



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 01:46 AM UTC

PDB ID : 9G08 / pdb_00009g08
EMDB ID : EMD-50913
Title : Structure of human RNF213 bound to the secreted effector IpaH1.4 from *Shigella flexneri*
Authors : Naydenova, K.; Randow, F.
Deposited on : 2024-07-07
Resolution : 3.30 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

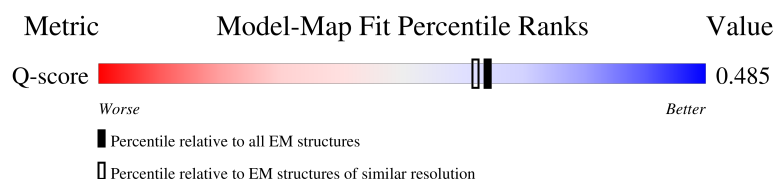
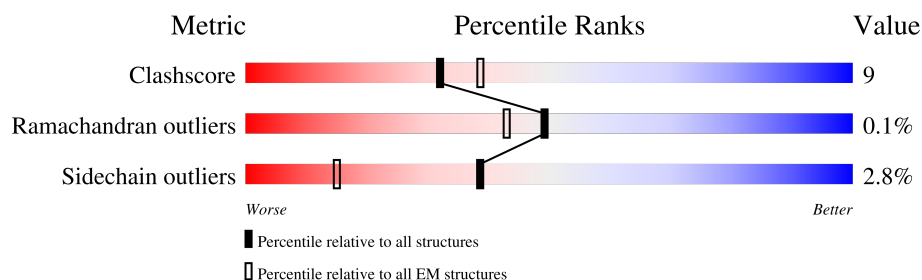
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	5247	
2	B	575	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 77075 atoms, of which 38644 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 E3 ubiquitin-protein ligase RNF213.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	4529	Total	C	H	N	O	S	0	0
			73234	23323	36721	6289	6681	220		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-39	MET	-	initiating methionine	UNP Q63HN8
A	-38	ALA	-	expression tag	UNP Q63HN8
A	-37	SER	-	expression tag	UNP Q63HN8
A	-36	TRP	-	expression tag	UNP Q63HN8
A	-35	SER	-	expression tag	UNP Q63HN8
A	-34	HIS	-	expression tag	UNP Q63HN8
A	-33	PRO	-	expression tag	UNP Q63HN8
A	-32	GLN	-	expression tag	UNP Q63HN8
A	-31	PHE	-	expression tag	UNP Q63HN8
A	-30	GLU	-	expression tag	UNP Q63HN8
A	-29	LYS	-	expression tag	UNP Q63HN8
A	-28	GLY	-	expression tag	UNP Q63HN8
A	-27	SER	-	expression tag	UNP Q63HN8
A	-26	ALA	-	expression tag	UNP Q63HN8
A	-25	GLY	-	expression tag	UNP Q63HN8
A	-24	SER	-	expression tag	UNP Q63HN8
A	-23	ALA	-	expression tag	UNP Q63HN8
A	-22	ALA	-	expression tag	UNP Q63HN8
A	-21	GLY	-	expression tag	UNP Q63HN8
A	-20	SER	-	expression tag	UNP Q63HN8
A	-19	GLY	-	expression tag	UNP Q63HN8
A	-18	ALA	-	expression tag	UNP Q63HN8
A	-17	GLY	-	expression tag	UNP Q63HN8
A	-16	TRP	-	expression tag	UNP Q63HN8
A	-15	SER	-	expression tag	UNP Q63HN8
A	-14	HIS	-	expression tag	UNP Q63HN8
A	-13	PRO	-	expression tag	UNP Q63HN8
A	-12	GLN	-	expression tag	UNP Q63HN8

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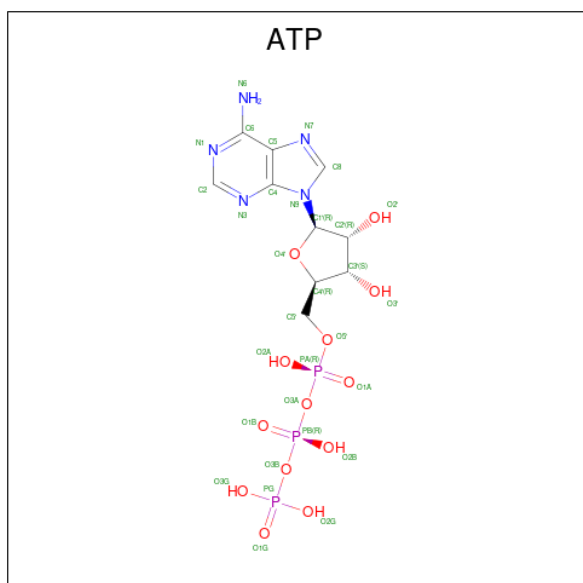
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	PHE	-	expression tag	UNP Q63HN8
A	-10	GLU	-	expression tag	UNP Q63HN8
A	-9	LYS	-	expression tag	UNP Q63HN8
A	-8	GLU	-	expression tag	UNP Q63HN8
A	-7	ASN	-	expression tag	UNP Q63HN8
A	-6	LEU	-	expression tag	UNP Q63HN8
A	-5	TYR	-	expression tag	UNP Q63HN8
A	-4	PHE	-	expression tag	UNP Q63HN8
A	-3	GLN	-	expression tag	UNP Q63HN8
A	-2	ALA	-	expression tag	UNP Q63HN8
A	-1	MET	-	expression tag	UNP Q63HN8
A	0	SER	-	expression tag	UNP Q63HN8

- Molecule 2 is a protein called E3 ubiquitin-protein ligase IpaH1.4.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	237	Total	C	H	N	O	S	0	0
			3794	1205	1911	322	349	7		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 1	Mg 1	0

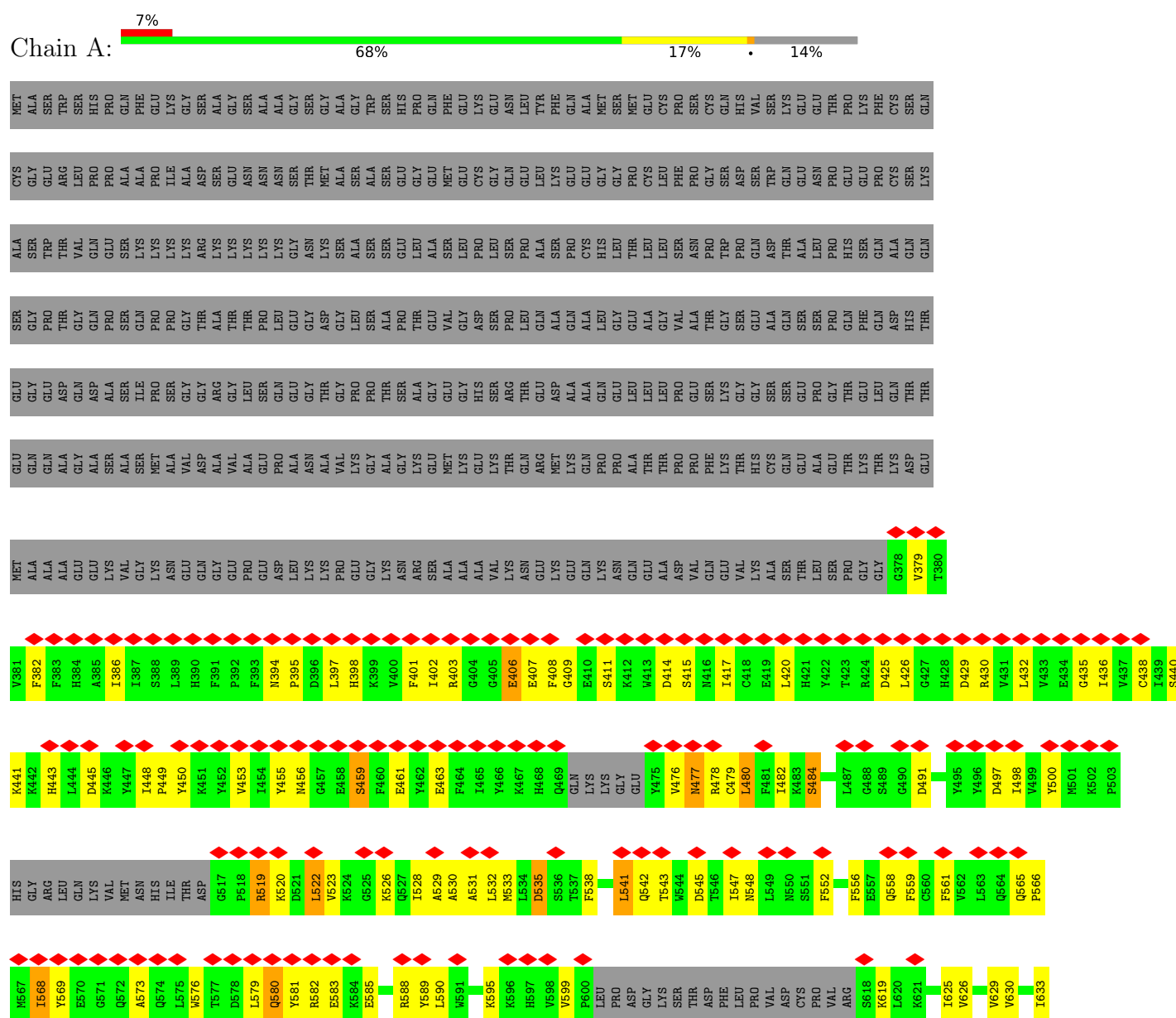
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	A	3	Total 3	Zn 3	0

3 Residue-property plots

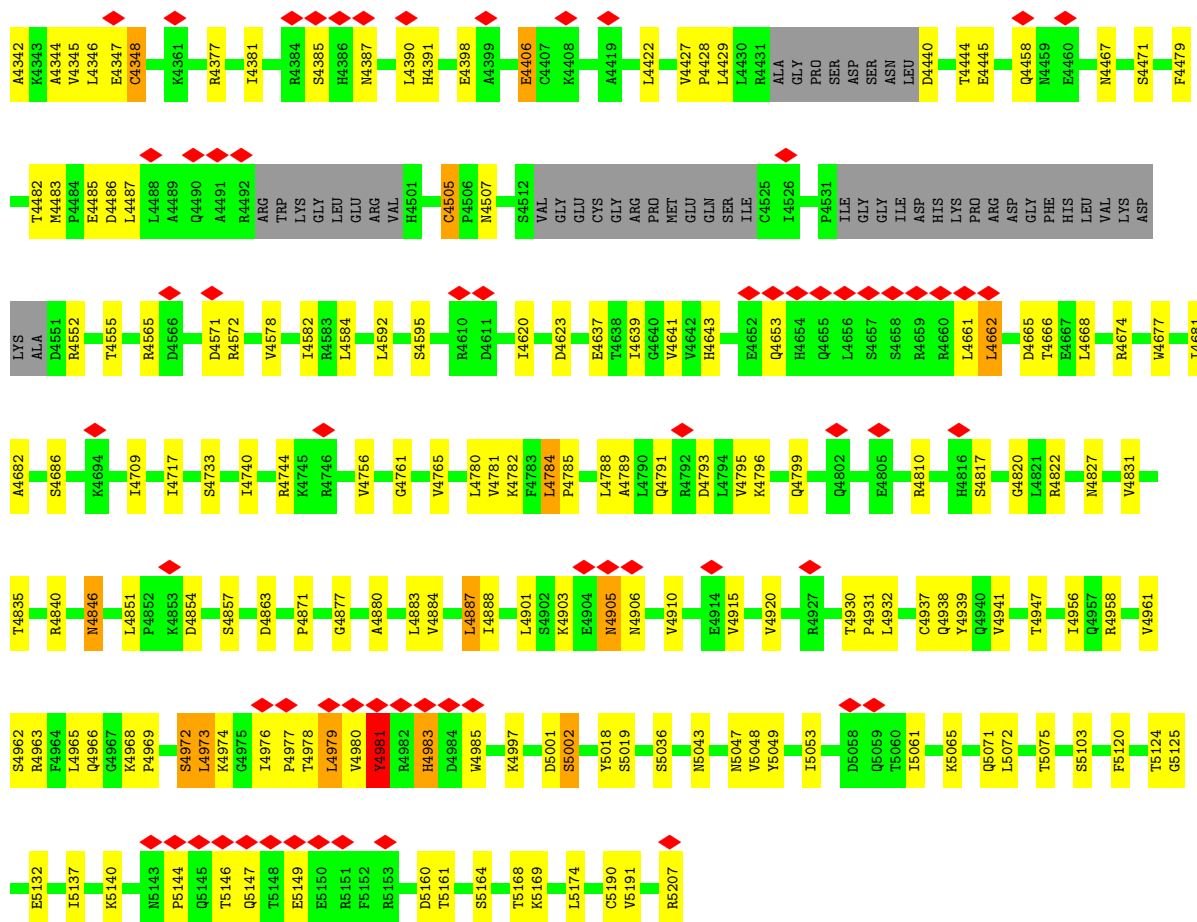
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: E3 ubiquitin-protein ligase RNF213

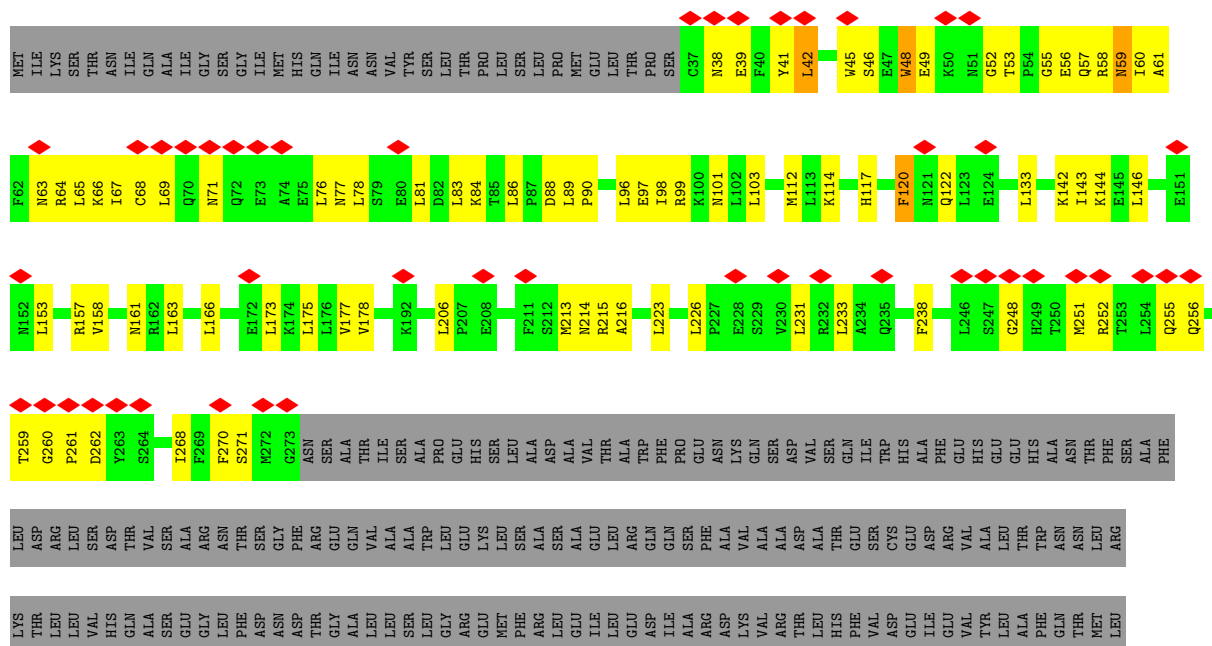








• Molecule 2: E3 ubiquitin-protein ligase IpaH1.4



ASP	ALA
ARG	GLU
TRP	LYS
ALA	LEU
GLN	GLN
LEU	LEU
SER	SER
GLU	THR
GLN	ALA
LYS	VAL
TYR	LYS
SER	GLU
ASN	MET
LEU	ARG
GLU	PHE
ASN	TYR
GLU	GLY
TYR	VAL
SER	SER
GLN	GLY
ARG	VAL
VAL	THR
ALA	ALA
ASP	ASN
ARG	ASP
LEU	LEU
LYS	ARG
ALA	THR
SER	ALA
GLY	GLU
LEU	ALA
SER	MET
GLY	VAL
ASP	ARG
ALA	SER
ASP	ARG
ALA	GLU
GLU	GLU
ARG	ASN
GLU	GLU
ALA	PHE
GLY	THR
ALA	ASP
GLN	TRP
VAL	PHE
MET	SER
ARG	LEU
GLU	TRP
THR	GLY
GLU	PRO
GLN	TRP
GLN	HIS
ILE	ALA
TYR	VAL
ARG	LEU
GLN	LYS
LEU	ARG
THR	THR
ASP	GLU
GLU	ALA

VAL
LEU
ALA
LEU
ARG
LEU
SER
GLU
ASN
GLY
SER
ASN
HIS
ILE
ALA

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	334921	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	8.673	Depositor
Minimum map value	0.000	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.103	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	471.552, 471.552, 471.552	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.228, 1.228, 1.228	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: MG, ATP, ZN

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	0.25	0/37285	0.43	0/50439
2	B	0.19	0/1927	0.44	0/2629
All	All	0.25	0/39212	0.43	0/53068

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	3
2	B	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2237	PRO	Peptide
1	A	4981	TYR	Peptide
1	A	580	GLN	Peptide
2	B	120	PHE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	36513	36721	36694	603	0
2	B	1883	1911	1910	64	0
3	A	31	12	12	1	0
4	A	1	0	0	0	0
5	A	3	0	0	0	0
All	All	38431	38644	38616	662	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 9.

All (662) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1511:ASP:OD1	1:A:1514:ARG:NH1	1.93	1.02
1:A:5061:ILE:O	1:A:5065:LYS:NZ	2.05	0.89
1:A:1198:ARG:NH1	1:A:1200:SER:OG	2.06	0.89
1:A:386:ILE:HD11	1:A:529:ALA:HB2	1.55	0.88
1:A:4817:SER:O	1:A:4822:ARG:NH2	2.05	0.88
1:A:4132:SER:OG	1:A:4177:CYS:SG	2.33	0.87
1:A:2365:PHE:O	1:A:2373:LYS:NZ	2.09	0.86
1:A:4036:LEU:HD22	2:B:175:LEU:HD13	1.56	0.85
1:A:4941:VAL:HG22	1:A:4947:THR:HG22	1.56	0.84
1:A:4901:LEU:O	1:A:4903:LYS:NZ	2.10	0.84
1:A:2074:LEU:O	1:A:2089:ARG:NH2	2.10	0.83
1:A:4176:ASN:OD1	1:A:4744:ARG:NE	2.10	0.83
1:A:916:GLU:OE2	1:A:916:GLU:N	2.13	0.81
1:A:2260:ARG:O	1:A:2264:THR:OG1	1.98	0.81
1:A:1594:LEU:O	1:A:3091:LYS:NZ	2.12	0.81
2:B:97:GLU:OE1	2:B:99:ARG:NH2	2.14	0.81
1:A:3117:ASN:OD1	1:A:3168:ARG:NE	2.14	0.80
2:B:213:MET:HE3	2:B:216:ALA:HB2	1.63	0.80
1:A:1181:ARG:NH2	1:A:1211:TYR:O	2.16	0.79
1:A:4016:HIS:NE2	1:A:4032:CYS:SG	2.56	0.79
2:B:78:LEU:O	2:B:101:ASN:ND2	2.15	0.79
1:A:3006:ALA:O	1:A:3009:SER:OG	2.01	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2142:GLU:OE1	1:A:2147:ARG:NH2	2.18	0.77
1:A:4015:VAL:O	1:A:4016:HIS:ND1	2.19	0.76
1:A:1118:ASP:OD2	1:A:1119:ILE:N	2.19	0.76
1:A:3103:LEU:O	1:A:3105:LEU:N	2.19	0.75
1:A:3674:LEU:O	1:A:3714:LYS:NZ	2.19	0.74
1:A:4592:LEU:O	1:A:4595:SER:OG	2.05	0.74
1:A:4194:GLU:OE2	1:A:4238:ARG:NH1	2.21	0.74
1:A:2166:ARG:NH2	1:A:2230:GLU:OE1	2.20	0.74
1:A:4406:GLU:N	1:A:4406:GLU:OE2	2.21	0.74
2:B:67:ILE:HD12	2:B:68:CYS:N	2.03	0.74
1:A:4941:VAL:CG2	1:A:4947:THR:HG22	2.18	0.73
1:A:545:ASP:OD1	1:A:547:ILE:HG22	1.88	0.73
2:B:213:MET:SD	2:B:215:ARG:N	2.61	0.73
1:A:3941:VAL:HG12	1:A:4057:LYS:CD	2.18	0.72
1:A:4031:ILE:HG22	1:A:4039:LEU:HB2	1.71	0.72
1:A:5043:ASN:O	1:A:5071:GLN:NE2	2.23	0.71
1:A:3645:ARG:O	1:A:3697:ASN:ND2	2.22	0.71
1:A:4784:LEU:HD21	1:A:4884:VAL:HA	1.72	0.71
1:A:1822:PRO:HD2	1:A:1825:LEU:HD12	1.71	0.71
1:A:2009:MET:HE3	1:A:2018:VAL:HG11	1.71	0.71
1:A:2975:SER:N	1:A:2978:ASP:OD2	2.24	0.71
1:A:4810:ARG:NH2	1:A:4863:ASP:OD1	2.23	0.71
1:A:3941:VAL:HG12	1:A:4057:LYS:HD3	1.73	0.70
1:A:456:ASN:OD1	1:A:459:SER:N	2.24	0.70
1:A:2268:HIS:O	1:A:2295:ARG:NH2	2.24	0.70
1:A:3069:ILE:HG22	1:A:3105:LEU:CD1	2.21	0.70
1:A:3345:THR:HG21	1:A:3365:CYS:SG	2.30	0.70
1:A:1375:LEU:HD21	1:A:1485:PHE:CZ	2.27	0.70
1:A:2176:GLN:OE1	1:A:2178:GLN:NE2	2.25	0.69
2:B:122:GLN:OE1	2:B:142:LYS:NZ	2.22	0.69
1:A:543:THR:HG1	1:A:548:ASN:CG	1.98	0.69
1:A:1768:LEU:O	1:A:1777:LYS:NZ	2.26	0.68
1:A:2618:VAL:CG2	1:A:2707:ILE:HG23	2.24	0.68
1:A:386:ILE:HD12	1:A:498:ILE:HD13	1.74	0.68
1:A:1913:HIS:O	1:A:1917:THR:HG23	1.92	0.68
1:A:2657:MET:HE2	1:A:2798:SER:OG	1.94	0.68
1:A:4965:LEU:O	1:A:4966:GLN:NE2	2.27	0.67
1:A:1280:GLN:OE1	1:A:1284:ARG:NE	2.28	0.67
1:A:1886:SER:OG	1:A:1921:ARG:NH2	2.28	0.67
1:A:2549:MET:O	1:A:2555:ARG:NH2	2.28	0.67
1:A:2370:ARG:NH1	1:A:2390:ASP:O	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:GLU:OE2	1:A:585:GLU:N	2.27	0.67
2:B:97:GLU:OE2	2:B:117:HIS:ND1	2.27	0.66
1:A:4035:CYS:SG	1:A:4037:THR:OG1	2.54	0.66
1:A:1332:GLN:O	1:A:1334:ASP:N	2.28	0.66
1:A:3095:GLU:OE1	1:A:3141:ARG:NH1	2.28	0.66
1:A:4000:CYS:SG	1:A:4005:LYS:NZ	2.68	0.66
1:A:3242:LEU:HD12	1:A:3243:THR:N	2.11	0.66
1:A:1029:LEU:HD11	1:A:1060:VAL:HG22	1.79	0.65
1:A:3948:VAL:O	1:A:3952:VAL:HG23	1.97	0.65
1:A:4036:LEU:HD22	2:B:175:LEU:CD1	2.25	0.65
1:A:925:SER:O	1:A:972:SER:OG	2.12	0.65
1:A:4784:LEU:HD22	1:A:4887:LEU:HD23	1.77	0.65
1:A:5001:ASP:OD2	1:A:5002:SER:N	2.30	0.65
2:B:48:TRP:O	2:B:58:ARG:NH2	2.30	0.65
1:A:4744:ARG:NH1	1:A:4939:TYR:OH	2.30	0.65
1:A:3717:ASP:OD2	1:A:4796:LYS:NZ	2.21	0.64
1:A:2392:THR:OG1	1:A:2428:ARG:NH1	2.30	0.64
1:A:719:TRP:O	1:A:759:ARG:NH2	2.30	0.64
1:A:4133:VAL:HG22	1:A:4938:GLN:NE2	2.13	0.64
1:A:530:ALA:HB3	1:A:590:LEU:HD21	1.79	0.64
1:A:1387:ASP:OD1	1:A:1388:PHE:N	2.30	0.63
1:A:1569:GLU:OE2	1:A:1577:SER:N	2.31	0.63
1:A:977:TYR:O	1:A:1024:LYS:NZ	2.31	0.63
2:B:60:ILE:HA	2:B:63:ASN:OD1	1.99	0.63
1:A:533:MET:HE2	1:A:559:PHE:CE2	2.33	0.63
1:A:1942:ALA:O	1:A:1945:GLN:NE2	2.32	0.63
1:A:3863:ALA:O	1:A:3867:THR:HG23	1.99	0.63
1:A:2618:VAL:HG23	1:A:2707:ILE:HG23	1.80	0.63
2:B:213:MET:CE	2:B:216:ALA:HB2	2.28	0.63
1:A:2009:MET:HE1	1:A:2053:LEU:HB2	1.81	0.62
2:B:158:VAL:O	2:B:161:ASN:ND2	2.32	0.62
1:A:535:ASP:OD1	1:A:535:ASP:N	2.28	0.62
1:A:976:ALA:O	1:A:980:SER:OG	2.17	0.62
1:A:1235:LEU:O	1:A:1237:TRP:N	2.33	0.62
1:A:2009:MET:HE3	1:A:2018:VAL:CG1	2.29	0.62
1:A:2133:ARG:NE	1:A:2151:GLU:OE1	2.31	0.62
1:A:2490:ASN:HA	1:A:2495:ILE:HD12	1.81	0.62
1:A:2268:HIS:O	1:A:2268:HIS:ND1	2.33	0.61
1:A:4584:LEU:HD11	1:A:4620:ILE:HG23	1.82	0.61
1:A:1976:ALA:O	1:A:1979:VAL:HG22	2.01	0.60
1:A:4565:ARG:NH1	1:A:4623:ASP:OD1	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4479:PHE:HD2	1:A:4483:MET:HE1	1.66	0.60
1:A:411:SER:OG	1:A:414:ASP:OD2	2.20	0.60
1:A:426:LEU:HD13	1:A:432:LEU:HB2	1.84	0.60
1:A:3964:ASP:O	1:A:3967:THR:OG1	2.18	0.60
1:A:379:VAL:HG23	1:A:441:LYS:HA	1.83	0.60
1:A:1548:ILE:HG23	1:A:1562:VAL:CG1	2.31	0.60
1:A:2186:GLN:O	1:A:2189:SER:OG	2.17	0.59
1:A:450:TYR:O	1:A:478:ARG:HB2	2.01	0.59
1:A:2539:GLU:OE2	1:A:2562:ARG:NH1	2.35	0.59
1:A:4062:ARG:NE	1:A:4122:ASP:OD2	2.36	0.59
1:A:2044:ASP:OD1	1:A:2045:ALA:N	2.35	0.59
1:A:2055:HIS:NE2	1:A:2098:GLU:OE1	2.36	0.59
1:A:619:LYS:NZ	1:A:649:THR:O	2.35	0.59
1:A:4781:VAL:HG13	1:A:4887:LEU:CD1	2.33	0.59
1:A:4485:GLU:OE2	1:A:4572:ARG:NH1	2.33	0.58
1:A:4979:LEU:HD23	1:A:4980:VAL:H	1.68	0.58
1:A:3743:PHE:O	1:A:3746:THR:OG1	2.20	0.58
2:B:55:GLY:O	2:B:57:GLN:NE2	2.36	0.58
1:A:4781:VAL:HG13	1:A:4887:LEU:HD13	1.84	0.58
1:A:4871:PRO:HD2	1:A:4973:LEU:HD11	1.84	0.58
1:A:2783:ALA:HB2	1:A:2804:LEU:HD11	1.86	0.58
1:A:5120:PHE:O	1:A:5124:THR:OG1	2.12	0.58
1:A:407:GLU:HB2	1:A:449:PRO:HD2	1.86	0.57
1:A:4130:ILE:HD11	1:A:4163:ILE:HD11	1.86	0.57
1:A:498:ILE:HG21	1:A:500:TYR:CZ	2.38	0.57
1:A:740:LEU:HD23	1:A:765:LEU:HD23	1.86	0.57
1:A:2602:VAL:O	1:A:2606:SER:N	2.35	0.57
1:A:1982:ASP:OD1	1:A:1982:ASP:N	2.35	0.57
1:A:3989:LEU:HD13	1:A:4057:LYS:HB2	1.85	0.57
1:A:4505:CYS:SG	1:A:4507:ASN:N	2.76	0.57
2:B:42:LEU:HA	2:B:45:TRP:CE3	2.39	0.57
1:A:386:ILE:HD12	1:A:498:ILE:CD1	2.35	0.57
1:A:398:HIS:HB3	1:A:455:TYR:O	2.05	0.57
1:A:1455:ASN:OD1	1:A:1456:ASP:N	2.38	0.57
1:A:637:LEU:HD11	1:A:644:LEU:HD23	1.85	0.57
1:A:3175:ASP:OD1	1:A:3176:ILE:N	2.38	0.57
2:B:252:ARG:O	2:B:255:GLN:HG3	2.05	0.57
1:A:2928:VAL:HG12	1:A:2932:PHE:CE1	2.39	0.57
2:B:213:MET:SD	2:B:214:ASN:N	2.78	0.57
1:A:1386:ASP:O	1:A:1390:ARG:NE	2.38	0.57
1:A:1860:ASP:OD1	1:A:1861:GLU:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3265:ASP:OD2	1:A:3269:ARG:NH2	2.37	0.57
1:A:4584:LEU:CD1	1:A:4620:ILE:HG23	2.35	0.56
1:A:2236:ASN:ND2	1:A:2237:PRO:O	2.39	0.56
1:A:3045:LEU:HD22	1:A:3157:VAL:HG21	1.87	0.56
1:A:630:VAL:HG21	1:A:637:LEU:HD21	1.88	0.56
1:A:4024:TRP:NE1	1:A:4029:GLN:O	2.39	0.56
1:A:4445:GLU:OE1	1:A:4643:HIS:NE2	2.38	0.56
2:B:206:LEU:HB3	2:B:226:LEU:HD22	1.88	0.56
1:A:3997:CYS:N	1:A:4002:GLY:O	2.35	0.56
1:A:531:ALA:O	1:A:535:ASP:OD1	2.24	0.56
1:A:4276:ARG:NE	1:A:4304:TRP:O	2.37	0.56
2:B:53:THR:OG1	2:B:84:LYS:NZ	2.36	0.56
1:A:633:ILE:HG22	1:A:633:ILE:O	2.05	0.56
1:A:3990:SER:O	1:A:3993:GLY:N	2.35	0.56
1:A:940:ARG:HH12	1:A:992:ALA:HB2	1.69	0.56
1:A:1376:ASN:O	1:A:1380:ASN:N	2.35	0.56
1:A:3941:VAL:HG12	1:A:4057:LYS:HD2	1.87	0.56
1:A:4888:ILE:HG12	1:A:4969:PRO:HG2	1.89	0.55
2:B:89:LEU:HB3	2:B:90:PRO:HD2	1.88	0.55
1:A:491:ASP:O	1:A:558:GLN:NE2	2.39	0.55
1:A:3069:ILE:HG22	1:A:3105:LEU:HD12	1.87	0.55
1:A:3087:ILE:HG12	1:A:3133:LEU:HD23	1.88	0.55
1:A:3982:LYS:HA	1:A:4061:PHE:CE1	2.43	0.54
1:A:3202:LYS:HG2	1:A:3270:LEU:HD21	1.89	0.54
1:A:3902:MET:HE2	1:A:3913:ILE:HD11	1.89	0.54
1:A:4139:LEU:HB3	1:A:4181:SER:HB2	1.89	0.54
1:A:5072:LEU:O	1:A:5075:THR:OG1	2.22	0.54
1:A:4387:ASN:HB3	1:A:4390:LEU:HD13	1.88	0.54
2:B:64:ARG:O	2:B:67:ILE:HG13	2.08	0.54
2:B:103:LEU:O	2:B:122:GLN:N	2.36	0.54
1:A:3556:ARG:NH2	1:A:3703:GLU:OE2	2.36	0.54
1:A:3709:VAL:HG23	1:A:3766:CYS:HB3	1.90	0.54
1:A:1051:LEU:O	1:A:1115:GLN:NE2	2.38	0.54
1:A:2787:GLN:O	1:A:2791:ALA:N	2.41	0.54
1:A:1293:LEU:O	1:A:1339:ARG:NE	2.40	0.54
1:A:674:LEU:O	1:A:677:VAL:HG12	2.08	0.53
1:A:2225:GLN:HB3	1:A:2255:MET:SD	2.48	0.53
1:A:1123:ARG:HD3	1:A:1123:ARG:C	2.34	0.53
1:A:1530:GLU:O	1:A:1532:SER:OG	2.27	0.53
2:B:223:LEU:HD22	2:B:226:LEU:HD21	1.90	0.53
1:A:3072:SER:O	1:A:3078:GLN:NE2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3806:GLU:OE2	1:A:3806:GLU:N	2.42	0.53
1:A:936:ILE:HG22	1:A:985:LYS:HE2	1.91	0.52
1:A:1235:LEU:O	1:A:1237:TRP:CD1	2.63	0.52
1:A:3102:LEU:HD12	1:A:3150:VAL:HG22	1.92	0.52
1:A:4980:VAL:O	1:A:4985:TRP:HA	2.08	0.52
1:A:414:ASP:OD2	1:A:415:SER:N	2.42	0.52
1:A:813:ASP:OD2	1:A:813:ASP:N	2.40	0.52
1:A:1407:LEU:HD12	1:A:1410:ILE:HD12	1.91	0.52
1:A:1909:GLU:OE2	1:A:5207:ARG:NH1	2.41	0.52
1:A:4019:ARG:NH1	1:A:4020:CYS:SG	2.82	0.52
1:A:4906:ASN:OD1	1:A:4906:ASN:N	2.42	0.52
2:B:83:LEU:N	2:B:101:ASN:OD1	2.34	0.52
1:A:595:LYS:O	1:A:599:VAL:HG13	2.10	0.52
1:A:630:VAL:HG21	1:A:637:LEU:CD2	2.40	0.52
1:A:2575:LEU:O	1:A:2579:VAL:HG23	2.08	0.52
1:A:3450:LEU:HD12	1:A:3451:MET:N	2.25	0.52
2:B:45:TRP:NE1	2:B:88:ASP:O	2.37	0.52
2:B:96:LEU:HG	2:B:98:ILE:HG23	1.92	0.52
1:A:4854:ASP:OD2	1:A:4854:ASP:N	2.42	0.52
1:A:940:ARG:NH1	1:A:992:ALA:HB2	2.25	0.52
1:A:2598:VAL:O	1:A:2602:VAL:HG23	2.10	0.52
1:A:3456:THR:HG22	1:A:3456:THR:O	2.10	0.52
1:A:408:PHE:HD1	1:A:448:ILE:HG21	1.74	0.52
2:B:260:GLY:O	2:B:262:ASP:N	2.43	0.52
1:A:3422:ARG:NE	1:A:3618:GLY:O	2.36	0.51
1:A:3585:ARG:NH1	1:A:3675:LEU:O	2.39	0.51
1:A:4781:VAL:HG22	1:A:4887:LEU:CD1	2.40	0.51
2:B:61:ALA:HB2	2:B:81:LEU:HD12	1.92	0.51
1:A:3458:LEU:CD2	1:A:3466:LEU:HD21	2.40	0.51
1:A:1548:ILE:HD11	1:A:1616:VAL:HG13	1.93	0.51
1:A:2610:ASN:OD1	1:A:2613:ARG:NH2	2.41	0.51
1:A:2729:GLN:NE2	1:A:2750:GLU:OE1	2.43	0.51
1:A:561:PHE:O	1:A:565:GLN:NE2	2.43	0.51
1:A:1005:SER:O	1:A:1008:GLN:HG3	2.11	0.51
1:A:4795:VAL:O	1:A:4799:GLN:N	2.43	0.51
1:A:4976:ILE:N	1:A:4977:PRO:CD	2.74	0.51
1:A:762:PHE:O	1:A:798:ARG:NH1	2.44	0.51
1:A:3379:THR:HG23	1:A:3418:THR:HG23	1.93	0.51
1:A:379:VAL:HG11	1:A:482:ILE:HD13	1.92	0.51
1:A:940:ARG:NH2	1:A:985:LYS:HB2	2.25	0.51
1:A:983:ASP:C	1:A:985:LYS:H	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3086:ASN:O	1:A:3090:VAL:HG23	2.11	0.51
1:A:1652:GLN:NE2	1:A:1662:GLU:OE1	2.44	0.50
1:A:867:LEU:HB2	1:A:868:PRO:HD3	1.94	0.50
1:A:406:GLU:HA	1:A:409:GLY:O	2.10	0.50
1:A:1291:GLN:O	1:A:1294:LYS:HG2	2.11	0.50
1:A:1401:ILE:O	1:A:1405:LYS:HG3	2.10	0.50
1:A:813:ASP:O	1:A:817:VAL:HG23	2.12	0.50
1:A:2686:MET:HE2	1:A:2725:ILE:HD11	1.94	0.50
1:A:4080:ASP:OD1	1:A:4082:ALA:N	2.44	0.50
1:A:568:ILE:O	1:A:573:ALA:HA	2.12	0.50
1:A:3536:LEU:O	1:A:3540:VAL:HG23	2.12	0.50
1:A:4324:MET:HA	1:A:4709:ILE:HD11	1.92	0.50
1:A:4458:GLN:N	1:A:4653:GLN:OE1	2.40	0.50
1:A:3908:LEU:O	1:A:3912:VAL:HG23	2.12	0.49
1:A:4143:PHE:CZ	1:A:4223:VAL:HG12	2.47	0.49
1:A:4440:ASP:O	1:A:4444:THR:OG1	2.29	0.49
1:A:4582:ILE:HG23	1:A:4677:TRP:HZ3	1.77	0.49
1:A:684:MET:O	1:A:687:ARG:NH2	2.45	0.49
1:A:2591:LYS:NZ	1:A:2617:GLU:OE2	2.42	0.49
1:A:1653:MET:HE2	1:A:1774:LEU:HD21	1.94	0.49
1:A:4050:ALA:O	1:A:4053:GLU:HG3	2.12	0.49
1:A:533:MET:HE2	1:A:559:PHE:CD2	2.47	0.49
1:A:876:CYS:SG	1:A:877:ARG:N	2.86	0.49
1:A:2254:PHE:CE2	1:A:2306:VAL:HG23	2.47	0.49
1:A:3038:GLU:OE1	1:A:3127:LYS:NZ	2.45	0.49
1:A:3268:VAL:HG11	1:A:3604:LEU:HD23	1.94	0.49
1:A:3589:PHE:HB2	1:A:3635:LEU:HD13	1.94	0.49
1:A:4377:ARG:HD3	1:A:4381:ILE:HD12	1.95	0.49
1:A:2221:PHE:CD2	1:A:2408:MET:HE2	2.48	0.49
1:A:2417:ILE:HD13	1:A:2578:LEU:HB2	1.94	0.49
1:A:4665:ASP:OD2	1:A:4666:THR:N	2.45	0.49
1:A:1939:LEU:N	1:A:1940:PRO:HD2	2.28	0.49
1:A:1536:LEU:HD23	1:A:1588:LEU:HD13	1.95	0.49
1:A:443:HIS:CG	1:A:448:ILE:HD11	2.48	0.49
1:A:545:ASP:CG	1:A:547:ILE:HG22	2.38	0.49
1:A:710:ASP:OD1	1:A:713:ARG:NE	2.43	0.49
1:A:1943:PHE:O	1:A:1946:HIS:N	2.46	0.49
1:A:538:PHE:O	1:A:541:LEU:HG	2.13	0.48
1:A:1679:GLN:HG3	1:A:1775:VAL:HG13	1.95	0.48
1:A:1976:ALA:HB1	1:A:2009:MET:SD	2.53	0.48
1:A:2975:SER:O	1:A:2979:ILE:HD12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3864:MET:SD	1:A:3919:GLN:NE2	2.86	0.48
1:A:862:LEU:HD11	1:A:938:VAL:HG21	1.94	0.48
1:A:1414:ARG:HD3	1:A:1496:TRP:CE2	2.49	0.48
1:A:1614:CYS:SG	1:A:3081:THR:HG21	2.53	0.48
1:A:2058:VAL:HG11	1:A:2066:ILE:HD13	1.94	0.48
1:A:5140:LYS:O	1:A:5146:THR:OG1	2.31	0.48
1:A:1485:PHE:CE1	1:A:1489:MET:HE3	2.48	0.48
1:A:1493:LYS:O	1:A:1496:TRP:HB2	2.13	0.48
1:A:4668:LEU:HD22	1:A:4674:ARG:HA	1.94	0.48
1:A:4997:LYS:NZ	1:A:5036:SER:O	2.43	0.48
1:A:2788:GLY:O	1:A:2797:ARG:HA	2.14	0.48
1:A:3307:ALA:HB1	1:A:3314:ILE:HD13	1.93	0.48
1:A:4827:ASN:O	1:A:4831:VAL:HG23	2.13	0.48
1:A:1482:SER:O	1:A:1482:SER:OG	2.30	0.48
1:A:5164:SER:O	1:A:5168:THR:HG23	2.14	0.48
1:A:1993:ARG:NH1	1:A:2209:ASN:O	2.44	0.48
1:A:2240:ILE:C	1:A:2240:ILE:HD12	2.38	0.48
1:A:2266:SER:O	1:A:2296:LYS:HB3	2.13	0.48
1:A:552:PHE:CE2	1:A:625:ILE:HG23	2.49	0.48
1:A:1096:LEU:HD12	1:A:1101:ILE:HD13	1.96	0.48
1:A:1548:ILE:HG23	1:A:1562:VAL:HG12	1.95	0.48
2:B:252:ARG:O	2:B:256:GLN:NE2	2.47	0.48
1:A:542:GLN:N	1:A:542:GLN:OE1	2.45	0.48
1:A:1294:LYS:HB2	1:A:1330:GLN:NE2	2.29	0.48
1:A:2216:ARG:HD2	3:A:5301:ATP:H1'	1.96	0.48
1:A:479:CYS:SG	1:A:569:TYR:HB2	2.54	0.48
1:A:1407:LEU:CD1	1:A:1410:ILE:HD12	2.44	0.48
1:A:671:SER:OG	1:A:674:LEU:HB3	2.14	0.47
1:A:4009:CYS:C	1:A:4010:LEU:HD12	2.38	0.47
1:A:4979:LEU:HD22	1:A:4981:TYR:HB3	1.95	0.47
1:A:3643:ILE:O	1:A:3648:ASN:ND2	2.45	0.47
1:A:401:PHE:CE2	1:A:455:TYR:HB2	2.49	0.47
1:A:498:ILE:HG21	1:A:500:TYR:CE1	2.49	0.47
1:A:2894:MET:HE1	1:A:2899:PHE:HB2	1.95	0.47
1:A:3612:ASP:O	1:A:3616:GLU:HG3	2.14	0.47
1:A:3859:ASP:OD2	1:A:3902:MET:HE1	2.13	0.47
1:A:4390:LEU:H	1:A:4390:LEU:HD12	1.79	0.47
1:A:4781:VAL:HG22	1:A:4887:LEU:HD13	1.96	0.47
1:A:2023:ILE:HD12	1:A:2056:LEU:CD2	2.45	0.47
1:A:4136:LYS:NZ	1:A:4937:CYS:O	2.42	0.47
1:A:4871:PRO:HA	1:A:4877:GLY:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:166:LEU:HD11	2:B:178:VAL:HG11	1.97	0.47
1:A:711:ALA:O	1:A:714:GLN:N	2.43	0.47
1:A:2416:VAL:HG12	1:A:2521:ILE:HG23	1.97	0.47
1:A:4277:VAL:HG13	1:A:4717:ILE:HG23	1.96	0.47
1:A:532:LEU:HA	1:A:535:ASP:OD1	2.15	0.47
1:A:2147:ARG:HG2	1:A:2147:ARG:HH21	1.80	0.47
1:A:4788:LEU:HD12	1:A:4915:VAL:HG11	1.95	0.47
1:A:1344:LYS:O	1:A:1348:HIS:ND1	2.41	0.47
1:A:2650:TRP:NE1	1:A:2760:GLU:HG2	2.29	0.47
1:A:2924:VAL:HG13	1:A:2967:ALA:HB3	1.96	0.47
1:A:2959:LEU:O	1:A:2963:VAL:HG23	2.14	0.47
1:A:3546:MET:O	1:A:3693:ILE:N	2.37	0.47
1:A:1369:ASN:N	1:A:1481:PRO:O	2.40	0.47
1:A:2488:GLU:O	1:A:2491:THR:OG1	2.19	0.47
1:A:3102:LEU:HG	1:A:3148:LEU:HD11	1.97	0.47
1:A:556:PHE:CZ	1:A:629:VAL:HG13	2.50	0.47
1:A:1029:LEU:CD1	1:A:1060:VAL:HG22	2.45	0.47
1:A:1743:ARG:NH2	1:A:1812:MET:SD	2.88	0.47
1:A:1935:GLU:HG2	1:A:1940:PRO:HB2	1.97	0.47
1:A:2493:GLU:C	1:A:2495:ILE:H	2.23	0.47
1:A:2237:PRO:O	1:A:2238:SER:C	2.58	0.46
1:A:543:THR:OG1	1:A:548:ASN:OD1	2.07	0.46
1:A:1126:SER:C	1:A:1127:LEU:HD22	2.41	0.46
1:A:3054:ILE:HD12	1:A:3054:ILE:H	1.79	0.46
1:A:4486:ASP:OD1	1:A:4552:ARG:NH1	2.47	0.46
1:A:3045:LEU:CD2	1:A:3157:VAL:HG21	2.44	0.46
1:A:3707:ASN:N	1:A:3707:ASN:OD1	2.48	0.46
1:A:4390:LEU:HD12	1:A:4390:LEU:N	2.30	0.46
1:A:4578:VAL:HG11	1:A:4682:ALA:CB	2.45	0.46
2:B:45:TRP:CZ3	2:B:65:LEU:HB3	2.50	0.46
1:A:2398:ASP:O	1:A:2402:LYS:HG3	2.16	0.46
1:A:3068:ILE:CG2	1:A:3103:LEU:HD22	2.46	0.46
2:B:49:GLU:O	2:B:52:GLY:N	2.41	0.46
2:B:213:MET:CG	2:B:233:LEU:HD13	2.46	0.46
1:A:382:PHE:CD2	1:A:436:ILE:CD1	2.98	0.46
1:A:582:ARG:CZ	1:A:582:ARG:HB3	2.45	0.46
1:A:2255:MET:HE1	1:A:2308:PHE:HE2	1.81	0.46
1:A:2372:LYS:HE2	1:A:2372:LYS:HA	1.96	0.46
1:A:3450:LEU:HD12	1:A:3450:LEU:C	2.40	0.46
1:A:4031:ILE:HD11	2:B:215:ARG:CD	2.45	0.46
1:A:4840:ARG:NH2	1:A:4857:SER:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:PHE:CE1	1:A:491:ASP:OD2	2.69	0.46
1:A:802:LEU:HD22	1:A:817:VAL:HG22	1.98	0.46
1:A:823:MET:SD	1:A:826:ARG:NH1	2.89	0.46
1:A:1069:LYS:O	1:A:1073:ASN:ND2	2.41	0.46
1:A:2166:ARG:HB3	1:A:2167:PRO:HD3	1.97	0.46
2:B:76:LEU:HD12	2:B:77:ASN:H	1.79	0.46
2:B:231:LEU:HD23	2:B:268:ILE:CD1	2.46	0.46
1:A:671:SER:OG	1:A:671:SER:O	2.26	0.46
1:A:5132:GLU:OE1	1:A:5169:LYS:NZ	2.43	0.46
1:A:532:LEU:O	1:A:535:ASP:OD1	2.33	0.46
1:A:4427:VAL:HG12	1:A:4428:PRO:O	2.16	0.46
2:B:166:LEU:CD1	2:B:178:VAL:HG11	2.46	0.46
1:A:425:ASP:OD2	1:A:426:LEU:N	2.49	0.45
1:A:3022:ILE:CG2	1:A:3099:MET:HE1	2.45	0.45
2:B:133:LEU:HD23	2:B:153:LEU:HD13	1.98	0.45
2:B:144:LYS:C	2:B:163:LEU:HD23	2.41	0.45
1:A:1015:GLN:HA	1:A:1015:GLN:OE1	2.15	0.45
1:A:2402:LYS:HE2	1:A:2582:PHE:CD1	2.51	0.45
1:A:2460:ILE:O	1:A:2464:VAL:HG23	2.16	0.45
1:A:3563:LEU:CD2	1:A:3653:THR:HG21	2.46	0.45
1:A:4637:GLU:O	1:A:4641:VAL:HG23	2.15	0.45
2:B:86:LEU:HD22	2:B:89:LEU:HD11	1.98	0.45
1:A:4961:VAL:HG22	1:A:4965:LEU:HD12	1.98	0.45
2:B:59:ASN:O	2:B:63:ASN:OD1	2.34	0.45
1:A:1287:ILE:HD13	1:A:1329:HIS:NE2	2.31	0.45
1:A:1700:TYR:CE2	1:A:1807:ALA:HA	2.52	0.45
1:A:3728:TYR:CD2	1:A:4820:GLY:HA2	2.52	0.45
1:A:1330:GLN:O	1:A:1330:GLN:HG3	2.17	0.45
1:A:1593:MET:HG3	1:A:3084:CYS:HB3	1.99	0.45
1:A:3937:THR:HG21	1:A:3945:GLN:HA	1.99	0.45
1:A:409:GLY:O	1:A:411:SER:N	2.49	0.45
1:A:1608:ARG:O	1:A:1611:GLU:HG2	2.16	0.45
1:A:4136:LYS:NZ	1:A:4180:ASP:OD2	2.46	0.45
1:A:4782:LYS:O	1:A:4785:PRO:HD2	2.16	0.45
1:A:4835:THR:HG22	1:A:4883:LEU:HD11	1.97	0.45
2:B:61:ALA:HB2	2:B:81:LEU:CD1	2.47	0.45
1:A:682:ARG:O	1:A:686:THR:OG1	2.33	0.45
1:A:2871:ASP:N	1:A:2871:ASP:OD1	2.49	0.45
1:A:3937:THR:HA	1:A:3941:VAL:HG22	1.99	0.45
1:A:4173:LEU:HD12	1:A:4939:TYR:HB2	1.98	0.45
1:A:4791:GLN:HG2	1:A:4871:PRO:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5160:ASP:OD2	1:A:5161:THR:N	2.50	0.45
1:A:1702:ASN:O	1:A:1876:LEU:HD22	2.16	0.45
1:A:4133:VAL:HG22	1:A:4938:GLN:HE22	1.81	0.45
1:A:394:ASN:O	1:A:395:PRO:C	2.59	0.45
1:A:982:TRP:O	1:A:985:LYS:HG3	2.17	0.45
1:A:3890:SER:HA	1:A:3920:TRP:CZ2	2.51	0.45
1:A:4983:HIS:CD2	1:A:4983:HIS:H	2.34	0.45
2:B:63:ASN:O	2:B:66:LYS:HG3	2.17	0.45
1:A:865:TYR:CG	1:A:938:VAL:HG22	2.52	0.45
1:A:2421:GLU:OE1	1:A:2566:TYR:OH	2.32	0.45
1:A:2686:MET:SD	1:A:2721:LEU:HB3	2.56	0.45
1:A:3811:LEU:N	1:A:3812:PRO:CD	2.80	0.45
1:A:4346:LEU:HD12	1:A:4347:GLU:HG2	1.98	0.45
1:A:1069:LYS:HE3	1:A:1069:LYS:HA	1.99	0.44
1:A:1454:GLU:HB3	1:A:1595:MET:SD	2.57	0.44
1:A:2493:GLU:C	1:A:2495:ILE:N	2.75	0.44
1:A:3799:LYS:HG2	1:A:3813:TRP:CE2	2.52	0.44
1:A:4930:THR:HB	1:A:4931:PRO:HD3	1.98	0.44
2:B:78:LEU:HD11	2:B:89:LEU:HD13	1.99	0.44
2:B:213:MET:HG3	2:B:233:LEU:HD13	1.99	0.44
1:A:526:LYS:HE2	1:A:579:LEU:HD21	1.99	0.44
1:A:2198:LEU:HD21	1:A:2212:TRP:CH2	2.52	0.44
1:A:4428:PRO:HB2	1:A:4595:SER:HB2	1.99	0.44
1:A:401:PHE:HB2	1:A:453:VAL:HG23	1.99	0.44
1:A:1950:VAL:HG12	1:A:1950:VAL:O	2.17	0.44
1:A:2504:ASP:OD1	1:A:2504:ASP:N	2.50	0.44
1:A:3066:PRO:CG	1:A:3101:LEU:HD13	2.47	0.44
1:A:3870:LEU:HD11	1:A:3889:LEU:HD12	1.99	0.44
1:A:3997:CYS:O	1:A:4001:LEU:N	2.44	0.44
1:A:4428:PRO:O	1:A:4429:LEU:HB3	2.18	0.44
1:A:568:ILE:HD13	1:A:568:ILE:H	1.83	0.44
1:A:1991:SER:HB2	1:A:1996:VAL:HG21	1.98	0.44
1:A:3709:VAL:HG23	1:A:3766:CYS:CB	2.47	0.44
1:A:4784:LEU:CB	1:A:4887:LEU:HD22	2.47	0.44
1:A:1898:ASP:HB2	1:A:1934:TRP:HB3	1.99	0.44
1:A:2078:TYR:HA	1:A:2087:TRP:O	2.17	0.44
1:A:4780:LEU:CD2	1:A:4835:THR:HG23	2.48	0.44
1:A:1375:LEU:HD21	1:A:1485:PHE:CE1	2.52	0.44
1:A:2715:TYR:HA	1:A:2720:LEU:HD23	1.99	0.44
1:A:5174:LEU:HD22	1:A:5174:LEU:H	1.82	0.44
2:B:157:ARG:HA	2:B:177:VAL:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:ARG:HA	1:A:522:LEU:HD12	1.99	0.44
1:A:1379:LEU:O	1:A:1383:ASP:OD2	2.36	0.44
1:A:2236:ASN:O	1:A:2237:PRO:C	2.60	0.44
1:A:2292:PHE:HZ	1:A:2564:LEU:HD22	1.81	0.44
1:A:2968:LYS:NZ	1:A:3035:GLU:OE2	2.51	0.44
2:B:252:ARG:HA	2:B:255:GLN:CG	2.48	0.44
1:A:1386:ASP:O	1:A:1390:ARG:NH1	2.50	0.44
1:A:2471:ALA:HB1	1:A:2516:SER:O	2.17	0.44
1:A:2894:MET:CE	1:A:2899:PHE:HB2	2.48	0.44
1:A:3455:VAL:HG12	1:A:3456:THR:N	2.33	0.44
1:A:4983:HIS:CD2	1:A:4983:HIS:N	2.85	0.44
1:A:476:VAL:HG22	1:A:477:ASN:N	2.33	0.44
1:A:2327:ASN:OD1	1:A:2327:ASN:N	2.51	0.44
1:A:2316:THR:HG22	1:A:2318:ILE:HD11	2.00	0.43
1:A:3054:ILE:HD12	1:A:3054:ILE:N	2.33	0.43
1:A:3394:ALA:O	1:A:3398:VAL:HG23	2.18	0.43
1:A:4795:VAL:HG22	1:A:4974:LYS:CG	2.47	0.43
2:B:259:THR:O	2:B:261:PRO:HD3	2.18	0.43
1:A:4582:ILE:HG12	1:A:4681:ILE:HG21	1.99	0.43
1:A:5140:LYS:O	1:A:5146:THR:CB	2.66	0.43
1:A:5144:PRO:HA	1:A:5147:GLN:HG2	2.00	0.43
1:A:588:ARG:HG3	1:A:589:TYR:N	2.33	0.43
1:A:1789:LEU:N	1:A:1790:PRO:CD	2.81	0.43
1:A:2805:VAL:HB	1:A:2825:CYS:SG	2.59	0.43
1:A:2994:GLN:O	1:A:2995:ALA:C	2.61	0.43
1:A:4962:SER:OG	1:A:4963:ARG:HD2	2.18	0.43
1:A:5174:LEU:HD22	1:A:5174:LEU:N	2.32	0.43
1:A:480:LEU:C	1:A:480:LEU:HD23	2.44	0.43
1:A:862:LEU:CD1	1:A:938:VAL:HG21	2.49	0.43
1:A:1146:GLU:OE2	1:A:1198:ARG:N	2.50	0.43
1:A:4756:VAL:HG13	1:A:4761:GLY:HA3	1.99	0.43
2:B:143:ILE:HG21	2:B:146:LEU:HD23	1.99	0.43
1:A:2179:ASP:O	1:A:2179:ASP:OD2	2.37	0.43
1:A:4979:LEU:HD23	1:A:4980:VAL:N	2.33	0.43
1:A:445:ASP:OD2	1:A:484:SER:OG	2.34	0.43
1:A:1290:HIS:CD2	1:A:1330:GLN:HB3	2.54	0.43
1:A:4029:GLN:HG2	2:B:238:PHE:CD2	2.53	0.43
1:A:4143:PHE:CE1	1:A:4223:VAL:HG12	2.53	0.43
1:A:4172:MET:SD	1:A:4740:ILE:HA	2.59	0.43
1:A:1451:SER:OG	1:A:1518:TRP:NE1	2.46	0.43
1:A:2239:PHE:O	1:A:2239:PHE:CG	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2351:TYR:CZ	1:A:2355:LEU:HD11	2.54	0.43
1:A:2861:HIS:HB3	1:A:2862:PRO:HD3	2.00	0.43
1:A:2991:ASP:OD1	1:A:2992:ASP:N	2.52	0.43
1:A:4130:ILE:HD13	1:A:4170:LEU:HD13	2.00	0.43
1:A:4347:GLU:OE1	1:A:4347:GLU:HA	2.19	0.43
1:A:4871:PRO:HG2	1:A:4973:LEU:HG	2.01	0.43
2:B:112:MET:O	2:B:114:LYS:N	2.52	0.43
1:A:1445:VAL:HG13	1:A:1462:VAL:CG1	2.49	0.43
1:A:2686:MET:HE3	1:A:2686:MET:HA	2.01	0.43
1:A:2783:ALA:HB2	1:A:2804:LEU:CD1	2.47	0.43
1:A:3270:LEU:HD13	1:A:3280:ALA:HB2	2.01	0.43
1:A:4973:LEU:HD13	1:A:4974:LYS:HG3	1.99	0.43
1:A:4977:PRO:O	1:A:4978:THR:C	2.62	0.43
1:A:1859:TYR:CZ	1:A:2086:MET:HE1	2.54	0.43
1:A:2147:ARG:HG3	1:A:2148:SER:H	1.84	0.43
1:A:2979:ILE:O	1:A:2983:VAL:HG23	2.19	0.43
1:A:3195:VAL:O	1:A:3199:ILE:HG12	2.19	0.43
1:A:4071:ASP:OD2	1:A:4958:ARG:NH1	2.52	0.43
1:A:4661:LEU:O	1:A:4662:LEU:HD13	2.19	0.43
1:A:407:GLU:HB2	1:A:449:PRO:CD	2.48	0.42
1:A:4141:TYR:O	1:A:4185:LYS:NZ	2.39	0.42
1:A:4483:MET:HE2	1:A:4485:GLU:HG2	2.00	0.42
2:B:153:LEU:O	2:B:173:LEU:HD12	2.19	0.42
2:B:248:GLY:HA2	2:B:251:MET:CE	2.48	0.42
1:A:737:THR:HG21	1:A:766:PRO:HG3	2.01	0.42
1:A:937:GLU:CG	1:A:985:LYS:NZ	2.82	0.42
1:A:1294:LYS:HB2	1:A:1330:GLN:CD	2.44	0.42
1:A:2024:ARG:NH2	1:A:2057:ASP:OD2	2.50	0.42
1:A:3992:PHE:C	2:B:120:PHE:CE2	2.97	0.42
1:A:4114:THR:HG21	1:A:4129:VAL:O	2.18	0.42
2:B:42:LEU:HA	2:B:45:TRP:CD2	2.54	0.42
2:B:76:LEU:HG	2:B:77:ASN:N	2.33	0.42
1:A:463:GLU:N	1:A:463:GLU:OE1	2.53	0.42
1:A:530:ALA:CB	1:A:590:LEU:HD21	2.49	0.42
1:A:1164:CYS:HA	1:A:1167:VAL:HG22	2.00	0.42
1:A:519:ARG:O	1:A:523:VAL:HG23	2.20	0.42
1:A:983:ASP:C	1:A:985:LYS:N	2.77	0.42
1:A:1866:THR:N	1:A:1869:THR:OG1	2.46	0.42
1:A:4639:ILE:HG22	1:A:4643:HIS:CD2	2.54	0.42
1:A:654:SER:HB2	1:A:655:PRO:CD	2.50	0.42
1:A:1062:ARG:O	1:A:1066:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1636:THR:OG1	1:A:1655:PHE:O	2.26	0.42
1:A:2036:LEU:HD23	1:A:2081:ASP:HB3	2.01	0.42
1:A:2650:TRP:CE2	1:A:2760:GLU:HG2	2.55	0.42
1:A:3405:ILE:O	1:A:3405:ILE:HG22	2.18	0.42
1:A:3673:MET:SD	1:A:3674:LEU:N	2.92	0.42
1:A:4016:HIS:CD2	1:A:4032:CYS:SG	3.13	0.42
1:A:4487:LEU:HD21	1:A:4571:ASP:OD2	2.19	0.42
1:A:420:LEU:CD2	1:A:435:GLY:HA3	2.50	0.42
1:A:626:VAL:O	1:A:630:VAL:HG23	2.19	0.42
1:A:1943:PHE:CD1	1:A:1943:PHE:N	2.88	0.42
1:A:3838:VAL:HG21	1:A:3866:CYS:SG	2.60	0.42
1:A:4761:GLY:O	1:A:4765:VAL:N	2.42	0.42
1:A:4761:GLY:HA2	1:A:4765:VAL:HG22	2.00	0.42
2:B:175:LEU:HD11	2:B:177:VAL:HG23	2.01	0.42
1:A:912:ARG:O	1:A:916:GLU:OE2	2.38	0.42
1:A:1608:ARG:HH21	1:A:1608:ARG:HG2	1.85	0.42
1:A:3237:GLN:O	1:A:3240:ARG:NE	2.48	0.42
1:A:3299:PHE:CZ	1:A:3440:VAL:HG21	2.55	0.42
1:A:4009:CYS:HG	1:A:4051:HIS:CE1	2.38	0.42
1:A:4042:GLU:HA	1:A:4042:GLU:OE1	2.20	0.42
1:A:4342:ALA:O	1:A:4345:VAL:HG12	2.20	0.42
1:A:532:LEU:C	1:A:535:ASP:OD1	2.62	0.42
1:A:934:LYS:O	1:A:938:VAL:HG23	2.20	0.42
1:A:2949:GLU:HB2	1:A:3163:ILE:HD13	2.00	0.42
1:A:3187:ILE:O	1:A:3191:LEU:HD23	2.19	0.42
1:A:3859:ASP:OD1	1:A:3860:ALA:N	2.53	0.42
1:A:4467:ASN:O	1:A:4471:SER:C	2.63	0.42
1:A:398:HIS:CB	1:A:455:TYR:O	2.67	0.42
1:A:566:PRO:HG2	1:A:576:TRP:CE3	2.55	0.42
1:A:580:GLN:O	1:A:581:TYR:C	2.63	0.42
1:A:737:THR:OG1	1:A:769:HIS:NE2	2.52	0.42
1:A:1277:TYR:O	1:A:1281:PRO:HD2	2.20	0.42
1:A:1396:ILE:O	1:A:1397:ASN:HB3	2.20	0.42
1:A:4871:PRO:HG2	1:A:4973:LEU:CG	2.50	0.42
1:A:4905:ASN:OD1	1:A:4905:ASN:N	2.52	0.42
2:B:38:ASN:HB3	2:B:69:LEU:HD21	2.02	0.42
1:A:1861:GLU:O	1:A:1892:TYR:HA	2.18	0.42
1:A:1977:ALA:HB1	1:A:1983:ARG:C	2.45	0.42
1:A:4173:LEU:CD1	1:A:4939:TYR:HB2	2.50	0.42
1:A:4781:VAL:HG12	1:A:4920:VAL:HB	2.01	0.42
1:A:4973:LEU:HD22	1:A:4973:LEU:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:983:ASP:O	1:A:985:LYS:N	2.53	0.41
1:A:3992:PHE:HD1	1:A:3992:PHE:O	2.03	0.41
1:A:1033:ILE:HG22	1:A:1081:LEU:HD12	2.02	0.41
1:A:2133:ARG:HE	1:A:2151:GLU:CD	2.25	0.41
1:A:2449:VAL:HG22	1:A:2463:ARG:HH21	1.85	0.41
1:A:2740:LYS:HB2	1:A:2920:SER:OG	2.20	0.41
1:A:2906:ASN:OD1	1:A:2908:THR:N	2.50	0.41
1:A:3453:SER:HB2	1:A:3529:ILE:HG23	2.01	0.41
1:A:3997:CYS:SG	1:A:3999:ILE:HB	2.60	0.41
1:A:4004:ALA:HA	1:A:4017:CYS:SG	2.60	0.41
1:A:4910:VAL:HB	1:A:4968:LYS:O	2.20	0.41
1:A:4932:LEU:CD2	1:A:4956:ILE:HG23	2.49	0.41
1:A:443:HIS:HB3	1:A:448:ILE:HD11	2.02	0.41
1:A:637:LEU:HD11	1:A:644:LEU:CD2	2.48	0.41
1:A:1106:LEU:HD11	1:A:1143:ARG:HB2	2.03	0.41
1:A:1514:ARG:HD2	1:A:2790:ALA:O	2.20	0.41
1:A:2594:ILE:O	1:A:2598:VAL:HG23	2.20	0.41
1:A:3269:ARG:NH2	1:A:3608:ALA:O	2.52	0.41
1:A:4846:ASN:OD1	1:A:4846:ASN:N	2.54	0.41
2:B:56:GLU:OE1	2:B:58:ARG:NH1	2.46	0.41
2:B:270:PHE:O	2:B:271:SER:OG	2.37	0.41
1:A:1332:GLN:O	1:A:1333:ARG:C	2.64	0.41
1:A:1534:LEU:HD23	1:A:1592:LEU:HD23	2.02	0.41
1:A:3000:LEU:O	1:A:3003:LEU:O	2.38	0.41
2:B:78:LEU:HD22	2:B:83:LEU:HD12	2.03	0.41
1:A:409:GLY:C	1:A:411:SER:H	2.29	0.41
1:A:1371:ASP:OD1	1:A:1373:SER:N	2.46	0.41
1:A:1601:ARG:NE	1:A:1601:ARG:HA	2.36	0.41
1:A:2378:CYS:O	1:A:2383:ILE:N	2.46	0.41
1:A:2643:ARG:O	1:A:2647:VAL:HG23	2.21	0.41
1:A:3764:LEU:HD23	1:A:3792:TRP:CZ3	2.55	0.41
1:A:408:PHE:HD2	1:A:417:ILE:HD13	1.86	0.41
1:A:430:ARG:NE	1:A:528:ILE:HD11	2.35	0.41
1:A:916:GLU:OE2	1:A:916:GLU:CA	2.69	0.41
1:A:2690:GLY:HA2	1:A:2694:HIS:HB3	2.02	0.41
1:A:2755:MET:HE1	1:A:2779:LYS:HA	2.02	0.41
1:A:4346:LEU:HD12	1:A:4347:GLU:N	2.35	0.41
1:A:5049:TYR:CD1	1:A:5053:ILE:HD12	2.56	0.41
1:A:426:LEU:CB	1:A:430:ARG:HB2	2.51	0.41
1:A:765:LEU:O	1:A:798:ARG:NH1	2.46	0.41
1:A:961:MET:HE1	1:A:991:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1366:LEU:HD22	1:A:1432:ARG:NH1	2.35	0.41
1:A:1383:ASP:OD2	1:A:1383:ASP:N	2.52	0.41
1:A:4132:SER:O	1:A:4136:LYS:HG2	2.21	0.41
2:B:41:TYR:HB3	2:B:45:TRP:CZ2	2.55	0.41
1:A:1236:PHE:O	1:A:1237:TRP:HB3	2.20	0.41
1:A:1319:SER:O	1:A:1323:ILE:HG13	2.20	0.41
1:A:3341:ALA:HB1	1:A:3342:PRO:HD2	2.03	0.41
1:A:3692:TYR:HB2	1:A:4978:THR:O	2.21	0.41
1:A:4114:THR:HG22	1:A:4115:LYS:N	2.36	0.41
1:A:4422:LEU:HD23	1:A:4427:VAL:HG21	2.02	0.41
1:A:429:ASP:C	1:A:430:ARG:CG	2.94	0.41
1:A:755:GLU:N	1:A:756:PRO:HD2	2.36	0.41
1:A:862:LEU:HD13	1:A:917:VAL:HG11	2.03	0.41
1:A:1172:GLN:O	1:A:1268:ILE:HG23	2.21	0.41
1:A:1286:PHE:CZ	1:A:1324:MET:HG2	2.55	0.41
1:A:1637:TRP:CZ2	1:A:1639:ALA:HB2	2.56	0.41
1:A:2036:LEU:O	1:A:2040:LEU:HG	2.20	0.41
1:A:2694:HIS:NE2	1:A:2700:LYS:HB3	2.36	0.41
1:A:2955:ASP:OD1	1:A:3040:ARG:NH2	2.47	0.41
1:A:3132:GLY:HA3	1:A:3137:ARG:HH21	1.85	0.41
1:A:3176:ILE:HG21	1:A:3227:ALA:HB1	2.03	0.41
1:A:3359:LEU:HD21	1:A:3397:SER:HB3	2.03	0.41
1:A:4289:MET:HE2	1:A:4324:MET:SD	2.60	0.41
1:A:4571:ASP:OD1	1:A:4571:ASP:N	2.53	0.41
1:A:4980:VAL:O	1:A:4981:TYR:O	2.39	0.41
1:A:5047:ASN:OD1	1:A:5048:VAL:N	2.53	0.41
1:A:5137:ILE:HG12	1:A:5190:CYS:SG	2.61	0.41
1:A:977:TYR:CE2	1:A:1024:LYS:HB3	2.55	0.41
1:A:1139:ALA:HA	1:A:1142:TRP:CE3	2.56	0.41
1:A:1388:PHE:CE2	1:A:1396:ILE:HG23	2.56	0.41
1:A:1450:ILE:HG23	1:A:1530:GLU:HA	2.03	0.41
1:A:3109:TYR:O	1:A:3113:TYR:N	2.54	0.41
1:A:1349:LEU:HD13	1:A:1349:LEU:C	2.46	0.40
1:A:2657:MET:HE3	1:A:2657:MET:HB3	1.97	0.40
1:A:3019:LYS:HB2	1:A:3059:PHE:CE1	2.57	0.40
1:A:4385:SER:O	1:A:4391:HIS:NE2	2.48	0.40
1:A:5124:THR:CG2	1:A:5125:GLY:N	2.83	0.40
1:A:2372:LYS:HA	1:A:2372:LYS:CE	2.51	0.40
1:A:2490:ASN:ND2	1:A:2525:ASN:O	2.53	0.40
1:A:2842:VAL:HA	1:A:2882:VAL:O	2.21	0.40
1:A:2861:HIS:HB3	1:A:2862:PRO:CD	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3538:SER:OG	1:A:3629:GLN:NE2	2.44	0.40
1:A:4344:ALA:O	1:A:4348:CYS:N	2.53	0.40
1:A:4791:GLN:HE21	1:A:4880:ALA:HB1	1.86	0.40
1:A:5190:CYS:SG	1:A:5191:VAL:N	2.93	0.40
2:B:46:SER:O	2:B:49:GLU:HB3	2.21	0.40
2:B:226:LEU:HD23	2:B:226:LEU:HA	1.95	0.40
1:A:2929:GLN:HA	1:A:2932:PHE:CD2	2.56	0.40
1:A:3827:ASN:OD1	1:A:3892:PRO:HB3	2.21	0.40
1:A:4789:ALA:O	1:A:4793:ASP:OD2	2.38	0.40
1:A:726:SER:O	1:A:726:SER:OG	2.36	0.40
1:A:1454:GLU:HG3	1:A:1533:SER:OG	2.21	0.40
1:A:1700:TYR:CZ	1:A:1810:ALA:CB	3.05	0.40
1:A:1748:CYS:SG	1:A:1801:THR:HG23	2.62	0.40
1:A:2701:ASP:OD1	1:A:2704:ARG:NH1	2.54	0.40
1:A:2825:CYS:HB3	1:A:2879:VAL:HG11	2.02	0.40
1:A:3563:LEU:HD22	1:A:3653:THR:HG21	2.02	0.40
1:A:3813:TRP:CE3	1:A:3816:LEU:HD12	2.57	0.40
1:A:4980:VAL:O	1:A:4985:TRP:N	2.55	0.40
1:A:1336:ILE:O	1:A:1340:VAL:HG23	2.22	0.40
1:A:1891:VAL:HG12	1:A:1892:TYR:N	2.36	0.40
1:A:2978:ASP:OD1	1:A:2979:ILE:N	2.54	0.40
1:A:3423:VAL:HG21	1:A:5018:TYR:CB	2.51	0.40
1:A:4008:VAL:N	1:A:4016:HIS:O	2.48	0.40
1:A:4784:LEU:HD22	1:A:4887:LEU:CD2	2.48	0.40
1:A:4972:SER:O	1:A:4973:LEU:HD23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	4479/5247 (85%)	4245 (95%)	228 (5%)	6 (0%)	48 75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	235/575 (41%)	203 (86%)	32 (14%)	0	100	100
All	All	4714/5822 (81%)	4448 (94%)	260 (6%)	6 (0%)	49	75

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1236	PHE
1	A	1333	ARG
1	A	3104	ASN
1	A	4981	TYR
1	A	1602	ASN
1	A	2494	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	4076/4653 (88%)	3960 (97%)	116 (3%)	38	62
2	B	216/501 (43%)	211 (98%)	5 (2%)	44	66
All	All	4292/5154 (83%)	4171 (97%)	121 (3%)	38	62

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	397	LEU
1	A	402	ILE
1	A	403	ARG
1	A	406	GLU
1	A	438	CYS
1	A	440	SER
1	A	459	SER
1	A	461	GLU
1	A	477	ASN
1	A	480	LEU

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Mol	Chain	Res	Type
1	A	484	SER
1	A	497	ASP
1	A	519	ARG
1	A	520	LYS
1	A	522	LEU
1	A	535	ASP
1	A	541	LEU
1	A	568	ILE
1	A	583	GLU
1	A	643	TRP
1	A	688	THR
1	A	768	SER
1	A	813	ASP
1	A	876	CYS
1	A	916	GLU
1	A	926	SER
1	A	962	GLU
1	A	989	ASP
1	A	1100	THR
1	A	1125	LYS
1	A	1175	PHE
1	A	1198	ARG
1	A	1204	ASN
1	A	1236	PHE
1	A	1281	PRO
1	A	1332	GLN
1	A	1368	LEU
1	A	1496	TRP
1	A	1509	LEU
1	A	1532	SER
1	A	1577	SER
1	A	1669	VAL
1	A	1696	MET
1	A	1717	ARG
1	A	1734	SER
1	A	1773	SER
1	A	1790	PRO
1	A	1838	SER
1	A	1982	ASP
1	A	1999	SER
1	A	2049	LYS
1	A	2082	ILE

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Mol	Chain	Res	Type
1	A	2147	ARG
1	A	2215	LEU
1	A	2222	LEU
1	A	2294	LEU
1	A	2318	ILE
1	A	2327	ASN
1	A	2554	ASP
1	A	2599	GLN
1	A	2604	SER
1	A	2609	GLU
1	A	2618	VAL
1	A	2640	ASP
1	A	2776	SER
1	A	2852	SER
1	A	2868	CYS
1	A	2870	GLU
1	A	3050	VAL
1	A	3082	GLN
1	A	3129	VAL
1	A	3133	LEU
1	A	3155	ASP
1	A	3245	GLU
1	A	3275	LEU
1	A	3303	HIS
1	A	3312	HIS
1	A	3319	THR
1	A	3421	SER
1	A	3451	MET
1	A	3780	THR
1	A	3835	TYR
1	A	3956	ASP
1	A	3963	SER
1	A	3965	VAL
1	A	3991	ARG
1	A	4005	LYS
1	A	4009	CYS
1	A	4014	HIS
1	A	4031	ILE
1	A	4039	LEU
1	A	4072	LEU
1	A	4219	ASN
1	A	4300	ARG

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Mol	Chain	Res	Type
1	A	4348	CYS
1	A	4398	GLU
1	A	4406	GLU
1	A	4482	THR
1	A	4505	CYS
1	A	4555	THR
1	A	4662	LEU
1	A	4686	SER
1	A	4733	SER
1	A	4784	LEU
1	A	4846	ASN
1	A	4851	LEU
1	A	4887	LEU
1	A	4905	ASN
1	A	4972	SER
1	A	4973	LEU
1	A	4979	LEU
1	A	4983	HIS
1	A	5002	SER
1	A	5019	SER
1	A	5103	SER
1	A	5149	GLU
2	B	39	GLU
2	B	42	LEU
2	B	48	TRP
2	B	59	ASN
2	B	71	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	597	HIS
1	A	816	ASN
1	A	921	ASN
1	A	979	ASN
1	A	1010	GLN
1	A	1184	GLN
1	A	1206	GLN
1	A	1395	GLN
1	A	1419	GLN
1	A	1491	HIS
1	A	1574	HIS

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Mol	Chain	Res	Type
1	A	1946	HIS
1	A	2478	HIS
1	A	2479	GLN
1	A	2505	HIS
1	A	2861	HIS
1	A	2994	GLN
1	A	3106	GLN
1	A	3122	HIS
1	A	3136	HIS
1	A	3200	ASN
1	A	3285	GLN
1	A	3294	ASN
1	A	3599	HIS
1	A	4081	ASN
1	A	4286	GLN
1	A	4313	GLN
1	A	4501	HIS
1	A	4655	GLN
1	A	4663	ASN
1	A	4770	HIS
1	A	4799	GLN
1	A	4826	HIS
1	A	4966	GLN
1	A	4983	HIS
1	A	5051	GLN
1	A	5062	HIS
2	B	57	GLN
2	B	256	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 5 ligands modelled in this entry, 4 are 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
3	ATP	A	5301	-	32,33,33	1.27	5 (15%)	48,52,52	1.74	10 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	5301	-	-	5/22/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5301	ATP	C5-C4	4.08	1.46	1.39
3	A	5301	ATP	C4-N9	-2.50	1.32	1.37
3	A	5301	ATP	C8-N7	2.46	1.36	1.31
3	A	5301	ATP	C5-N7	-2.38	1.34	1.39
3	A	5301	ATP	C5-C6	2.27	1.47	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	5301	ATP	C5-C4-N3	-4.97	119.87	126.72
3	A	5301	ATP	N3-C4-N9	3.96	133.90	127.17
3	A	5301	ATP	C2-N3-C4	3.42	120.19	111.83
3	A	5301	ATP	C4-N9-C8	3.39	109.30	105.74
3	A	5301	ATP	C4-C5-N7	-3.18	106.94	110.58
3	A	5301	ATP	N3-C2-N1	-3.12	123.86	128.58
3	A	5301	ATP	N9-C8-N7	-2.63	110.20	113.94
3	A	5301	ATP	C5-N7-C8	2.47	107.33	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	5301	ATP	C6-C5-N7	2.46	136.82	132.09
3	A	5301	ATP	C3'-C2'-C1'	2.02	105.29	101.46

There are no chirality outliers.

All (5) torsion outliers are listed below:

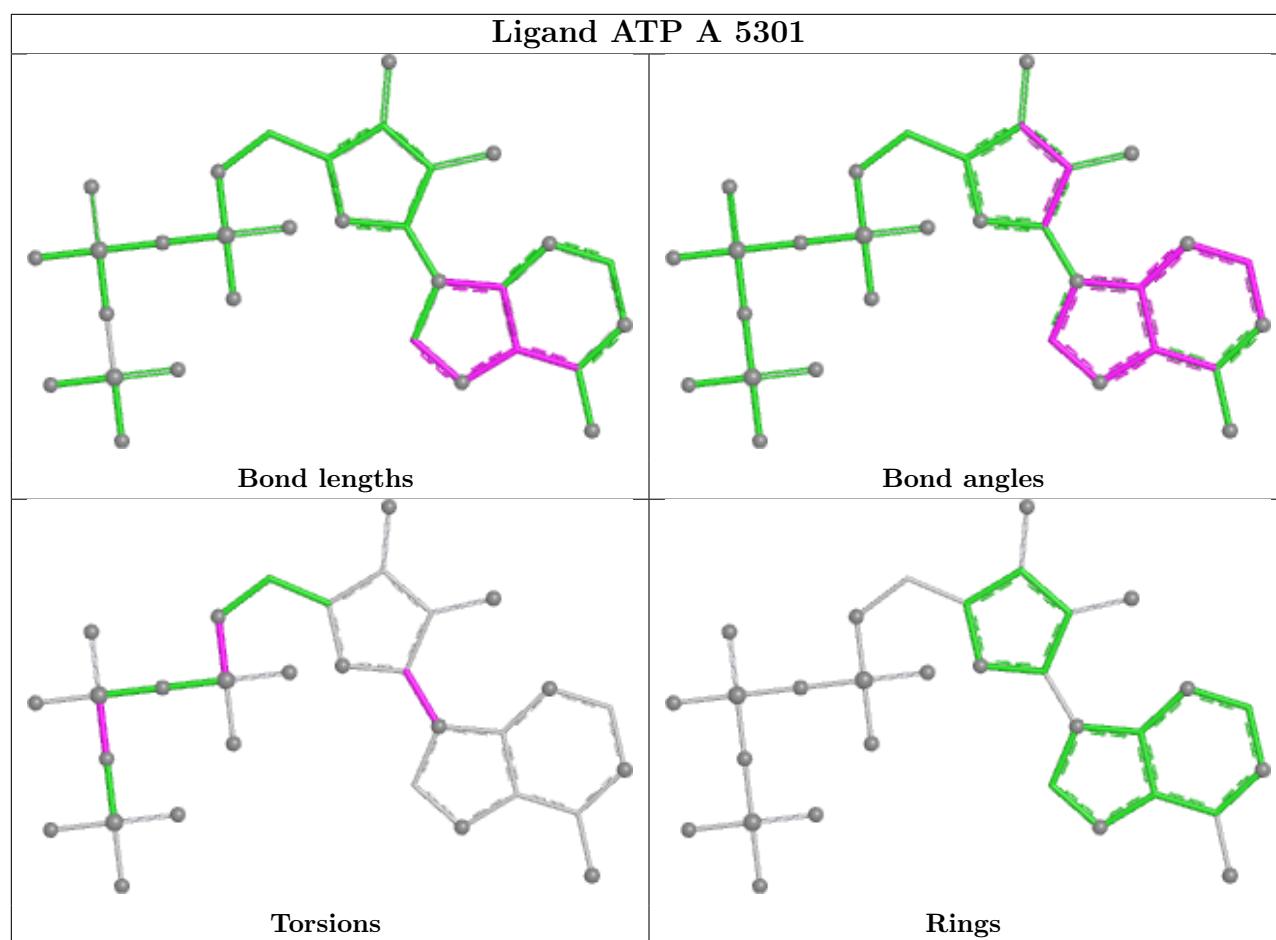
Mol	Chain	Res	Type	Atoms
3	A	5301	ATP	C5'-O5'-PA-O2A
3	A	5301	ATP	O4'-C1'-N9-C8
3	A	5301	ATP	O4'-C1'-N9-C4
3	A	5301	ATP	PG-O3B-PB-O2B
3	A	5301	ATP	PG-O3B-PB-O1B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5301	ATP	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.

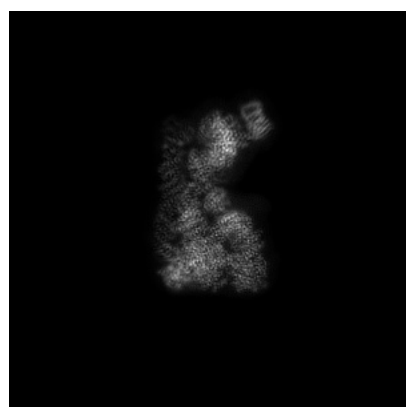
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50913. These allow visual inspection of the internal detail of the map and identification of artifacts.

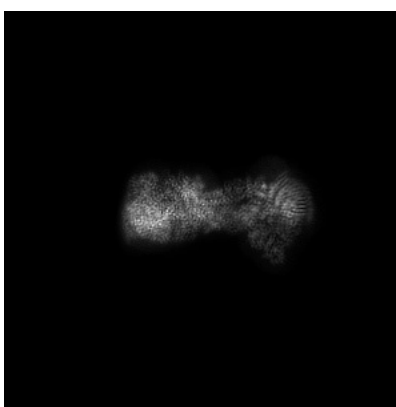
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

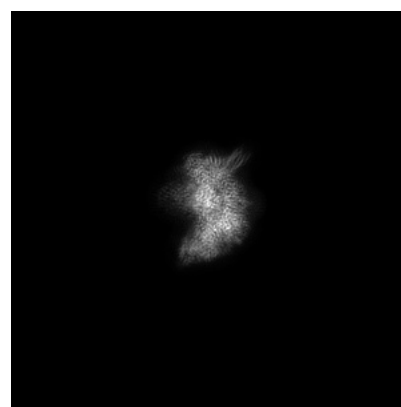
6.1.1 Primary map



X



Y

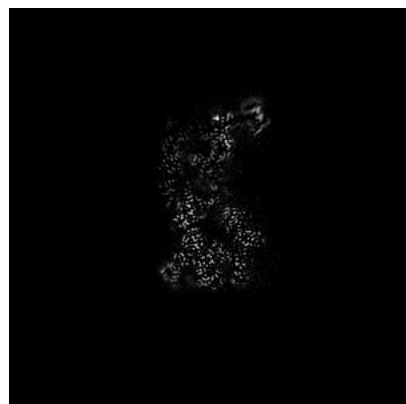


Z

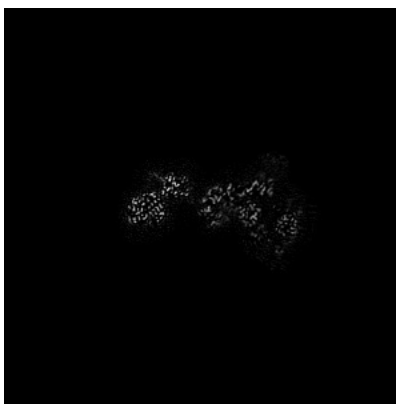
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

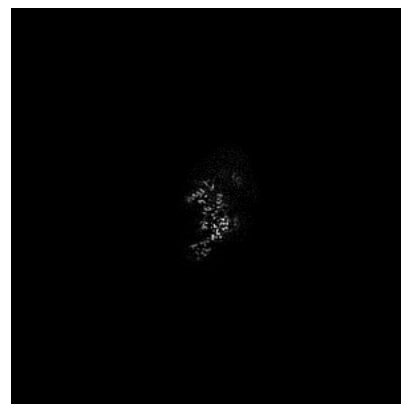
6.2.1 Primary map



X Index: 192



Y Index: 192

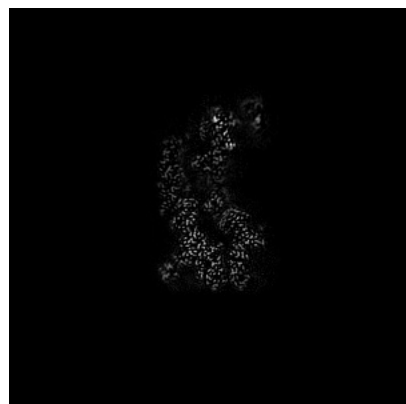


Z Index: 192

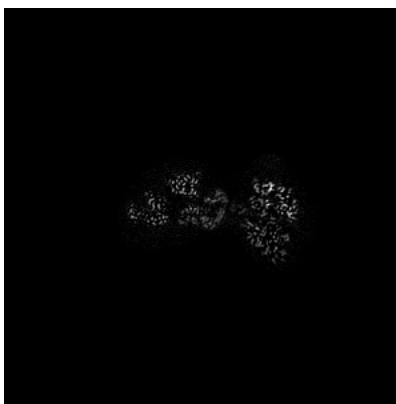
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

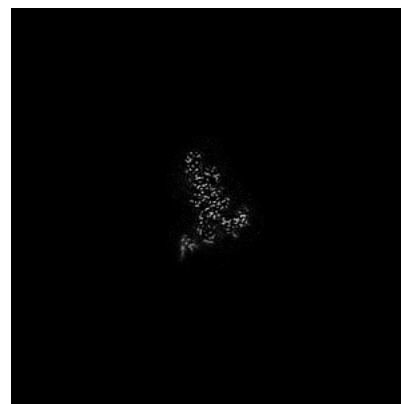
6.3.1 Primary map



X Index: 189



Y Index: 205

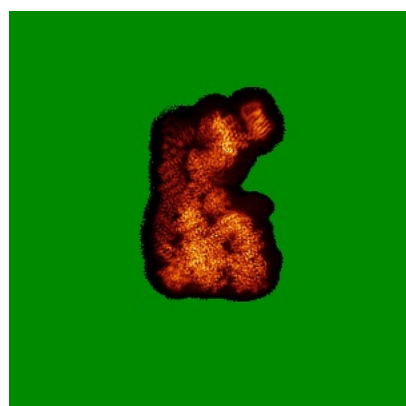


Z Index: 144

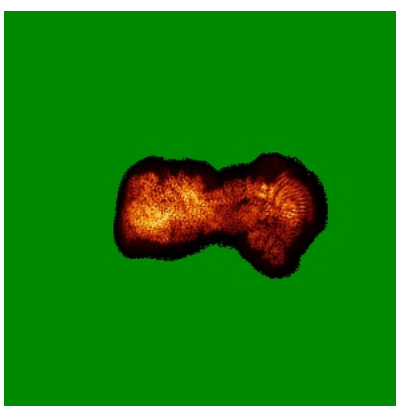
The images above show the largest variance slices of the map in three orthogonal directions.

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

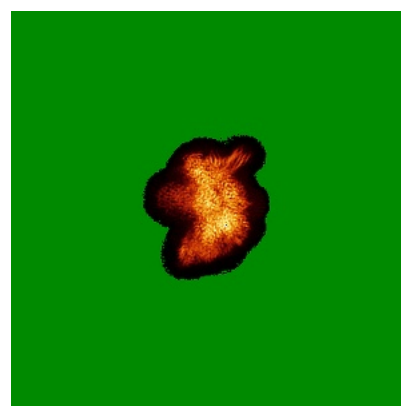
6.4.1 Primary map



X



Y



Z

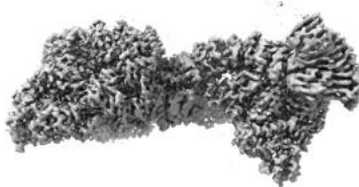
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

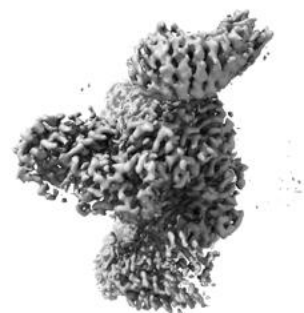
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

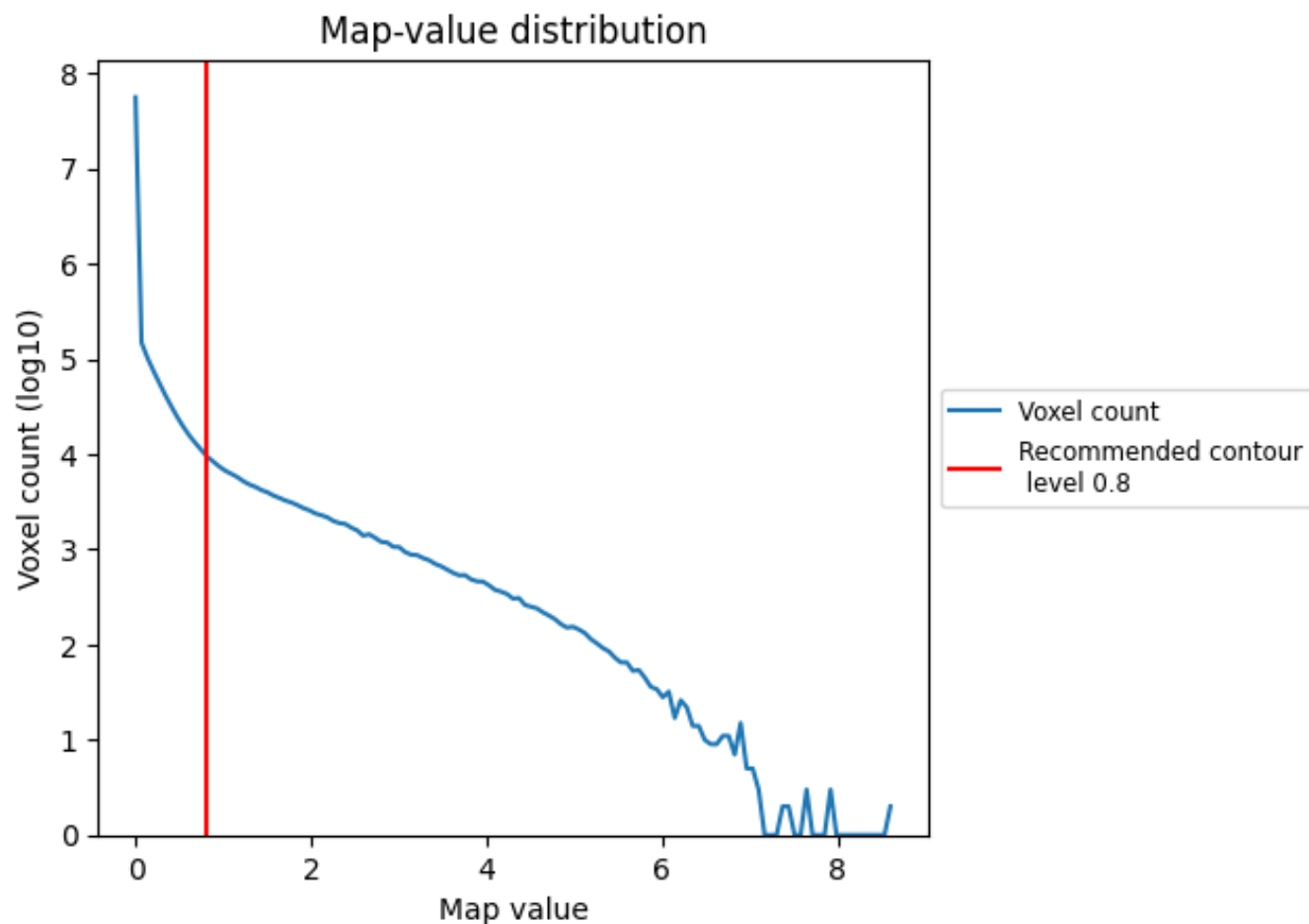
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

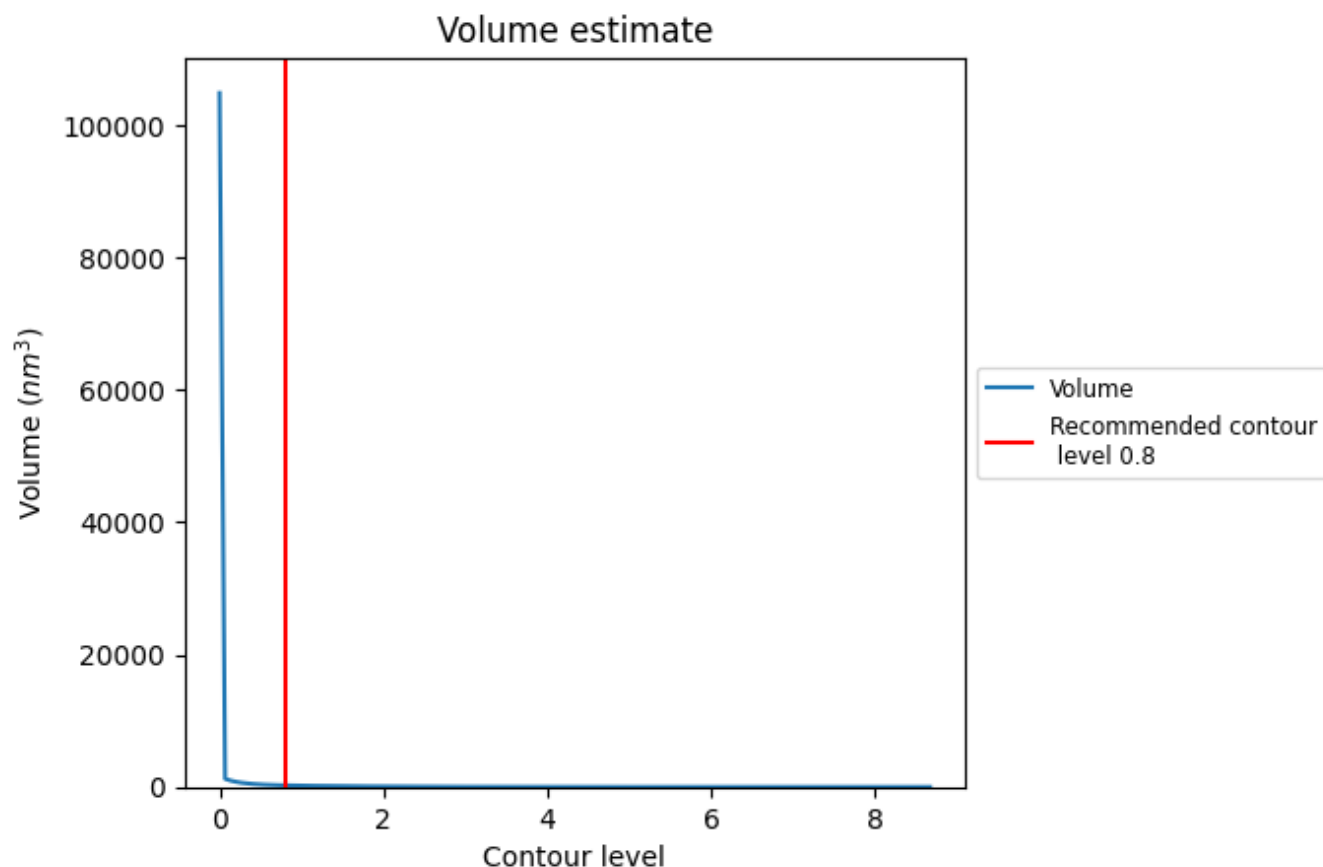
This section contains the results of statistical analysis of the map.

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.

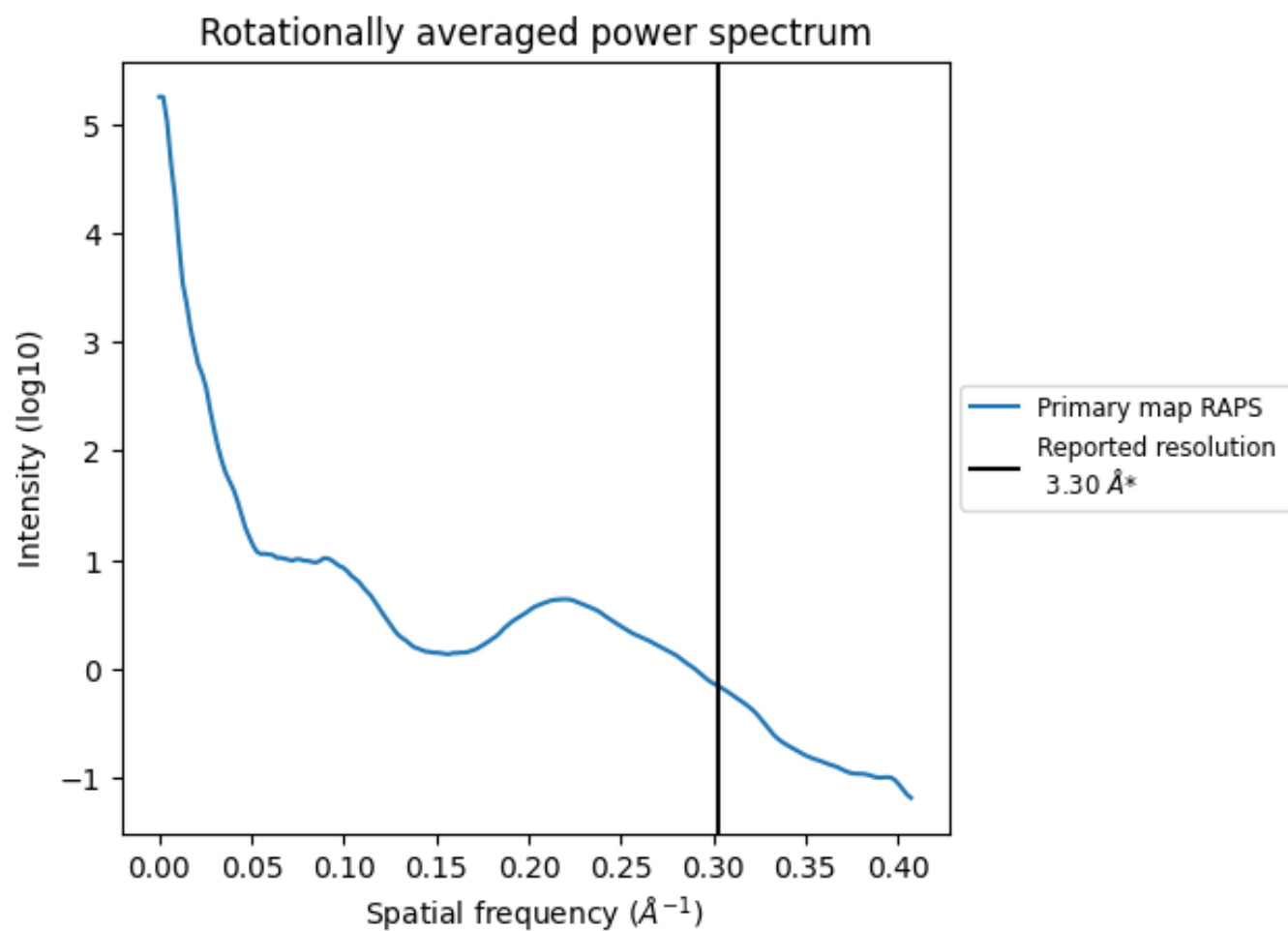
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 241 nm^3 ; this corresponds to an approximate mass of 218 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 0.303 Å⁻¹

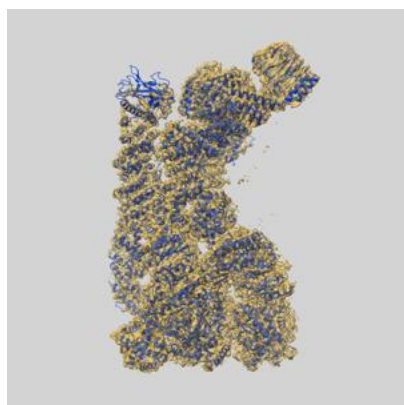
8 Fourier-Shell correlation ⓘ

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

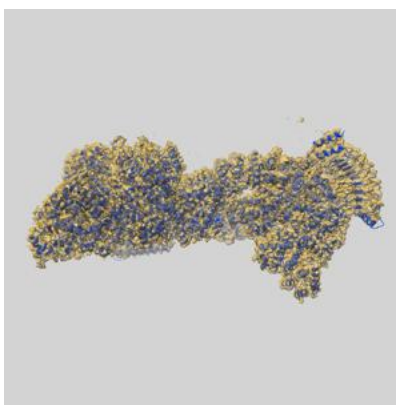
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50913 and PDB model 9G08. Per-residue inclusion information can be found in section [3](#) on page [6](#).

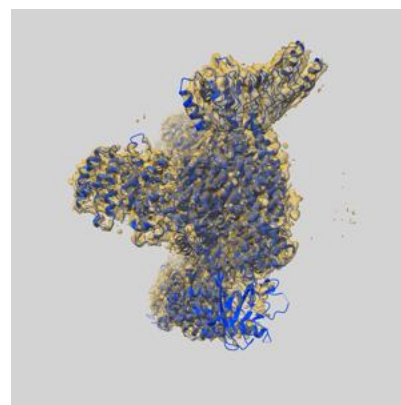
9.1 Map-model overlay [i](#)



X



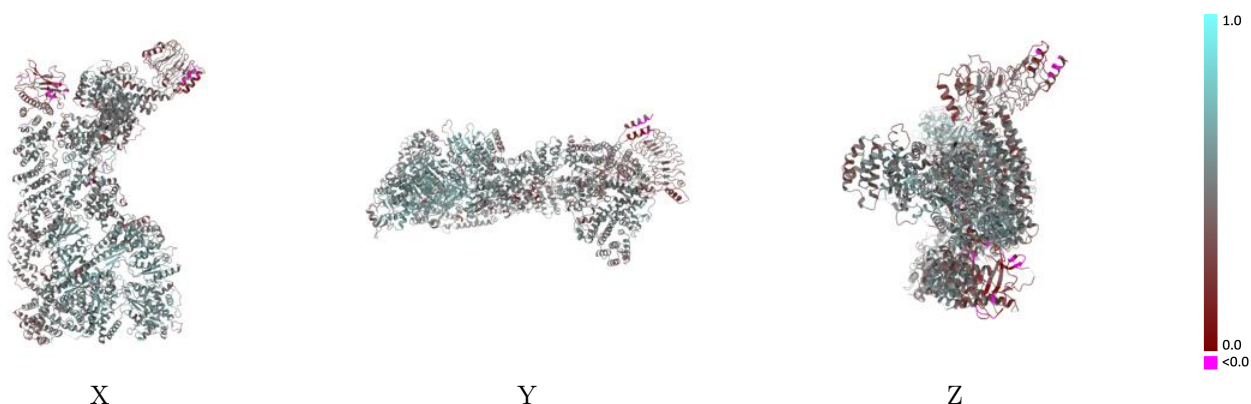
Y



Z

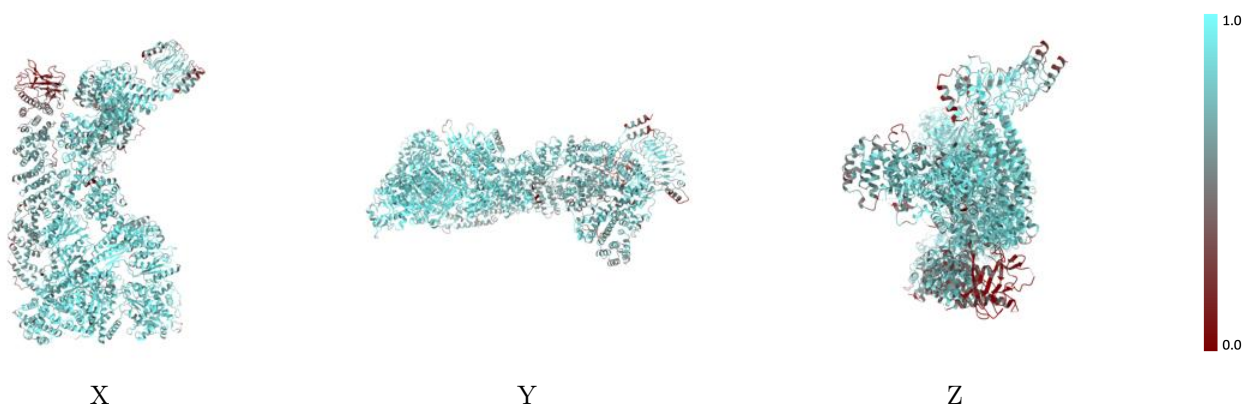
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



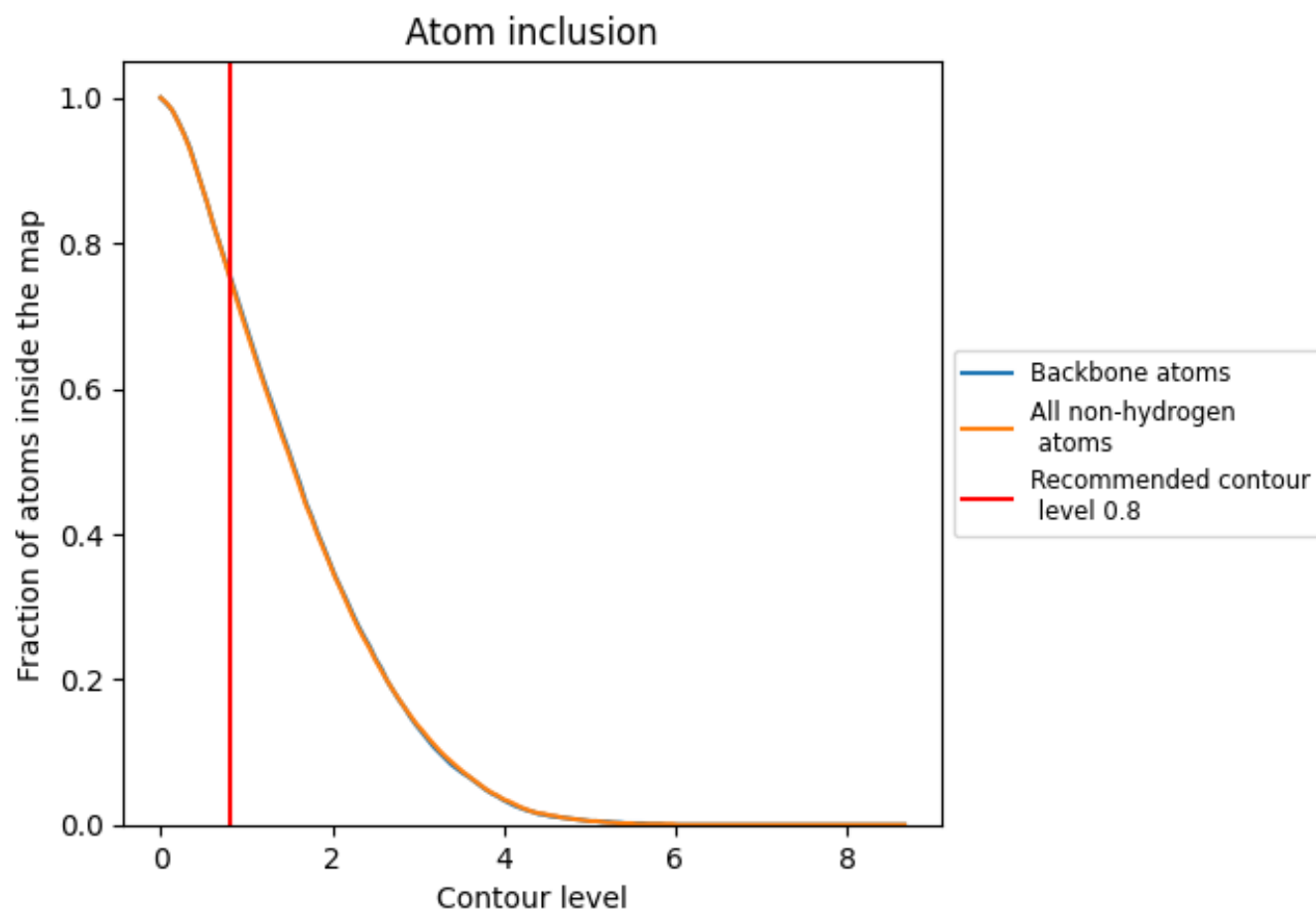
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7550	0.4850
A	0.7710	0.4940
B	0.6110	0.3240

