



## Full wwPDB EM Validation Report ⓘ

Oct 12, 2024 – 10:48 AM EDT

PDB ID : 6VEJ  
EMDB ID : EMD-21363  
Title : TriABC transporter from *Pseudomonas aeruginosa*  
Authors : Sygusch, J.; Fabre, L.; Rouiller, I.; Bhattacharyya, S.  
Deposited on : 2020-01-02  
Resolution : 4.50 Å (reported)  
Based on initial models : 3LNN, 2V4D, 3NE5

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

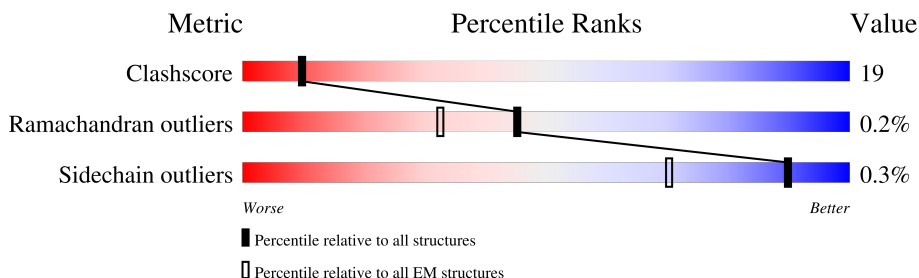
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.50 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1022	<div> <div>40%</div> <div>59%</div> <div>41%</div> </div>
1	B	1022	<div> <div>38%</div> <div>59%</div> <div>41%</div> </div>
1	C	1022	<div> <div>39%</div> <div>59%</div> <div>41%</div> </div>
2	P	695	<div> <div>27%</div> <div>20%</div> <div>11%</div> <div>69%</div> </div>
2	Q	695	<div> <div>27%</div> <div>19%</div> <div>12%</div> <div>69%</div> </div>
2	R	695	<div> <div>27%</div> <div>20%</div> <div>11%</div> <div>69%</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 28983 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 Probable Resistance-Nodulation-Cell Division (RND) efflux transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1022	Total	C	N	O	S	0	0
			7955	5116	1356	1454	29		
1	B	1022	Total	C	N	O	S	0	0
			7955	5116	1356	1454	29		
1	C	1022	Total	C	N	O	S	0	0
			7955	5116	1356	1454	29		

- Molecule 2 is a protein called Probable Resistance-Nodulation-Cell Division (RND) efflux membrane fusion protein, Probable Resistance-Nodulation-Cell Division (RND) efflux membrane fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	217	Total	C	N	O	S	0	0
			1612	1001	298	311	2		
2	Q	217	Total	C	N	O	S	0	0
			1612	1001	298	311	2		
2	R	217	Total	C	N	O	S	0	0
			1612	1001	298	311	2		

There are 15 discrepancies between the modelled and reference sequences:

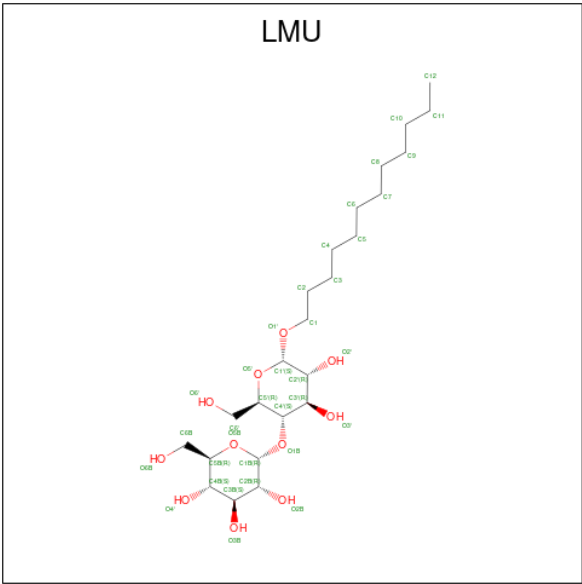
Chain	Residue	Modelled	Actual	Comment	Reference
P	354	GLY	-	linker	UNP Q9I6X6
P	355	ASN	-	linker	UNP Q9I6X6
P	356	SER	-	linker	UNP Q9I6X6
P	357	ARG	-	linker	UNP Q9I6X6
P	358	GLY	-	linker	UNP Q9I6X6
Q	354	GLY	-	linker	UNP Q9I6X6
Q	355	ASN	-	linker	UNP Q9I6X6
Q	356	SER	-	linker	UNP Q9I6X6
Q	357	ARG	-	linker	UNP Q9I6X6
Q	358	GLY	-	linker	UNP Q9I6X6

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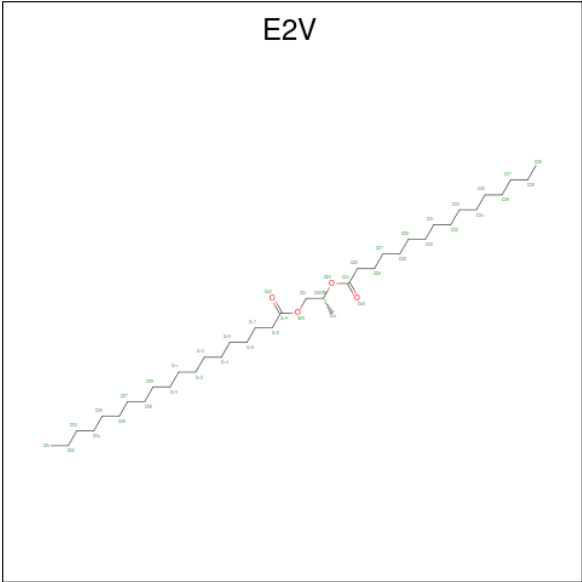
Chain	Residue	Modelled	Actual	Comment	Reference
R	354	GLY	-	linker	UNP Q9I6X6
R	355	ASN	-	linker	UNP Q9I6X6
R	356	SER	-	linker	UNP Q9I6X6
R	357	ARG	-	linker	UNP Q9I6X6
R	358	GLY	-	linker	UNP Q9I6X6

- Molecule 3 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



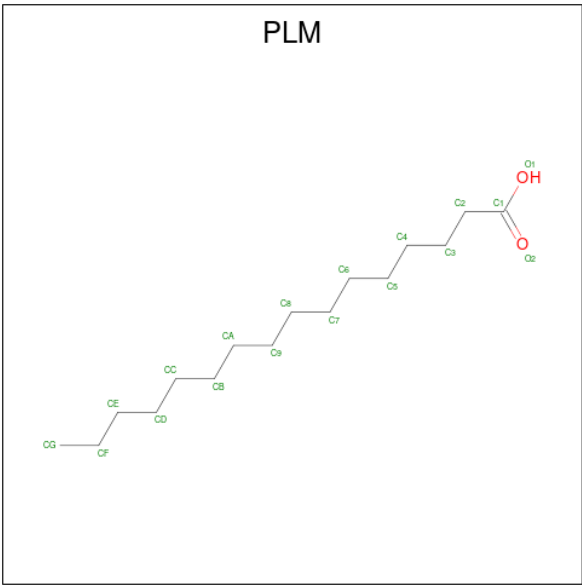
Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			35	24	11	
3	B	1	Total	C	O	0
			35	24	11	
3	C	1	Total	C	O	0
			35	24	11	

- Molecule 4 is (2R)-2-(hexadecanoyloxy)propyl nonadecanoate (three-letter code: E2V) (formula: C<sub>38</sub>H<sub>74</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			AltConf
4	P	1	Total	C	O	0
			42	38	4	
4	Q	1	Total	C	O	0
			42	38	4	
4	R	1	Total	C	O	0
			42	38	4	

- Molecule 5 is PALMITIC ACID (three-letter code: PLM) (formula: C<sub>16</sub>H<sub>32</sub>O<sub>2</sub>).



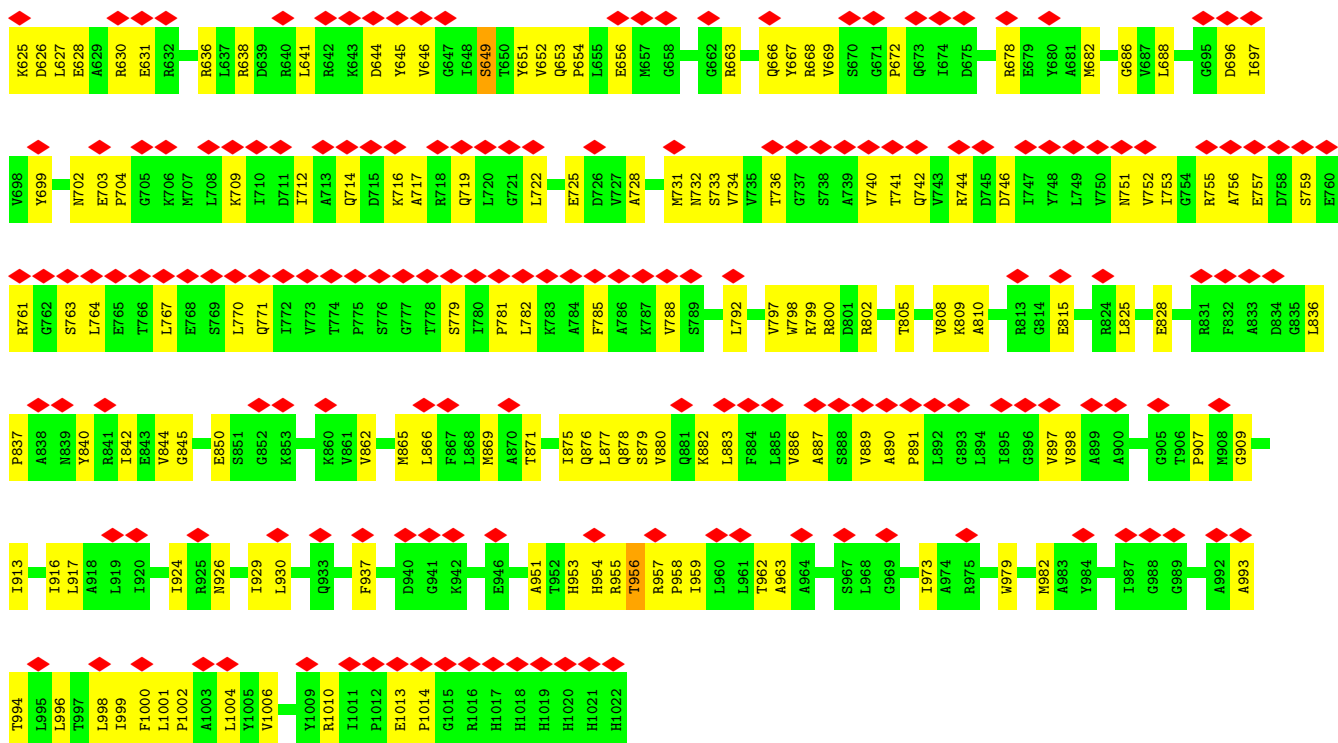
Mol	Chain	Residues	Atoms			AltConf
5	P	1	Total	C	O	0
			17	16	1	

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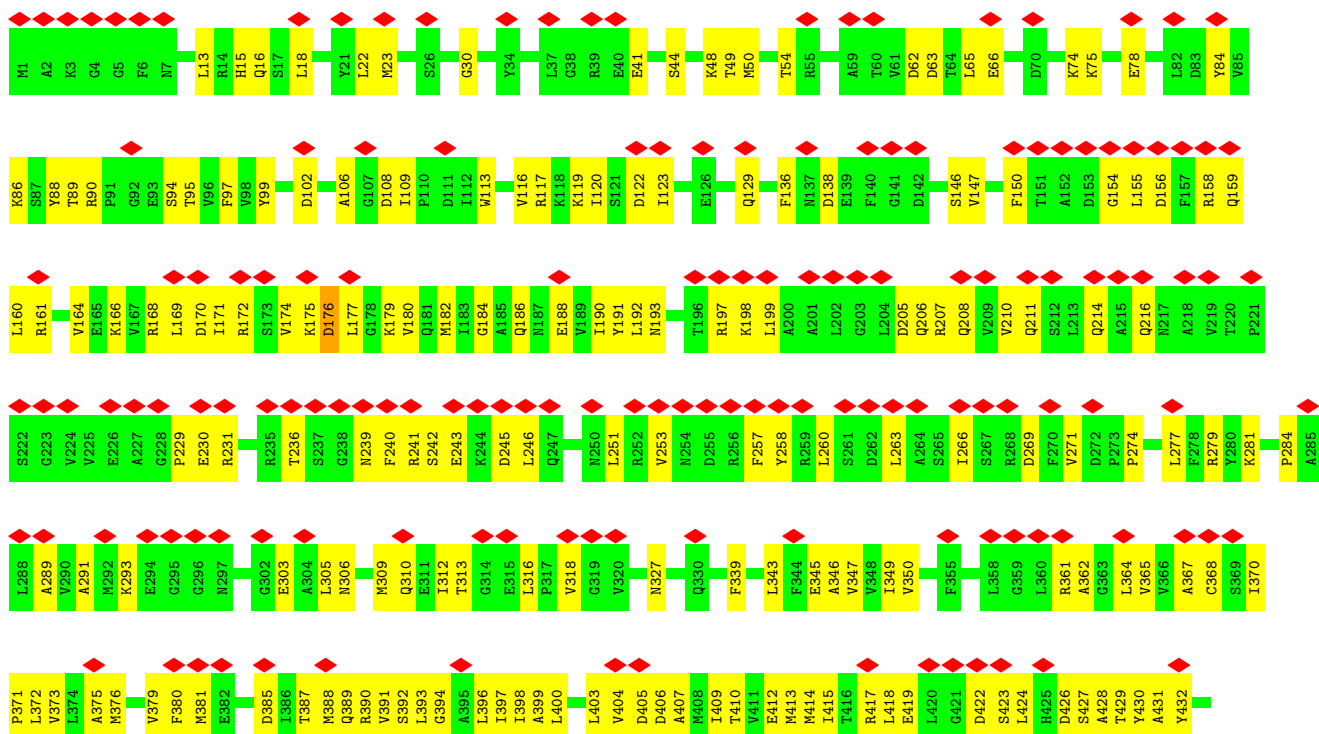
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Mol	Chain	Residues	Atoms			AltConf
5	Q	1	Total	C	O	0
			17	16	1	
5	R	1	Total	C	O	0
			17	16	1	

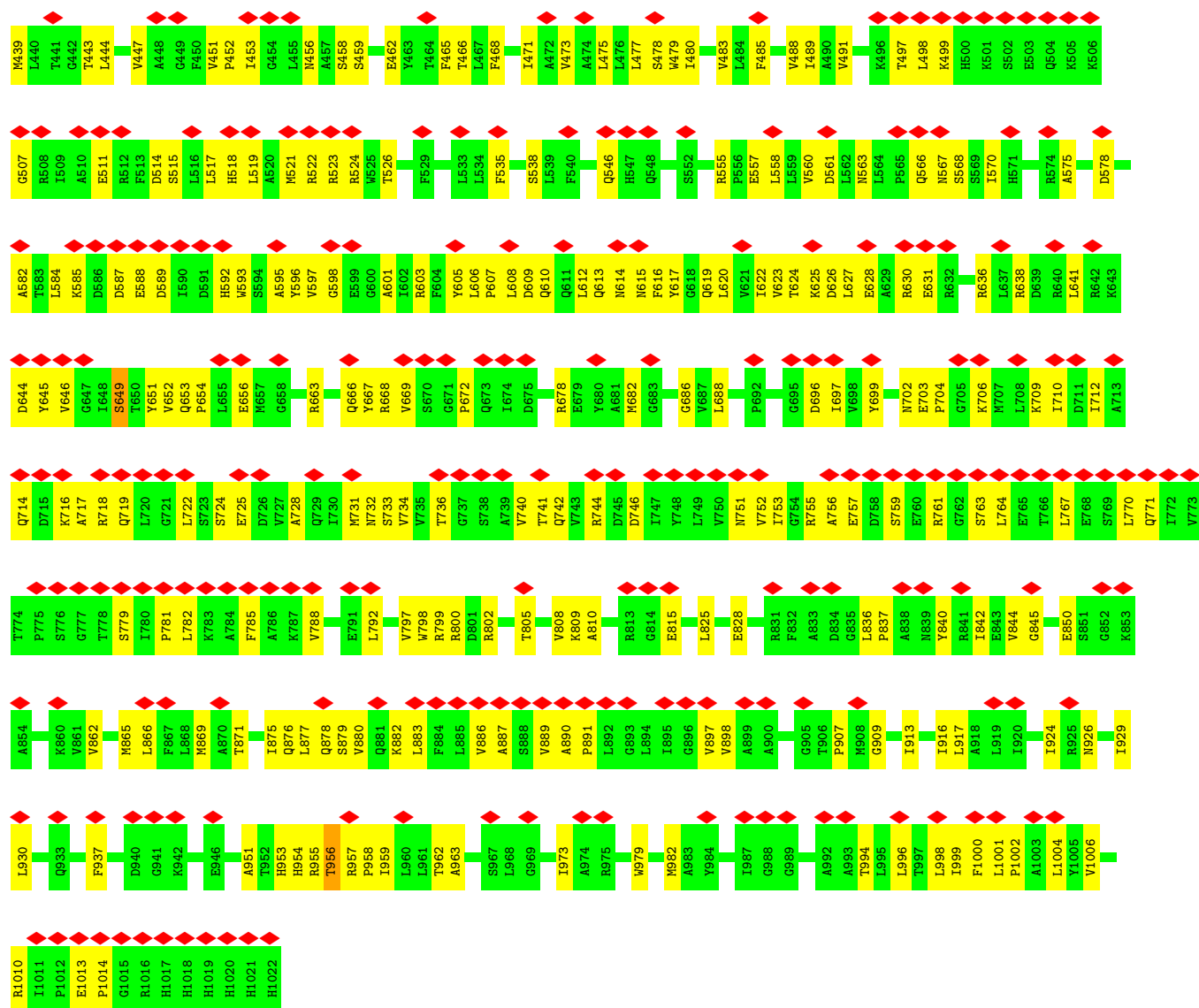




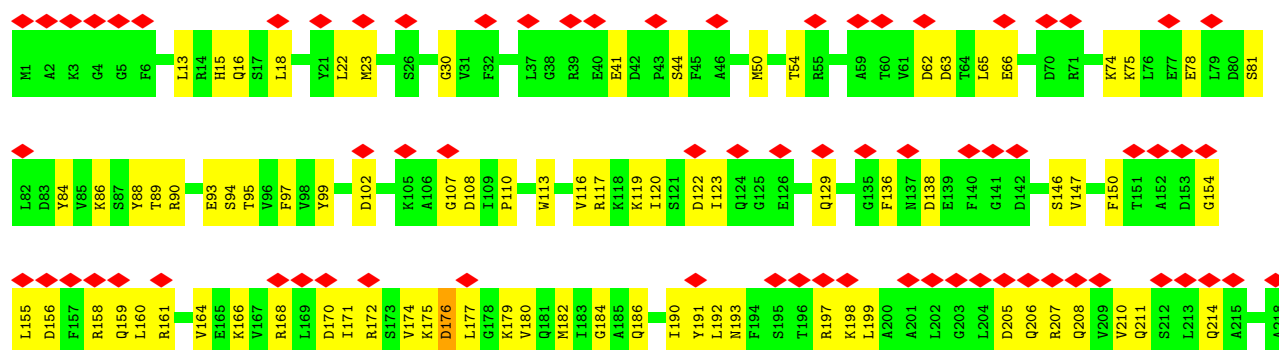
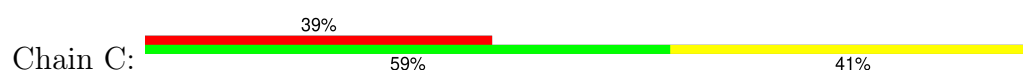
• Molecule 1: Probable Resistance-Nodulation-Cell Division (RND) efflux transporter

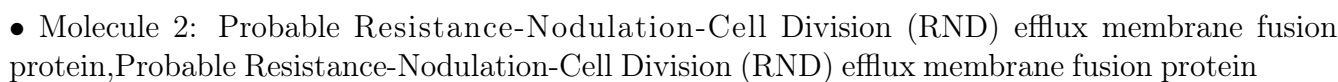


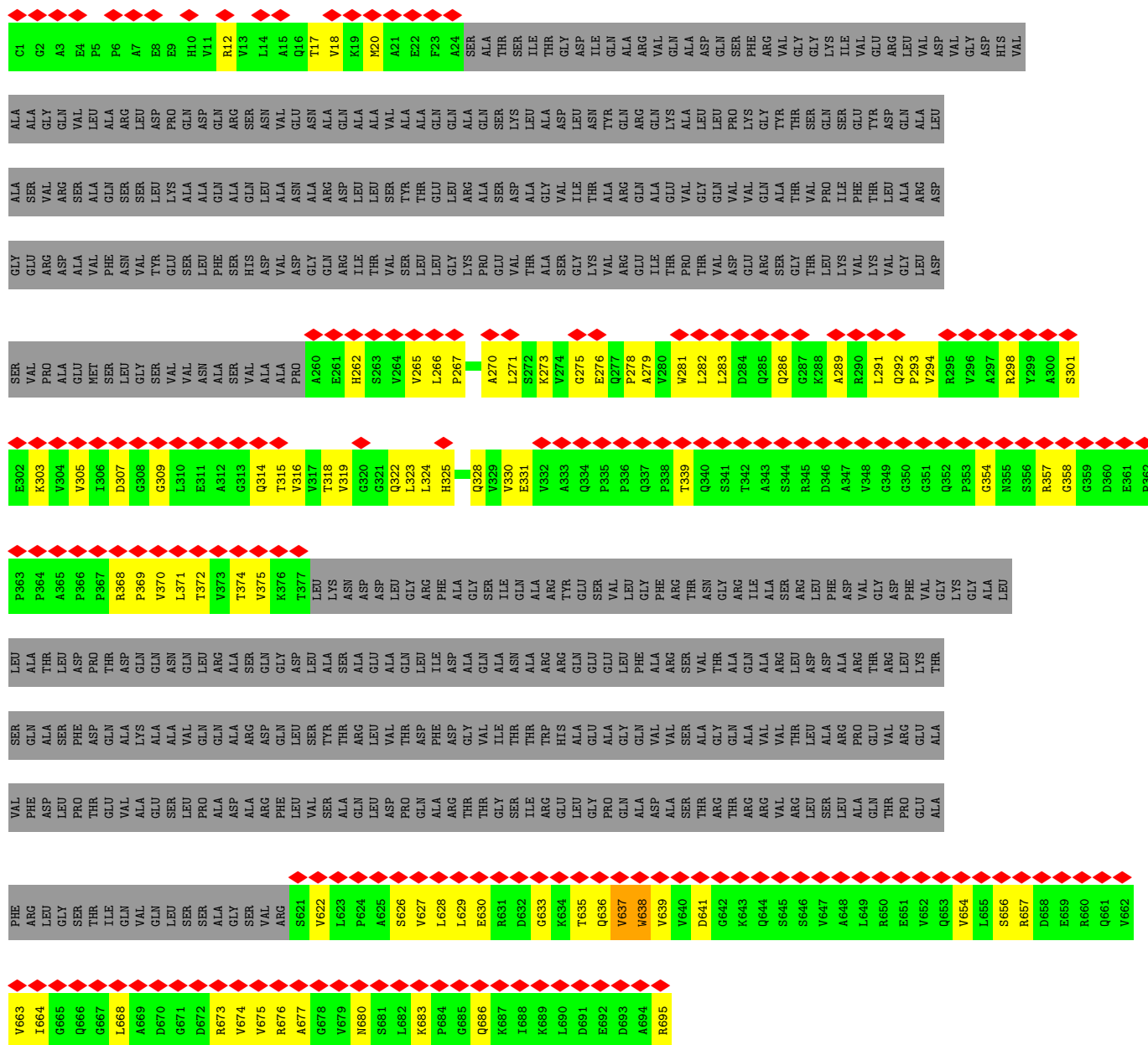




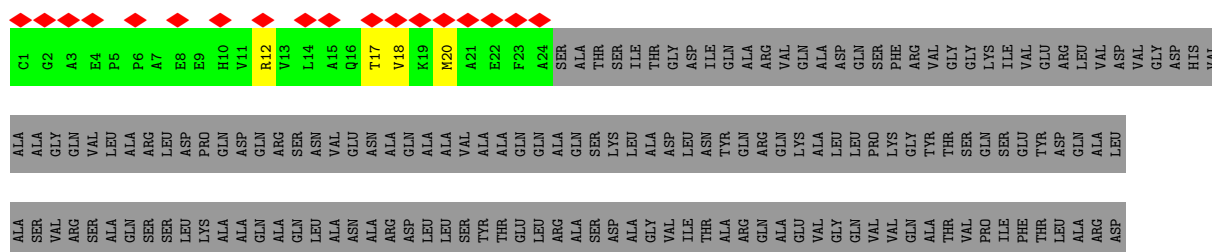
● Molecule 1: Probable Resistance-Nodulation-Cell Division (RND) efflux transporter

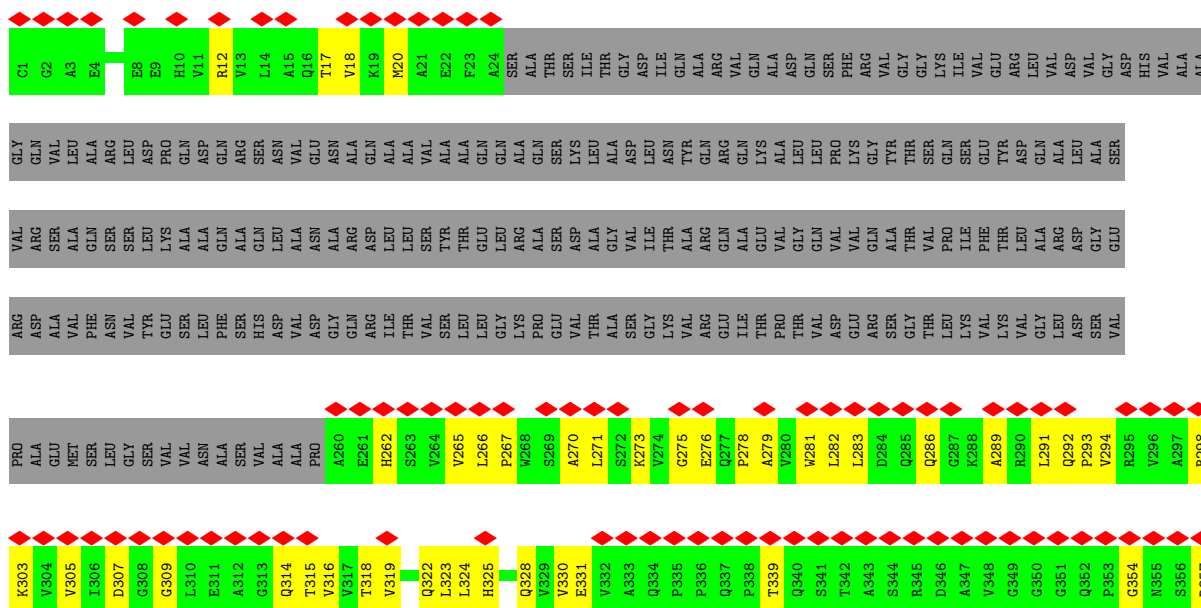






- Molecule 2: Probable Resistance-Nodulation-Cell Division (RND) efflux membrane fusion protein, Probable Resistance-Nodulation-Cell Division (RND) efflux membrane fusion protein





G665	G666	G667	L668	A669	D670	G671	D672	R673	G674	V675	R676	A677	G678	V679	N680	S681	L682	K683	P684	G685	Q686	K687	I688	K689	L690	D691	E692	D693	A694	R695																													
LEU	GLY	SER	THR	ILE	GLN	VAL	GLN	SER	SER	ALA	GLY	SER	VAL	ARG	ARG	S621	V622	L623	P624	A625	S626	V627	L628	L629	E630	R631	D632	G633	K634	T635	Q636	V637	W638	V639	V640	D641	G642	K643	Q644	S645	S646	V647	A648	L649	R650	E651	V652	Q653	V654	L655	S656	R657	D658	E659	R660	Q661	V662	V663	V664
THR	LEU	ASP	PRO	THR	GLU	VAL	ALA	GLN	PRO	ALA	ASP	ALA	ARG	PHE	LEU	VAL	SER	THR	THR	ARG	GLN	ALA	THR	THR	GLY	ILE	VAL	ASP	GLY	ALA	GLU	PRO	ALA	ALA	ASP	THR	SER	SER	ALA	GLY	GLN	ALA	VAL	ARG	THR	GLN	PRO	VAL	ARG	LEU	THR	LYS	THR	GLY	SER	GLN	LEU	ALA	

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35220	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.598	Depositor
Minimum map value	-0.271	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.158	Depositor
Map size (Å)	217.434, 217.434, 217.434	wwPDB
Map dimensions	140, 140, 140	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.5531, 1.5531, 1.5531	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMU, E2V, PLM

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	0.30	0/8115	0.49	0/11022
1	B	0.30	0/8115	0.49	0/11022
1	C	0.30	0/8115	0.49	0/11022
2	P	0.28	0/1638	0.53	0/2228
2	Q	0.28	0/1638	0.53	0/2228
2	R	0.28	0/1638	0.53	0/2228
All	All	0.30	0/29259	0.50	0/39750

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	7955	0	8136	316	0
1	B	7955	0	8136	319	0
1	C	7955	0	8136	324	0
2	P	1612	0	1638	74	0
2	Q	1612	0	1638	76	0
2	R	1612	0	1638	73	0
3	A	35	0	46	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	35	0	46	1	0
3	C	35	0	46	1	0
4	P	42	0	0	0	0
4	Q	42	0	0	0	0
4	R	42	0	0	0	0
5	P	17	0	31	0	0
5	Q	17	0	31	0	0
5	R	17	0	31	0	0
All	All	28983	0	29553	1127	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 19.

All (1127) 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:C:889:VAL:HG13	1:C:996:LEU:HD11	1.66	0.78
1:B:889:VAL:HG13	1:B:996:LEU:HD11	1.66	0.78
1:A:889:VAL:HG13	1:A:996:LEU:HD11	1.66	0.76
1:B:179:LYS:HG3	1:C:78:GLU:HG3	1.69	0.75
1:C:174:VAL:HB	1:C:177:LEU:HD11	1.74	0.70
1:A:930:LEU:HD13	1:A:1001:LEU:HD21	1.75	0.69
1:B:930:LEU:HD13	1:B:1001:LEU:HD21	1.75	0.69
1:C:930:LEU:HD13	1:C:1001:LEU:HD21	1.75	0.69
1:A:174:VAL:HB	1:A:177:LEU:HD11	1.74	0.69
1:B:174:VAL:HB	1:B:177:LEU:HD11	1.74	0.69
2:P:20:MET:HG3	2:P:262:HIS:HA	1.75	0.69
1:C:179:LYS:H	1:C:291:ALA:HB3	1.59	0.68
1:A:361:ARG:HA	1:A:364:LEU:HD13	1.76	0.68
1:B:179:LYS:H	1:B:291:ALA:HB3	1.59	0.68
2:R:20:MET:HG3	2:R:262:HIS:HA	1.75	0.68
2:Q:20:MET:HG3	2:Q:262:HIS:HA	1.75	0.67
2:Q:628:LEU:HA	2:Q:637:VAL:HG11	1.76	0.67
1:B:293:LYS:NZ	1:C:81:SER:H	1.92	0.67
1:C:361:ARG:HA	1:C:364:LEU:HD13	1.76	0.67
2:P:628:LEU:HA	2:P:637:VAL:HG11	1.76	0.67
1:A:179:LYS:H	1:A:291:ALA:HB3	1.59	0.67
1:A:569:SER:N	1:C:229:PRO:O	2.27	0.67
2:Q:273:LYS:NZ	2:Q:275:GLY:O	2.28	0.67
2:R:273:LYS:NZ	2:R:275:GLY:O	2.28	0.67
1:B:361:ARG:HA	1:B:364:LEU:HD13	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:273:LYS:NZ	2:P:275:GLY:O	2.28	0.67
1:B:184:GLY:O	1:B:186:GLN:NE2	2.28	0.66
1:A:184:GLY:O	1:A:186:GLN:NE2	2.28	0.66
1:C:184:GLY:O	1:C:186:GLN:NE2	2.28	0.66
1:C:456:ASN:ND2	1:C:458:SER:OG	2.29	0.66
1:A:236:THR:HA	1:B:710:ILE:O	1.96	0.66
2:R:628:LEU:HA	2:R:637:VAL:HG11	1.76	0.66
1:B:456:ASN:ND2	1:B:458:SER:OG	2.29	0.66
1:C:84:TYR:HB2	1:C:99:TYR:HB2	1.77	0.66
2:R:654:VAL:HG12	2:R:656:SER:H	1.61	0.65
1:B:84:TYR:HB2	1:B:99:TYR:HB2	1.77	0.65
1:B:277:LEU:HB2	1:B:597:VAL:HB	1.79	0.65
1:A:686:GLY:HA2	2:P:324:LEU:HD21	1.79	0.65
1:A:277:LEU:HB2	1:A:597:VAL:HB	1.79	0.65
2:Q:654:VAL:HG12	2:Q:656:SER:H	1.61	0.65
2:P:654:VAL:HG12	2:P:656:SER:H	1.61	0.65
1:A:84:TYR:HB2	1:A:99:TYR:HB2	1.77	0.65
1:A:456:ASN:ND2	1:A:458:SER:OG	2.29	0.64
1:B:65:LEU:HD13	1:B:799:ARG:HD2	1.80	0.64
1:C:277:LEU:HB2	1:C:597:VAL:HB	1.79	0.64
1:A:65:LEU:HD13	1:A:799:ARG:HD2	1.79	0.64
1:C:570:ILE:HD13	1:C:614:ASN:HB2	1.80	0.64
1:C:65:LEU:HD13	1:C:799:ARG:HD2	1.80	0.64
1:B:570:ILE:HD13	1:B:614:ASN:HB2	1.80	0.64
1:A:624:THR:HG21	1:A:628:GLU:HA	1.80	0.64
1:A:23:MET:HB2	1:A:485:PHE:HE1	1.63	0.64
1:A:570:ILE:HD13	1:A:614:ASN:HB2	1.80	0.64
2:P:627:VAL:HA	2:P:676:ARG:HA	1.80	0.64
1:B:429:THR:HA	1:B:432:TYR:CD2	2.33	0.64
1:B:686:GLY:HA2	2:Q:324:LEU:HD21	1.80	0.64
2:Q:627:VAL:HA	2:Q:676:ARG:HA	1.80	0.64
1:A:429:THR:HA	1:A:432:TYR:CD2	2.33	0.63
1:B:23:MET:HB2	1:B:485:PHE:HE1	1.63	0.63
1:B:624:THR:HG21	1:B:628:GLU:HA	1.80	0.63
1:B:771:GLN:HA	1:B:781:PRO:HA	1.80	0.63
1:C:686:GLY:HA2	2:R:324:LEU:HD21	1.80	0.63
1:A:568:SER:HA	1:C:230:GLU:HA	1.79	0.63
1:C:23:MET:HB2	1:C:485:PHE:HE1	1.63	0.63
1:C:624:THR:HG21	1:C:628:GLU:HA	1.80	0.63
2:R:18:VAL:HB	2:R:314:GLN:H	1.64	0.63
2:Q:18:VAL:HB	2:Q:314:GLN:H	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LYS:NZ	1:A:170:ASP:OD2	2.32	0.63
1:A:865:MET:SD	1:A:865:MET:N	2.72	0.63
1:C:86:LYS:HB2	1:C:97:PHE:HB2	1.80	0.63
1:C:771:GLN:HA	1:C:781:PRO:HA	1.80	0.63
1:C:865:MET:SD	1:C:865:MET:N	2.72	0.63
1:A:86:LYS:HB2	1:A:97:PHE:HB2	1.80	0.62
1:C:429:THR:HA	1:C:432:TYR:CD2	2.34	0.62
1:C:653:GLN:NE2	1:C:654:PRO:O	2.32	0.62
1:A:560:VAL:HG23	1:A:620:LEU:HB2	1.82	0.62
1:A:771:GLN:HA	1:A:781:PRO:HA	1.80	0.62
1:B:653:GLN:NE2	1:B:654:PRO:O	2.32	0.62
1:C:587:ASP:OD1	1:C:588:GLU:N	2.32	0.62
1:C:890:ALA:HB2	1:C:924:ILE:HD11	1.81	0.62
1:C:560:VAL:HG23	1:C:620:LEU:HB2	1.82	0.62
1:A:589:ASP:HA	1:A:625:LYS:HG3	1.82	0.62
1:B:560:VAL:HG23	1:B:620:LEU:HB2	1.81	0.62
1:B:587:ASP:OD1	1:B:588:GLU:N	2.32	0.62
1:B:712:ILE:O	1:B:714:GLN:NE2	2.33	0.62
1:C:589:ASP:HA	1:C:625:LYS:HG3	1.82	0.62
2:P:270:ALA:HB2	2:P:318:THR:HA	1.82	0.62
1:A:646:VAL:HG23	2:P:319:VAL:HG11	1.81	0.62
2:R:627:VAL:HA	2:R:676:ARG:HA	1.80	0.62
1:A:712:ILE:O	1:A:714:GLN:NE2	2.33	0.62
1:B:644:ASP:OD1	1:B:645:TYR:N	2.28	0.62
1:C:646:VAL:HG23	2:R:319:VAL:HG11	1.80	0.62
2:P:18:VAL:HB	2:P:314:GLN:H	1.64	0.62
1:C:712:ILE:O	1:C:714:GLN:NE2	2.33	0.62
2:Q:270:ALA:HB2	2:Q:318:THR:HA	1.82	0.62
1:B:86:LYS:HB2	1:B:97:PHE:HB2	1.80	0.61
1:B:890:ALA:HB2	1:B:924:ILE:HD11	1.81	0.61
1:C:166:LYS:NZ	1:C:170:ASP:OD2	2.32	0.61
1:A:587:ASP:OD1	1:A:588:GLU:N	2.32	0.61
1:A:890:ALA:HB2	1:A:924:ILE:HD11	1.81	0.61
1:B:865:MET:SD	1:B:865:MET:N	2.72	0.61
2:R:270:ALA:HB2	2:R:318:THR:HA	1.82	0.61
1:A:403:LEU:HB2	1:A:478:SER:HB2	1.82	0.61
1:B:208:GLN:OE1	1:B:208:GLN:N	2.31	0.61
1:B:589:ASP:HA	1:B:625:LYS:HG3	1.82	0.61
2:Q:674:VAL:HG22	2:Q:675:VAL:H	1.66	0.61
1:B:646:VAL:HG23	2:Q:319:VAL:HG11	1.80	0.61
2:R:674:VAL:HG22	2:R:675:VAL:H	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:ASP:OD1	1:A:645:TYR:N	2.28	0.61
1:B:166:LYS:NZ	1:B:170:ASP:OD2	2.32	0.61
1:B:293:LYS:HZ1	1:C:81:SER:H	1.47	0.60
1:B:403:LEU:HB2	1:B:478:SER:HB2	1.82	0.60
1:C:403:LEU:HB2	1:C:478:SER:HB2	1.82	0.60
1:A:916:ILE:HG13	1:A:917:LEU:HD12	1.84	0.60
2:P:674:VAL:HG22	2:P:675:VAL:H	1.66	0.60
1:B:158:ARG:NH2	1:B:746:ASP:OD2	2.34	0.60
1:B:879:SER:HB3	1:B:882:LYS:HE2	1.83	0.60
1:C:158:ARG:NH2	1:C:746:ASP:OD2	2.34	0.60
1:C:669:VAL:HG12	1:C:842:ILE:HG22	1.84	0.60
1:B:916:ILE:HG13	1:B:917:LEU:HD12	1.84	0.60
2:R:322:GLN:OE1	2:R:322:GLN:N	2.35	0.60
1:A:653:GLN:NE2	1:A:654:PRO:O	2.31	0.59
2:Q:265:VAL:HG12	2:Q:305:VAL:HG22	1.84	0.59
1:A:158:ARG:NH2	1:A:746:ASP:OD2	2.34	0.59
2:P:265:VAL:HG12	2:P:305:VAL:HG22	1.84	0.59
2:Q:322:GLN:N	2:Q:322:GLN:OE1	2.35	0.59
1:A:669:VAL:HG12	1:A:842:ILE:HG22	1.84	0.59
1:A:514:ASP:OD1	1:A:518:HIS:NE2	2.36	0.59
1:B:362:ALA:O	1:B:365:VAL:HG22	2.02	0.59
1:B:669:VAL:HG12	1:B:842:ILE:HG22	1.84	0.59
2:R:683:LYS:HG3	2:R:686:GLN:HB2	1.85	0.59
1:A:362:ALA:O	1:A:365:VAL:HG22	2.02	0.59
1:C:916:ILE:HG13	1:C:917:LEU:HD12	1.84	0.59
1:C:1001:LEU:HG	1:C:1002:PRO:HD3	1.85	0.59
2:Q:283:LEU:HD22	2:Q:330:VAL:HG11	1.85	0.59
1:C:514:ASP:OD1	1:C:518:HIS:NE2	2.36	0.59
2:P:322:GLN:N	2:P:322:GLN:OE1	2.35	0.59
2:P:683:LYS:HG3	2:P:686:GLN:HB2	1.85	0.59
1:A:879:SER:HB3	1:A:882:LYS:HE2	1.83	0.59
1:C:208:GLN:N	1:C:208:GLN:OE1	2.31	0.59
2:R:637:VAL:CG1	2:R:674:VAL:HG11	2.33	0.59
1:C:362:ALA:O	1:C:365:VAL:HG22	2.02	0.59
2:R:265:VAL:HG12	2:R:305:VAL:HG22	1.84	0.59
1:A:30:GLY:HA3	1:A:375:ALA:HB1	1.85	0.58
2:P:637:VAL:CG1	2:P:674:VAL:HG11	2.33	0.58
1:B:514:ASP:OD1	1:B:518:HIS:NE2	2.36	0.58
1:B:30:GLY:HA3	1:B:375:ALA:HB1	1.85	0.58
1:B:566:GLN:NE2	1:B:704:PRO:O	2.36	0.58
1:C:879:SER:HB3	1:C:882:LYS:HE2	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:683:LYS:HG3	2:Q:686:GLN:HB2	1.85	0.58
1:B:672:PRO:HD2	1:B:840:TYR:CE1	2.39	0.58
1:B:1001:LEU:HG	1:B:1002:PRO:HD3	1.84	0.58
1:A:406:ASP:O	1:A:409:ILE:HG13	2.04	0.58
1:C:672:PRO:HD2	1:C:840:TYR:CE1	2.39	0.58
2:Q:637:VAL:CG1	2:Q:674:VAL:HG11	2.33	0.58
1:A:208:GLN:N	1:A:208:GLN:OE1	2.31	0.58
1:A:606:LEU:HB2	1:A:607:PRO:HD3	1.86	0.58
1:B:757:GLU:HG3	1:B:759:SER:H	1.69	0.58
1:C:644:ASP:OD1	1:C:645:TYR:N	2.28	0.58
2:P:283:LEU:HD22	2:P:330:VAL:HG11	1.85	0.57
1:A:682:MET:HB3	2:P:325:HIS:HB3	1.86	0.57
2:Q:628:LEU:HD13	2:Q:637:VAL:HG22	1.86	0.57
1:B:90:ARG:NH2	1:B:612:LEU:O	2.38	0.57
2:R:283:LEU:HD22	2:R:330:VAL:HG11	1.85	0.57
1:A:672:PRO:HD2	1:A:840:TYR:CE1	2.39	0.57
1:A:757:GLU:HG3	1:A:759:SER:H	1.69	0.57
1:C:566:GLN:NE2	1:C:704:PRO:O	2.36	0.57
1:A:566:GLN:NE2	1:A:704:PRO:O	2.36	0.57
1:B:406:ASP:O	1:B:409:ILE:HG13	2.04	0.57
1:B:606:LEU:HB2	1:B:607:PRO:HD3	1.86	0.57
1:A:90:ARG:NH2	1:A:612:LEU:O	2.38	0.57
1:A:699:TYR:HA	1:A:808:VAL:HG12	1.87	0.57
1:A:1001:LEU:HG	1:A:1002:PRO:HD3	1.85	0.57
1:C:90:ARG:NH2	1:C:612:LEU:O	2.38	0.57
1:C:757:GLU:HG3	1:C:759:SER:H	1.69	0.57
2:P:628:LEU:HD13	2:P:637:VAL:HG22	1.86	0.57
2:Q:12:ARG:HA	2:Q:331:GLU:HB3	1.86	0.57
1:A:631:GLU:HB3	1:A:636:ARG:HH12	1.70	0.57
1:C:30:GLY:HA3	1:C:375:ALA:HB1	1.85	0.57
2:R:628:LEU:HD13	2:R:637:VAL:HG22	1.86	0.57
1:C:699:TYR:HA	1:C:808:VAL:HG12	1.87	0.57
1:B:608:LEU:HD23	1:B:609:ASP:H	1.70	0.57
1:C:606:LEU:HB2	1:C:607:PRO:HD3	1.86	0.57
2:P:12:ARG:HA	2:P:331:GLU:HB3	1.87	0.56
1:C:406:ASP:O	1:C:409:ILE:HG13	2.04	0.56
1:C:613:GLN:O	1:C:617:TYR:N	2.39	0.56
2:P:282:LEU:HG	2:P:316:VAL:HG12	1.87	0.56
1:A:339:PHE:HB3	1:A:393:LEU:HD13	1.88	0.56
2:Q:282:LEU:HG	2:Q:316:VAL:HG12	1.87	0.56
1:B:230:GLU:HA	1:C:568:SER:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:GLN:O	1:A:617:TYR:N	2.39	0.56
1:B:631:GLU:HB3	1:B:636:ARG:HH12	1.70	0.56
1:C:171:ILE:HG22	1:C:177:LEU:HD21	1.88	0.56
1:A:608:LEU:HD23	1:A:609:ASP:H	1.70	0.56
1:B:613:GLN:O	1:B:617:TYR:N	2.39	0.56
2:R:282:LEU:HG	2:R:316:VAL:HG12	1.87	0.56
1:C:279:ARG:HB3	1:C:595:ALA:HB3	1.88	0.56
1:C:419:GLU:O	1:C:497:THR:OG1	2.23	0.56
1:B:596:TYR:HB2	1:B:619:GLN:HB2	1.88	0.56
1:B:627:LEU:HB3	1:B:630:ARG:HB2	1.88	0.56
1:C:310:GLN:O	1:C:313:THR:OG1	2.21	0.56
1:C:627:LEU:HB3	1:C:630:ARG:HB2	1.88	0.56
2:R:17:THR:HA	2:R:315:THR:HA	1.88	0.56
1:A:279:ARG:HB3	1:A:595:ALA:HB3	1.88	0.55
1:A:596:TYR:HB2	1:A:619:GLN:HB2	1.88	0.55
1:B:716:LYS:HA	1:B:719:GLN:HB3	1.89	0.55
1:C:742:GLN:HG2	1:C:751:ASN:HB3	1.88	0.55
2:R:12:ARG:HA	2:R:331:GLU:HB3	1.87	0.55
2:R:370:VAL:HG13	2:R:372:THR:H	1.71	0.55
1:A:410:THR:O	1:A:413:MET:HG3	2.06	0.55
1:A:716:LYS:HA	1:A:719:GLN:HB3	1.89	0.55
1:B:419:GLU:O	1:B:497:THR:OG1	2.23	0.55
1:C:631:GLU:HB3	1:C:636:ARG:HH12	1.70	0.55
2:P:370:VAL:HG13	2:P:372:THR:H	1.71	0.55
2:R:664:ILE:HG13	2:R:668:LEU:HD23	1.89	0.55
1:A:313:THR:HA	1:A:316:LEU:HD23	1.88	0.55
1:B:410:THR:O	1:B:413:MET:HG3	2.06	0.55
1:B:682:MET:HB3	2:Q:325:HIS:HB3	1.87	0.55
1:C:567:ASN:HB3	1:C:616:PHE:CE2	2.42	0.55
1:C:850:GLU:OE1	1:C:850:GLU:N	2.34	0.55
1:A:419:GLU:O	1:A:497:THR:OG1	2.23	0.55
1:B:171:ILE:HG22	1:B:177:LEU:HD21	1.88	0.55
1:B:850:GLU:OE1	1:B:850:GLU:N	2.34	0.55
1:C:608:LEU:HD23	1:C:609:ASP:H	1.70	0.55
2:R:266:LEU:HG	2:R:318:THR:HG22	1.89	0.55
1:A:627:LEU:HB3	1:A:630:ARG:HB2	1.88	0.55
1:B:414:MET:HG2	1:B:432:TYR:HE1	1.72	0.55
1:A:937:PHE:HZ	1:A:951:ALA:HB2	1.71	0.55
1:B:339:PHE:HB3	1:B:393:LEU:HD13	1.88	0.55
1:B:699:TYR:HA	1:B:808:VAL:HG12	1.87	0.55
1:C:339:PHE:HB3	1:C:393:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:370:VAL:HG13	2:Q:372:THR:H	1.71	0.55
1:A:567:ASN:HB3	1:A:616:PHE:CE2	2.42	0.55
1:C:410:THR:O	1:C:413:MET:HG3	2.06	0.55
1:C:596:TYR:HB2	1:C:619:GLN:HB2	1.88	0.55
1:A:414:MET:HG2	1:A:432:TYR:HE1	1.72	0.55
2:P:17:THR:HA	2:P:315:THR:HA	1.88	0.55
2:P:633:GLY:HA2	2:P:636:GLN:HE21	1.72	0.55
1:B:229:PRO:O	1:C:569:SER:N	2.32	0.55
1:C:682:MET:HB3	2:R:325:HIS:HB3	1.87	0.55
1:C:937:PHE:HZ	1:C:951:ALA:HB2	1.71	0.55
1:A:260:LEU:HB3	1:A:266:ILE:HD11	1.89	0.55
1:A:878:GLN:HG2	1:C:18:LEU:HD21	1.89	0.55
2:P:664:ILE:HG13	2:P:668:LEU:HD23	1.89	0.55
1:A:310:GLN:O	1:A:313:THR:OG1	2.21	0.54
1:B:260:LEU:HB3	1:B:266:ILE:HD11	1.90	0.54
1:B:742:GLN:HG2	1:B:751:ASN:HB3	1.88	0.54
1:C:716:LYS:HA	1:C:719:GLN:HB3	1.89	0.54
2:Q:633:GLY:HA2	2:Q:636:GLN:HE21	1.72	0.54
1:A:171:ILE:HG22	1:A:177:LEU:HD21	1.88	0.54
2:Q:664:ILE:HG13	2:Q:668:LEU:HD23	1.89	0.54
1:A:850:GLU:OE1	1:A:850:GLU:N	2.34	0.54
1:C:313:THR:HA	1:C:316:LEU:HD23	1.88	0.54
1:C:414:MET:HG2	1:C:432:TYR:HE1	1.72	0.54
2:Q:270:ALA:CB	2:Q:318:THR:HA	2.38	0.54
1:B:279:ARG:HB3	1:B:595:ALA:HB3	1.88	0.54
1:B:937:PHE:HZ	1:B:951:ALA:HB2	1.71	0.54
1:C:198:LYS:O	1:C:198:LYS:NZ	2.35	0.54
1:C:260:LEU:HB3	1:C:266:ILE:HD11	1.89	0.54
2:Q:17:THR:HA	2:Q:315:THR:HA	1.88	0.54
2:Q:266:LEU:HG	2:Q:318:THR:HG22	1.89	0.54
2:R:270:ALA:CB	2:R:318:THR:HA	2.38	0.54
1:A:742:GLN:HG2	1:A:751:ASN:HB3	1.88	0.54
1:B:310:GLN:O	1:B:313:THR:OG1	2.21	0.54
1:B:313:THR:HA	1:B:316:LEU:HD23	1.88	0.54
2:P:266:LEU:HG	2:P:318:THR:HG22	1.89	0.54
2:R:664:ILE:HD11	2:R:668:LEU:HB3	1.90	0.54
1:B:444:LEU:O	1:B:447:VAL:HG12	2.08	0.54
1:C:199:LEU:HD21	1:C:206:GLN:N	2.23	0.54
2:P:270:ALA:CB	2:P:318:THR:HA	2.38	0.54
1:A:303:GLU:HA	1:A:306:ASN:HD21	1.73	0.54
1:B:205:ASP:HB3	1:B:208:GLN:HE22	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:485:PHE:O	1:C:489:ILE:HG12	2.08	0.54
2:R:633:GLY:HA2	2:R:636:GLN:HE21	1.72	0.54
1:A:444:LEU:O	1:A:447:VAL:HG12	2.08	0.53
1:B:485:PHE:O	1:B:489:ILE:HG12	2.09	0.53
1:B:567:ASN:HB3	1:B:616:PHE:CE2	2.42	0.53
1:C:108:ASP:OD1	1:C:108:ASP:N	2.41	0.53
1:C:452:PRO:HB3	1:C:862:VAL:HG12	1.90	0.53
2:Q:664:ILE:HD11	2:Q:668:LEU:HB3	1.90	0.53
2:P:639:VAL:HB	2:P:674:VAL:HG23	1.90	0.53
2:P:664:ILE:HD11	2:P:668:LEU:HB3	1.90	0.53
2:Q:633:GLY:HA2	2:Q:636:GLN:NE2	2.24	0.53
2:R:630:GLU:OE2	2:R:657:ARG:NH1	2.41	0.53
1:A:452:PRO:HB3	1:A:862:VAL:HG12	1.91	0.53
1:B:732:ASN:ND2	1:B:736:THR:O	2.42	0.53
2:P:630:GLU:OE2	2:P:657:ARG:NH1	2.41	0.53
2:R:633:GLY:HA2	2:R:636:GLN:NE2	2.24	0.53
1:B:303:GLU:HA	1:B:306:ASN:HD21	1.73	0.53
1:B:303:GLU:HA	1:B:306:ASN:ND2	2.24	0.53
2:Q:630:GLU:OE2	2:Q:657:ARG:NH1	2.41	0.53
1:B:568:SER:O	1:B:615:ASN:ND2	2.42	0.53
1:B:871:THR:O	1:B:875:ILE:HG13	2.09	0.53
1:C:318:VAL:HA	2:R:368:ARG:HD3	1.91	0.53
1:A:161:ARG:HE	1:A:182:MET:HE1	1.74	0.53
1:A:303:GLU:HA	1:A:306:ASN:ND2	2.24	0.53
1:A:485:PHE:O	1:A:489:ILE:HG12	2.09	0.53
1:C:75:LYS:HZ1	1:C:119:LYS:HD2	1.73	0.53
1:C:399:ALA:HB2	1:C:471:ILE:HD13	1.91	0.53
1:C:444:LEU:O	1:C:447:VAL:HG12	2.08	0.53
2:P:375:VAL:O	2:P:673:ARG:NH1	2.42	0.53
1:A:199:LEU:HD21	1:A:206:GLN:N	2.23	0.53
1:A:318:VAL:HA	2:P:368:ARG:HD3	1.90	0.53
1:A:732:ASN:ND2	1:A:736:THR:O	2.42	0.53
1:A:871:THR:O	1:A:875:ILE:HG13	2.09	0.53
1:B:742:GLN:HA	1:B:751:ASN:HA	1.91	0.53
2:Q:371:LEU:HD22	2:Q:676:ARG:N	2.24	0.53
1:A:443:THR:HB	1:A:475:LEU:HD21	1.90	0.53
1:B:169:LEU:HD21	1:C:802:ARG:CZ	2.40	0.53
1:C:303:GLU:HA	1:C:306:ASN:HD21	1.73	0.53
1:C:568:SER:O	1:C:615:ASN:ND2	2.42	0.53
1:C:880:VAL:HG23	1:C:883:LEU:HD23	1.91	0.53
2:P:633:GLY:HA2	2:P:636:GLN:NE2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:637:VAL:HG11	2:P:674:VAL:HG11	1.91	0.53
1:A:197:ARG:HH12	1:A:779:SER:HB3	1.74	0.52
1:A:568:SER:O	1:A:615:ASN:ND2	2.42	0.52
1:B:558:LEU:HB3	1:B:622:ILE:HD11	1.91	0.52
1:C:166:LYS:HD3	2:R:695:ARG:HD3	1.91	0.52
1:C:210:VAL:HG13	1:C:740:VAL:HG12	1.91	0.52
1:A:90:ARG:HH22	1:A:613:GLN:HA	1.75	0.52
1:B:23:MET:HB2	1:B:485:PHE:CE1	2.44	0.52
1:B:199:LEU:HD21	1:B:206:GLN:N	2.23	0.52
1:B:318:VAL:HA	2:Q:368:ARG:HD3	1.91	0.52
1:C:546:GLN:HG2	1:C:907:PRO:HA	1.91	0.52
2:Q:639:VAL:HB	2:Q:674:VAL:HG23	1.90	0.52
2:R:639:VAL:HB	2:R:674:VAL:HG23	1.90	0.52
1:A:880:VAL:HG23	1:A:883:LEU:HD23	1.91	0.52
1:B:90:ARG:HH22	1:B:613:GLN:HA	1.75	0.52
1:B:880:VAL:HG23	1:B:883:LEU:HD23	1.91	0.52
1:C:175:LYS:NZ	1:C:176:ASP:OD1	2.30	0.52
1:C:197:ARG:HH12	1:C:779:SER:HB3	1.74	0.52
2:R:307:ASP:OD1	2:R:307:ASP:N	2.42	0.52
1:C:443:THR:HB	1:C:475:LEU:HD21	1.90	0.52
1:C:732:ASN:ND2	1:C:736:THR:O	2.42	0.52
1:C:742:GLN:HA	1:C:751:ASN:HA	1.91	0.52
1:C:871:THR:O	1:C:875:ILE:HG13	2.09	0.52
2:P:307:ASP:N	2:P:307:ASP:OD1	2.42	0.52
2:R:371:LEU:HD22	2:R:676:ARG:N	2.24	0.52
1:A:518:HIS:O	1:A:522:ARG:HG2	2.10	0.52
1:A:558:LEU:HB3	1:A:622:ILE:HD11	1.91	0.52
1:B:210:VAL:HG13	1:B:740:VAL:HG12	1.91	0.52
1:C:205:ASP:HB3	1:C:208:GLN:HE22	1.73	0.52
2:Q:375:VAL:O	2:Q:673:ARG:NH1	2.42	0.52
2:R:375:VAL:O	2:R:673:ARG:NH1	2.42	0.52
1:A:399:ALA:HB2	1:A:471:ILE:HD13	1.91	0.52
1:A:717:ALA:O	1:A:722:LEU:N	2.42	0.52
1:B:102:ASP:OD2	1:B:459:SER:N	2.42	0.52
1:B:166:LYS:HD3	2:Q:695:ARG:HD3	1.91	0.52
1:B:546:GLN:HG2	1:B:907:PRO:HA	1.91	0.52
2:P:371:LEU:HD22	2:P:676:ARG:N	2.24	0.52
1:A:703:GLU:OE1	1:A:703:GLU:N	2.43	0.52
1:A:742:GLN:HA	1:A:751:ASN:HA	1.91	0.52
1:B:399:ALA:HB2	1:B:471:ILE:HD13	1.91	0.52
1:C:122:ASP:OD1	1:C:122:ASP:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:GLU:HA	1:C:306:ASN:ND2	2.24	0.52
1:A:75:LYS:HZ1	1:A:119:LYS:HD2	1.73	0.52
1:A:122:ASP:OD1	1:A:122:ASP:N	2.43	0.52
1:A:205:ASP:HB3	1:A:208:GLN:HE22	1.73	0.52
1:C:389:GLN:HE22	1:C:466:THR:HG21	1.75	0.52
1:C:558:LEU:HB3	1:C:622:ILE:HD11	1.91	0.52
1:C:703:GLU:OE1	1:C:703:GLU:N	2.43	0.52
2:Q:637:VAL:HG11	2:Q:674:VAL:HG11	1.91	0.52
1:B:389:GLN:HE22	1:B:466:THR:HG21	1.75	0.52
1:C:13:LEU:O	1:C:16:GLN:NE2	2.43	0.52
1:C:242:SER:H	1:C:245:ASP:HB2	1.75	0.52
1:C:518:HIS:O	1:C:522:ARG:HG2	2.10	0.52
2:Q:627:VAL:HG22	2:Q:676:ARG:HD3	1.92	0.52
1:A:712:ILE:HG22	1:A:714:GLN:H	1.75	0.51
1:A:878:GLN:H	1:A:882:LYS:NZ	2.09	0.51
1:B:452:PRO:HB3	1:B:862:VAL:HG12	1.91	0.51
1:B:518:HIS:O	1:B:522:ARG:HG2	2.10	0.51
1:B:563:ASN:HB2	1:B:649:SER:OG	2.10	0.51
1:B:926:ASN:HA	1:B:929:ILE:HD12	1.92	0.51
1:B:994:THR:O	1:B:998:LEU:HG	2.11	0.51
1:C:90:ARG:HH22	1:C:613:GLN:HA	1.75	0.51
2:P:289:ALA:HB3	2:P:328:GLN:HB3	1.93	0.51
1:A:23:MET:HB2	1:A:485:PHE:CE1	2.44	0.51
1:A:563:ASN:HB2	1:A:649:SER:OG	2.10	0.51
1:B:197:ARG:HH12	1:B:779:SER:HB3	1.74	0.51
2:Q:307:ASP:OD1	2:Q:307:ASP:N	2.42	0.51
1:A:242:SER:H	1:A:245:ASP:HB2	1.75	0.51
1:B:703:GLU:N	1:B:703:GLU:OE1	2.43	0.51
2:P:279:ALA:HA	2:P:294:VAL:HG22	1.92	0.51
2:Q:279:ALA:HA	2:Q:294:VAL:HG22	1.92	0.51
1:A:546:GLN:HG2	1:A:907:PRO:HA	1.91	0.51
1:B:368:CYS:O	1:B:371:PRO:HD2	2.11	0.51
1:B:443:THR:HB	1:B:475:LEU:HD21	1.90	0.51
2:P:622:VAL:HG12	2:P:663:VAL:HB	1.93	0.51
2:Q:289:ALA:HB3	2:Q:328:GLN:HB3	1.93	0.51
2:Q:622:VAL:HG12	2:Q:663:VAL:HB	1.93	0.51
2:R:637:VAL:HG11	2:R:674:VAL:HG11	1.91	0.51
1:A:368:CYS:O	1:A:371:PRO:HD2	2.11	0.51
1:B:242:SER:H	1:B:245:ASP:HB2	1.75	0.51
1:C:88:TYR:HB3	1:C:95:THR:HB	1.92	0.51
1:C:704:PRO:HB2	1:C:792:LEU:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:289:ALA:HB3	2:R:328:GLN:HB3	1.93	0.51
1:A:50:MET:HB2	1:A:113:TRP:CZ3	2.46	0.51
1:A:645:TYR:HA	2:P:339:THR:HG21	1.93	0.51
1:A:954:HIS:O	1:A:955:ARG:NH2	2.44	0.51
1:A:994:THR:O	1:A:998:LEU:HG	2.11	0.51
1:B:50:MET:HB2	1:B:113:TRP:CZ3	2.46	0.51
1:B:161:ARG:HE	1:B:182:MET:HE1	1.75	0.51
1:C:155:LEU:HB2	1:C:159:GLN:NE2	2.26	0.51
1:C:712:ILE:HG22	1:C:714:GLN:H	1.75	0.51
1:A:704:PRO:HB2	1:A:792:LEU:HB3	1.92	0.51
1:B:704:PRO:HB2	1:B:792:LEU:HB3	1.92	0.51
1:A:147:VAL:HG12	1:A:289:ALA:HA	1.93	0.51
1:A:155:LEU:HB2	1:A:159:GLN:NE2	2.26	0.51
1:A:175:LYS:NZ	1:A:176:ASP:OD1	2.30	0.51
1:C:563:ASN:HB2	1:C:649:SER:OG	2.11	0.51
1:C:628:GLU:OE1	1:C:628:GLU:N	2.41	0.51
2:P:630:GLU:HA	2:P:635:THR:O	2.11	0.51
2:R:627:VAL:HG22	2:R:676:ARG:HD3	1.92	0.51
1:B:13:LEU:O	1:B:16:GLN:NE2	2.43	0.51
1:B:88:TYR:HB3	1:B:95:THR:HB	1.92	0.51
2:P:271:LEU:HD11	2:P:278:PRO:HB2	1.93	0.51
2:Q:630:GLU:HA	2:Q:635:THR:O	2.11	0.51
1:A:166:LYS:HD3	2:P:695:ARG:HD3	1.93	0.51
1:A:190:ILE:HB	1:A:752:VAL:HG22	1.93	0.51
1:A:210:VAL:HG13	1:A:740:VAL:HG12	1.91	0.51
1:A:598:GLY:HA2	1:A:614:ASN:HA	1.93	0.51
1:A:926:ASN:HA	1:A:929:ILE:HD12	1.92	0.51
1:B:155:LEU:HB2	1:B:159:GLN:NE2	2.26	0.51
1:B:712:ILE:HG22	1:B:714:GLN:H	1.75	0.51
1:A:13:LEU:O	1:A:16:GLN:NE2	2.43	0.50
1:B:453:ILE:HD11	1:B:468:PHE:HB2	1.94	0.50
2:R:630:GLU:HA	2:R:635:THR:O	2.11	0.50
1:C:102:ASP:OD2	1:C:459:SER:N	2.42	0.50
1:C:926:ASN:HA	1:C:929:ILE:HD12	1.92	0.50
1:C:994:THR:O	1:C:998:LEU:HG	2.10	0.50
2:R:622:VAL:HG12	2:R:663:VAL:HB	1.93	0.50
1:A:389:GLN:HE22	1:A:466:THR:HG21	1.75	0.50
1:B:122:ASP:N	1:B:122:ASP:OD1	2.43	0.50
1:B:190:ILE:HB	1:B:752:VAL:HG22	1.93	0.50
1:C:368:CYS:O	1:C:371:PRO:HD2	2.11	0.50
1:A:88:TYR:HB3	1:A:95:THR:HB	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:598:GLY:HA2	1:B:614:ASN:HA	1.93	0.50
1:C:50:MET:HB2	1:C:113:TRP:CZ3	2.46	0.50
1:C:563:ASN:O	1:C:649:SER:OG	2.28	0.50
1:C:598:GLY:HA2	1:C:614:ASN:HA	1.93	0.50
1:C:954:HIS:O	1:C:955:ARG:NH2	2.44	0.50
2:P:627:VAL:HG22	2:P:676:ARG:HD3	1.92	0.50
2:R:271:LEU:HD11	2:R:278:PRO:HB2	1.93	0.50
2:R:279:ALA:HA	2:R:294:VAL:HG22	1.92	0.50
1:B:156:ASP:O	1:B:159:GLN:HG2	2.11	0.50
1:B:214:GLN:OE1	1:B:741:THR:OG1	2.28	0.50
1:B:645:TYR:HA	2:Q:339:THR:HG21	1.94	0.50
1:A:453:ILE:HD11	1:A:468:PHE:HB2	1.94	0.50
1:A:610:GLN:OE1	1:A:610:GLN:N	2.44	0.50
1:C:147:VAL:HG12	1:C:289:ALA:HA	1.93	0.50
1:C:190:ILE:HB	1:C:752:VAL:HG22	1.93	0.50
1:B:954:HIS:O	1:B:955:ARG:NH2	2.44	0.50
1:C:23:MET:HB2	1:C:485:PHE:CE1	2.44	0.50
1:C:453:ILE:HD11	1:C:468:PHE:HB2	1.94	0.50
1:A:563:ASN:O	1:A:649:SER:OG	2.28	0.50
1:B:78:GLU:OE1	1:B:119:LYS:NZ	2.39	0.50
1:C:663:ARG:HG3	1:C:809:LYS:HD3	1.94	0.50
2:Q:628:LEU:HD12	2:Q:637:VAL:HG13	1.94	0.50
1:A:376:MET:O	1:A:379:VAL:HG12	2.12	0.50
1:B:108:ASP:N	1:B:108:ASP:OD1	2.41	0.50
1:B:147:VAL:HG12	1:B:289:ALA:HA	1.93	0.50
1:C:156:ASP:O	1:C:159:GLN:HG2	2.11	0.50
1:C:645:TYR:HA	2:R:339:THR:HG21	1.94	0.50
1:C:878:GLN:H	1:C:882:LYS:NZ	2.09	0.50
2:Q:266:LEU:HG	2:Q:267:PRO:HD2	1.94	0.50
1:A:156:ASP:O	1:A:159:GLN:HG2	2.11	0.49
1:A:230:GLU:HB3	2:Q:268:TRP:CE3	2.47	0.49
1:C:610:GLN:HB2	1:C:617:TYR:CE2	2.47	0.49
1:B:717:ALA:O	1:B:722:LEU:N	2.43	0.49
1:A:250:ASN:OD1	1:B:718:ARG:HD2	2.13	0.49
1:B:155:LEU:HD12	1:B:159:GLN:HE21	1.78	0.49
1:B:878:GLN:H	1:B:882:LYS:NZ	2.09	0.49
2:Q:271:LEU:HD11	2:Q:278:PRO:HB2	1.93	0.49
1:A:610:GLN:HB2	1:A:617:TYR:CE2	2.47	0.49
1:A:999:ILE:O	1:A:1002:PRO:HD2	2.13	0.49
1:B:18:LEU:HD21	1:C:878:GLN:HG2	1.94	0.49
1:B:555:ARG:HG3	1:B:557:GLU:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:LEU:HB2	1:A:257:PHE:HA	1.94	0.49
1:A:281:LYS:HA	1:A:593:TRP:CE2	2.48	0.49
1:B:610:GLN:HB2	1:B:617:TYR:CE2	2.47	0.49
1:C:696:ASP:OD1	1:C:697:ILE:N	2.46	0.49
1:A:609:ASP:N	1:A:609:ASP:OD1	2.45	0.49
1:A:725:GLU:OE1	1:A:725:GLU:N	2.40	0.49
1:B:376:MET:O	1:B:379:VAL:HG12	2.12	0.49
1:B:696:ASP:OD1	1:B:697:ILE:N	2.46	0.49
1:A:897:VAL:HG23	1:A:898:VAL:HG13	1.95	0.49
2:R:266:LEU:CG	2:R:318:THR:HG22	2.43	0.49
1:A:628:GLU:OE1	1:A:628:GLU:N	2.42	0.49
1:B:281:LYS:HA	1:B:593:TRP:CE2	2.48	0.49
1:C:155:LEU:HD12	1:C:159:GLN:HE21	1.77	0.49
1:C:376:MET:O	1:C:379:VAL:HG12	2.12	0.49
1:C:555:ARG:HG3	1:C:557:GLU:H	1.77	0.49
1:C:609:ASP:OD1	1:C:609:ASP:N	2.45	0.49
2:P:266:LEU:CG	2:P:318:THR:HG22	2.43	0.49
2:P:279:ALA:HB2	2:P:293:PRO:HA	1.94	0.49
2:P:374:THR:HB	2:P:641:ASP:CB	2.43	0.49
2:P:628:LEU:HD12	2:P:637:VAL:HG13	1.94	0.49
1:C:251:LEU:HB2	1:C:257:PHE:HA	1.94	0.49
1:C:876:GLN:O	1:C:876:GLN:NE2	2.46	0.49
1:A:555:ARG:HG3	1:A:557:GLU:H	1.77	0.48
1:A:876:GLN:O	1:A:876:GLN:NE2	2.46	0.48
1:B:609:ASP:OD1	1:B:609:ASP:N	2.45	0.48
1:B:663:ARG:HG3	1:B:809:LYS:HD3	1.94	0.48
1:C:305:LEU:O	1:C:309:MET:HG2	2.13	0.48
2:Q:286:GLN:N	2:Q:286:GLN:OE1	2.46	0.48
1:B:62:ASP:OD1	1:B:63:ASP:N	2.46	0.48
1:A:696:ASP:OD1	1:A:697:ILE:N	2.46	0.48
1:C:62:ASP:O	1:C:65:LEU:HG	2.14	0.48
2:P:286:GLN:OE1	2:P:286:GLN:N	2.47	0.48
2:Q:374:THR:HB	2:Q:641:ASP:CB	2.43	0.48
1:A:412:GLU:O	1:A:415:ILE:HG13	2.14	0.48
1:B:999:ILE:O	1:B:1002:PRO:HD2	2.13	0.48
1:C:281:LYS:HA	1:C:593:TRP:CE2	2.48	0.48
1:C:582:ALA:HA	1:C:585:LYS:HE3	1.96	0.48
1:C:725:GLU:OE1	1:C:725:GLU:N	2.40	0.48
1:C:999:ILE:O	1:C:1002:PRO:HD2	2.13	0.48
2:P:266:LEU:HG	2:P:267:PRO:HD2	1.94	0.48
2:R:374:THR:HB	2:R:641:ASP:CB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:LEU:O	1:A:309:MET:HG2	2.13	0.48
1:A:958:PRO:O	1:A:962:THR:HG23	2.14	0.48
2:P:674:VAL:HG13	2:P:675:VAL:O	2.14	0.48
1:C:214:GLN:OE1	1:C:741:THR:OG1	2.28	0.48
1:C:897:VAL:HG23	1:C:898:VAL:HG13	1.95	0.48
2:Q:279:ALA:HB2	2:Q:293:PRO:HA	1.94	0.48
2:R:266:LEU:HG	2:R:267:PRO:HD2	1.94	0.48
2:R:628:LEU:HD12	2:R:637:VAL:HG13	1.94	0.48
1:A:129:GLN:OE1	1:A:129:GLN:N	2.39	0.48
1:A:155:LEU:HD12	1:A:159:GLN:HE21	1.77	0.48
1:A:235:ARG:O	1:B:709:LYS:HD2	2.13	0.48
1:A:507:GLY:O	1:A:511:GLU:HG3	2.14	0.48
1:B:198:LYS:O	1:B:198:LYS:NZ	2.35	0.48
1:B:897:VAL:HG23	1:B:898:VAL:HG13	1.95	0.48
1:C:517:LEU:HD12	1:C:521:MET:HE3	1.95	0.48
1:C:717:ALA:O	1:C:722:LEU:N	2.43	0.48
2:P:636:GLN:HB2	2:P:638:TRP:NE1	2.29	0.48
2:R:286:GLN:N	2:R:286:GLN:OE1	2.47	0.48
1:A:582:ALA:HA	1:A:585:LYS:HE3	1.96	0.48
1:B:75:LYS:HZ1	1:B:119:LYS:HD2	1.78	0.48
1:B:305:LEU:O	1:B:309:MET:HG2	2.13	0.48
2:R:279:ALA:HB2	2:R:293:PRO:HA	1.94	0.48
1:B:507:GLY:O	1:B:511:GLU:HG3	2.13	0.48
1:C:78:GLU:OE1	1:C:119:LYS:NZ	2.39	0.48
1:C:242:SER:OG	1:C:243:GLU:N	2.47	0.48
1:C:412:GLU:O	1:C:415:ILE:HG13	2.14	0.48
1:A:108:ASP:OD1	1:A:108:ASP:N	2.41	0.48
1:A:663:ARG:HG3	1:A:809:LYS:HD3	1.94	0.48
1:A:953:HIS:ND1	1:A:953:HIS:O	2.47	0.48
1:B:876:GLN:O	1:B:876:GLN:NE2	2.46	0.48
1:B:958:PRO:O	1:B:962:THR:HG23	2.14	0.48
1:C:797:VAL:HG12	1:C:798:TRP:H	1.79	0.48
2:R:281:TRP:CD1	2:R:323:LEU:HD21	2.49	0.48
2:R:674:VAL:HG13	2:R:675:VAL:O	2.14	0.48
1:B:62:ASP:O	1:B:65:LEU:HG	2.14	0.47
1:B:175:LYS:NZ	1:B:176:ASP:OD1	2.30	0.47
1:B:584:LEU:O	1:B:584:LEU:HD12	2.14	0.47
2:P:292:GLN:NE2	2:P:309:GLY:O	2.44	0.47
1:B:129:GLN:OE1	1:B:129:GLN:N	2.39	0.47
1:B:242:SER:OG	1:B:243:GLU:N	2.47	0.47
1:B:412:GLU:O	1:B:415:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:601:ALA:HB3	1:B:603:ARG:HH12	1.78	0.47
1:C:601:ALA:HB3	1:C:603:ARG:HH12	1.79	0.47
2:R:292:GLN:NE2	2:R:309:GLY:O	2.44	0.47
1:A:62:ASP:O	1:A:65:LEU:HG	2.14	0.47
1:A:62:ASP:OD1	1:A:63:ASP:N	2.46	0.47
1:A:172:ARG:HD3	1:A:177:LEU:HD22	1.96	0.47
1:A:584:LEU:HD12	1:A:584:LEU:O	2.14	0.47
1:B:251:LEU:HB2	1:B:257:PHE:HA	1.94	0.47
1:B:582:ALA:HA	1:B:585:LYS:HE3	1.96	0.47
1:A:198:LYS:O	1:A:198:LYS:NZ	2.35	0.47
1:B:953:HIS:O	1:B:953:HIS:ND1	2.47	0.47
1:C:241:ARG:NH1	1:C:744:ARG:O	2.47	0.47
1:C:316:LEU:O	2:R:369:PRO:HD2	2.14	0.47
1:C:397:ILE:O	1:C:400:LEU:HG	2.15	0.47
1:C:584:LEU:HD12	1:C:584:LEU:O	2.14	0.47
1:C:953:HIS:O	1:C:953:HIS:ND1	2.47	0.47
2:Q:266:LEU:CG	2:Q:318:THR:HG22	2.43	0.47
2:Q:636:GLN:HB2	2:Q:638:TRP:NE1	2.29	0.47
1:A:242:SER:OG	1:A:243:GLU:N	2.47	0.47
1:C:65:LEU:HB3	1:C:89:THR:HG21	1.97	0.47
1:A:214:GLN:OE1	1:A:741:THR:OG1	2.28	0.47
1:B:563:ASN:O	1:B:649:SER:OG	2.28	0.47
2:P:281:TRP:CH2	2:P:291:LEU:HD12	2.50	0.47
1:A:102:ASP:OD2	1:A:459:SER:N	2.42	0.47
1:A:316:LEU:O	2:P:369:PRO:HD2	2.15	0.47
1:A:797:VAL:HG12	1:A:798:TRP:H	1.79	0.47
1:B:316:LEU:O	2:Q:369:PRO:HD2	2.14	0.47
1:B:558:LEU:HD12	1:B:654:PRO:HA	1.96	0.47
1:B:561:ASP:OD1	1:B:651:TYR:HB3	2.15	0.47
1:C:62:ASP:OD1	1:C:63:ASP:N	2.46	0.47
1:C:198:LYS:HA	1:C:198:LYS:HD2	1.80	0.47
1:C:507:GLY:O	1:C:511:GLU:HG3	2.14	0.47
2:P:281:TRP:CD1	2:P:323:LEU:HD21	2.49	0.47
2:Q:281:TRP:CH2	2:Q:291:LEU:HD12	2.50	0.47
2:Q:674:VAL:HG13	2:Q:675:VAL:O	2.14	0.47
2:R:281:TRP:CH2	2:R:291:LEU:HD12	2.50	0.47
1:A:168:ARG:HH21	1:A:180:VAL:HB	1.80	0.47
1:A:241:ARG:NH1	1:A:744:ARG:O	2.47	0.47
1:A:963:ALA:HB2	1:A:994:THR:HG21	1.96	0.47
1:B:608:LEU:HD23	1:B:609:ASP:N	2.30	0.47
1:C:172:ARG:HD3	1:C:177:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:477:LEU:O	1:C:480:ILE:HG22	2.15	0.47
1:A:65:LEU:HB3	1:A:89:THR:HG21	1.97	0.47
1:A:828:GLU:H	1:A:828:GLU:CD	2.18	0.47
1:B:65:LEU:HB3	1:B:89:THR:HG21	1.97	0.47
1:B:241:ARG:NH1	1:B:744:ARG:O	2.47	0.47
1:B:367:ALA:HA	1:B:370:ILE:HG12	1.97	0.47
1:B:815:GLU:OE1	1:B:815:GLU:N	2.48	0.47
1:C:558:LEU:HD12	1:C:654:PRO:HA	1.96	0.47
1:C:958:PRO:O	1:C:962:THR:HG23	2.14	0.47
2:R:636:GLN:HB2	2:R:638:TRP:NE1	2.29	0.47
1:A:387:THR:OG1	1:A:388:MET:N	2.49	0.47
1:A:477:LEU:O	1:A:480:ILE:HG22	2.15	0.47
1:A:667:TYR:HB2	1:A:808:VAL:HG23	1.97	0.47
1:B:979:TRP:HD1	1:B:982:MET:SD	2.38	0.47
1:C:815:GLU:N	1:C:815:GLU:OE1	2.48	0.47
2:R:279:ALA:CB	2:R:293:PRO:HA	2.45	0.47
1:A:601:ALA:HB3	1:A:603:ARG:HH12	1.79	0.46
1:A:614:ASN:OD1	1:A:614:ASN:N	2.48	0.46
1:A:764:LEU:HD23	1:A:767:LEU:HD12	1.97	0.46
1:B:725:GLU:OE1	1:B:725:GLU:N	2.40	0.46
1:B:764:LEU:HD23	1:B:767:LEU:HD12	1.97	0.46
1:B:963:ALA:HB2	1:B:994:THR:HG21	1.96	0.46
1:C:963:ALA:HB2	1:C:994:THR:HG21	1.96	0.46
1:B:136:PHE:HB3	1:B:138:ASP:O	2.16	0.46
1:B:477:LEU:O	1:B:480:ILE:HG22	2.15	0.46
1:B:797:VAL:HG12	1:B:798:TRP:H	1.79	0.46
1:C:381:MET:O	1:C:385:ASP:N	2.48	0.46
1:C:389:GLN:O	1:C:393:LEU:HG	2.15	0.46
2:P:279:ALA:CB	2:P:293:PRO:HA	2.45	0.46
2:Q:636:GLN:HB2	2:Q:638:TRP:CD1	2.51	0.46
1:A:50:MET:SD	1:A:116:VAL:HG11	2.55	0.46
1:A:561:ASP:OD1	1:A:651:TYR:HB3	2.15	0.46
1:B:389:GLN:O	1:B:393:LEU:HG	2.15	0.46
1:C:50:MET:SD	1:C:116:VAL:HG11	2.55	0.46
1:C:608:LEU:HD23	1:C:609:ASP:N	2.30	0.46
1:B:628:GLU:OE1	1:B:628:GLU:N	2.42	0.46
1:C:764:LEU:HD23	1:C:767:LEU:HD12	1.97	0.46
2:Q:281:TRP:CD1	2:Q:323:LEU:HD21	2.49	0.46
1:A:198:LYS:HA	1:A:198:LYS:HD2	1.80	0.46
1:A:397:ILE:O	1:A:400:LEU:HG	2.15	0.46
1:A:447:VAL:O	1:A:451:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:815:GLU:N	1:A:815:GLU:OE1	2.48	0.46
1:B:50:MET:SD	1:B:116:VAL:HG11	2.55	0.46
1:B:168:ARG:HH21	1:B:180:VAL:HB	1.80	0.46
1:B:231:ARG:HG3	1:C:567:ASN:HB2	1.97	0.46
1:B:381:MET:O	1:B:385:ASP:N	2.48	0.46
1:B:387:THR:OG1	1:B:388:MET:N	2.48	0.46
1:C:561:ASP:OD1	1:C:651:TYR:HB3	2.15	0.46
2:Q:292:GLN:NE2	2:Q:309:GLY:O	2.44	0.46
1:A:558:LEU:HD12	1:A:654:PRO:HA	1.96	0.46
1:B:48:LYS:O	1:B:49:THR:OG1	2.33	0.46
1:C:979:TRP:HD1	1:C:982:MET:SD	2.38	0.46
1:A:179:LYS:HG3	1:B:78:GLU:HG3	1.98	0.46
1:A:389:GLN:O	1:A:393:LEU:HG	2.15	0.46
1:A:979:TRP:HD1	1:A:982:MET:SD	2.38	0.46
1:B:397:ILE:O	1:B:400:LEU:HG	2.15	0.46
1:B:517:LEU:HD12	1:B:521:MET:HE3	1.98	0.46
1:B:836:LEU:HG	1:B:837:PRO:HD2	1.98	0.46
1:C:447:VAL:O	1:C:451:VAL:HG23	2.15	0.46
1:C:627:LEU:HB2	1:C:630:ARG:HH21	1.81	0.46
2:P:636:GLN:HB2	2:P:638:TRP:CD1	2.51	0.46
2:Q:279:ALA:CB	2:Q:293:PRO:HA	2.45	0.46
1:A:136:PHE:HB3	1:A:138:ASP:O	2.16	0.46
1:C:136:PHE:HB3	1:C:138:ASP:O	2.16	0.46
1:C:168:ARG:HH21	1:C:180:VAL:HB	1.80	0.46
1:C:697:ILE:HG22	1:C:810:ALA:HB2	1.98	0.46
2:P:628:LEU:HD11	2:P:630:GLU:HB3	1.98	0.46
1:A:381:MET:O	1:A:385:ASP:N	2.48	0.46
1:B:709:LYS:O	1:B:788:VAL:HA	2.16	0.46
1:C:367:ALA:HA	1:C:370:ILE:HG12	1.97	0.46
1:C:387:THR:OG1	1:C:388:MET:N	2.49	0.46
2:Q:628:LEU:HD11	2:Q:630:GLU:HB3	1.98	0.46
2:R:301:SER:C	2:R:303:LYS:H	2.19	0.46
1:A:627:LEU:HB2	1:A:630:ARG:HH21	1.81	0.46
1:B:154:GLY:O	2:Q:626:SER:OG	2.33	0.46
1:B:172:ARG:HD3	1:B:177:LEU:HD22	1.96	0.46
1:B:216:GLN:OE1	1:C:725:GLU:HA	2.15	0.46
1:B:258:TYR:HD2	1:B:263:LEU:HD21	1.81	0.46
1:B:596:TYR:OH	1:B:603:ARG:NH2	2.48	0.46
1:C:667:TYR:HB2	1:C:808:VAL:HG23	1.97	0.46
1:A:367:ALA:HA	1:A:370:ILE:HG12	1.97	0.45
1:C:380:PHE:CE2	1:C:473:VAL:HG21	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LEU:HD21	1:A:206:GLN:H	1.82	0.45
1:B:389:GLN:NE2	1:B:466:THR:HG21	2.32	0.45
1:B:627:LEU:HB2	1:B:630:ARG:HH21	1.81	0.45
2:Q:301:SER:C	2:Q:303:LYS:H	2.19	0.45
2:Q:637:VAL:HB	2:Q:674:VAL:CB	2.47	0.45
1:A:258:TYR:HD2	1:A:263:LEU:HD21	1.81	0.45
1:A:397:ILE:HD13	1:A:973:ILE:HG21	1.99	0.45
1:B:614:ASN:OD1	1:B:614:ASN:N	2.48	0.45
1:B:828:GLU:H	1:B:828:GLU:CD	2.18	0.45
1:C:258:TYR:HD2	1:C:263:LEU:HD21	1.81	0.45
1:C:614:ASN:N	1:C:614:ASN:OD1	2.48	0.45
2:R:273:LYS:NZ	2:R:276:GLU:HA	2.32	0.45
1:B:236:THR:HG21	1:C:731:MET:SD	2.57	0.45
2:P:637:VAL:HB	2:P:674:VAL:CB	2.47	0.45
1:A:697:ILE:HG22	1:A:810:ALA:HB2	1.98	0.45
1:A:709:LYS:O	1:A:788:VAL:HA	2.16	0.45
1:B:447:VAL:O	1:B:451:VAL:HG23	2.15	0.45
1:B:877:LEU:HD13	1:B:882:LYS:HB2	1.99	0.45
1:C:161:ARG:HE	1:C:182:MET:HE1	1.81	0.45
1:C:459:SER:O	1:C:462:GLU:HG2	2.16	0.45
1:C:709:LYS:O	1:C:788:VAL:HA	2.16	0.45
2:R:636:GLN:HB2	2:R:638:TRP:CD1	2.51	0.45
1:A:154:GLY:O	2:P:626:SER:OG	2.34	0.45
1:A:407:ALA:O	1:A:410:THR:OG1	2.29	0.45
1:B:890:ALA:HB3	1:B:891:PRO:HD3	1.99	0.45
1:C:113:TRP:O	1:C:117:ARG:HG2	2.17	0.45
1:C:309:MET:HA	1:C:312:ILE:HD12	1.99	0.45
1:C:836:LEU:HG	1:C:837:PRO:HD2	1.98	0.45
1:A:390:ARG:HG3	1:A:391:VAL:H	1.82	0.45
1:A:666:GLN:HG2	1:A:809:LYS:HB3	1.99	0.45
1:B:610:GLN:OE1	1:B:610:GLN:N	2.44	0.45
1:B:697:ILE:HG22	1:B:810:ALA:HB2	1.98	0.45
1:C:154:GLY:O	2:R:626:SER:OG	2.34	0.45
1:C:828:GLU:H	1:C:828:GLU:CD	2.18	0.45
1:C:1000:PHE:CZ	1:C:1004:LEU:HD22	2.52	0.45
2:P:301:SER:C	2:P:303:LYS:H	2.19	0.45
2:Q:637:VAL:HB	2:Q:674:VAL:HB	1.99	0.45
1:A:251:LEU:O	1:A:257:PHE:HB3	2.17	0.45
1:A:389:GLN:NE2	1:A:466:THR:HG21	2.32	0.45
1:A:836:LEU:HG	1:A:837:PRO:HD2	1.98	0.45
1:A:999:ILE:C	1:A:1002:PRO:HD2	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1000:PHE:CZ	1:A:1004:LEU:HD22	2.52	0.45
1:B:172:ARG:HD3	1:B:172:ARG:HA	1.81	0.45
1:B:309:MET:HA	1:B:312:ILE:HD12	1.99	0.45
1:B:397:ILE:HD13	1:B:973:ILE:HG21	1.99	0.45
2:P:637:VAL:HB	2:P:674:VAL:HB	1.99	0.45
2:R:637:VAL:HB	2:R:674:VAL:CB	2.47	0.45
1:A:78:GLU:HG3	1:C:179:LYS:HG3	1.99	0.45
1:A:608:LEU:HD23	1:A:609:ASP:N	2.30	0.45
1:A:890:ALA:HB3	1:A:891:PRO:HD3	1.99	0.45
1:B:243:GLU:O	1:B:246:LEU:HG	2.17	0.45
1:B:380:PHE:CE2	1:B:473:VAL:HG21	2.51	0.45
1:B:459:SER:O	1:B:462:GLU:HG2	2.16	0.45
1:C:407:ALA:O	1:C:410:THR:OG1	2.29	0.45
1:A:15:HIS:HB3	1:A:18:LEU:HD12	1.98	0.45
1:A:413:MET:SD	1:A:431:ALA:HB1	2.57	0.45
1:A:459:SER:O	1:A:462:GLU:HG2	2.16	0.45
1:A:877:LEU:HD13	1:A:882:LYS:HB2	1.99	0.45
1:B:251:LEU:O	1:B:257:PHE:HB3	2.17	0.45
1:B:451:VAL:HA	1:B:468:PHE:CE1	2.52	0.45
1:B:667:TYR:HB2	1:B:808:VAL:HG23	1.97	0.45
1:B:955:ARG:HD3	1:B:955:ARG:HA	1.78	0.45
1:C:451:VAL:HA	1:C:468:PHE:CE1	2.52	0.45
1:C:558:LEU:HD13	1:C:628:GLU:HG3	1.99	0.45
1:C:610:GLN:HB3	1:C:613:GLN:OE1	2.17	0.45
2:P:273:LYS:NZ	2:P:276:GLU:HA	2.32	0.45
1:A:515:SER:O	1:A:519:LEU:HG	2.17	0.44
1:A:955:ARG:HA	1:A:955:ARG:HD3	1.78	0.44
1:B:44:SER:HA	1:B:605:TYR:CZ	2.53	0.44
1:C:251:LEU:O	1:C:257:PHE:HB3	2.17	0.44
2:R:637:VAL:HB	2:R:674:VAL:HB	1.99	0.44
1:A:345:GLU:O	1:A:349:ILE:HG23	2.17	0.44
1:A:380:PHE:CE2	1:A:473:VAL:HG21	2.51	0.44
1:A:610:GLN:HB3	1:A:613:GLN:OE1	2.17	0.44
1:B:199:LEU:HD21	1:B:206:GLN:H	1.82	0.44
1:B:999:ILE:C	1:B:1002:PRO:HD2	2.38	0.44
1:B:1000:PHE:CZ	1:B:1004:LEU:HD22	2.52	0.44
3:B:1101:LMU:H62	1:C:465:PHE:HE1	1.82	0.44
2:R:628:LEU:HD11	2:R:630:GLU:HB3	1.98	0.44
1:A:113:TRP:O	1:A:117:ARG:HG2	2.17	0.44
1:A:451:VAL:HA	1:A:468:PHE:CE1	2.52	0.44
1:B:113:TRP:O	1:B:117:ARG:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:LYS:NZ	1:B:593:TRP:HE1	2.15	0.44
1:B:499:LYS:HA	1:B:499:LYS:HD3	1.78	0.44
1:B:558:LEU:HD13	1:B:628:GLU:HG3	1.99	0.44
1:B:733:SER:HB2	1:B:756:ALA:HB2	2.00	0.44
1:C:15:HIS:HB3	1:C:18:LEU:HD12	1.98	0.44
1:C:389:GLN:NE2	1:C:466:THR:HG21	2.32	0.44
1:A:150:PHE:HD2	1:A:164:VAL:HG22	1.83	0.44
1:A:243:GLU:O	1:A:246:LEU:HG	2.17	0.44
1:B:15:HIS:HB3	1:B:18:LEU:HD12	1.98	0.44
1:B:405:ASP:O	1:B:409:ILE:HG23	2.18	0.44
1:B:909:GLY:O	1:B:913:ILE:HG13	2.18	0.44
1:C:397:ILE:HD13	1:C:973:ILE:HG21	1.99	0.44
1:A:309:MET:HA	1:A:312:ILE:HD12	1.99	0.44
1:A:405:ASP:O	1:A:409:ILE:HG23	2.18	0.44
1:A:427:SER:O	1:A:430:TYR:HE1	2.01	0.44
1:B:138:ASP:OD1	1:B:138:ASP:N	2.50	0.44
1:B:345:GLU:O	1:B:349:ILE:HG23	2.17	0.44
1:B:515:SER:O	1:B:519:LEU:HG	2.17	0.44
1:C:243:GLU:O	1:C:246:LEU:HG	2.17	0.44
1:C:405:ASP:O	1:C:409:ILE:HG23	2.18	0.44
1:C:427:SER:O	1:C:430:TYR:HE1	2.01	0.44
1:A:418:LEU:HG	1:A:423:SER:HA	1.99	0.44
1:A:422:ASP:OD2	1:A:427:SER:OG	2.36	0.44
1:B:422:ASP:OD2	1:B:427:SER:OG	2.36	0.44
1:B:535:PHE:O	1:B:538:SER:OG	2.32	0.44
1:C:239:ASN:OD1	1:C:240:PHE:N	2.51	0.44
1:C:494:LEU:HD23	1:C:494:LEU:HA	1.85	0.44
1:A:423:SER:HB2	1:A:497:THR:H	1.82	0.44
1:A:499:LYS:HA	1:A:499:LYS:HD3	1.78	0.44
1:A:955:ARG:O	1:A:959:ILE:HG12	2.18	0.44
1:C:150:PHE:HD2	1:C:164:VAL:HG22	1.83	0.44
1:C:733:SER:HB2	1:C:756:ALA:HB2	1.99	0.44
1:C:877:LEU:HD13	1:C:882:LYS:HB2	1.99	0.44
2:Q:273:LYS:NZ	2:Q:276:GLU:HA	2.32	0.44
1:A:239:ASN:OD1	1:A:240:PHE:N	2.51	0.44
1:A:465:PHE:HE1	3:C:1101:LMU:H62	1.82	0.44
1:A:567:ASN:HB2	1:C:231:ARG:HG3	1.98	0.44
1:A:751:ASN:OD1	1:A:751:ASN:N	2.45	0.44
1:A:866:LEU:O	1:A:869:MET:HG2	2.18	0.44
3:A:1101:LMU:H62	1:B:465:PHE:HE1	1.82	0.44
1:B:239:ASN:OD1	1:B:240:PHE:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:MET:SD	1:B:431:ALA:HB1	2.57	0.44
1:B:418:LEU:HG	1:B:423:SER:HA	1.99	0.44
1:B:937:PHE:CZ	1:B:951:ALA:HB2	2.53	0.44
1:B:955:ARG:O	1:B:959:ILE:HG12	2.18	0.44
1:C:199:LEU:HD21	1:C:206:GLN:H	1.82	0.44
1:C:413:MET:SD	1:C:431:ALA:HB1	2.57	0.44
1:C:479:TRP:CZ2	1:C:483:VAL:HG11	2.53	0.44
1:C:666:GLN:HG2	1:C:809:LYS:HB3	1.99	0.44
1:C:866:LEU:O	1:C:869:MET:HG2	2.18	0.44
1:C:955:ARG:O	1:C:959:ILE:HG12	2.18	0.44
2:P:358:GLY:HA2	2:P:680:ASN:HB2	2.00	0.44
1:A:909:GLY:O	1:A:913:ILE:HG13	2.18	0.44
1:C:370:ILE:O	1:C:373:VAL:HG22	2.18	0.44
1:C:515:SER:O	1:C:519:LEU:HG	2.17	0.44
1:C:596:TYR:OH	1:C:603:ARG:NH2	2.48	0.44
1:C:688:LEU:HD12	1:C:825:LEU:HD23	2.00	0.44
1:A:44:SER:HA	1:A:605:TYR:CZ	2.53	0.43
1:A:231:ARG:HG3	1:B:567:ASN:HB2	1.99	0.43
1:A:479:TRP:CZ2	1:A:483:VAL:HG11	2.53	0.43
1:B:150:PHE:HD2	1:B:164:VAL:HG22	1.83	0.43
1:B:390:ARG:HG3	1:B:391:VAL:H	1.82	0.43
1:B:423:SER:HB2	1:B:497:THR:H	1.82	0.43
1:C:44:SER:HA	1:C:605:TYR:CZ	2.53	0.43
1:C:129:GLN:OE1	1:C:129:GLN:N	2.39	0.43
1:C:890:ALA:HB3	1:C:891:PRO:HD3	1.99	0.43
1:C:955:ARG:HD3	1:C:955:ARG:HA	1.78	0.43
1:B:18:LEU:O	1:B:22:LEU:HG	2.18	0.43
1:C:63:ASP:HA	1:C:66:GLU:CD	2.39	0.43
1:C:138:ASP:N	1:C:138:ASP:OD1	2.51	0.43
1:C:390:ARG:HG3	1:C:391:VAL:H	1.82	0.43
1:C:422:ASP:OD2	1:C:427:SER:OG	2.36	0.43
1:C:524:ARG:HD3	1:C:1006:VAL:HG13	2.00	0.43
1:C:999:ILE:C	1:C:1002:PRO:HD2	2.38	0.43
2:Q:358:GLY:HA2	2:Q:680:ASN:HB2	2.00	0.43
1:B:610:GLN:HB3	1:B:613:GLN:OE1	2.17	0.43
1:B:666:GLN:HG2	1:B:809:LYS:HB3	1.99	0.43
1:C:306:ASN:O	1:C:310:GLN:HG2	2.19	0.43
1:C:345:GLU:O	1:C:349:ILE:HG23	2.17	0.43
1:C:426:ASP:C	1:C:428:ALA:H	2.21	0.43
2:P:281:TRP:CE3	2:P:323:LEU:HD11	2.53	0.43
2:P:282:LEU:HD13	2:P:292:GLN:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:LEU:O	1:A:782:LEU:N	2.52	0.43
1:B:370:ILE:O	1:B:373:VAL:HG22	2.18	0.43
1:B:479:TRP:CZ2	1:B:483:VAL:HG11	2.53	0.43
1:C:281:LYS:NZ	1:C:593:TRP:HE1	2.15	0.43
1:C:423:SER:HB2	1:C:497:THR:H	1.82	0.43
1:C:638:ARG:HH11	1:C:652:VAL:HG21	1.83	0.43
1:A:63:ASP:HA	1:A:66:GLU:CD	2.39	0.43
1:A:306:ASN:O	1:A:310:GLN:HG2	2.18	0.43
1:A:535:PHE:O	1:A:538:SER:OG	2.32	0.43
1:B:422:ASP:OD1	1:B:423:SER:N	2.51	0.43
1:C:417:ARG:HD3	1:C:430:TYR:CZ	2.54	0.43
1:C:418:LEU:HG	1:C:423:SER:HA	1.99	0.43
1:C:488:VAL:HA	1:C:491:VAL:HG12	2.00	0.43
1:C:770:LEU:O	1:C:782:LEU:N	2.52	0.43
2:Q:281:TRP:CE3	2:Q:323:LEU:HD11	2.53	0.43
1:C:909:GLY:O	1:C:913:ILE:HG13	2.18	0.43
1:C:937:PHE:CZ	1:C:951:ALA:HB2	2.53	0.43
1:A:18:LEU:O	1:A:22:LEU:HG	2.18	0.43
1:A:422:ASP:OD1	1:A:423:SER:N	2.51	0.43
1:A:1013:GLU:HB2	1:A:1014:PRO:HD3	2.01	0.43
1:B:306:ASN:O	1:B:310:GLN:HG2	2.19	0.43
1:B:427:SER:O	1:B:430:TYR:HE1	2.01	0.43
1:C:191:TYR:O	1:C:192:LEU:HD12	2.19	0.43
2:Q:374:THR:HB	2:Q:641:ASP:HB3	2.01	0.43
2:R:281:TRP:CE3	2:R:323:LEU:HD11	2.53	0.43
1:A:426:ASP:C	1:A:428:ALA:H	2.21	0.43
1:B:312:ILE:O	1:B:316:LEU:N	2.52	0.43
1:B:350:VAL:HG11	1:B:404:VAL:HG11	2.01	0.43
1:B:638:ARG:HH11	1:B:652:VAL:HG21	1.83	0.43
1:B:770:LEU:O	1:B:782:LEU:N	2.52	0.43
2:R:689:LYS:HE3	2:R:689:LYS:HB2	1.77	0.43
1:A:558:LEU:HD13	1:A:628:GLU:HG3	1.99	0.43
1:A:575:ALA:HA	1:A:578:ASP:OD2	2.19	0.43
1:B:243:GLU:OE2	1:B:269:ASP:N	2.52	0.43
1:A:138:ASP:N	1:A:138:ASP:OD1	2.51	0.43
1:A:243:GLU:OE2	1:A:269:ASP:N	2.52	0.43
1:A:312:ILE:O	1:A:316:LEU:N	2.52	0.43
1:A:733:SER:HB2	1:A:756:ALA:HB2	1.99	0.43
1:B:488:VAL:HA	1:B:491:VAL:HG12	2.01	0.43
1:C:172:ARG:HD3	1:C:172:ARG:HA	1.81	0.43
1:C:575:ALA:HA	1:C:578:ASP:OD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:374:THR:HB	2:P:641:ASP:HB3	2.01	0.43
1:A:207:ARG:HG2	1:A:211:GLN:OE1	2.19	0.42
1:A:417:ARG:HD3	1:A:430:TYR:CZ	2.54	0.42
1:C:41:GLU:O	1:C:389:GLN:HB2	2.19	0.42
1:C:193:ASN:HA	1:C:755:ARG:O	2.19	0.42
1:C:243:GLU:OE2	1:C:269:ASP:N	2.52	0.42
1:C:424:LEU:HB2	1:C:427:SER:OG	2.19	0.42
1:C:488:VAL:O	1:C:491:VAL:HG12	2.19	0.42
1:C:566:GLN:HG2	1:C:567:ASN:H	1.84	0.42
1:C:610:GLN:OE1	1:C:610:GLN:N	2.45	0.42
2:R:374:THR:HB	2:R:641:ASP:HB3	2.01	0.42
1:A:216:GLN:NE2	1:B:724:SER:HB2	2.34	0.42
1:A:281:LYS:NZ	1:A:593:TRP:HE1	2.15	0.42
1:A:410:THR:O	1:A:414:MET:HG3	2.19	0.42
1:B:488:VAL:O	1:B:491:VAL:HG12	2.19	0.42
1:B:524:ARG:HD3	1:B:1006:VAL:HG13	2.00	0.42
1:B:866:LEU:O	1:B:869:MET:HG2	2.18	0.42
1:C:343:LEU:O	1:C:347:VAL:HG23	2.19	0.42
2:P:357:ARG:NH1	2:P:677:ALA:O	2.52	0.42
1:A:172:ARG:HD3	1:A:172:ARG:HA	1.81	0.42
1:A:596:TYR:OH	1:A:603:ARG:NH2	2.48	0.42
1:A:809:LYS:HB3	1:A:809:LYS:HE2	1.79	0.42
1:A:882:LYS:HB2	1:A:882:LYS:HE3	1.89	0.42
1:A:882:LYS:O	1:A:886:VAL:HG22	2.19	0.42
1:B:63:ASP:HA	1:B:66:GLU:CD	2.39	0.42
1:B:343:LEU:O	1:B:347:VAL:HG23	2.20	0.42
1:B:585:LYS:HB2	2:Q:354:GLY:HA3	2.01	0.42
1:B:666:GLN:HB2	1:B:845:GLY:O	2.19	0.42
1:B:678:ARG:NH2	1:B:702:ASN:O	2.53	0.42
1:B:763:SER:O	1:B:767:LEU:HG	2.19	0.42
1:B:1013:GLU:HB2	1:B:1014:PRO:HD3	2.01	0.42
1:C:422:ASP:OD1	1:C:423:SER:N	2.51	0.42
1:C:882:LYS:O	1:C:886:VAL:HG22	2.19	0.42
1:A:253:VAL:HA	1:A:257:PHE:CD2	2.54	0.42
1:A:523:ARG:O	1:A:526:THR:OG1	2.34	0.42
1:A:524:ARG:HD3	1:A:1006:VAL:HG13	2.00	0.42
1:A:566:GLN:HG2	1:A:567:ASN:H	1.84	0.42
1:A:688:LEU:HD12	1:A:825:LEU:HD23	2.00	0.42
1:B:253:VAL:HA	1:B:257:PHE:CD2	2.54	0.42
1:B:346:ALA:HA	1:B:349:ILE:HG12	2.01	0.42
1:B:417:ARG:HD3	1:B:430:TYR:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:LEU:O	1:C:22:LEU:HG	2.18	0.42
1:C:253:VAL:HA	1:C:257:PHE:CD2	2.54	0.42
1:A:346:ALA:HA	1:A:349:ILE:HG12	2.01	0.42
1:A:488:VAL:O	1:A:491:VAL:HG12	2.19	0.42
1:A:488:VAL:HA	1:A:491:VAL:HG12	2.01	0.42
1:A:524:ARG:HH22	1:A:1010:ARG:HG3	1.84	0.42
1:A:763:SER:O	1:A:767:LEU:HG	2.19	0.42
1:B:41:GLU:O	1:B:389:GLN:HB2	2.19	0.42
1:B:523:ARG:O	1:B:526:THR:OG1	2.34	0.42
1:B:688:LEU:HD12	1:B:825:LEU:HD23	2.00	0.42
1:B:882:LYS:O	1:B:886:VAL:HG22	2.19	0.42
1:C:279:ARG:HH12	1:C:284:PRO:HG3	1.84	0.42
1:C:666:GLN:HB2	1:C:845:GLY:O	2.20	0.42
1:A:279:ARG:HH12	1:A:284:PRO:HG3	1.85	0.42
1:A:370:ILE:O	1:A:373:VAL:HG22	2.18	0.42
1:A:517:LEU:HD12	1:A:521:MET:HE3	2.01	0.42
3:A:1101:LMU:H102	3:A:1101:LMU:H71	1.92	0.42
1:B:191:TYR:O	1:B:192:LEU:HD12	2.19	0.42
1:B:193:ASN:HA	1:B:755:ARG:O	2.19	0.42
1:B:372:LEU:O	1:B:376:MET:HG3	2.20	0.42
1:B:407:ALA:O	1:B:410:THR:OG1	2.29	0.42
2:R:357:ARG:NH1	2:R:677:ALA:O	2.52	0.42
1:A:193:ASN:HA	1:A:755:ARG:O	2.19	0.42
1:A:343:LEU:O	1:A:347:VAL:HG23	2.20	0.42
1:A:350:VAL:HG11	1:A:404:VAL:HG11	2.01	0.42
1:A:678:ARG:NH2	1:A:702:ASN:O	2.53	0.42
1:B:426:ASP:C	1:B:428:ALA:H	2.21	0.42
1:C:312:ILE:O	1:C:316:LEU:N	2.52	0.42
1:C:410:THR:O	1:C:414:MET:HG3	2.19	0.42
1:A:366:VAL:O	1:A:369:SER:OG	2.25	0.42
1:A:424:LEU:HB2	1:A:427:SER:OG	2.20	0.42
1:A:638:ARG:HH11	1:A:652:VAL:HG21	1.83	0.42
1:B:575:ALA:HA	1:B:578:ASP:OD2	2.19	0.42
1:B:656:GLU:N	1:B:656:GLU:OE1	2.53	0.42
1:C:350:VAL:HG11	1:C:404:VAL:HG11	2.01	0.42
1:C:372:LEU:O	1:C:376:MET:HG3	2.20	0.42
1:C:523:ARG:O	1:C:526:THR:OG1	2.34	0.42
1:A:232:ILE:HG21	1:B:764:LEU:HD11	2.00	0.42
1:B:293:LYS:HZ1	1:C:81:SER:N	2.15	0.42
1:B:524:ARG:HH22	1:B:1010:ARG:HG3	1.84	0.42
1:B:566:GLN:HG2	1:B:567:ASN:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:638:ARG:O	1:B:641:LEU:HG	2.20	0.42
1:B:882:LYS:HB2	1:B:882:LYS:HE3	1.89	0.42
2:R:282:LEU:HD23	2:R:314:GLN:HG2	2.02	0.42
1:A:54:THR:HB	1:A:94:SER:OG	2.20	0.42
1:A:439:MET:HB2	1:A:479:TRP:HE1	1.85	0.42
1:A:585:LYS:HB2	2:P:354:GLY:HA3	2.00	0.42
1:B:146:SER:OG	1:B:327:ASN:HA	2.20	0.42
1:B:424:LEU:HB2	1:B:427:SER:OG	2.19	0.42
1:B:626:ASP:OD2	1:B:630:ARG:NE	2.53	0.42
1:C:146:SER:OG	1:C:327:ASN:HA	2.20	0.42
1:C:497:THR:OG1	1:C:498:LEU:N	2.53	0.42
1:C:763:SER:O	1:C:767:LEU:HG	2.19	0.42
1:C:1013:GLU:HB2	1:C:1014:PRO:HD3	2.01	0.42
2:Q:282:LEU:HD13	2:Q:292:GLN:HB3	2.01	0.42
2:Q:357:ARG:NH1	2:Q:677:ALA:O	2.52	0.42
1:A:543:LYS:HB3	1:A:543:LYS:HE2	1.84	0.41
1:A:666:GLN:HB2	1:A:845:GLY:O	2.19	0.41
1:B:392:SER:O	1:B:396:LEU:HG	2.20	0.41
1:C:54:THR:HB	1:C:94:SER:OG	2.20	0.41
1:C:567:ASN:OD1	1:C:567:ASN:N	2.53	0.41
1:C:585:LYS:HB2	2:R:354:GLY:HA3	2.01	0.41
2:R:282:LEU:HD13	2:R:292:GLN:HB3	2.01	0.41
1:A:81:SER:H	1:C:293:LYS:HZ1	1.68	0.41
1:A:392:SER:O	1:A:396:LEU:HG	2.20	0.41
1:A:656:GLU:N	1:A:656:GLU:OE1	2.53	0.41
1:A:799:ARG:NH1	1:A:802:ARG:HA	2.35	0.41
1:A:956:THR:HG23	1:A:957:ARG:H	1.85	0.41
1:B:120:ILE:HA	1:B:123:ILE:HG22	2.02	0.41
1:B:279:ARG:HH12	1:B:284:PRO:HG3	1.84	0.41
1:B:417:ARG:HH11	1:B:431:ALA:HA	1.85	0.41
1:B:592:HIS:HB2	1:B:623:VAL:HB	2.02	0.41
1:B:638:ARG:NH1	1:B:652:VAL:HG21	2.35	0.41
1:C:207:ARG:HG2	1:C:211:GLN:OE1	2.19	0.41
1:C:274:PRO:HB3	1:C:277:LEU:HD21	2.03	0.41
1:C:394:GLY:O	1:C:398:ILE:HG12	2.20	0.41
1:C:524:ARG:HH22	1:C:1010:ARG:HG3	1.84	0.41
2:R:358:GLY:HA2	2:R:680:ASN:HB2	2.00	0.41
1:A:41:GLU:O	1:A:389:GLN:HB2	2.19	0.41
1:A:638:ARG:O	1:A:641:LEU:HG	2.20	0.41
1:B:734:VAL:HA	1:B:761:ARG:HD3	2.02	0.41
1:C:191:TYR:CE1	1:C:753:ILE:HD11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:ARG:HH11	1:C:431:ALA:HA	1.85	0.41
1:C:638:ARG:NH1	1:C:652:VAL:HG21	2.36	0.41
1:C:667:TYR:CD1	1:C:844:VAL:HA	2.55	0.41
1:A:274:PRO:HB3	1:A:277:LEU:HD21	2.03	0.41
1:A:417:ARG:HH11	1:A:431:ALA:HA	1.85	0.41
1:A:592:HIS:HB2	1:A:623:VAL:HB	2.02	0.41
1:B:54:THR:HB	1:B:94:SER:OG	2.20	0.41
1:B:74:LYS:HB2	1:B:802:ARG:CZ	2.50	0.41
1:B:207:ARG:HG2	1:B:211:GLN:OE1	2.19	0.41
1:B:497:THR:OG1	1:B:498:LEU:N	2.53	0.41
1:B:667:TYR:CD1	1:B:844:VAL:HA	2.55	0.41
1:B:956:THR:HG23	1:B:957:ARG:H	1.85	0.41
1:C:120:ILE:HA	1:C:123:ILE:HG22	2.02	0.41
1:C:678:ARG:NH2	1:C:702:ASN:O	2.53	0.41
1:C:699:TYR:HB2	1:C:702:ASN:OD1	2.21	0.41
1:C:728:ALA:HA	1:C:731:MET:HE2	2.03	0.41
1:C:956:THR:HG23	1:C:957:ARG:H	1.85	0.41
2:P:298:ARG:HB3	2:P:305:VAL:HB	2.02	0.41
2:Q:282:LEU:HD23	2:Q:314:GLN:HG2	2.02	0.41
1:A:74:LYS:HB2	1:A:802:ARG:CZ	2.50	0.41
1:A:101:LYS:HE2	1:A:101:LYS:HB3	1.86	0.41
1:A:626:ASP:OD2	1:A:630:ARG:NE	2.53	0.41
1:A:734:VAL:HA	1:A:761:ARG:HD3	2.02	0.41
1:B:198:LYS:HD2	1:B:198:LYS:HA	1.80	0.41
1:B:410:THR:O	1:B:414:MET:HG3	2.19	0.41
1:C:439:MET:HB2	1:C:479:TRP:HE1	1.85	0.41
1:C:592:HIS:HB2	1:C:623:VAL:HB	2.02	0.41
1:C:799:ARG:NH1	1:C:802:ARG:HA	2.35	0.41
1:C:924:ILE:HD13	1:C:924:ILE:HA	1.95	0.41
2:P:273:LYS:HZ1	2:P:276:GLU:HA	1.86	0.41
1:A:181:GLN:OE1	1:A:182:MET:N	2.54	0.41
1:A:638:ARG:NH1	1:A:652:VAL:HG21	2.35	0.41
1:B:251:LEU:O	1:C:723:SER:HB2	2.20	0.41
1:B:394:GLY:O	1:B:398:ILE:HG12	2.20	0.41
1:C:346:ALA:HA	1:C:349:ILE:HG12	2.01	0.41
2:P:637:VAL:HB	2:P:674:VAL:HG11	2.03	0.41
1:A:191:TYR:CE1	1:A:753:ILE:HD11	2.56	0.41
1:A:394:GLY:O	1:A:398:ILE:HG12	2.21	0.41
1:A:667:TYR:CD1	1:A:844:VAL:HA	2.55	0.41
1:B:274:PRO:HB3	1:B:277:LEU:HD21	2.03	0.41
1:C:517:LEU:O	1:C:521:MET:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:638:ARG:O	1:C:641:LEU:HG	2.20	0.41
1:C:668:ARG:NH2	1:C:800:ARG:HH22	2.19	0.41
1:A:191:TYR:O	1:A:192:LEU:HD12	2.19	0.41
1:B:475:LEU:O	1:B:478:SER:OG	2.26	0.41
1:B:668:ARG:NH2	1:B:800:ARG:HH22	2.19	0.41
1:C:626:ASP:OD2	1:C:630:ARG:NE	2.53	0.41
2:P:282:LEU:HD23	2:P:314:GLN:HG2	2.02	0.41
1:A:81:SER:H	1:C:293:LYS:NZ	2.18	0.41
1:A:146:SER:OG	1:A:327:ASN:HA	2.20	0.41
1:A:188:GLU:OE2	1:A:271:VAL:HG13	2.21	0.41
1:A:190:ILE:HG12	1:A:269:ASP:HB3	2.03	0.41
1:A:390:ARG:HA	1:A:393:LEU:HD12	2.03	0.41
1:A:497:THR:OG1	1:A:498:LEU:N	2.53	0.41
1:A:567:ASN:OD1	1:A:567:ASN:N	2.53	0.41
1:A:728:ALA:HA	1:A:731:MET:HE2	2.03	0.41
1:A:785:PHE:N	1:A:785:PHE:CD1	2.88	0.41
1:A:993:ALA:O	1:A:996:LEU:HG	2.21	0.41
1:B:106:ALA:HA	1:B:109:ILE:HD11	2.03	0.41
1:B:191:TYR:CE1	1:B:753:ILE:HD11	2.56	0.41
1:B:785:PHE:N	1:B:785:PHE:CD1	2.88	0.41
1:B:799:ARG:NH1	1:B:802:ARG:HA	2.35	0.41
1:B:800:ARG:HB3	1:B:805:THR:HG21	2.03	0.41
1:C:74:LYS:HB2	1:C:802:ARG:CZ	2.50	0.41
1:C:390:ARG:HA	1:C:393:LEU:HD12	2.03	0.41
1:C:392:SER:O	1:C:396:LEU:HG	2.20	0.41
1:C:535:PHE:O	1:C:538:SER:OG	2.32	0.41
1:C:800:ARG:HB3	1:C:805:THR:HG21	2.03	0.41
1:C:887:ALA:O	1:C:891:PRO:HD3	2.21	0.41
2:Q:689:LYS:HE3	2:Q:689:LYS:HB2	1.77	0.41
2:R:636:GLN:C	2:R:638:TRP:H	2.24	0.41
2:R:637:VAL:HB	2:R:674:VAL:HG11	2.03	0.41
1:A:298:ILE:HG12	1:A:299:LEU:H	1.86	0.41
1:A:668:ARG:NH2	1:A:800:ARG:HH22	2.19	0.41
1:B:109:ILE:H	1:B:109:ILE:HG12	1.60	0.41
1:C:160:LEU:O	1:C:164:VAL:HG23	2.21	0.41
1:C:298:ILE:HG12	1:C:299:LEU:H	1.86	0.41
1:C:785:PHE:N	1:C:785:PHE:CD1	2.89	0.41
2:Q:298:ARG:HB3	2:Q:305:VAL:HB	2.02	0.41
1:A:235:ARG:HD2	1:B:709:LYS:HD3	2.03	0.40
1:B:176:ASP:C	1:B:177:LEU:HD12	2.42	0.40
1:B:728:ALA:HA	1:B:731:MET:HE2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:ILE:HG12	1:C:269:ASP:HB3	2.03	0.40
1:C:656:GLU:OE1	1:C:656:GLU:N	2.53	0.40
2:Q:637:VAL:HB	2:Q:674:VAL:HG11	2.03	0.40
2:Q:683:LYS:H	2:Q:683:LYS:HG2	1.71	0.40
1:A:230:GLU:HG3	1:B:706:LYS:HZ3	1.86	0.40
1:A:372:LEU:O	1:A:376:MET:HG3	2.20	0.40
1:B:160:LEU:O	1:B:164:VAL:HG23	2.21	0.40
1:B:390:ARG:HA	1:B:393:LEU:HD12	2.03	0.40
1:B:570:ILE:HD12	1:B:570:ILE:HA	1.83	0.40
1:C:90:ARG:HB2	1:C:93:GLU:HB3	2.03	0.40
1:C:499:LYS:HA	1:C:499:LYS:HD3	1.78	0.40
1:C:570:ILE:HA	1:C:570:ILE:HD12	1.83	0.40
1:C:734:VAL:HA	1:C:761:ARG:HD3	2.02	0.40
1:A:120:ILE:HA	1:A:123:ILE:HG22	2.02	0.40
1:A:699:TYR:HB2	1:A:702:ASN:OD1	2.21	0.40
1:B:699:TYR:HB2	1:B:702:ASN:OD1	2.21	0.40
1:C:313:THR:HA	1:C:316:LEU:HB3	2.04	0.40
1:C:526:THR:O	1:C:530:LEU:HG	2.21	0.40
1:C:882:LYS:HB2	1:C:882:LYS:HE3	1.89	0.40
1:C:993:ALA:O	1:C:996:LEU:HG	2.21	0.40
1:A:800:ARG:HB3	1:A:805:THR:HG21	2.03	0.40
1:A:887:ALA:O	1:A:891:PRO:HD3	2.21	0.40
1:B:409:ILE:HD11	1:B:439:MET:SD	2.62	0.40
1:B:439:MET:HB2	1:B:479:TRP:HE1	1.85	0.40
1:C:633:VAL:O	1:C:637:LEU:HG	2.22	0.40
1:C:751:ASN:OD1	1:C:751:ASN:N	2.45	0.40
1:C:809:LYS:HB3	1:C:809:LYS:HE2	1.79	0.40
2:P:636:GLN:C	2:P:638:TRP:H	2.24	0.40
2:Q:636:GLN:C	2:Q:638:TRP:H	2.24	0.40
2:R:298:ARG:HB3	2:R:305:VAL:HB	2.02	0.40
1:A:409:ILE:HD11	1:A:439:MET:SD	2.62	0.40
1:B:188:GLU:OE2	1:B:271:VAL:HG13	2.21	0.40
1:B:887:ALA:O	1:B:891:PRO:HD3	2.21	0.40
1:C:107:GLY:O	1:C:110:PRO:HD2	2.21	0.40
2:P:629:LEU:HD23	2:P:680:ASN:H	1.87	0.40
2:Q:281:TRP:CZ3	2:Q:323:LEU:HD11	2.57	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	1020/1022 (100%)	939 (92%)	81 (8%)	0	100	100
1	B	1020/1022 (100%)	937 (92%)	83 (8%)	0	100	100
1	C	1020/1022 (100%)	937 (92%)	83 (8%)	0	100	100
2	P	211/695 (30%)	184 (87%)	25 (12%)	2 (1%)	14	51
2	Q	211/695 (30%)	184 (87%)	25 (12%)	2 (1%)	14	51
2	R	211/695 (30%)	185 (88%)	24 (11%)	2 (1%)	14	51
All	All	3693/5151 (72%)	3366 (91%)	321 (9%)	6 (0%)	45	78

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	P	637	VAL
2	P	638	TRP
2	Q	637	VAL
2	Q	638	TRP
2	R	637	VAL
2	R	638	TRP

### 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	856/856 (100%)	853 (100%)	3 (0%)	89	90
1	B	856/856 (100%)	853 (100%)	3 (0%)	89	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	856/856 (100%)	853 (100%)	3 (0%)	89	90
2	P	174/551 (32%)	174 (100%)	0	100	100
2	Q	174/551 (32%)	174 (100%)	0	100	100
2	R	174/551 (32%)	174 (100%)	0	100	100
All	All	3090/4221 (73%)	3081 (100%)	9 (0%)	90	91

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	ASP
1	A	649	SER
1	A	956	THR
1	B	176	ASP
1	B	649	SER
1	B	956	THR
1	C	176	ASP
1	C	649	SER
1	C	956	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	A	159	GLN
1	A	456	ASN
1	A	933	GLN
1	B	137	ASN
1	B	159	GLN
1	B	456	ASN
1	B	933	GLN
1	C	159	GLN
1	C	456	ASN
1	C	933	GLN
2	P	636	GLN
2	P	644	GLN
2	Q	636	GLN
2	Q	644	GLN
2	R	636	GLN
2	R	644	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 ⓘ

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	E2V	Q	701	2	41,41,41	0.96	4 (9%)	43,43,43	1.07	4 (9%)
4	E2V	P	701	2	41,41,41	0.96	4 (9%)	43,43,43	1.07	4 (9%)
5	PLM	R	702	2	15,16,17	0.20	0	14,15,17	0.22	0
3	LMU	A	1101	-	36,36,36	1.54	6 (16%)	47,47,47	0.79	1 (2%)
5	PLM	Q	702	2	15,16,17	0.21	0	14,15,17	0.22	0
4	E2V	R	701	2	41,41,41	0.97	4 (9%)	43,43,43	1.07	4 (9%)
3	LMU	C	1101	-	36,36,36	1.54	6 (16%)	47,47,47	0.79	1 (2%)
5	PLM	P	702	2	15,16,17	0.21	0	14,15,17	0.22	0
3	LMU	B	1101	-	36,36,36	1.54	6 (16%)	47,47,47	0.79	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	E2V	Q	701	2	-	28/42/42/42	-
4	E2V	P	701	2	-	28/42/42/42	-
5	PLM	R	702	2	-	5/14/14/15	-
3	LMU	A	1101	-	-	11/21/61/61	0/2/2/2
5	PLM	Q	702	2	-	5/14/14/15	-
4	E2V	R	701	2	-	28/42/42/42	-
3	LMU	C	1101	-	-	11/21/61/61	0/2/2/2
5	PLM	P	702	2	-	5/14/14/15	-
3	LMU	B	1101	-	-	11/21/61/61	0/2/2/2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1101	LMU	O5'-C5'	4.43	1.55	1.44
3	B	1101	LMU	O5'-C5'	4.42	1.55	1.44
3	A	1101	LMU	O5'-C5'	4.42	1.55	1.44
4	R	701	E2V	O23-C22	-3.89	1.40	1.47
4	Q	701	E2V	O23-C22	-3.89	1.40	1.47
4	P	701	E2V	O23-C22	-3.87	1.40	1.47
3	B	1101	LMU	O5B-C1B	3.56	1.51	1.41
3	C	1101	LMU	O5B-C1B	3.55	1.51	1.41
3	A	1101	LMU	O5B-C1B	3.54	1.50	1.41
3	A	1101	LMU	C6'-C5'	-3.19	1.41	1.51
3	B	1101	LMU	C6'-C5'	-3.18	1.41	1.51
3	C	1101	LMU	C6'-C5'	-3.17	1.41	1.51
4	Q	701	E2V	O20-C19	2.36	1.40	1.33
4	P	701	E2V	O20-C19	2.36	1.40	1.33
4	R	701	E2V	O20-C19	2.35	1.40	1.33
3	C	1101	LMU	O5'-C1'	2.32	1.47	1.41
3	A	1101	LMU	O5'-C1'	2.32	1.47	1.41
3	B	1101	LMU	O5'-C1'	2.31	1.47	1.41
3	A	1101	LMU	O3'-C3'	2.21	1.48	1.43
3	C	1101	LMU	O3'-C3'	2.20	1.48	1.43
4	R	701	E2V	O20-C21	-2.18	1.40	1.45
3	B	1101	LMU	O3'-C3'	2.18	1.48	1.43
4	P	701	E2V	O20-C21	-2.16	1.40	1.45
4	Q	701	E2V	O20-C21	-2.16	1.40	1.45
4	R	701	E2V	O23-C24	2.12	1.40	1.34
4	P	701	E2V	O23-C24	2.10	1.40	1.34
4	Q	701	E2V	O23-C24	2.10	1.40	1.34
3	C	1101	LMU	C3'-C2'	-2.07	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1101	LMU	C3'-C2'	-2.07	1.47	1.52
3	A	1101	LMU	C3'-C2'	-2.06	1.47	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	701	E2V	O23-C24-C25	3.94	120.00	111.48
4	P	701	E2V	O23-C24-C25	3.93	119.99	111.48
4	R	701	E2V	O23-C24-C25	3.92	119.95	111.48
4	R	701	E2V	C22-O23-C24	-2.88	113.62	117.78
4	Q	701	E2V	C22-O23-C24	-2.88	113.63	117.78
4	P	701	E2V	C22-O23-C24	-2.86	113.65	117.78
4	Q	701	E2V	O20-C19-C18	2.66	119.94	111.83
4	R	701	E2V	O20-C19-C18	2.65	119.91	111.83
4	P	701	E2V	O20-C19-C18	2.65	119.90	111.83
4	Q	701	E2V	O23-C22-C21	2.31	111.53	106.21
4	P	701	E2V	O23-C22-C21	2.31	111.51	106.21
4	R	701	E2V	O23-C22-C21	2.28	111.45	106.21
3	A	1101	LMU	C1B-O1B-C4'	-2.17	112.83	117.98
3	C	1101	LMU	C1B-O1B-C4'	-2.17	112.84	117.98
3	B	1101	LMU	C1B-O1B-C4'	-2.17	112.84	117.98

There are no chirality outliers.

All (132) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	P	701	E2V	C18-C19-O20-C21
4	P	701	E2V	O42-C19-O20-C21
4	P	701	E2V	O20-C21-C22-O23
4	P	701	E2V	C25-C24-O23-C22
4	P	701	E2V	O40-C24-O23-C22
4	Q	701	E2V	C18-C19-O20-C21
4	Q	701	E2V	O42-C19-O20-C21
4	Q	701	E2V	O20-C21-C22-O23
4	Q	701	E2V	C25-C24-O23-C22
4	Q	701	E2V	O40-C24-O23-C22
4	R	701	E2V	C18-C19-O20-C21
4	R	701	E2V	O42-C19-O20-C21
4	R	701	E2V	O20-C21-C22-O23
4	R	701	E2V	C25-C24-O23-C22
4	R	701	E2V	O40-C24-O23-C22
5	P	702	PLM	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	Q	702	PLM	O2-C1-C2-C3
5	R	702	PLM	O2-C1-C2-C3
3	A	1101	LMU	O5'-C5'-C6'-O6'
3	B	1101	LMU	O5'-C5'-C6'-O6'
3	C	1101	LMU	O5'-C5'-C6'-O6'
3	A	1101	LMU	C4'-C5'-C6'-O6'
3	B	1101	LMU	C4'-C5'-C6'-O6'
3	C	1101	LMU	C4'-C5'-C6'-O6'
3	A	1101	LMU	C3'-C4'-O1B-C1B
3	B	1101	LMU	C3'-C4'-O1B-C1B
3	C	1101	LMU	C3'-C4'-O1B-C1B
3	A	1101	LMU	C7-C8-C9-C10
3	B	1101	LMU	C7-C8-C9-C10
3	C	1101	LMU	C7-C8-C9-C10
3	A	1101	LMU	O1'-C1-C2-C3
3	B	1101	LMU	O1'-C1-C2-C3
3	C	1101	LMU	O1'-C1-C2-C3
3	A	1101	LMU	C4-C5-C6-C7
3	B	1101	LMU	C4-C5-C6-C7
3	C	1101	LMU	C4-C5-C6-C7
4	P	701	E2V	C07-C08-C09-C10
4	Q	701	E2V	C07-C08-C09-C10
4	R	701	E2V	C07-C08-C09-C10
4	R	701	E2V	C30-C31-C32-C33
4	P	701	E2V	C30-C31-C32-C33
4	Q	701	E2V	C30-C31-C32-C33
4	R	701	E2V	C15-C16-C17-C18
4	P	701	E2V	C15-C16-C17-C18
4	Q	701	E2V	C15-C16-C17-C18
4	P	701	E2V	C02-C03-C04-C05
4	Q	701	E2V	C02-C03-C04-C05
4	R	701	E2V	C02-C03-C04-C05
4	P	701	E2V	C04-C05-C06-C07
4	Q	701	E2V	C04-C05-C06-C07
4	R	701	E2V	C04-C05-C06-C07
4	P	701	E2V	C13-C14-C15-C16
4	Q	701	E2V	C13-C14-C15-C16
4	R	701	E2V	C13-C14-C15-C16
3	A	1101	LMU	C5'-C4'-O1B-C1B
3	C	1101	LMU	C5'-C4'-O1B-C1B
3	B	1101	LMU	C5'-C4'-O1B-C1B
4	R	701	E2V	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
4	P	701	E2V	C10-C11-C12-C13
4	Q	701	E2V	C10-C11-C12-C13
4	R	701	E2V	C10-C11-C12-C13
4	P	701	E2V	C16-C17-C18-C19
4	P	701	E2V	C24-C25-C26-C27
4	Q	701	E2V	C16-C17-C18-C19
4	Q	701	E2V	C24-C25-C26-C27
4	R	701	E2V	C24-C25-C26-C27
3	A	1101	LMU	C2-C3-C4-C5
3	B	1101	LMU	C2-C3-C4-C5
3	C	1101	LMU	C2-C3-C4-C5
4	P	701	E2V	C25-C26-C27-C28
4	Q	701	E2V	C25-C26-C27-C28
4	R	701	E2V	C25-C26-C27-C28
4	R	701	E2V	C28-C29-C30-C31
4	P	701	E2V	C11-C12-C13-C14
4	P	701	E2V	C28-C29-C30-C31
4	Q	701	E2V	C28-C29-C30-C31
4	Q	701	E2V	C11-C12-C13-C14
4	R	701	E2V	C11-C12-C13-C14
5	R	702	PLM	C2-C3-C4-C5
5	P	702	PLM	C2-C3-C4-C5
5	Q	702	PLM	C2-C3-C4-C5
4	P	701	E2V	C29-C30-C31-C32
4	Q	701	E2V	C29-C30-C31-C32
4	R	701	E2V	C29-C30-C31-C32
4	P	701	E2V	C03-C04-C05-C06
4	Q	701	E2V	C03-C04-C05-C06
4	R	701	E2V	C03-C04-C05-C06
3	A	1101	LMU	C1-C2-C3-C4
3	B	1101	LMU	C1-C2-C3-C4
3	C	1101	LMU	C1-C2-C3-C4
3	A	1101	LMU	C6-C7-C8-C9
3	B	1101	LMU	C6-C7-C8-C9
3	C	1101	LMU	C6-C7-C8-C9
4	Q	701	E2V	C08-C09-C10-C11
4	P	701	E2V	C08-C09-C10-C11
4	R	701	E2V	C08-C09-C10-C11
5	P	702	PLM	C9-CA-CB-CC
5	Q	702	PLM	C9-CA-CB-CC
5	R	702	PLM	C9-CA-CB-CC
4	P	701	E2V	O20-C21-C22-C41

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Mol	Chain	Res	Type	Atoms
4	Q	701	E2V	O20-C21-C22-C41
4	R	701	E2V	O20-C21-C22-C41
4	P	701	E2V	C36-C37-C38-C39
4	Q	701	E2V	C36-C37-C38-C39
4	R	701	E2V	C36-C37-C38-C39
5	P	702	PLM	C7-C8-C9-CA
5	Q	702	PLM	C7-C8-C9-CA
5	R	702	PLM	C7-C8-C9-CA
4	P	701	E2V	C32-C33-C34-C35
4	R	701	E2V	C32-C33-C34-C35
4	Q	701	E2V	C32-C33-C34-C35
4	P	701	E2V	C09-C10-C11-C12
4	Q	701	E2V	C09-C10-C11-C12
4	R	701	E2V	C09-C10-C11-C12
3	A	1101	LMU	C4B-C5B-C6B-O6B
3	B	1101	LMU	C4B-C5B-C6B-O6B
3	C	1101	LMU	C4B-C5B-C6B-O6B
4	P	701	E2V	C01-C02-C03-C04
4	Q	701	E2V	C01-C02-C03-C04
4	R	701	E2V	C01-C02-C03-C04
4	P	701	E2V	C35-C36-C37-C38
4	Q	701	E2V	C35-C36-C37-C38
4	R	701	E2V	C35-C36-C37-C38
4	P	701	E2V	C12-C13-C14-C15
4	Q	701	E2V	C12-C13-C14-C15
4	R	701	E2V	C12-C13-C14-C15
5	P	702	PLM	C5-C6-C7-C8
5	Q	702	PLM	C5-C6-C7-C8
5	R	702	PLM	C5-C6-C7-C8
4	P	701	E2V	O23-C24-C25-C26
4	Q	701	E2V	O23-C24-C25-C26
4	R	701	E2V	O23-C24-C25-C26

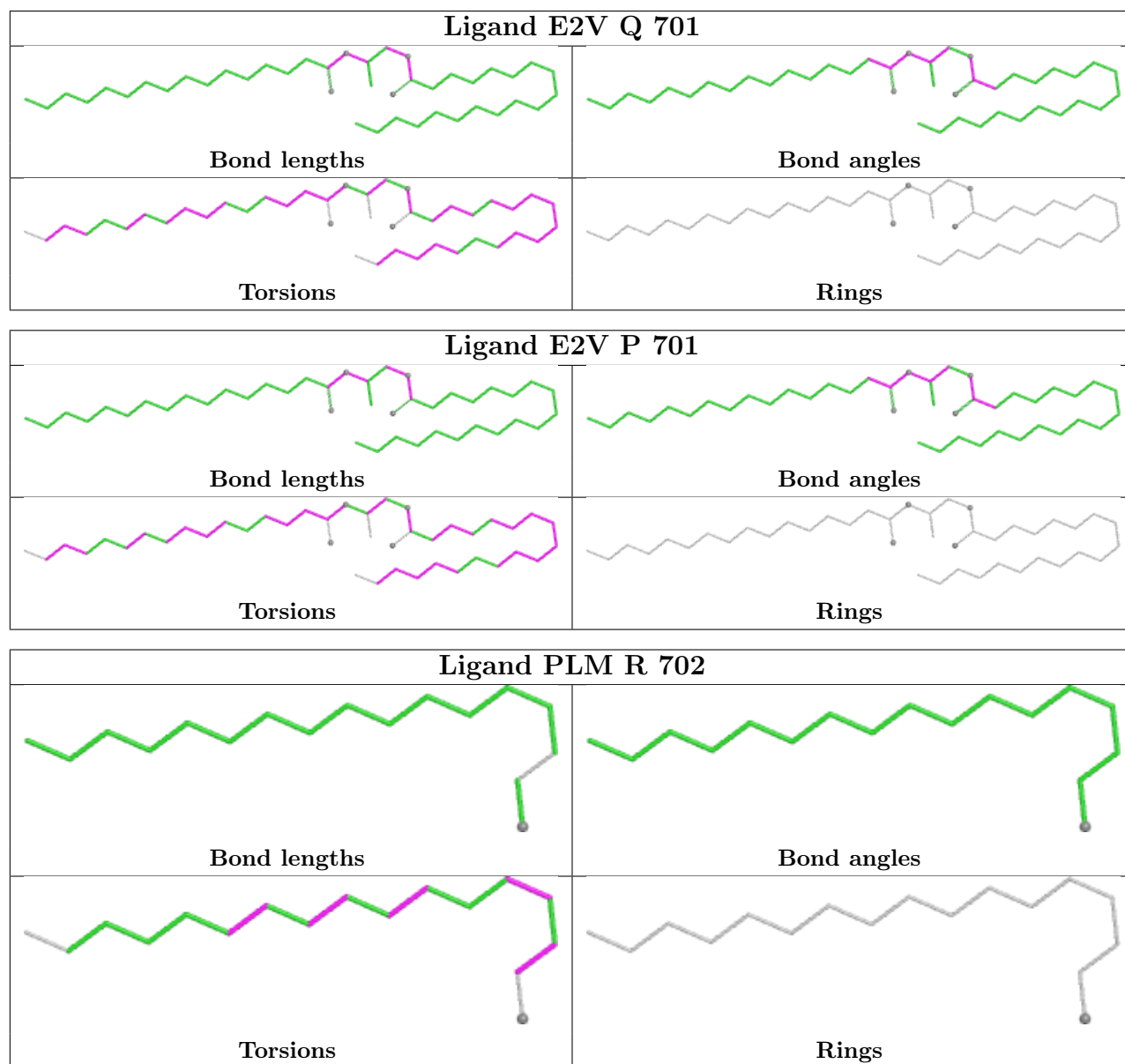
There are no ring outliers.

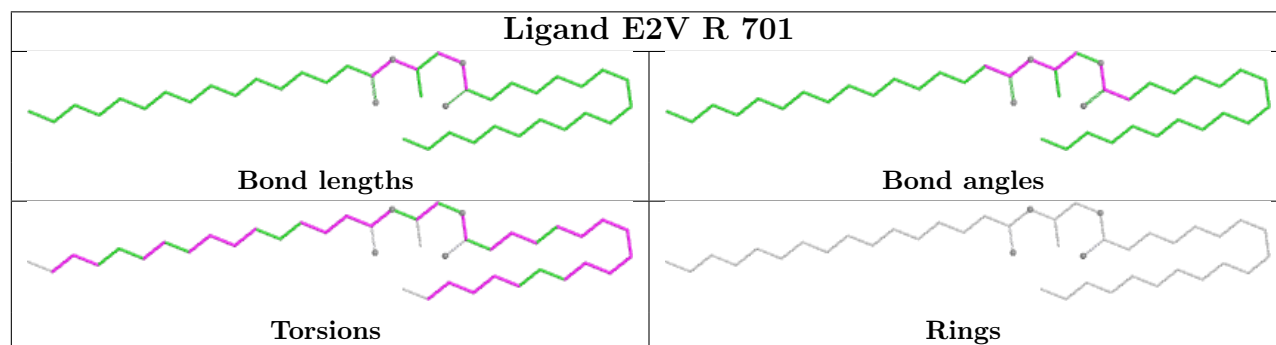
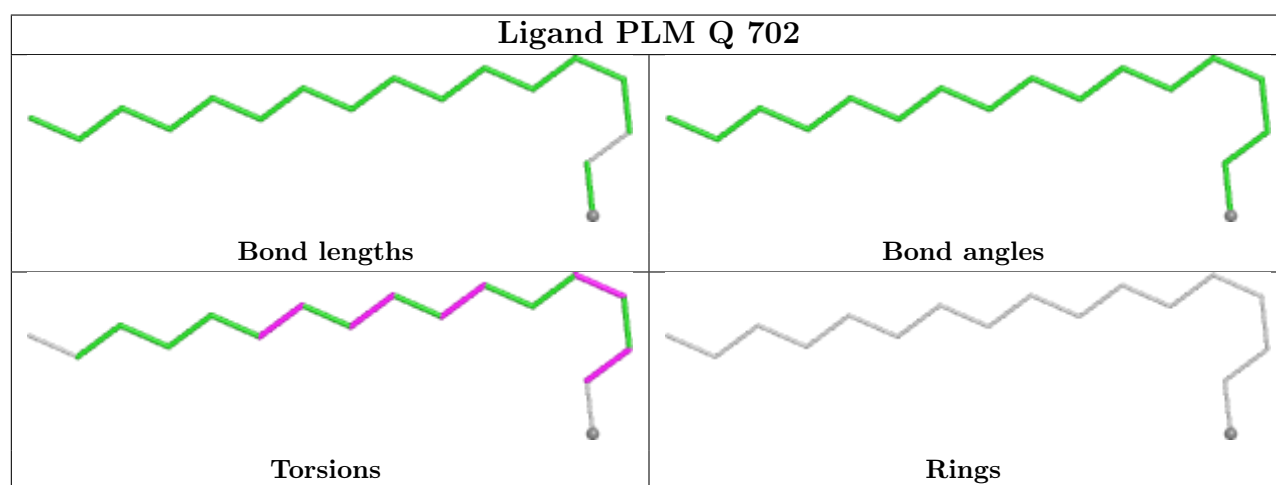
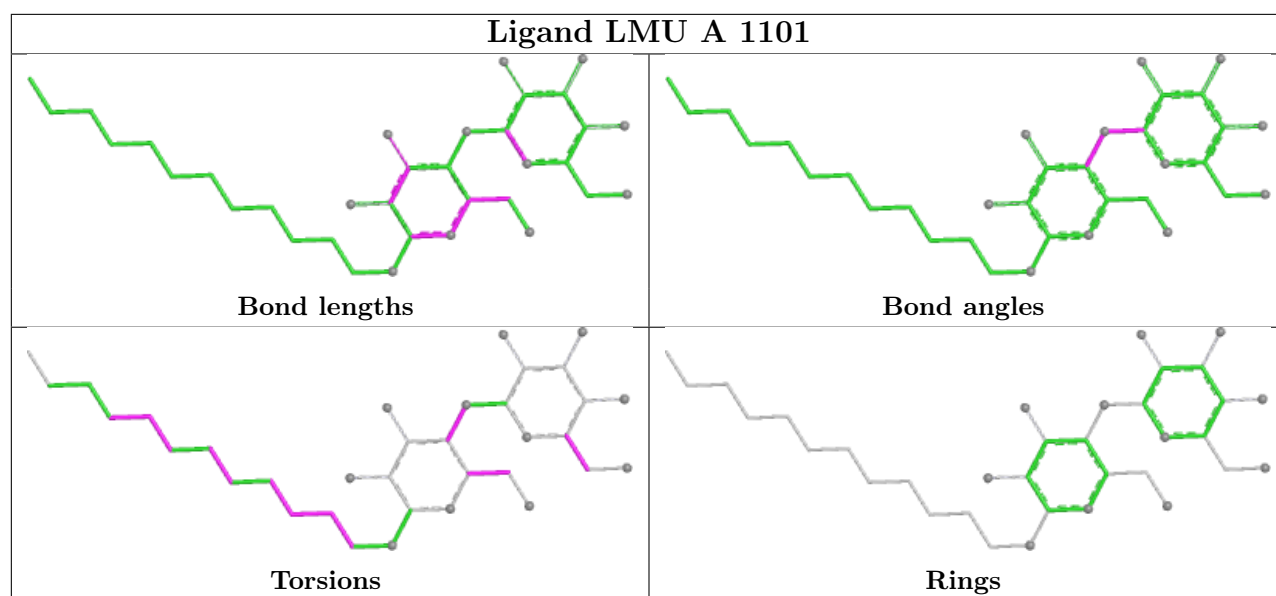
3 monomers are involved in 4 short contacts:

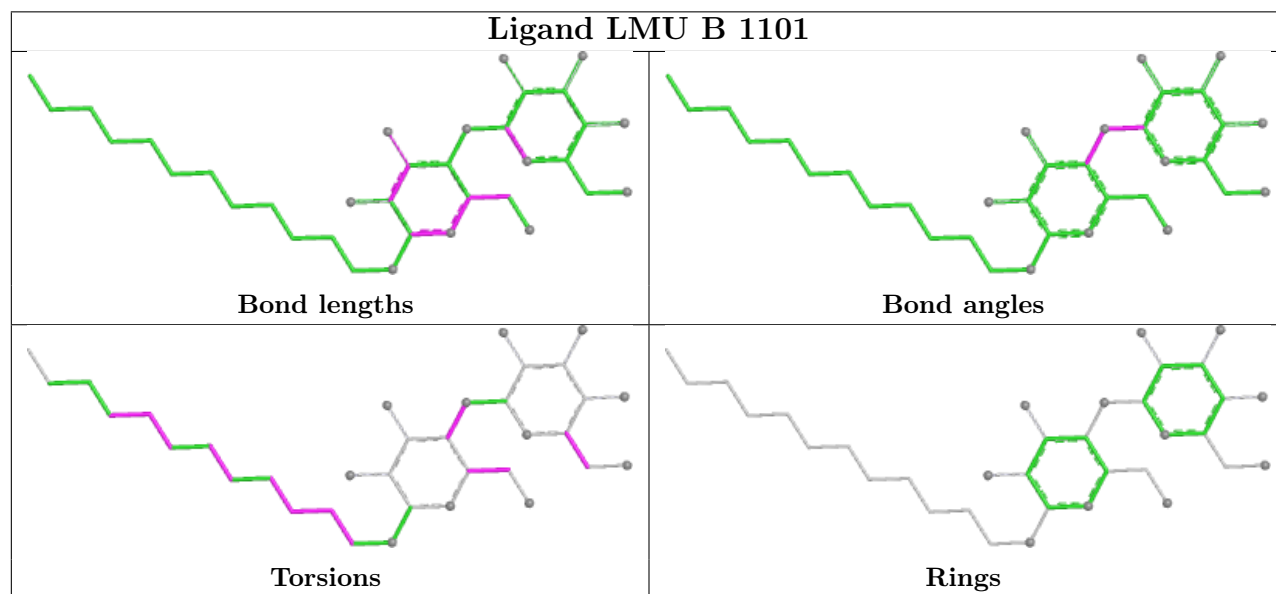
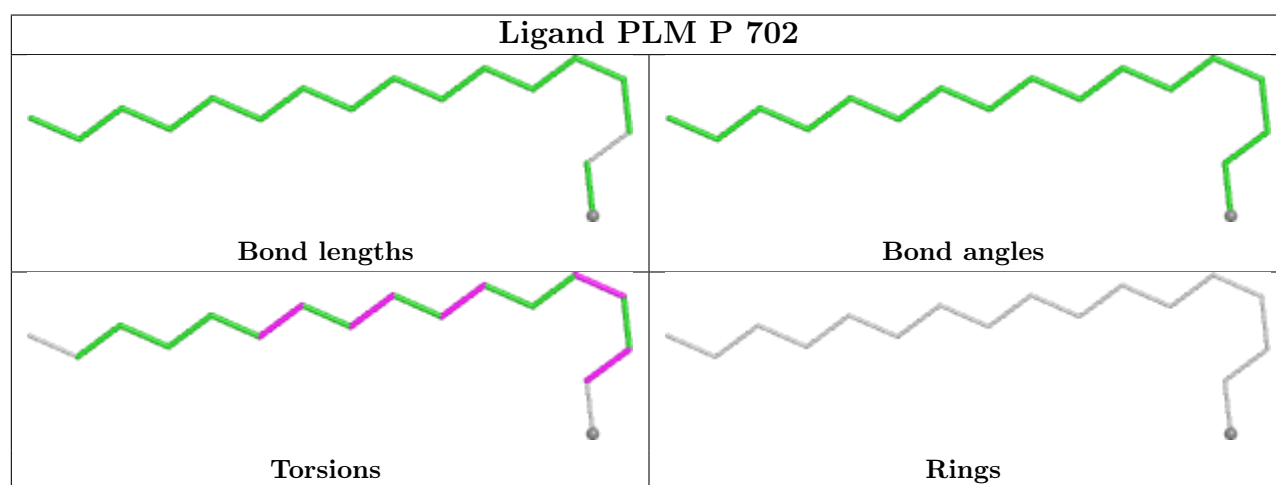
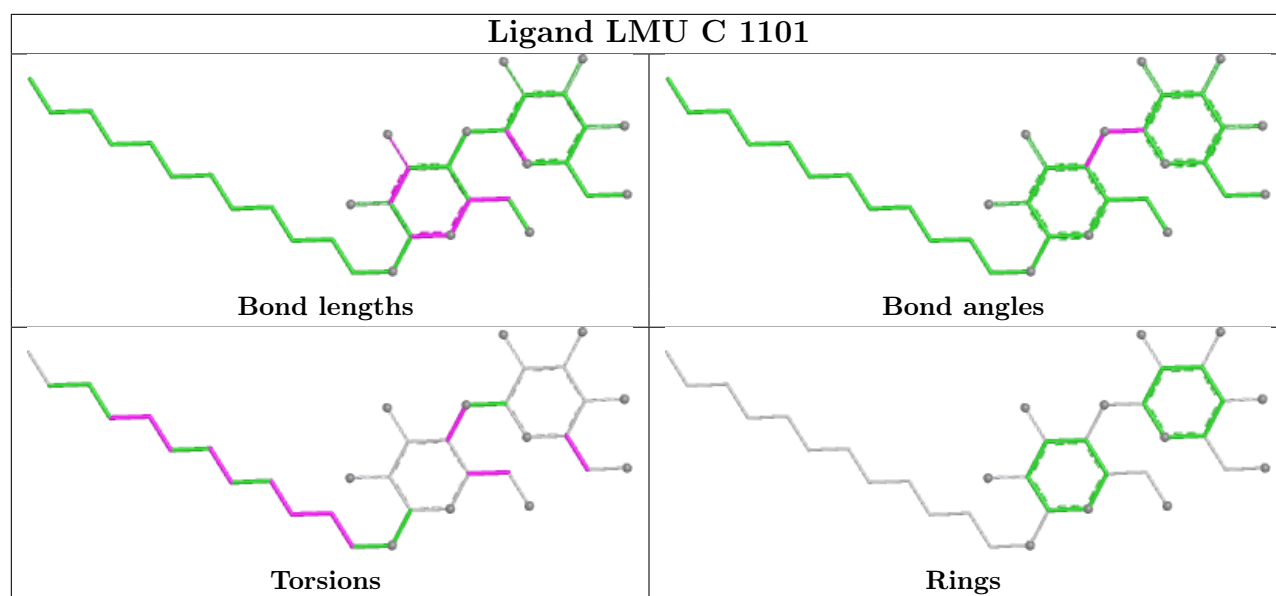
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1101	LMU	2	0
3	C	1101	LMU	1	0
3	B	1101	LMU	1	0

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.

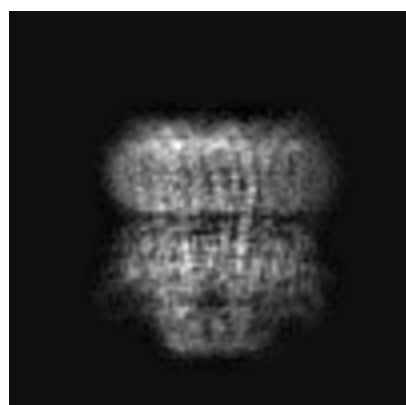
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21363. These allow visual inspection of the internal detail of the map and identification of artifacts.

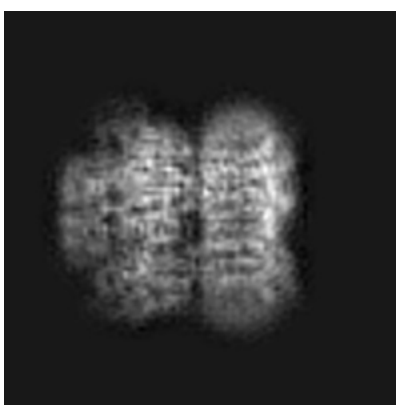
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

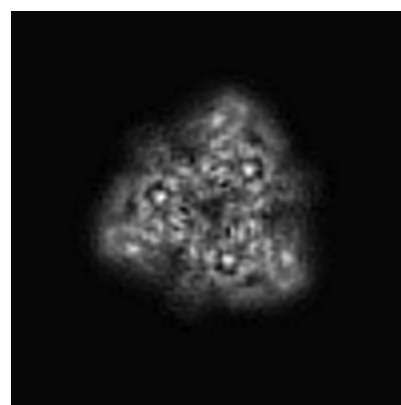
#### 6.1.1 Primary map



X



Y

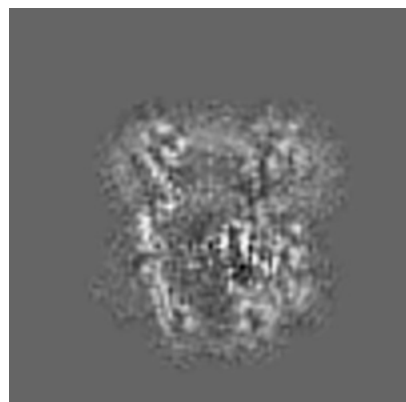


Z

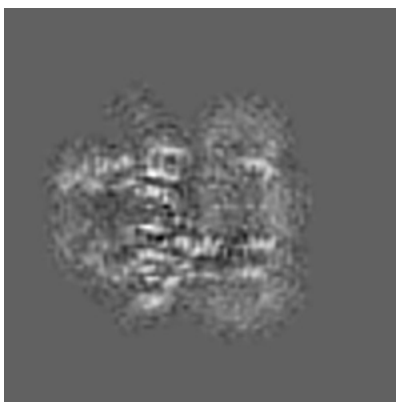
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

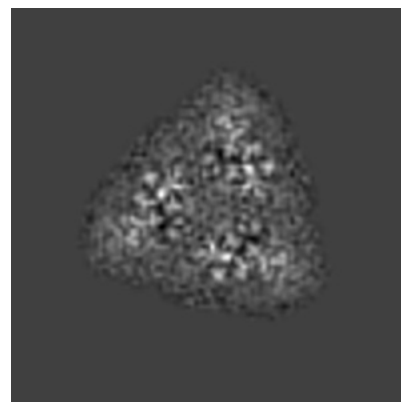
#### 6.2.1 Primary map



X Index: 70



Y Index: 70



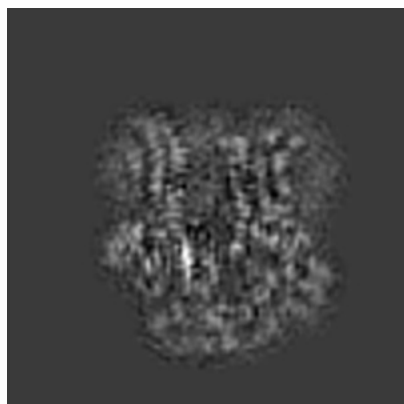
Z Index: 70



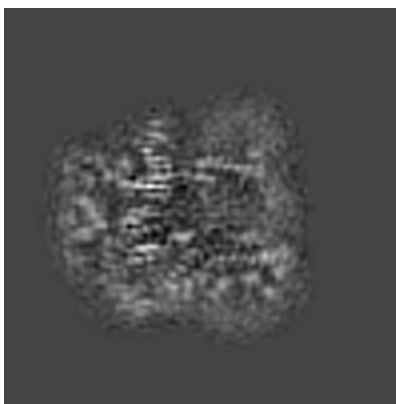
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

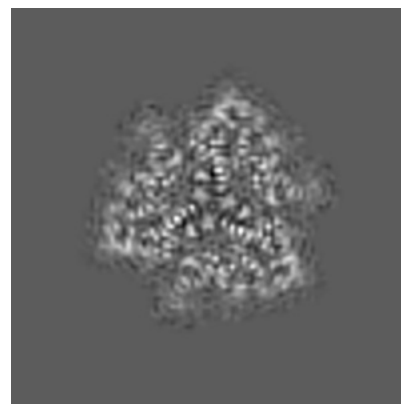
### 6.3.1 Primary map



X Index: 77



Y Index: 63

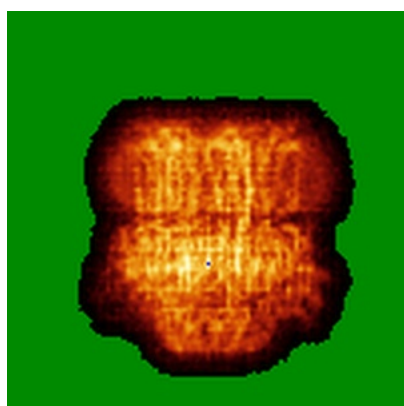


Z Index: 49

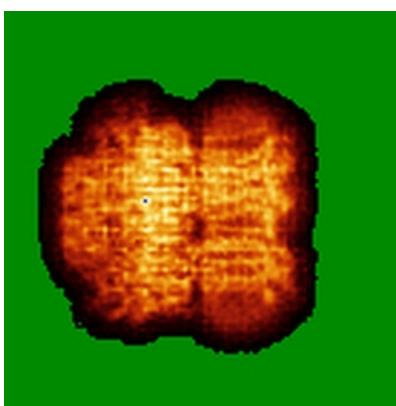
The images above show the largest variance slices of the map in three orthogonal directions.

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

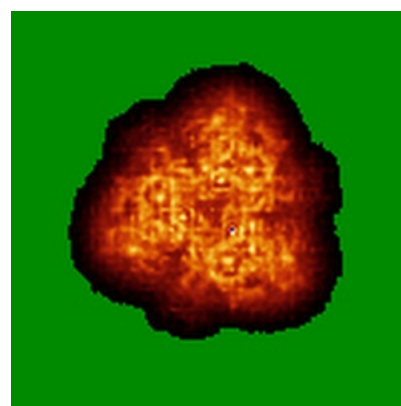
### 6.4.1 Primary map



X



Y

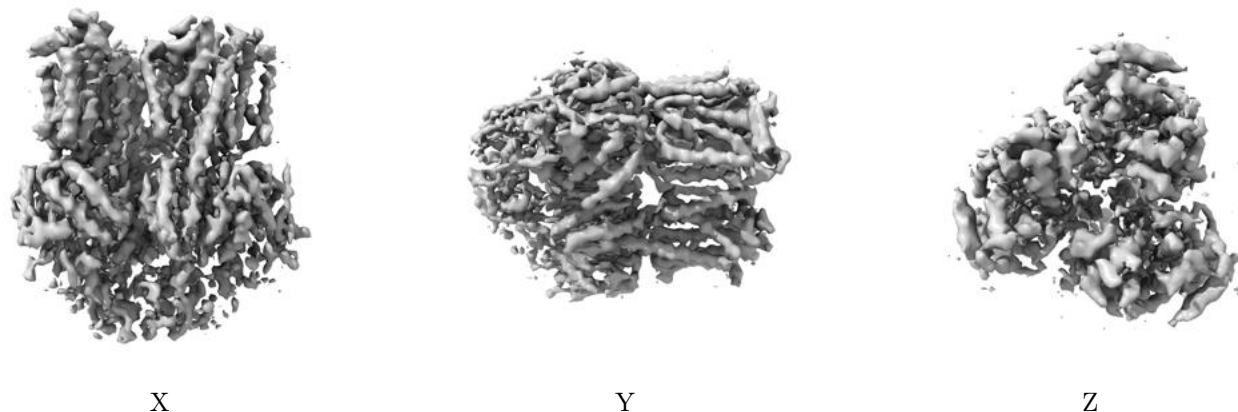


Z

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 0.158. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

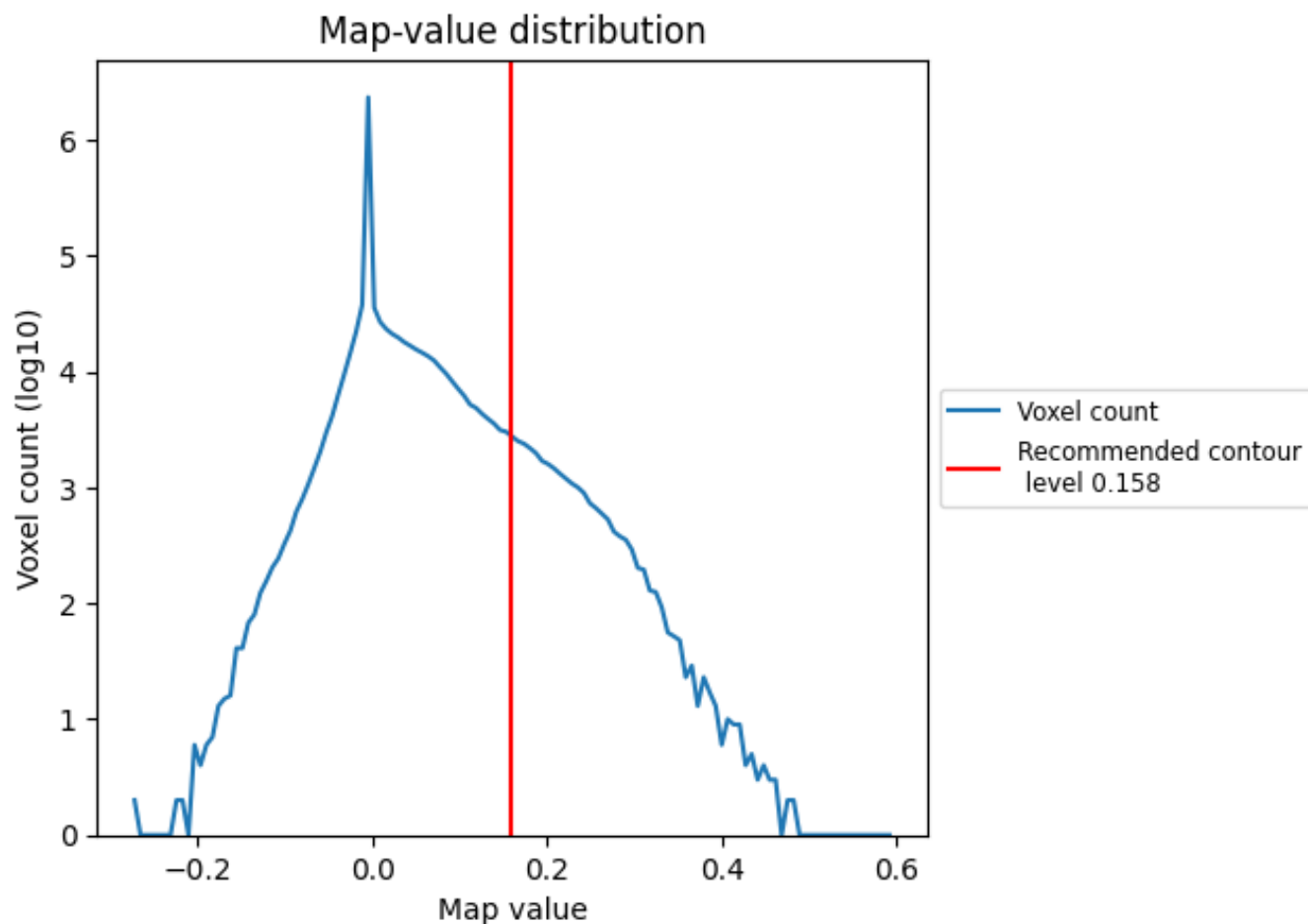
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

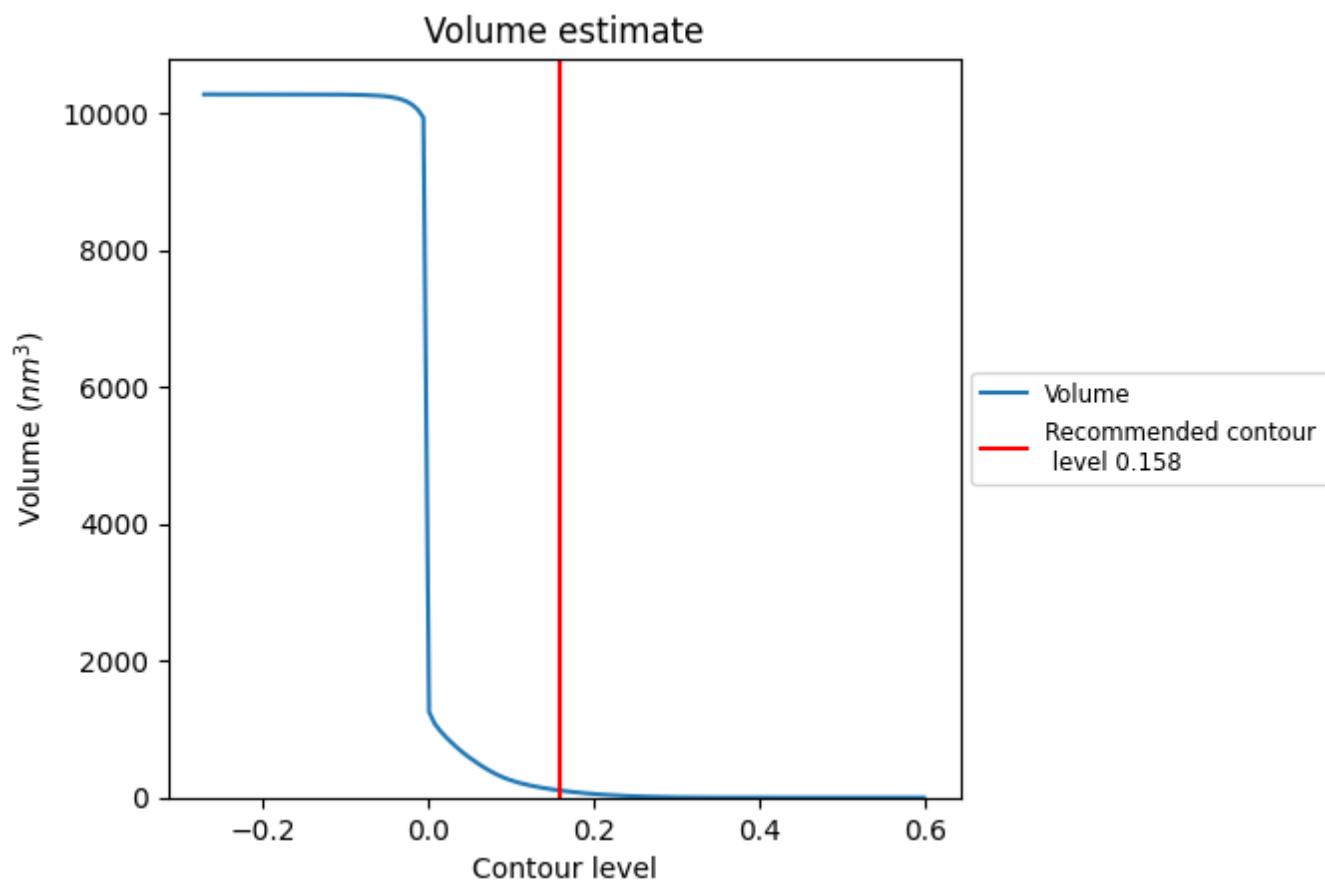
This section contains the results of statistical analysis of the map.

### 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.

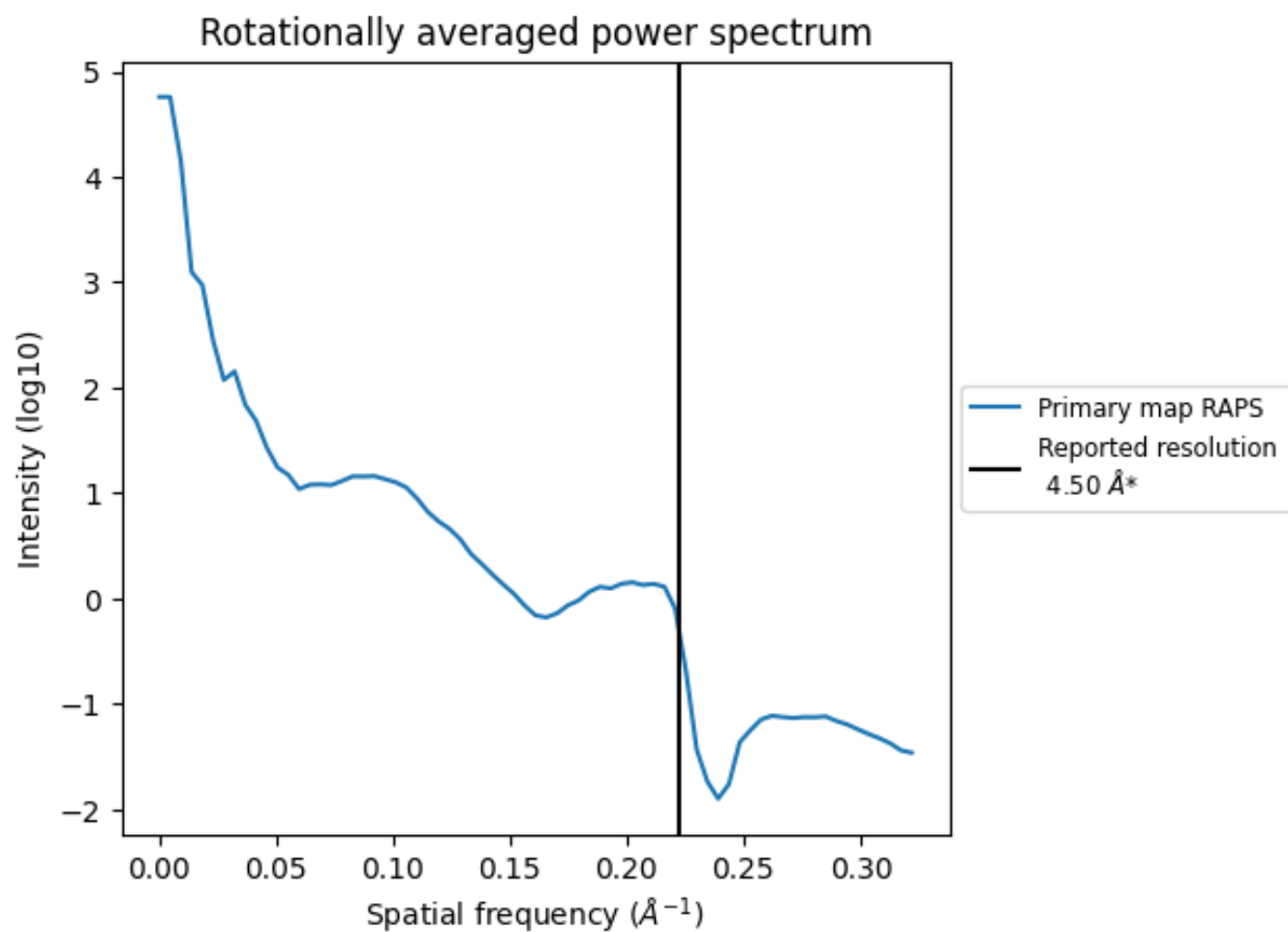
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 105 nm<sup>3</sup>; this corresponds to an approximate mass of 95 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of 0.222 Å<sup>-1</sup>

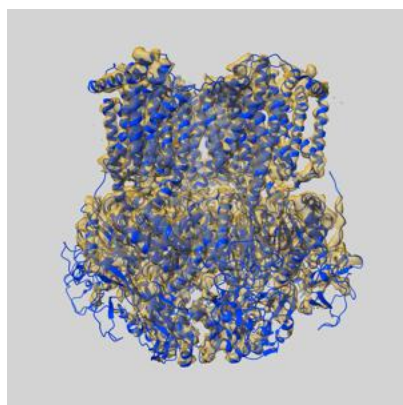
## 8 Fourier-Shell correlation ⓘ

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

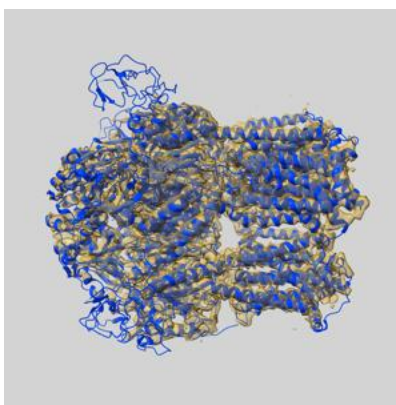
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21363 and PDB model 6VEJ. Per-residue inclusion information can be found in section [3](#) on page [7](#).

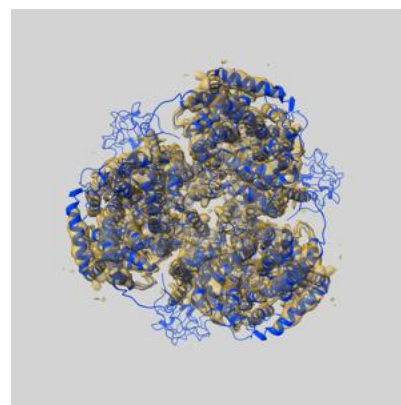
### 9.1 Map-model overlay [i](#)



X



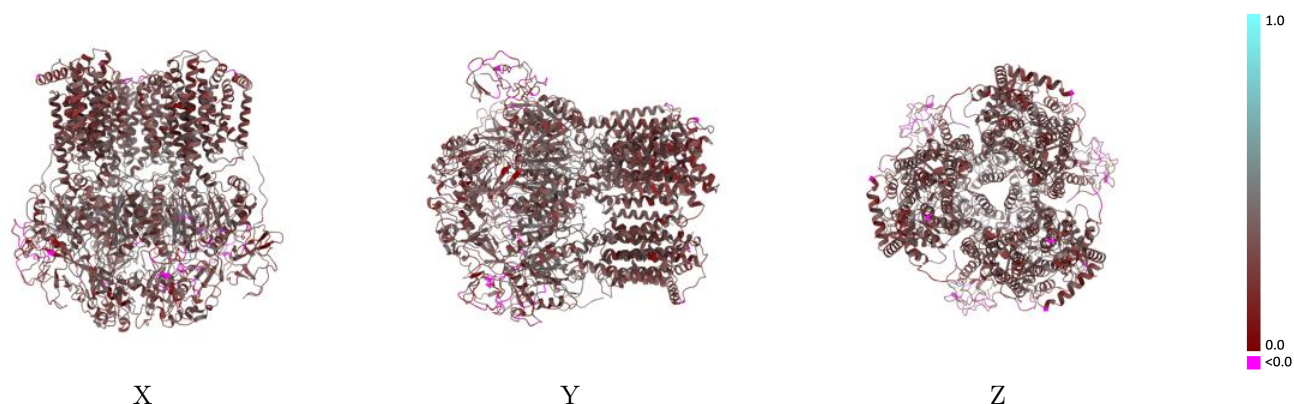
Y



Z

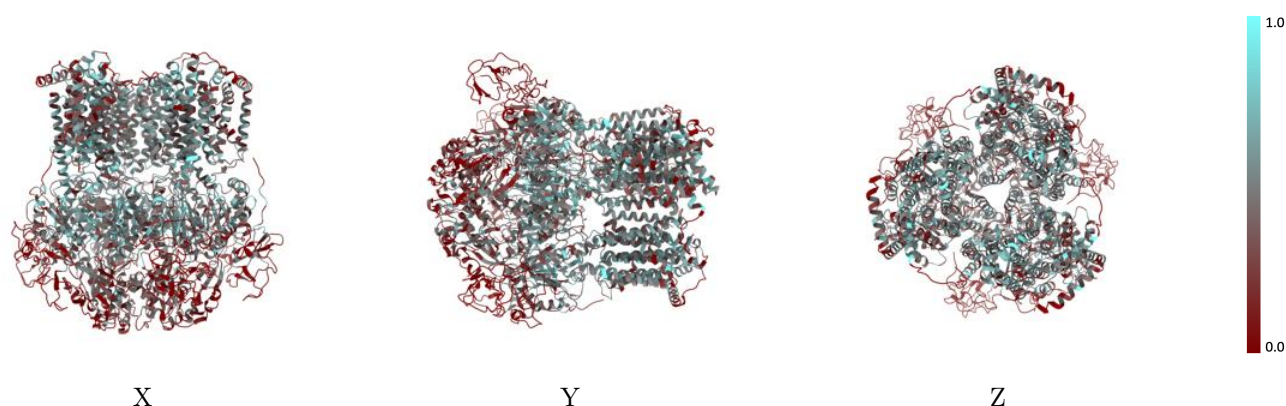
The images above show the 3D surface view of the map at the recommended contour level 0.158 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

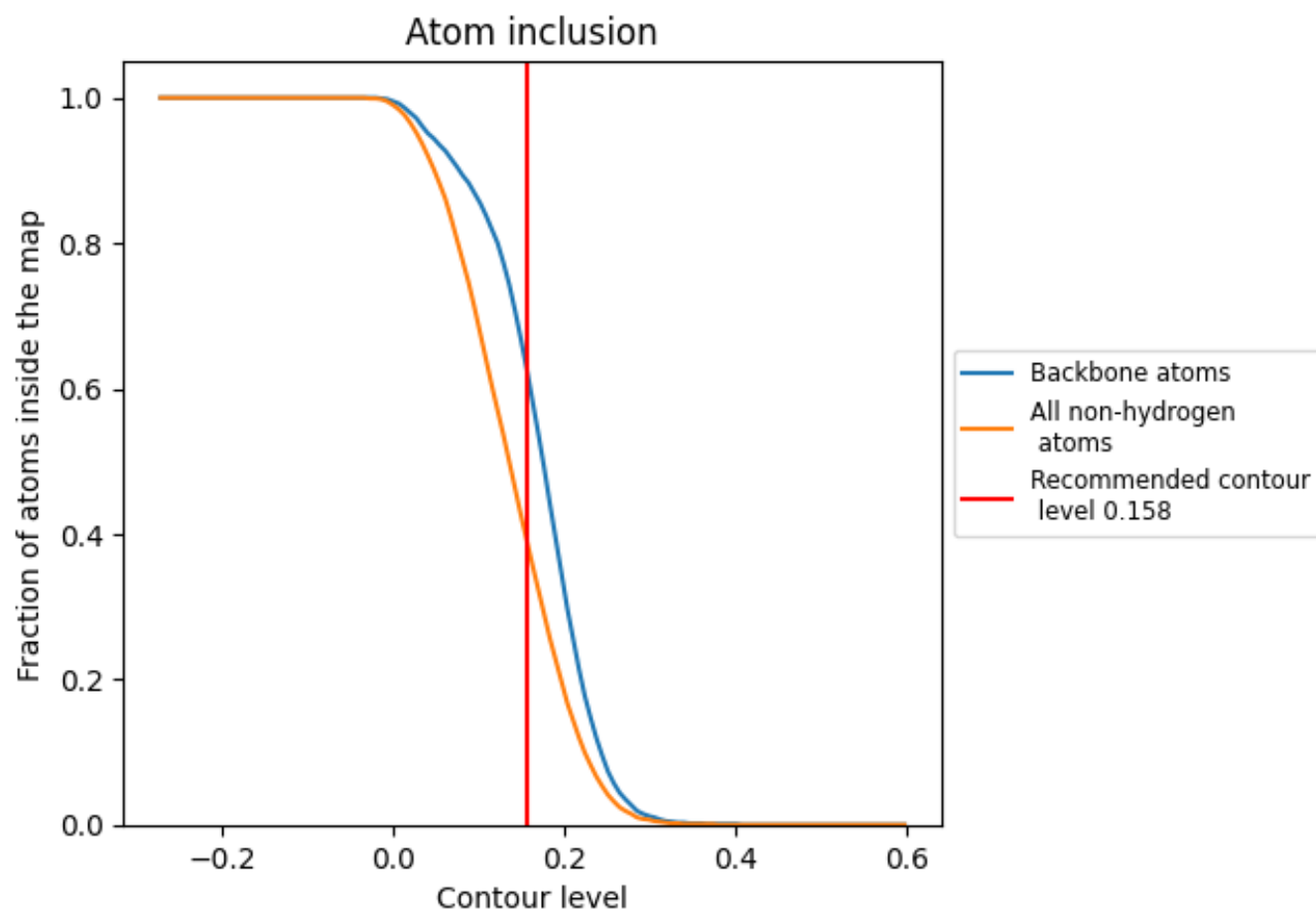
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.158).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 38% 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 (0.158) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.3850	<div><div></div></div> 0.3130
A	<div><div></div></div> 0.4410	<div><div></div></div> 0.3260
B	<div><div></div></div> 0.4450	<div><div></div></div> 0.3270
C	<div><div></div></div> 0.4400	<div><div></div></div> 0.3270
P	<div><div></div></div> 0.1120	<div><div></div></div> 0.2460
Q	<div><div></div></div> 0.1160	<div><div></div></div> 0.2470
R	<div><div></div></div> 0.1170	<div><div></div></div> 0.2500

1.0

0.0

<0.0