55
2:C:251:ILE:HB	2:C:286:LEU:HD13	1.87	0.55
3:D:141:LEU:HD23	3:D:144:LEU:HD12	1.88	0.55
1:B:558:VAL:HG21	1:B:564:ALA:HB2	1.87	0.55
1:B:658:MET:H	1:B:695:GLN:NE2	2.04	0.55
2:C:69:ILE:HG13	2:C:223:TYR:CD1	2.42	0.55
2:C:821:VAL:HG23	2:C:1034:PRO:HD2	1.88	0.55
3:D:271:ALA:N	3:D:295:LEU:O	2.26	0.55
3:D:440:LEU:HD23	3:D:550:ALA:HB3	1.89	0.55
1:B:458:ASN:HD22	1:B:475:PHE:HZ	1.54	0.55
1:B:518:MET:HE2	1:B:816:GLY:HA3	1.89	0.55
1:B:1138:VAL:O	1:B:1157:THR:HA	2.07	0.55
2:C:1087:ASP:O	2:C:1091:GLN:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:464:ARG:HD3	2:C:504:TRP:CZ3	2.41	0.55
3:D:514:MET:HE3	3:D:520:LYS:HD2	1.89	0.55
3:D:573:ALA:HB1	3:D:576:ARG:O	2.06	0.55
1:B:1003:ASN:CG	1:B:1004:GLU:H	2.14	0.54
1:B:44:LEU:HD21	1:B:104:ILE:HG12	1.88	0.54
1:B:974:ARG:HB2	1:B:987:GLU:HG3	1.89	0.54
1:B:531:GLN:HG2	1:B:535:ARG:HH12	1.72	0.54
1:B:1003:ASN:OD1	1:B:1004:GLU:N	2.40	0.54
2:C:179:LEU:HD22	2:C:627:GLN:HG3	1.88	0.54
2:C:397:LEU:HD23	2:C:403:LEU:HD23	1.89	0.54
3:D:74:GLU:O	3:D:78:LEU:HD23	2.07	0.54
3:D:279:MET:HE3	3:D:283:ILE:HD11	1.88	0.54
1:B:741:ILE:O	1:B:744:SER:OG	2.15	0.54
2:C:114:TYR:HD2	2:C:115:LEU:HD12	1.72	0.54
2:C:355:ILE:HA	2:C:358:PHE:HB3	1.89	0.54
2:C:1060:ASP:N	2:C:1060:ASP:OD1	2.36	0.54
3:D:309:VAL:O	3:D:313:ILE:HG12	2.06	0.54
3:D:584:ARG:HD2	3:D:584:ARG:H	1.70	0.54
1:B:464:THR:HG21	1:B:844:LYS:HA	1.89	0.54
1:B:1130:ASP:H	1:B:1134:HIS:HD2	1.54	0.54
2:C:185:HIS:CD2	2:C:187:ALA:HB3	2.43	0.54
2:C:433:ARG:HH12	2:C:804:ARG:H	1.55	0.54
1:B:22:GLU:O	1:B:442:THR:HA	2.08	0.54
1:B:168:TRP:CD1	1:B:172:CYS:HG	2.26	0.54
1:B:472:GLU:N	1:B:472:GLU:OE1	2.41	0.54
1:B:1020:GLU:HA	1:B:1066:ILE:O	2.08	0.54
3:D:239:THR:HG22	3:D:241:HIS:H	1.72	0.54
1:B:992:GLU:HG3	1:B:993:TRP:N	2.23	0.53
1:B:84:ARG:HE	1:B:115:LEU:HB2	1.73	0.53
2:C:10:LEU:O	2:C:13:LEU:N	2.41	0.53
1:B:403:HIS:CG	1:B:404:GLN:H	2.26	0.53
2:C:944:ASP:HA	2:C:952:ILE:O	2.08	0.53
1:B:282:LEU:HD21	1:B:317:LEU:HD12	1.91	0.53
1:B:501:MET:HE3	1:B:857:ILE:HG23	1.90	0.53
1:B:977:LEU:HD13	1:B:986:TRP:HB2	1.91	0.53
3:D:269:ASP:HA	3:D:295:LEU:HB2	1.90	0.53
1:B:146:MET:SD	1:B:357:ARG:NH1	2.81	0.53
1:B:307:HIS:HD2	1:B:309:LEU:HG	1.72	0.53
2:C:251:ILE:HD12	2:C:256:TYR:HD2	1.73	0.53
2:C:930:ARG:NH2	2:C:1003:ASP:HA	2.22	0.53
3:D:297:ASP:HB3	3:D:300:GLN:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:388:GLN:C	3:D:390:PHE:H	2.16	0.53
1:B:405:PRO:O	1:B:406:GLU:HG2	2.08	0.53
1:B:550:ARG:HD3	1:B:734:HIS:CD2	2.44	0.53
1:B:798:ASP:HB3	1:B:837:ALA:HB2	1.91	0.53
2:C:109:THR:HG23	2:C:110:LEU:N	2.24	0.53
2:C:264:GLN:HG2	2:C:322:GLU:CD	2.34	0.53
3:D:67:LEU:HA	3:D:70:THR:HB	1.90	0.53
3:D:170:SER:HB2	3:D:354:LEU:HD13	1.90	0.53
1:B:522:CYS:SG	1:B:526:ILE:HD11	2.49	0.53
1:B:904:THR:O	1:B:1062:LEU:HA	2.08	0.53
2:C:72:MET:HE2	2:C:207:LEU:HD22	1.90	0.53
2:C:146:LEU:HD22	2:C:169:TRP:CE2	2.44	0.53
2:C:204:PRO:HG2	2:C:207:LEU:HD12	1.91	0.53
2:C:367:LEU:O	2:C:762:PRO:HD3	2.09	0.53
2:C:849:PHE:HD2	2:C:1089:TRP:HE3	1.57	0.53
3:D:55:LEU:HD23	3:D:58:LEU:HD21	1.90	0.53
3:D:442:CYS:O	3:D:537:THR:HA	2.09	0.53
1:B:556:VAL:HB	1:B:738:ILE:HG12	1.91	0.53
2:C:97:THR:O	2:C:100:PRO:HD2	2.09	0.53
1:B:1082:LYS:HB2	1:B:1142:PHE:CD1	2.44	0.53
2:C:390:HIS:HD2	2:C:426:PHE:CD1	2.26	0.53
1:B:168:TRP:O	1:B:172:CYS:HB2	2.10	0.52
1:B:233:LYS:HB3	1:B:266:ILE:HG23	1.91	0.52
1:B:325:ASP:OD1	1:B:326:LEU:N	2.42	0.52
1:B:668:ARG:HB3	1:B:670:ILE:HG23	1.91	0.52
1:B:880:VAL:HG22	1:B:882:ASP:H	1.74	0.52
2:C:544:TRP:CD2	2:C:545:GLN:HG2	2.45	0.52
1:B:862:ASP:O	1:B:864:ASP:N	2.40	0.52
1:B:854:ARG:O	1:B:858:GLU:HG3	2.10	0.52
1:B:83:LEU:HD13	1:B:97:TYR:HD1	1.73	0.52
2:C:946:ALA:HB2	2:C:951:GLN:HE22	1.75	0.52
1:B:253:ASP:HB2	4:X:25:DA:H5"	1.91	0.52
1:B:940:LEU:N	1:B:940:LEU:CD1	2.73	0.52
2:C:921:CYS:O	2:C:925:GLN:HB2	2.09	0.52
3:D:584:ARG:N	3:D:584:ARG:CD	2.70	0.52
1:B:128:THR:O	1:B:132:PHE:N	2.42	0.52
1:B:809:SER:HB3	1:B:813:CYS:HB3	1.92	0.52
1:B:1071:ARG:HB3	1:B:1076:TYR:CE1	2.45	0.52
2:C:245:ARG:NH1	2:C:328:ASP:OD1	2.42	0.52
4:X:18:DT:H2"	4:X:19:DG:H8	1.74	0.52
1:B:950:SER:HB3	1:B:951:PRO:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:242:ARG:HB2	4:X:6:DT:H5''	1.91	0.52
1:B:367:GLY:O	1:B:370:LEU:HB3	2.10	0.52
1:B:760:PHE:HB2	1:B:794:ARG:HH21	1.75	0.52
2:C:501:GLY:HA2	2:C:503:ARG:NH1	2.24	0.52
1:B:1008:SER:HB3	1:B:1011:GLN:HG3	1.92	0.52
2:C:488:GLU:HA	2:C:491:ARG:HH11	1.73	0.52
3:D:297:ASP:OD1	3:D:298:ARG:N	2.42	0.52
1:B:911:GLN:CG	1:B:912:ARG:H	2.03	0.51
2:C:798:GLU:OE1	2:C:799:ARG:HG3	2.09	0.51
4:X:6:DT:H2'	4:X:7:DT:H71	1.92	0.51
1:B:838:LEU:HD21	1:B:842:LEU:HD11	1.92	0.51
1:B:1050:CYS:HB3	1:B:1051:PRO:HD2	1.92	0.51
4:X:59:DC:H2''	4:X:60:DG:H8	1.73	0.51
1:B:226:VAL:HG13	1:B:269:ILE:HD13	1.92	0.51
1:B:490:VAL:O	1:B:538:ALA:HA	2.11	0.51
2:C:570:GLN:HB3	2:C:598:PHE:HE1	1.75	0.51
3:D:519:ILE:O	3:D:519:ILE:HG13	2.09	0.51
1:B:657:VAL:O	1:B:660:MET:N	2.43	0.51
2:C:408:ILE:HG12	2:C:674:VAL:HB	1.93	0.51
3:D:475:ARG:O	3:D:475:ARG:HG3	2.10	0.51
1:B:901:TRP:CE2	2:C:406:ARG:NH1	2.78	0.51
1:B:100:LEU:O	1:B:104:ILE:HG13	2.10	0.51
1:B:204:GLU:OE1	1:B:392:GLN:NE2	2.44	0.51
1:B:497:PRO:HB2	1:B:864:ASP:O	2.10	0.51
1:B:503:LEU:HD21	1:B:854:ARG:HG3	1.91	0.51
2:C:142:ARG:CZ	2:C:702:LYS:HD3	2.40	0.51
3:D:364:ASP:OD1	3:D:365:SER:N	2.44	0.51
2:C:524:TRP:CE3	2:C:568:LEU:HD21	2.45	0.51
2:C:960:GLN:HG2	2:C:963:GLY:O	2.11	0.51
1:B:644:GLU:HG3	1:B:645:PHE:N	2.25	0.51
2:C:819:GLU:HG3	2:C:821:VAL:HG12	1.92	0.51
3:D:241:HIS:O	3:D:245:GLY:N	2.44	0.51
1:B:94:ASN:OD1	1:B:95:PRO:HD2	2.11	0.51
1:B:862:ASP:C	1:B:864:ASP:H	2.19	0.51
2:C:776:VAL:O	2:C:779:HIS:N	2.43	0.51
3:D:137:LEU:O	3:D:140:THR:OG1	2.25	0.51
1:B:1093:TYR:CD2	1:B:1145:GLY:HA2	2.46	0.51
3:D:82:GLU:HG3	3:D:102:LEU:HD21	1.93	0.51
1:B:89:ARG:HH22	2:C:770:ASP:CG	2.19	0.50
1:B:652:TRP:CZ3	1:B:657:VAL:HG13	2.46	0.50
2:C:35:ILE:HB	2:C:62:PHE:HE1	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:558:VAL:HB	1:B:563:GLU:HG2	1.94	0.50
2:C:544:TRP:CE3	2:C:545:GLN:HG2	2.45	0.50
3:D:389:ASP:C	3:D:391:THR:H	2.19	0.50
1:B:1114:TYR:O	1:B:1117:ALA:N	2.44	0.50
2:C:253:ASP:H	2:C:256:TYR:HB3	1.77	0.50
3:D:181:VAL:HG21	3:D:295:LEU:HD11	1.92	0.50
4:X:22:DA:H2''	4:X:23:DG:H8	1.76	0.50
1:B:61:VAL:HG22	1:B:382:MET:HE3	1.93	0.50
1:B:254:ARG:HH12	4:X:59:DC:H4'	1.77	0.50
1:B:500:LYS:HG3	1:B:866:ALA:O	2.12	0.50
1:B:1161:ASN:C	1:B:1163:GLY:H	2.20	0.50
1:B:461:PHE:CE2	1:B:803:TYR:HD1	2.26	0.50
2:C:10:LEU:HD21	2:C:42:MET:HE1	1.94	0.50
1:B:306:ARG:HG3	1:B:307:HIS:H	1.77	0.50
1:B:391:PRO:O	1:B:395:ARG:HG3	2.12	0.50
1:B:728:ARG:HE	1:B:735:LEU:HD12	1.76	0.50
1:B:1072:HIS:CD2	1:B:1073:GLU:HG3	2.46	0.50
3:D:202:ALA:O	3:D:268:VAL:HA	2.11	0.50
1:B:350:GLY:O	1:B:354:MET:HG3	2.11	0.50
1:B:458:ASN:HD21	1:B:478:VAL:HG22	1.76	0.50
2:C:240:PHE:CE2	2:C:242:ASN:HB3	2.46	0.50
3:D:3:LEU:HD13	3:D:33:PRO:HB3	1.94	0.50
3:D:328:GLN:HA	3:D:331:ARG:HE	1.77	0.50
3:D:407:MET:HG3	3:D:580:TYR:CE1	2.47	0.50
1:B:39:ARG:NH2	1:B:45:GLY:HA3	2.27	0.50
2:C:411:MET:HA	2:C:662:CYS:O	2.11	0.50
2:C:839:ARG:NH1	2:C:851:MET:SD	2.75	0.50
1:B:188:LYS:HB3	2:C:871:ILE:HG21	1.94	0.49
1:B:523:ALA:HB1	1:B:574:LEU:HD12	1.94	0.49
1:B:901:TRP:CZ2	2:C:406:ARG:NH1	2.80	0.49
3:D:396:ARG:HB2	3:D:580:TYR:CD1	2.47	0.49
3:D:539:HIS:CB	4:X:3:DT:H5''	2.42	0.49
1:B:843:GLN:C	1:B:844:LYS:HD2	2.38	0.49
2:C:847:ALA:O	2:C:851:MET:N	2.45	0.49
3:D:213:THR:HG22	3:D:237:ALA:H	1.78	0.49
4:X:55:DT:H2''	4:X:56:DG:H8	1.77	0.49
2:C:681:ASN:ND2	2:C:732:ILE:HB	2.18	0.49
3:D:200:ARG:HB2	3:D:263:LEU:HD22	1.94	0.49
1:B:464:THR:HG22	1:B:844:LYS:HA	1.91	0.49
2:C:479:LEU:HD12	2:C:599:PHE:HE1	1.76	0.49
2:C:565:ALA:HB1	3:D:22:GLN:HE21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:582:ARG:O	2:C:632:VAL:N	2.42	0.49
3:D:440:LEU:HD22	3:D:552:ILE:HD11	1.94	0.49
3:D:3:LEU:O	3:D:6:GLN:HB3	2.12	0.49
3:D:67:LEU:HD22	3:D:81:TRP:HH2	1.77	0.49
2:C:70:TRP:HA	2:C:73:PHE:HD2	1.78	0.49
2:C:384:ARG:NH1	2:C:788:PRO:HA	2.28	0.49
2:C:430:PRO:HD2	2:C:433:ARG:HD2	1.94	0.49
4:X:52:DC:H2''	4:X:53:DA:C8	2.48	0.49
1:B:281:GLN:OE1	1:B:281:GLN:N	2.46	0.49
1:B:519:ALA:HB2	1:B:756:PHE:CZ	2.46	0.49
1:B:1027:ILE:HG13	1:B:1027:ILE:O	2.11	0.49
2:C:118:ASP:O	2:C:119:SER:OG	2.24	0.49
2:C:166:ALA:HB3	2:C:167:PRO:HD3	1.95	0.49
2:C:240:PHE:CE2	2:C:311:ILE:HD13	2.48	0.49
2:C:305:LYS:HA	2:C:308:ARG:HG3	1.95	0.49
1:B:894:GLN:HG3	1:B:895:ARG:H	1.78	0.49
1:B:970:PRO:HB3	1:B:987:GLU:OE2	2.13	0.49
1:B:1081:TYR:O	1:B:1082:LYS:HD3	2.13	0.49
2:C:501:GLY:HA2	2:C:503:ARG:HH12	1.76	0.49
3:D:145:PHE:HE2	3:D:155:LYS:HA	1.77	0.49
1:B:177:ARG:HH12	2:C:914:GLU:HB3	1.77	0.48
1:B:1091:SER:C	1:B:1093:TYR:N	2.71	0.48
2:C:257:LEU:O	2:C:261:LEU:HG	2.13	0.48
2:C:1040:GLU:HB3	2:C:1084:GLU:OE1	2.13	0.48
1:B:496:GLN:OE1	1:B:497:PRO:HD2	2.13	0.48
1:B:613:ARG:HG2	2:C:855:VAL:HG22	1.94	0.48
2:C:1033:ALA:O	2:C:1035:LEU:N	2.46	0.48
3:D:226:THR:HB	3:D:229:GLN:OE1	2.13	0.48
4:X:21:DG:H2''	4:X:22:DA:C8	2.47	0.48
2:C:974:VAL:HB	2:C:1039:PRO:O	2.13	0.48
2:C:680:MET:O	2:C:745:SER:N	2.46	0.48
1:B:446:ASN:OD1	1:B:448:ARG:N	2.38	0.48
1:B:1018:GLN:HG2	2:C:59:ASN:HD21	1.79	0.48
1:B:1028:SER:O	1:B:1059:ARG:HG3	2.13	0.48
1:B:1056:MET:O	1:B:1058:VAL:HG23	2.14	0.48
4:X:16:DA:H2''	4:X:17:DA:C8	2.48	0.48
1:B:760:PHE:HZ	1:B:822:ARG:HB2	1.78	0.48
1:B:1111:TYR:O	1:B:1115:THR:HG23	2.14	0.48
2:C:1087:ASP:OD1	2:C:1088:ILE:N	2.47	0.48
3:D:226:THR:HG22	3:D:227:ASP:H	1.78	0.48
3:D:582:ASP:HB2	3:D:585:ILE:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:LEU:HD23	1:B:103:GLU:CD	2.39	0.48
2:C:433:ARG:NH1	2:C:804:ARG:H	2.12	0.48
1:B:233:LYS:O	1:B:266:ILE:HD13	2.14	0.48
1:B:306:ARG:HG3	1:B:307:HIS:CE1	2.48	0.48
2:C:430:PRO:O	2:C:434:TYR:N	2.44	0.48
2:C:656:ALA:HB3	2:C:658:PRO:HD3	1.95	0.48
2:C:896:ARG:HA	2:C:899:ARG:HH21	1.78	0.48
3:D:61:ASN:OD1	3:D:62:GLU:N	2.47	0.48
3:D:301:LEU:HB3	3:D:542:GLN:NE2	2.28	0.48
4:X:56:DG:H1'	4:X:57:DC:H5'	1.95	0.48
2:C:941:MET:CE	2:C:987:TYR:CD1	2.87	0.48
1:B:59:LEU:O	1:B:125:ALA:HB3	2.14	0.47
2:C:220:PRO:HD2	2:C:223:TYR:CD2	2.49	0.47
2:C:1088:ILE:HD11	2:C:1089:TRP:CE2	2.49	0.47
3:D:117:ARG:O	3:D:121:ARG:HG2	2.13	0.47
3:D:511:TRP:CE3	3:D:519:ILE:HD12	2.49	0.47
1:B:1130:ASP:H	1:B:1134:HIS:CD2	2.31	0.47
2:C:120:ASP:O	2:C:633:PRO:HG3	2.14	0.47
3:D:155:LYS:HG2	3:D:333:THR:HG22	1.96	0.47
2:C:984:HIS:NE2	2:C:988:CYS:SG	2.88	0.47
3:D:145:PHE:HE1	3:D:183:LYS:HG3	1.79	0.47
3:D:230:LYS:HA	3:D:233:ILE:HD12	1.96	0.47
2:C:265:ARG:HA	2:C:271:ASP:HA	1.95	0.47
2:C:382:PRO:HB2	2:C:421:PHE:CE2	2.50	0.47
2:C:654:PHE:O	2:C:660:ASN:ND2	2.47	0.47
1:B:595:GLU:OE1	1:B:620:MET:HB2	2.14	0.47
1:B:838:LEU:CD2	1:B:842:LEU:HD11	2.45	0.47
2:C:406:ARG:HG3	2:C:657:GLY:HA2	1.96	0.47
3:D:437:GLU:O	3:D:548:HIS:N	2.38	0.47
3:D:262:HIS:O	3:D:263:LEU:HD23	2.14	0.47
3:D:412:LEU:CD2	3:D:462:MET:HE1	2.44	0.47
1:B:307:HIS:CD2	1:B:309:LEU:HG	2.49	0.47
1:B:1111:TYR:HB3	1:B:1140:TYR:HE2	1.78	0.47
2:C:390:HIS:HD2	2:C:426:PHE:CE1	2.32	0.47
2:C:432:ASP:OD1	2:C:433:ARG:N	2.47	0.47
2:C:593:ASP:O	2:C:597:ALA:CB	2.61	0.47
2:C:833:PRO:O	2:C:836:THR:N	2.46	0.47
3:D:175:THR:HA	3:D:358:SER:HA	1.96	0.47
3:D:398:LEU:HD11	3:D:404:TYR:HB2	1.95	0.47
1:B:136:MET:HE1	1:B:140:ASN:ND2	2.29	0.47
1:B:180:ALA:HB1	2:C:912:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:561:ARG:HH12	1:B:584:ARG:NH1	2.12	0.47
1:B:979:LEU:HD12	1:B:979:LEU:O	2.14	0.47
1:B:258:ASN:HB3	1:B:277:THR:HB	1.97	0.47
1:B:1053:LEU:HD22	1:B:1109:LEU:HD22	1.97	0.47
2:C:73:PHE:HB3	2:C:80:ILE:HD13	1.97	0.47
2:C:506:ILE:HG12	2:C:507:ASP:OD1	2.15	0.47
2:C:550:TYR:CE2	2:C:552:GLU:HB2	2.49	0.47
2:C:1114:LEU:HD21	2:C:1118:ARG:NH1	2.29	0.47
3:D:55:LEU:HG	3:D:105:ASP:O	2.15	0.47
3:D:390:PHE:O	3:D:391:THR:OG1	2.25	0.47
3:D:485:ALA:HB3	3:D:529:GLU:HB3	1.96	0.47
1:B:460:LEU:HD21	1:B:841:LEU:CD1	2.44	0.46
1:B:706:ALA:O	1:B:709:ARG:HB3	2.15	0.46
1:B:754:LEU:HD21	1:B:805:ALA:HB1	1.97	0.46
2:C:351:ALA:HB3	2:C:353:VAL:HG23	1.97	0.46
2:C:940:SER:OG	2:C:957:PRO:HA	2.15	0.46
1:B:265:TRP:CD1	1:B:275:GLU:HG2	2.50	0.46
2:C:385:GLU:OE2	2:C:730:SER:OG	2.27	0.46
2:C:530:ARG:NH2	2:C:548:LEU:O	2.48	0.46
3:D:175:THR:HG22	3:D:358:SER:HB3	1.98	0.46
1:B:722:ALA:O	1:B:725:GLN:HB2	2.15	0.46
2:C:857:PHE:HB2	2:C:1088:ILE:HD13	1.97	0.46
1:B:401:TRP:HD1	1:B:407:THR:HB	1.80	0.46
2:C:109:THR:HA	2:C:112:ARG:NH2	2.31	0.46
3:D:538:VAL:O	3:D:541:SER:OG	2.33	0.46
1:B:501:MET:HE2	1:B:865:ILE:HG21	1.97	0.46
1:B:831:THR:HG22	1:B:848:GLN:O	2.15	0.46
1:B:1120:ARG:NE	1:B:1169:ASP:OD1	2.49	0.46
2:C:1046:LEU:HD21	2:C:1114:LEU:HA	1.98	0.46
3:D:5:LYS:HA	3:D:8:LEU:HD12	1.98	0.46
3:D:425:ARG:NH2	3:D:504:ARG:HA	2.29	0.46
1:B:464:THR:HG22	1:B:844:LYS:CA	2.46	0.46
2:C:86:PHE:CZ	2:C:176:THR:HG21	2.51	0.46
2:C:376:PHE:HE1	2:C:729:ILE:HD12	1.80	0.46
2:C:504:TRP:CG	2:C:505:GLY:N	2.84	0.46
4:X:22:DA:H2''	4:X:23:DG:C8	2.49	0.46
1:B:689:HIS:CG	1:B:727:MET:HE2	2.51	0.46
2:C:121:LYS:NZ	2:C:631:ALA:O	2.48	0.46
4:X:11:DT:C2'	4:X:12:DT:H5''	2.44	0.46
2:C:297:ASN:HD22	2:C:342:ILE:HA	1.80	0.46
2:C:457:LEU:HA	2:C:460:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:467:SER:HA	2:C:524:TRP:HZ2	1.79	0.46
2:C:966:ARG:O	2:C:998:LEU:HD12	2.16	0.46
2:C:998:LEU:HG	2:C:1000:LEU:HD11	1.97	0.46
1:B:86:ALA:O	1:B:90:GLU:N	2.48	0.46
1:B:894:GLN:HG3	1:B:895:ARG:N	2.31	0.46
1:B:1018:GLN:O	1:B:1068:LEU:HD12	2.16	0.46
2:C:248:TRP:CD1	2:C:248:TRP:H	2.33	0.46
3:D:226:THR:HG22	3:D:227:ASP:N	2.31	0.46
1:B:645:PHE:HD1	1:B:648:TYR:CD2	2.34	0.45
1:B:710:TRP:CE2	1:B:714:HIS:CD2	3.04	0.45
1:B:1110:GLN:NE2	1:B:1114:TYR:OH	2.44	0.45
2:C:310:TYR:CE2	2:C:314:LEU:HD11	2.51	0.45
2:C:538:GLU:HG2	2:C:540:ALA:H	1.81	0.45
1:B:611:THR:O	1:B:611:THR:CG2	2.65	0.45
1:B:1125:ARG:HG2	2:C:29:PRO:HA	1.98	0.45
2:C:209:SER:O	2:C:234:ILE:HG23	2.17	0.45
2:C:105:ARG:O	2:C:106:GLU:HB2	2.17	0.45
1:B:254:ARG:HH22	4:X:59:DC:H5'	1.81	0.45
1:B:494:GLU:N	1:B:494:GLU:OE1	2.50	0.45
1:B:500:LYS:HA	1:B:866:ALA:O	2.16	0.45
1:B:1077:TYR:CE1	1:B:1136:GLY:HA3	2.51	0.45
2:C:409:ILE:HD12	2:C:672:PHE:HE2	1.81	0.45
2:C:411:MET:HE3	2:C:677:LEU:HD21	1.98	0.45
1:B:712:SER:HB2	2:C:860:GLU:HG2	1.97	0.45
2:C:35:ILE:HB	2:C:62:PHE:CE1	2.52	0.45
2:C:943:ILE:HG21	2:C:986:VAL:HG22	1.99	0.45
3:D:474:SER:O	3:D:475:ARG:CB	2.64	0.45
1:B:636:HIS:O	1:B:640:VAL:HG23	2.17	0.45
2:C:89:GLN:O	2:C:92:SER:HB3	2.17	0.45
1:B:243:LEU:HD21	1:B:247:ILE:HD11	1.98	0.45
1:B:514:TYR:CE1	1:B:518:MET:HG3	2.51	0.45
1:B:833:VAL:O	1:B:836:SER:OG	2.31	0.45
2:C:43:ALA:HB1	2:C:62:PHE:CD2	2.51	0.45
2:C:941:MET:CG	2:C:959:VAL:HG21	2.46	0.45
3:D:543:GLY:H	3:D:572:ARG:HH12	1.64	0.45
1:B:465:ASP:OD1	1:B:466:ASP:N	2.50	0.45
1:B:692:GLU:OE2	2:C:383:GLN:HG2	2.16	0.45
1:B:751:LEU:HD22	1:B:812:HIS:HB3	1.98	0.45
2:C:682:ASP:HA	2:C:745:SER:HA	1.99	0.45
2:C:848:PHE:CD2	2:C:1034:PRO:HB3	2.51	0.45
2:C:875:LEU:HD21	4:X:11:DT:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:881:ASN:OD1	2:C:920:GLN:NE2	2.49	0.45
3:D:140:THR:O	3:D:144:LEU:HG	2.16	0.45
1:B:187:TRP:CZ2	1:B:327:VAL:HG11	2.51	0.45
1:B:1115:THR:HG21	1:B:1160:PRO:HG2	1.98	0.45
2:C:923:GLU:HG2	2:C:924:MET:HE2	1.98	0.45
1:B:60:LEU:HB2	1:B:378:PHE:CD1	2.52	0.44
1:B:63:THR:HG22	1:B:64:PHE:N	2.32	0.44
1:B:716:LEU:O	1:B:718:PRO:HD3	2.17	0.44
2:C:273:GLU:CG	2:C:274:LEU:H	2.27	0.44
2:C:388:VAL:HG11	2:C:784:HIS:CD2	2.52	0.44
3:D:256:HIS:HD2	3:D:258:GLY:H	1.59	0.44
2:C:522:HIS:CE1	2:C:905:GLY:O	2.70	0.44
2:C:941:MET:HG2	2:C:959:VAL:CG2	2.44	0.44
1:B:25:ALA:HB2	1:B:417:GLN:HE21	1.83	0.44
2:C:84:SER:OG	2:C:85:ALA:N	2.51	0.44
2:C:162:GLN:O	2:C:165:GLN:N	2.46	0.44
2:C:245:ARG:HD2	2:C:343:LEU:HD21	1.99	0.44
2:C:471:LEU:HD13	2:C:494:ARG:HD2	2.00	0.44
2:C:583:PRO:HD2	2:C:586:GLU:OE1	2.18	0.44
1:B:24:SER:C	1:B:27:THR:HG1	2.24	0.44
1:B:973:VAL:HG21	1:B:991:THR:HB	1.99	0.44
2:C:207:LEU:HD23	2:C:207:LEU:HA	1.82	0.44
1:B:456:SER:OG	1:B:499:MET:SD	2.76	0.44
2:C:956:LEU:HD23	2:C:956:LEU:HA	1.82	0.44
2:C:1057:MET:HE1	2:C:1110:GLN:HE21	1.81	0.44
3:D:393:ILE:HD13	3:D:577:LEU:HD23	1.99	0.44
2:C:479:LEU:HD12	2:C:599:PHE:CE1	2.52	0.44
2:C:657:GLY:N	2:C:658:PRO:CD	2.80	0.44
3:D:144:LEU:HD11	3:D:187:ALA:HB2	1.99	0.44
1:B:169:ARG:NH2	2:C:867:THR:OG1	2.50	0.44
1:B:956:HIS:O	1:B:960:GLU:HG3	2.18	0.44
3:D:444:LEU:HD22	4:X:1:DT:H4'	1.98	0.44
1:B:169:ARG:HA	1:B:173:TYR:CE2	2.52	0.44
2:C:233:HIS:HB2	2:C:234:ILE:HD12	2.00	0.44
3:D:42:LEU:HD11	3:D:108:TYR:HA	2.00	0.44
1:B:503:LEU:O	1:B:870:ALA:N	2.49	0.44
1:B:530:LEU:O	1:B:533:GLY:N	2.48	0.44
1:B:9:ASP:HB2	1:B:12:ARG:HB2	2.00	0.43
1:B:487:LEU:C	1:B:488:ARG:HG3	2.43	0.43
1:B:631:LEU:HD21	1:B:638:TRP:CE3	2.53	0.43
3:D:50:HIS:HD2	3:D:597:ARG:H	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:537:THR:HG21	4:X:3:DT:OP1	2.18	0.43
1:B:258:ASN:O	1:B:261:ASN:HB2	2.18	0.43
2:C:251:ILE:HG21	2:C:286:LEU:HD22	1.91	0.43
2:C:276:LEU:HB2	2:C:280:SER:HB3	1.99	0.43
2:C:872:LEU:HD12	2:C:916:PHE:CE2	2.53	0.43
3:D:407:MET:HG3	3:D:580:TYR:CZ	2.53	0.43
1:B:580:TYR:HD2	1:B:583:ASN:HB2	1.83	0.43
2:C:125:PHE:CG	2:C:636:LEU:HD11	2.54	0.43
1:B:840:ARG:HG3	1:B:845:GLY:HA2	2.00	0.43
1:B:760:PHE:O	1:B:822:ARG:NH2	2.51	0.43
2:C:69:ILE:HG22	2:C:73:PHE:CE2	2.53	0.43
2:C:111:LEU:HD11	2:C:164:TRP:CE3	2.54	0.43
2:C:253:ASP:O	2:C:256:TYR:N	2.43	0.43
3:D:405:ILE:O	3:D:409:GLU:HG3	2.18	0.43
3:D:445:ARG:HD2	4:X:3:DT:OP2	2.18	0.43
1:B:906:TYR:O	1:B:909:LEU:HB2	2.18	0.43
2:C:386:VAL:HG11	2:C:422:ILE:HD13	2.00	0.43
2:C:531:MET:HE2	2:C:561:VAL:HG22	2.01	0.43
1:B:77:ARG:NH1	1:B:81:HIS:HB2	2.33	0.43
2:C:109:THR:HG23	2:C:110:LEU:H	1.83	0.43
2:C:939:GLN:CD	2:C:939:GLN:H	2.27	0.43
2:C:998:LEU:HG	2:C:1000:LEU:CD1	2.48	0.43
3:D:55:LEU:O	3:D:59:GLU:HG2	2.19	0.43
3:D:165:ARG:HG2	3:D:166:ILE:HD12	1.99	0.43
3:D:545:GLU:HB3	3:D:574:ARG:CG	2.49	0.43
1:B:31:PHE:CD2	1:B:31:PHE:C	2.97	0.43
1:B:143:GLU:OE1	1:B:143:GLU:N	2.47	0.43
2:C:120:ASP:O	2:C:121:LYS:HB2	2.19	0.43
2:C:149:TRP:CD1	2:C:149:TRP:N	2.86	0.43
2:C:794:TYR:CE1	2:C:801:SER:HB3	2.53	0.43
2:C:942:GLU:HG3	2:C:954:GLY:O	2.19	0.43
1:B:575:GLU:O	1:B:575:GLU:HG2	2.18	0.43
1:B:683:ARG:NH1	2:C:1095:ARG:HG3	2.33	0.43
1:B:1067:ASP:HB2	1:B:1079:LEU:O	2.19	0.43
1:B:1090:SER:O	1:B:1092:ALA:N	2.52	0.43
2:C:454:PHE:O	2:C:457:LEU:HB2	2.18	0.43
2:C:878:TYR:CD1	4:X:11:DT:H4'	2.54	0.43
3:D:275:ASP:OD2	3:D:305:GLU:HB2	2.19	0.43
2:C:99:LEU:HB2	2:C:100:PRO:HD3	2.00	0.43
2:C:295:VAL:HG12	2:C:295:VAL:O	2.19	0.43
2:C:524:TRP:HB3	2:C:568:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:794:TYR:CE2	2:C:807:LEU:HA	2.53	0.43
3:D:154:GLN:NE2	3:D:359:TYR:HE2	2.17	0.43
3:D:225:LEU:HB3	3:D:229:GLN:HB2	2.00	0.43
3:D:265:VAL:HA	3:D:291:ARG:O	2.18	0.43
4:X:4:DT:H2''	4:X:5:DT:O5'	2.19	0.43
1:B:421:ALA:HA	1:B:425:ALA:O	2.19	0.42
1:B:652:TRP:CZ3	1:B:657:VAL:HG22	2.54	0.42
3:D:165:ARG:HH22	3:D:288:ASP:HA	1.84	0.42
4:X:19:DG:H2''	4:X:20:DC:C6	2.54	0.42
1:B:18:GLU:CG	1:B:409:LEU:HD23	2.44	0.42
1:B:588:PHE:CD2	1:B:714:HIS:HB3	2.54	0.42
2:C:135:PHE:CE1	2:C:169:TRP:HB2	2.53	0.42
2:C:245:ARG:HA	2:C:326:PHE:CZ	2.54	0.42
2:C:362:ASP:HB3	2:C:765:GLU:O	2.19	0.42
2:C:534:GLY:HA3	2:C:550:TYR:O	2.18	0.42
3:D:86:LEU:HD11	3:D:93:ARG:HG2	2.00	0.42
3:D:333:THR:OG1	3:D:335:THR:OG1	2.34	0.42
3:D:387:GLN:C	3:D:389:ASP:H	2.27	0.42
3:D:510:VAL:O	3:D:521:SER:HA	2.19	0.42
1:B:420:TYR:HD1	1:B:422:PHE:CE2	2.37	0.42
1:B:587:VAL:HG21	1:B:689:HIS:ND1	2.34	0.42
1:B:592:GLU:CD	1:B:683:ARG:HG3	2.43	0.42
1:B:877:PRO:O	1:B:878:TRP:HB2	2.19	0.42
2:C:70:TRP:HA	2:C:73:PHE:CD2	2.53	0.42
2:C:251:ILE:CB	2:C:286:LEU:HD13	2.50	0.42
2:C:332:ASP:OD1	2:C:332:ASP:N	2.51	0.42
2:C:619:ILE:HD11	2:C:644:ARG:HG3	2.01	0.42
2:C:146:LEU:HA	2:C:146:LEU:HD23	1.84	0.42
3:D:253:LEU:HD11	3:D:281:ARG:HE	1.85	0.42
1:B:15:LEU:C	1:B:16:GLN:HG3	2.44	0.42
2:C:107:ASP:C	2:C:109:THR:H	2.26	0.42
3:D:145:PHE:CE2	3:D:155:LYS:HA	2.54	0.42
1:B:265:TRP:CZ2	1:B:274:GLU:HA	2.55	0.42
2:C:265:ARG:O	2:C:323:LEU:HA	2.19	0.42
3:D:67:LEU:HD23	3:D:70:THR:HB	2.02	0.42
3:D:406:ALA:O	3:D:409:GLU:HB2	2.20	0.42
3:D:584:ARG:H	3:D:584:ARG:CD	2.31	0.42
1:B:558:VAL:O	1:B:740:THR:HA	2.20	0.42
3:D:418:TYR:CZ	3:D:422:LEU:HD11	2.55	0.42
4:X:53:DA:H2''	4:X:54:DG:C8	2.55	0.42
1:B:254:ARG:HH22	4:X:59:DC:C4'	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1036:LEU:O	1:B:1039:LEU:N	2.53	0.42
1:B:1090:SER:C	1:B:1092:ALA:H	2.28	0.42
2:C:1050:TYR:HA	2:C:1057:MET:HA	2.00	0.42
3:D:438:TYR:HD1	3:D:548:HIS:CD2	2.38	0.42
1:B:94:ASN:HD22	1:B:97:TYR:HD2	1.66	0.42
1:B:1031:LEU:HD12	1:B:1171:MET:HE2	2.01	0.42
1:B:504:MET:HA	1:B:870:ALA:HB3	2.01	0.42
2:C:483:PHE:O	2:C:484:ASP:OD1	2.37	0.42
3:D:53:LEU:HG	3:D:58:LEU:HD23	2.01	0.42
3:D:511:TRP:CZ3	3:D:519:ILE:CD1	3.03	0.42
1:B:147:LEU:HD22	2:C:126:GLN:HG3	2.02	0.41
1:B:1124:HIS:O	2:C:25:ARG:NH2	2.52	0.41
2:C:998:LEU:O	2:C:1005:GLU:HA	2.20	0.41
3:D:65:HIS:CG	3:D:66:PRO:HD2	2.55	0.41
3:D:599:GLY:O	3:D:603:LEU:N	2.47	0.41
2:C:523:THR:O	2:C:526:PHE:N	2.52	0.41
3:D:301:LEU:HB3	3:D:542:GLN:HE21	1.85	0.41
3:D:549:ALA:HB3	3:D:573:ALA:HB2	2.02	0.41
1:B:1041:ARG:HA	1:B:1047:SER:HB3	2.02	0.41
2:C:880:ILE:HG23	2:C:901:PHE:HE2	1.85	0.41
3:D:497:ASP:OD1	3:D:498:ILE:N	2.53	0.41
1:B:134:GLN:NE2	1:B:152:LEU:HD11	2.36	0.41
1:B:403:HIS:CD2	1:B:404:GLN:H	2.38	0.41
1:B:947:ARG:C	1:B:951:PRO:HG2	2.46	0.41
2:C:72:MET:SD	2:C:230:LEU:HD11	2.60	0.41
2:C:649:ARG:HA	2:C:649:ARG:HD3	1.88	0.41
2:C:960:GLN:HE21	2:C:962:ASP:HB2	1.85	0.41
3:D:50:HIS:CD2	3:D:597:ARG:H	2.38	0.41
3:D:425:ARG:HD2	3:D:425:ARG:HA	1.78	0.41
1:B:760:PHE:CZ	1:B:822:ARG:HB2	2.55	0.41
2:C:115:LEU:O	2:C:117:ASP:N	2.53	0.41
2:C:272:ARG:HG3	2:C:273:GLU:N	2.34	0.41
3:D:229:GLN:OE1	3:D:229:GLN:N	2.44	0.41
1:B:64:PHE:HD2	1:B:65:THR:HG23	1.85	0.41
1:B:170:ARG:HG3	1:B:171:HIS:ND1	2.34	0.41
1:B:563:GLU:CG	1:B:756:PHE:HD2	2.31	0.41
1:B:672:GLU:CD	2:C:808:PRO:HB2	2.46	0.41
1:B:901:TRP:HA	1:B:1059:ARG:O	2.21	0.41
2:C:98:LEU:HD11	2:C:172:LEU:HA	2.01	0.41
2:C:260:LEU:HD23	2:C:260:LEU:HA	1.93	0.41
2:C:1061:ASP:HA	2:C:1064:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:ALA:HB2	1:B:443:LEU:H	1.86	0.41
1:B:674:LEU:HD22	1:B:683:ARG:HD2	2.02	0.41
1:B:689:HIS:CD2	1:B:727:MET:HE2	2.55	0.41
1:B:945:PHE:HB3	1:B:1144:ARG:HH21	1.85	0.41
2:C:311:ILE:HD12	2:C:311:ILE:HA	1.93	0.41
2:C:963:GLY:HA3	2:C:995:GLU:O	2.20	0.41
1:B:240:VAL:HA	1:B:259:ARG:NH1	2.35	0.41
1:B:652:TRP:NE1	1:B:704:GLU:HB3	2.27	0.41
1:B:694:LEU:HD23	1:B:694:LEU:HA	1.86	0.41
2:C:147:ALA:O	2:C:151:THR:HG23	2.20	0.41
2:C:502:ILE:HD11	2:C:527:GLY:HA3	2.03	0.41
2:C:749:GLN:O	2:C:752:ILE:HG13	2.21	0.41
2:C:749:GLN:OE1	2:C:752:ILE:HD11	2.20	0.41
2:C:820:PHE:CE2	2:C:849:PHE:HE1	2.39	0.41
3:D:113:TRP:CZ2	3:D:117:ARG:HD2	2.56	0.41
3:D:438:TYR:CD1	3:D:548:HIS:CD2	3.08	0.41
1:B:245:ALA:HA	1:B:306:ARG:HH22	1.85	0.41
1:B:325:ASP:HA	1:B:780:LEU:HD13	2.03	0.41
1:B:328:ILE:O	1:B:332:LEU:HB2	2.21	0.41
1:B:453:MET:HE2	1:B:809:SER:OG	2.21	0.41
1:B:582:SER:OG	1:B:743:LYS:HG3	2.21	0.41
1:B:607:GLU:H	1:B:607:GLU:HG3	1.75	0.41
1:B:1085:TRP:CD1	1:B:1093:TYR:HE1	2.39	0.41
2:C:109:THR:O	2:C:112:ARG:N	2.54	0.41
2:C:185:HIS:HD2	2:C:187:ALA:H	1.67	0.41
2:C:204:PRO:HA	2:C:205:PRO:HD3	1.89	0.41
2:C:411:MET:HB3	2:C:664:LEU:CD1	2.51	0.41
2:C:1114:LEU:N	2:C:1115:PRO:HD2	2.36	0.41
3:D:412:LEU:HD21	3:D:462:MET:HE1	2.03	0.41
3:D:498:ILE:H	3:D:498:ILE:HG13	1.73	0.41
4:X:57:DC:H2"	4:X:58:DT:C6	2.56	0.41
4:X:64:DT:H2"	4:X:65:DA:C8	2.56	0.41
1:B:645:PHE:HD1	1:B:648:TYR:HD2	1.68	0.41
2:C:89:GLN:N	2:C:89:GLN:OE1	2.54	0.41
2:C:875:LEU:HA	2:C:878:TYR:HB3	2.03	0.41
3:D:367:ILE:HD11	3:D:577:LEU:HB3	2.03	0.41
3:D:390:PHE:C	3:D:392:ASP:H	2.29	0.41
1:B:50:PHE:CG	1:B:51:PRO:HD2	2.56	0.40
1:B:283:PRO:HD3	1:B:310:PHE:O	2.21	0.40
2:C:251:ILE:HB	2:C:286:LEU:CD1	2.51	0.40
2:C:324:ASP:OD1	2:C:324:ASP:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:62:GLU:HG2	3:D:67:LEU:HD12	2.03	0.40
1:B:461:PHE:CD1	1:B:841:LEU:CD1	3.04	0.40
1:B:986:TRP:O	1:B:989:VAL:N	2.54	0.40
1:B:1098:MET:O	1:B:1102:MET:HG2	2.22	0.40
2:C:403:LEU:HD12	2:C:403:LEU:HA	1.80	0.40
2:C:685:TYR:HA	2:C:686:PRO:C	2.45	0.40
3:D:209:ALA:O	3:D:213:THR:HG23	2.21	0.40
3:D:389:ASP:O	3:D:391:THR:N	2.55	0.40
4:X:24:DC:H2''	4:X:25:DA:C8	2.56	0.40
1:B:306:ARG:HD3	1:B:306:ARG:HA	1.79	0.40
1:B:820:LEU:HD23	1:B:821:VAL:N	2.36	0.40
2:C:50:LEU:O	2:C:53:LYS:N	2.54	0.40
1:B:89:ARG:C	1:B:91:THR:H	2.29	0.40
2:C:365:ARG:HB2	2:C:759:HIS:ND1	2.36	0.40
2:C:965:LEU:O	2:C:966:ARG:NH2	2.45	0.40
2:C:1087:ASP:OD2	2:C:1089:TRP:HD1	2.04	0.40
3:D:112:MET:O	3:D:116:GLU:CB	2.68	0.40
3:D:378:ASP:OD1	3:D:378:ASP:N	2.54	0.40
3:D:432:ILE:HG12	3:D:500:ILE:HD12	2.03	0.40
3:D:480:ARG:HH21	3:D:482:VAL:HG12	1.86	0.40
1:B:514:TYR:CE2	1:B:756:PHE:HA	2.57	0.40
2:C:104:GLU:OE1	2:C:112:ARG:NH2	2.53	0.40
2:C:394:LEU:HD21	2:C:433:ARG:HG3	2.04	0.40
2:C:567:LEU:HG	2:C:568:LEU:HD12	2.03	0.40
2:C:602:ASP:O	2:C:606:GLU:HG3	2.21	0.40
4:X:21:DG:H2''	4:X:22:DA:H8	1.85	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	B	1126/1181 (95%)	1054 (94%)	70 (6%)	2 (0%)	43	74
2	C	1119/1122 (100%)	1058 (94%)	58 (5%)	3 (0%)	36	69
3	D	603/609 (99%)	566 (94%)	35 (6%)	2 (0%)	36	69
All	All	2848/2912 (98%)	2678 (94%)	163 (6%)	7 (0%)	44	74

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1091	SER
2	C	282	ASN
1	B	1090	SER
3	D	389	ASP
2	C	295	VAL
2	C	659	VAL
3	D	528	PRO

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	960/980 (98%)	957 (100%)	3 (0%)	86	85
2	C	976/977 (100%)	976 (100%)	0	100	100
3	D	489/492 (99%)	486 (99%)	3 (1%)	78	80
All	All	2425/2449 (99%)	2419 (100%)	6 (0%)	85	87

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	158	LEU
1	B	979	LEU
1	B	1032	ILE
3	D	354	LEU
3	D	398	LEU
3	D	430	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	134	GLN
1	B	140	ASN
1	B	150	GLN
1	B	261	ASN
1	B	262	GLN
1	B	307	HIS
1	B	402	HIS
1	B	458	ASN
1	B	484	ASN
1	B	566	GLN
1	B	695	GLN
1	B	765	GLN
1	B	769	HIS
1	B	781	ASN
1	B	848	GLN
1	B	879	GLN
1	B	943	HIS
1	B	944	GLN
1	B	1072	HIS
1	B	1095	GLN
1	B	1133	HIS
1	B	1134	HIS
1	B	1150	HIS
2	C	6	HIS
2	C	87	ASN
2	C	126	GLN
2	C	162	GLN
2	C	185	HIS
2	C	237	HIS
2	C	336	HIS
2	C	390	HIS
2	C	510	ASN
2	C	660	ASN
2	C	768	ASN
2	C	793	ASN
2	C	881	ASN
2	C	920	GLN
2	C	925	GLN
2	C	951	GLN
2	C	993	ASN
2	C	1078	ASN

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Mol	Chain	Res	Type
2	C	1110	GLN
3	D	13	HIS
3	D	22	GLN
3	D	50	HIS
3	D	115	ASN
3	D	247	GLN
3	D	262	HIS
3	D	473	HIS
3	D	523	GLN
3	D	548	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	ANP	B	1501	6	33,33,33	2.71	11 (33%)	45,52,52	2.11	14 (31%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ANP	B	1501	6	-	2/18/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1501	ANP	PA-O3A	-8.44	1.50	1.59
5	B	1501	ANP	C5-C4	5.38	1.48	1.39
5	B	1501	ANP	PG-N3B	5.28	1.77	1.63
5	B	1501	ANP	PB-O1B	-5.26	1.38	1.46
5	B	1501	ANP	PB-N3B	4.19	1.74	1.63
5	B	1501	ANP	PB-O3A	-3.20	1.55	1.59
5	B	1501	ANP	PG-O1G	3.14	1.50	1.46
5	B	1501	ANP	C5-N7	-2.97	1.33	1.39
5	B	1501	ANP	C5-C6	2.96	1.49	1.41
5	B	1501	ANP	C8-N7	2.24	1.36	1.31
5	B	1501	ANP	PG-O3G	-2.09	1.51	1.56

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1501	ANP	C5-C4-N3	-6.86	117.27	126.72
5	B	1501	ANP	N3-C4-N9	5.09	135.83	127.17
5	B	1501	ANP	C4-C5-N7	-3.98	106.03	110.58
5	B	1501	ANP	O2G-PG-O3G	3.62	117.33	107.59
5	B	1501	ANP	C2-N3-C4	3.58	120.58	111.83
5	B	1501	ANP	O1G-PG-N3B	-2.65	107.86	111.77
5	B	1501	ANP	O2B-PB-O3A	2.52	113.05	104.64
5	B	1501	ANP	C5-N7-C8	2.50	107.38	103.45
5	B	1501	ANP	O3'-C3'-C4'	-2.50	103.90	111.08
5	B	1501	ANP	O3'-C3'-C2'	2.46	119.70	111.82
5	B	1501	ANP	N3-C2-N1	-2.39	124.97	128.58
5	B	1501	ANP	O2'-C2'-C3'	2.26	119.06	111.82
5	B	1501	ANP	C3'-C2'-C1'	2.03	105.30	101.46
5	B	1501	ANP	C4'-O4'-C1'	2.02	113.92	109.47

There are no chirality outliers.

All (2) torsion outliers are listed below:

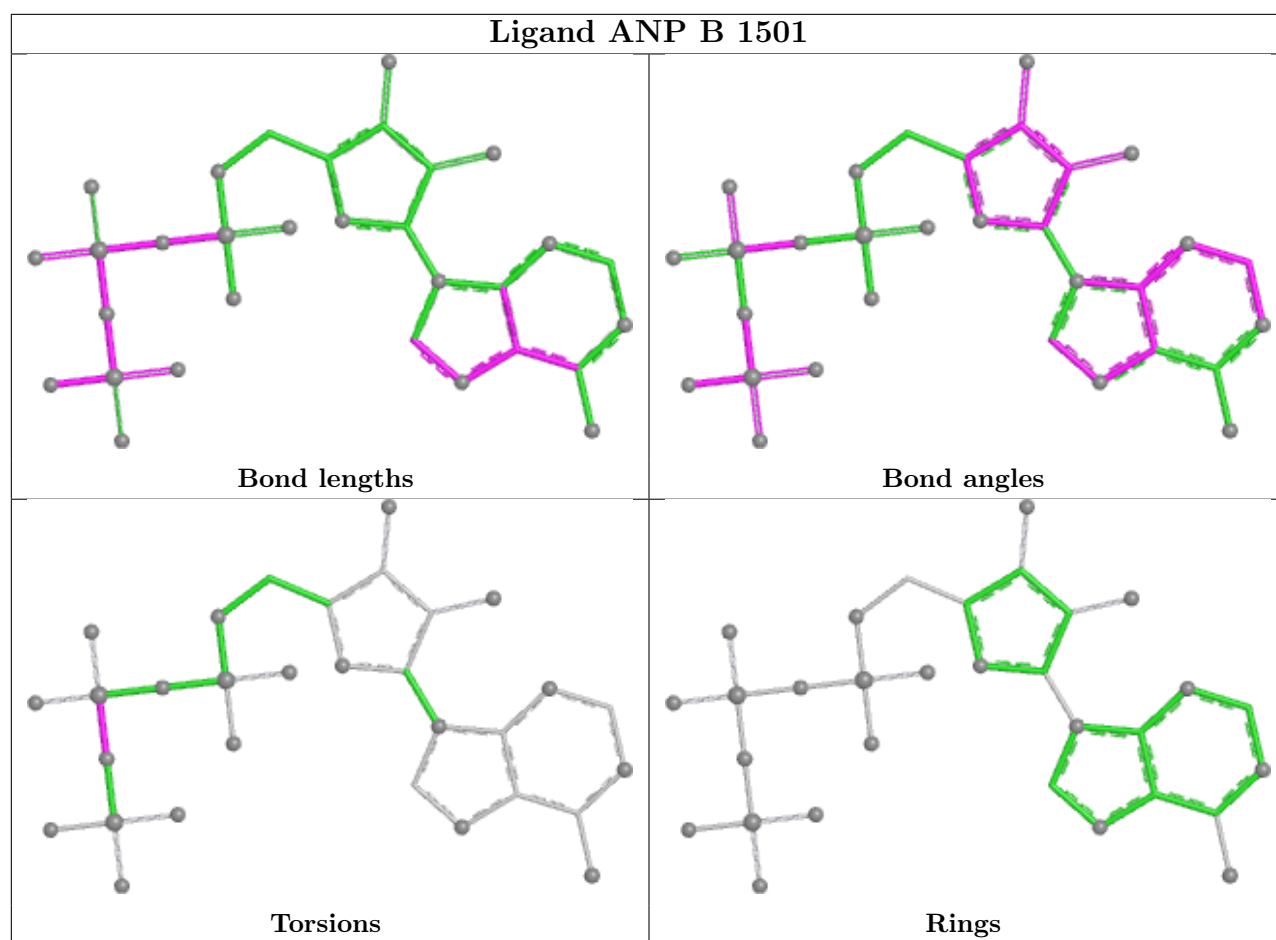
Mol	Chain	Res	Type	Atoms
5	B	1501	ANP	PG-N3B-PB-O1B
5	B	1501	ANP	PG-N3B-PB-O3A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1501	ANP	1	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.

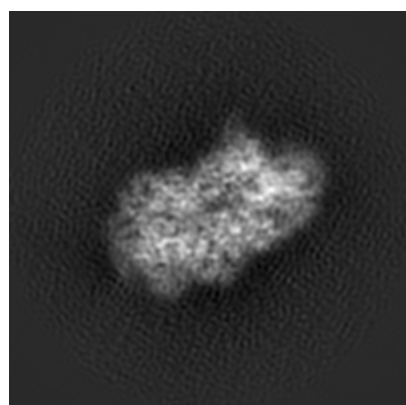
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4038. These allow visual inspection of the internal detail of the map and identification of artifacts.

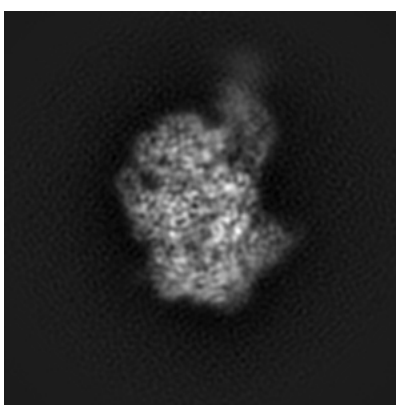
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

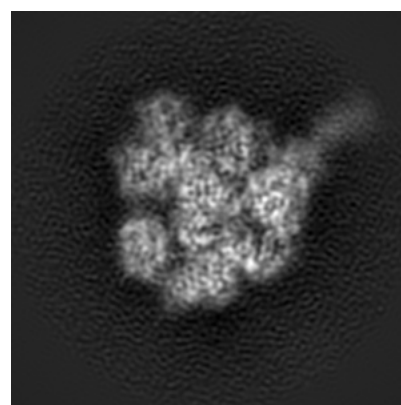
6.1.1 Primary map



X



Y

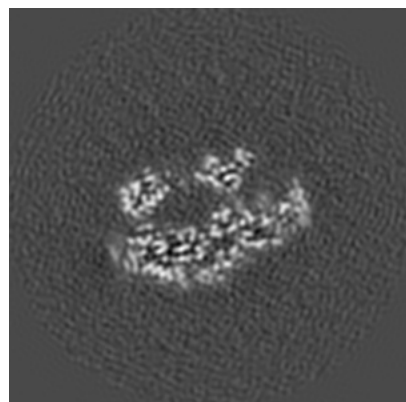


Z

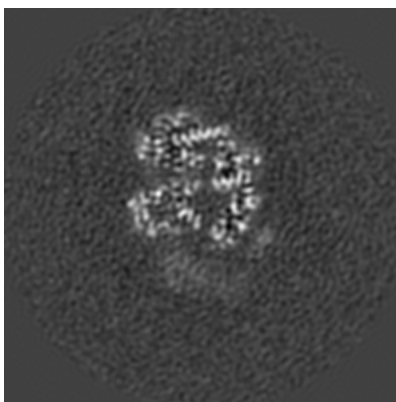
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

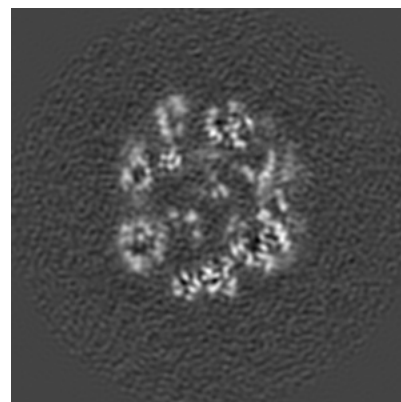
6.2.1 Primary map



X Index: 90



Y Index: 90

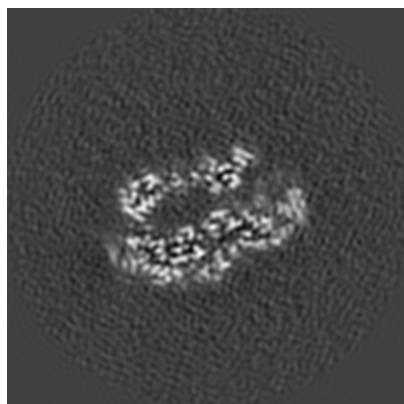


Z Index: 90

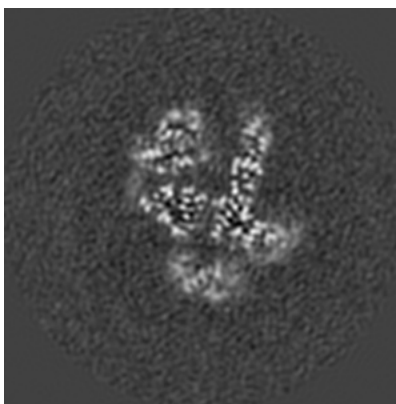
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

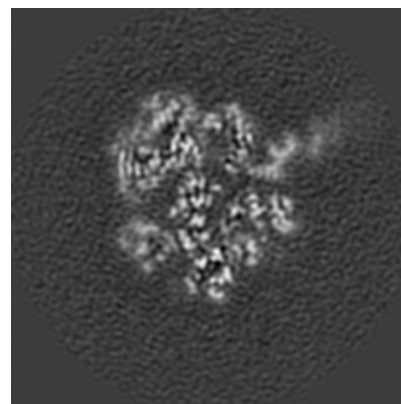
6.3.1 Primary map



X Index: 89



Y Index: 99

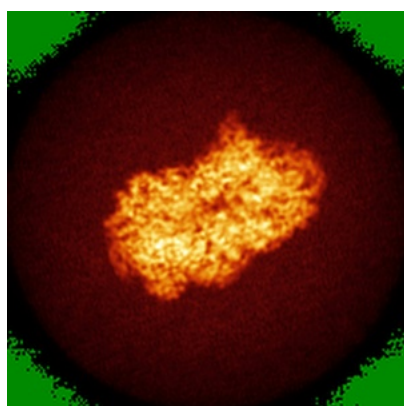


Z Index: 97

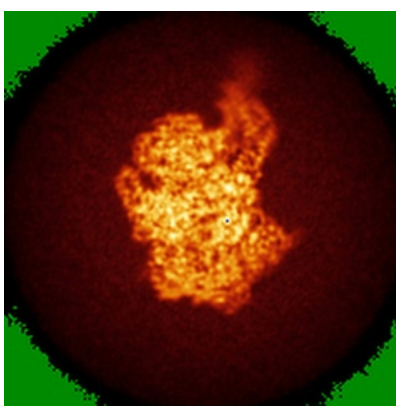
The images above show the largest variance slices of the map in three orthogonal directions.

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

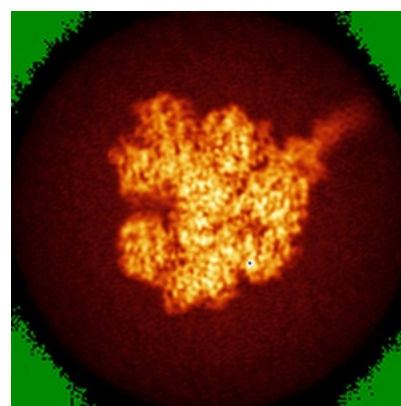
6.4.1 Primary map



X



Y

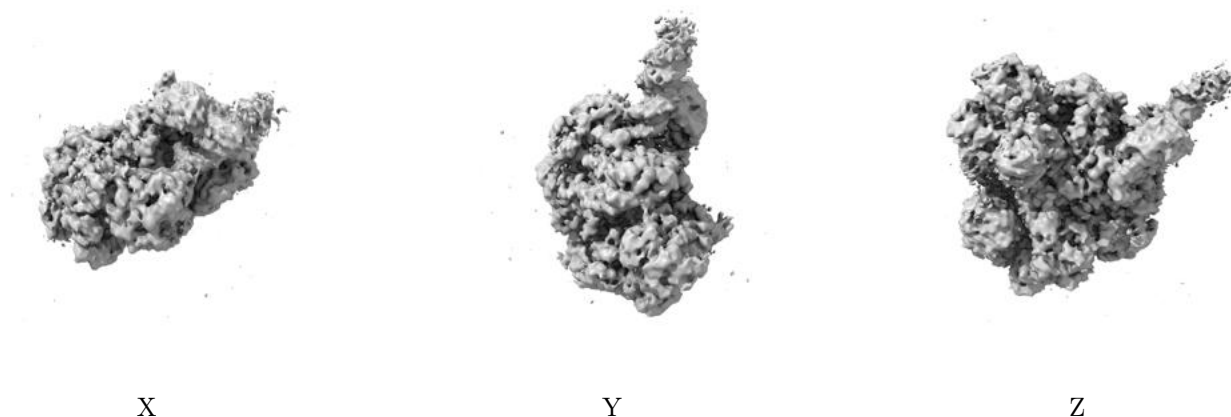


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

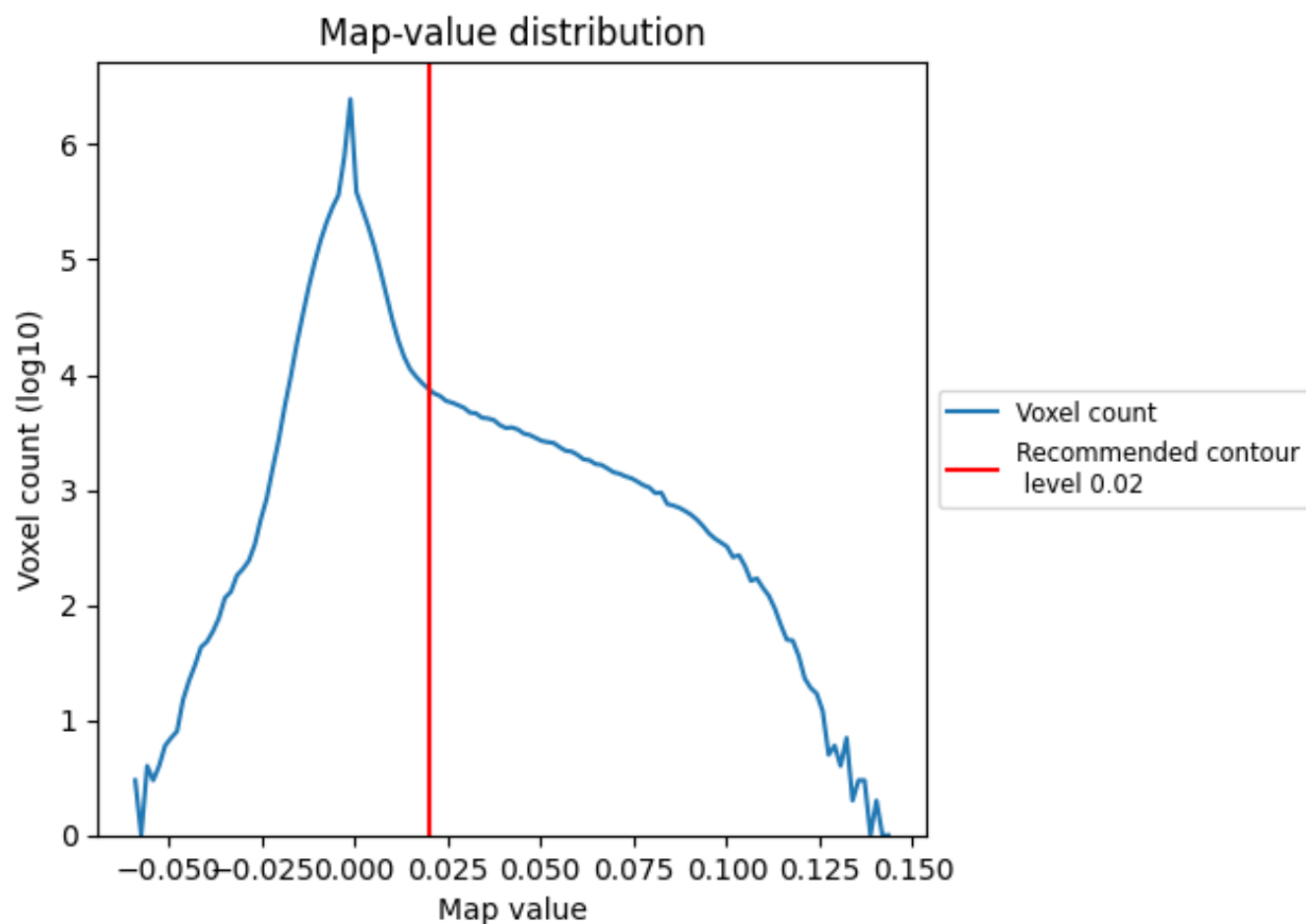
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

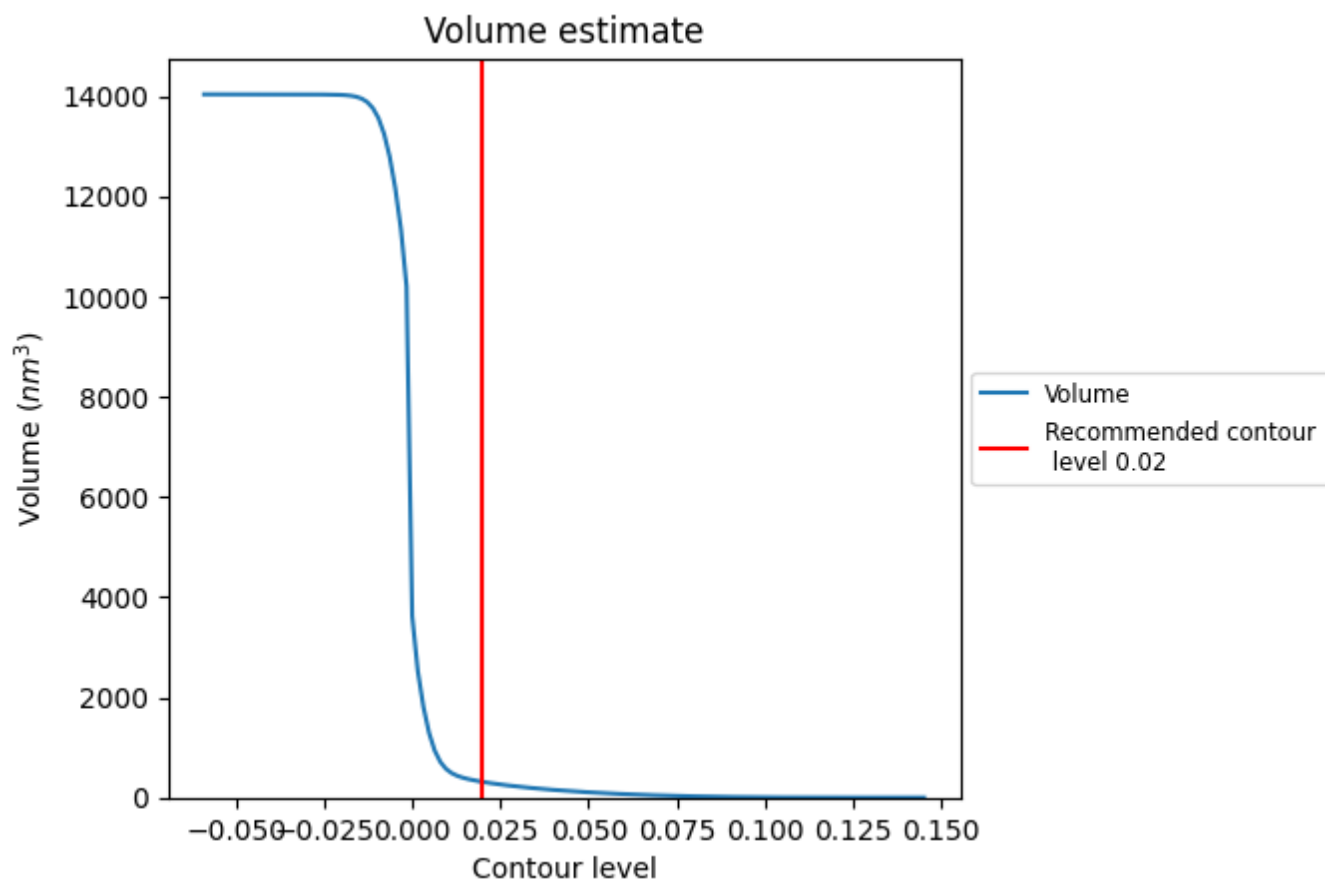
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

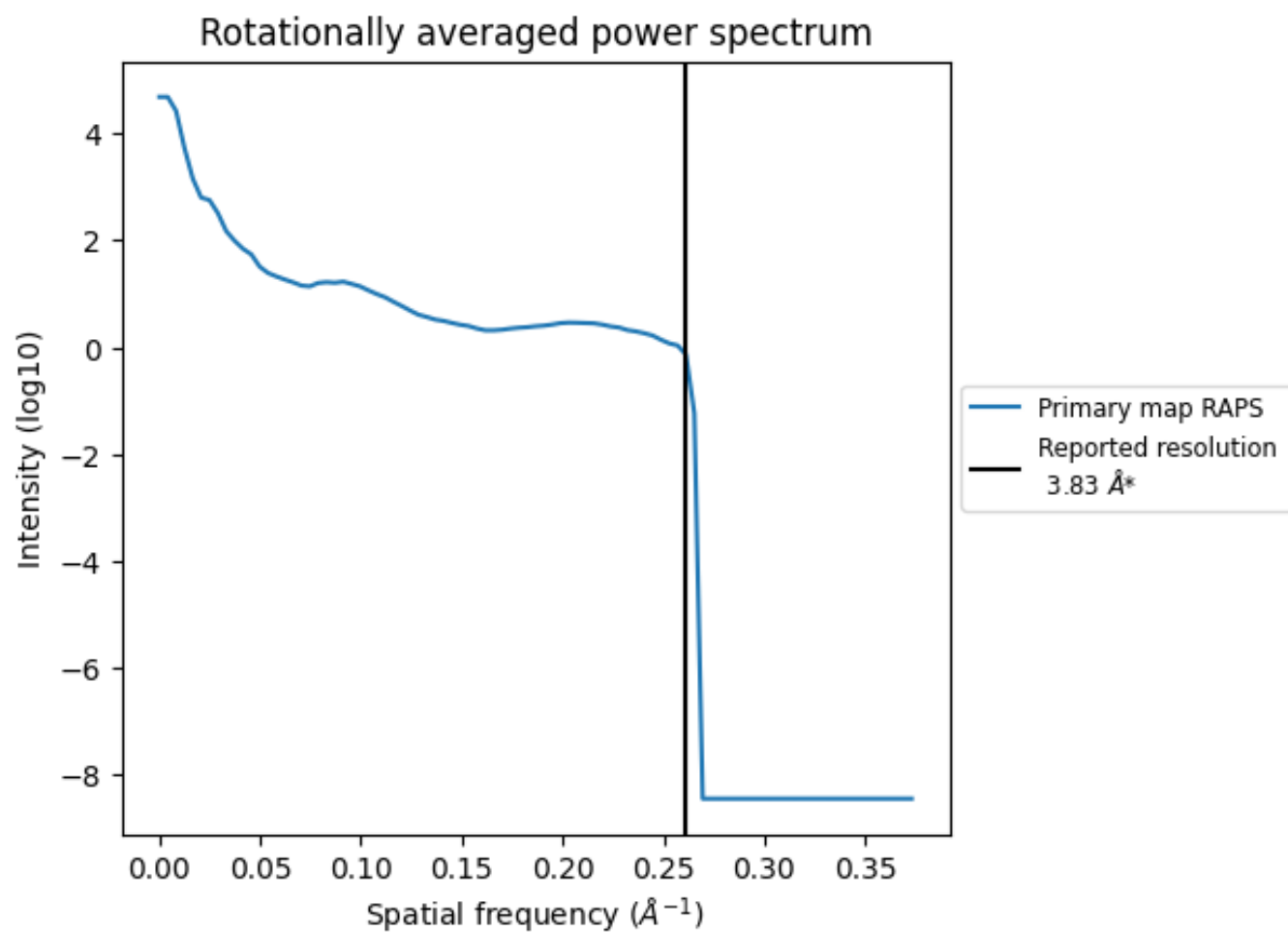
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 313 nm³; this corresponds to an approximate mass of 283 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 0.261 Å⁻¹

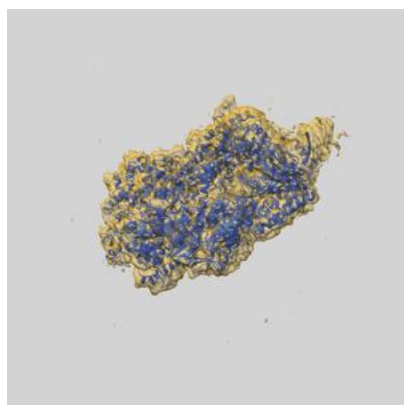
8 Fourier-Shell correlation ⓘ

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

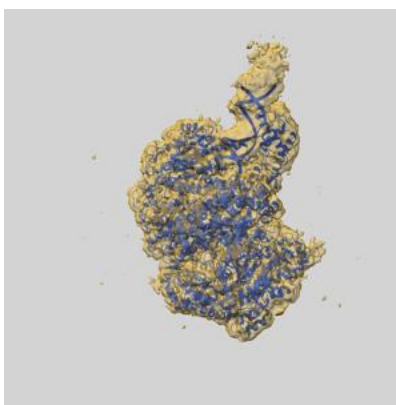
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4038 and PDB model 5LD2. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

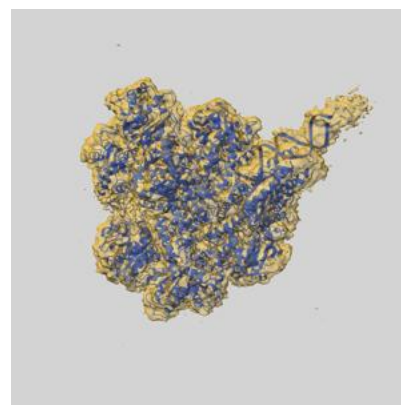
9.1 Map-model overlay [i](#)



X



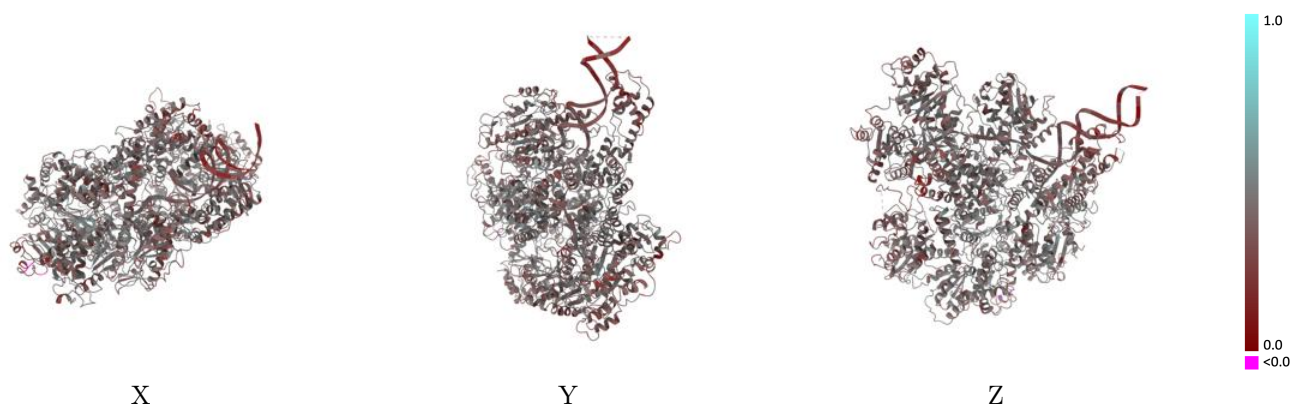
Y



Z

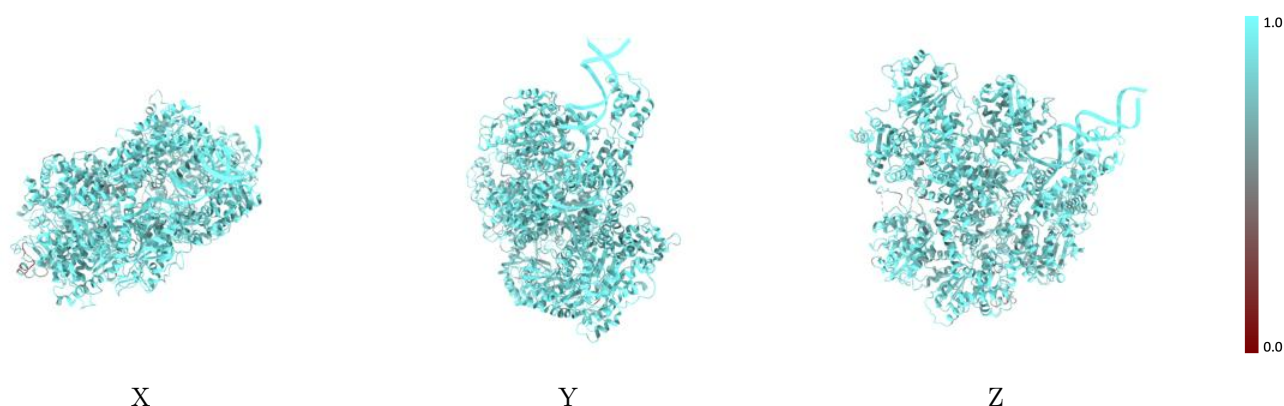
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



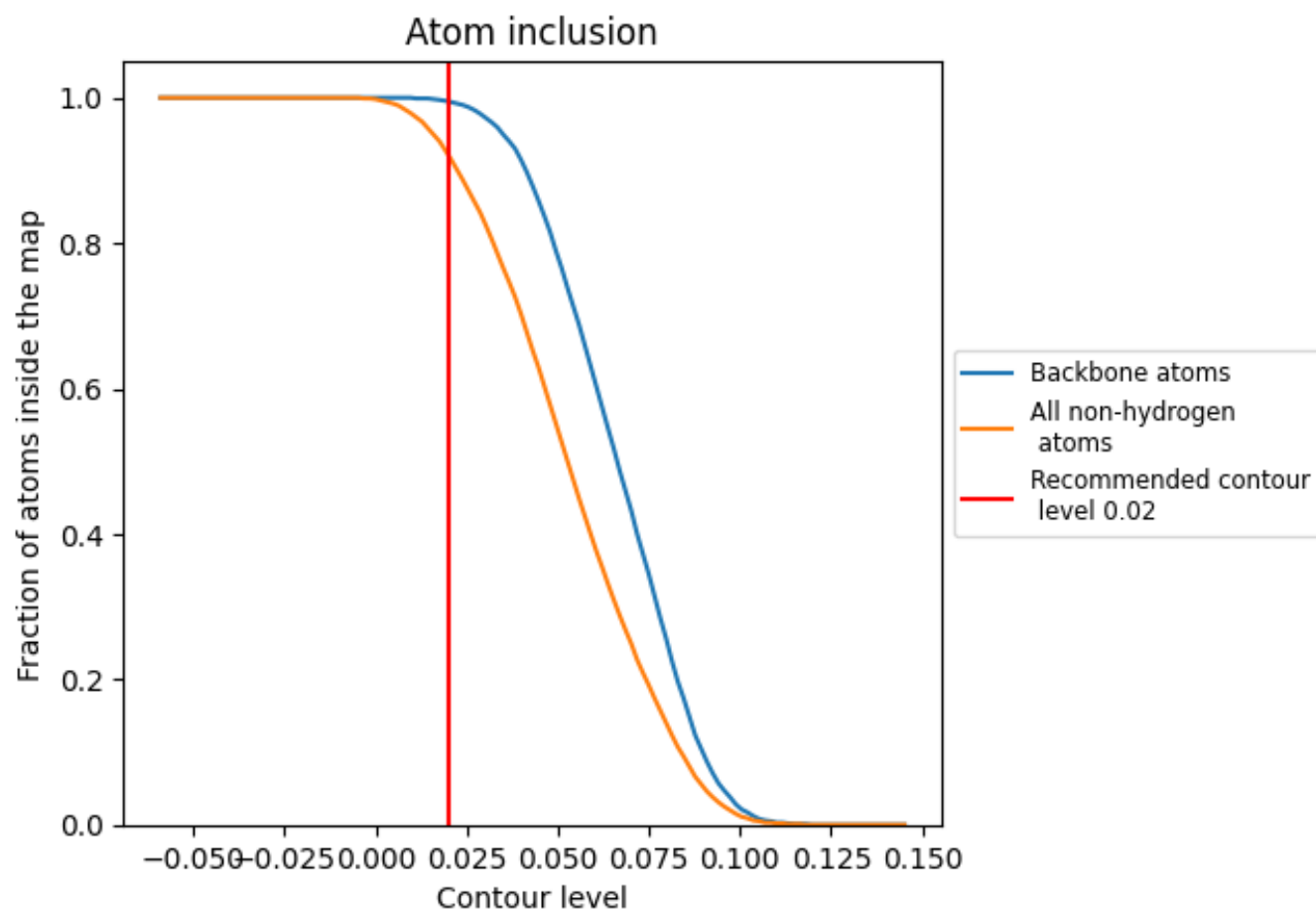
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 92% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9210	0.4010
B	0.9220	0.3950
C	0.9150	0.4190
D	0.9190	0.3930
X	0.9750	0.3200

