



Preliminary Full wwPDB EM Validation Report ⓘ

Mar 25, 2023 – 02:53 PM EDT

This wwPDB validation report is NOT for manuscript review

This is a Preliminary Full wwPDB EM Validation Report.

This report is produced by the standalone wwPDB validation server.
The structure in question has not been deposited to the wwPDB.
This report should not be submitted to journals.

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.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

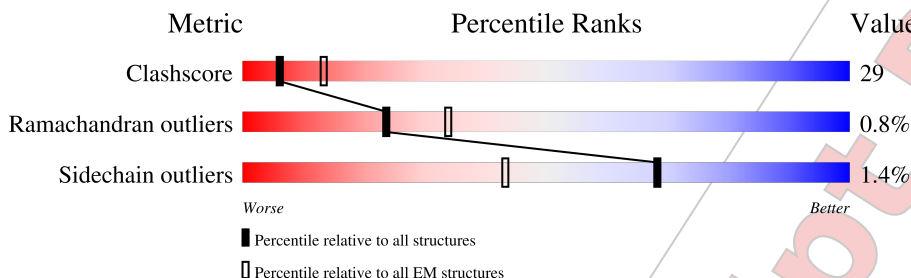
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	619	<div> <div>13%</div> <div>46%</div> <div>53%</div> <div>.</div> </div>
1	C	619	<div> <div>15%</div> <div>47%</div> <div>52%</div> <div>.</div> </div>
2	B	636	<div> <div>8%</div> <div>47%</div> <div>51%</div> <div>.</div> </div>
2	D	636	<div> <div>8%</div> <div>48%</div> <div>50%</div> <div>.</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 20730 atoms, of which 290 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.

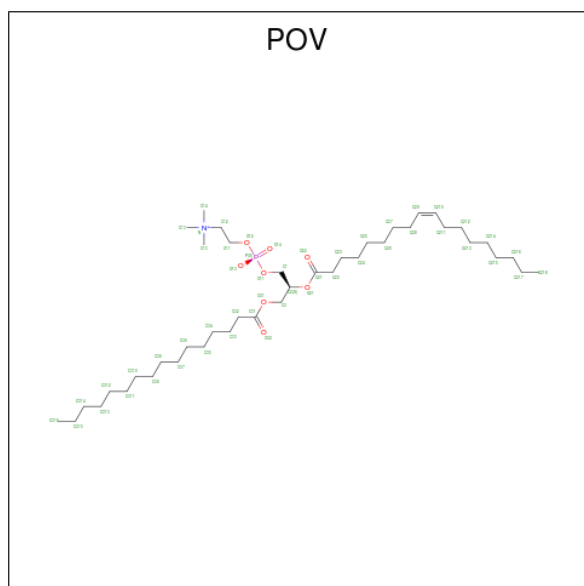
- Molecule 1 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	619	Total	C	N	O	S	0	0
			4990	3248	829	889	24		
1	C	619	Total	C	N	O	S	0	0
			4990	3248	829	889	24		

- Molecule 2 is a protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	636	Total	C	N	O	S	0	0
			5116	3326	850	914	26		
2	D	636	Total	C	N	O	S	0	0
			5116	3326	850	914	26		

- Molecule 3 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: C₄₂H₈₂NO₈P).



Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	H	N	O	P	0
			62	18	34	1	8	1	
3	B	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	
3	C	1	Total	C	H	N	O	P	0
			62	18	34	1	8	1	
3	D	1	Total	C	H	N	O	P	0
			134	42	82	1	8	1	

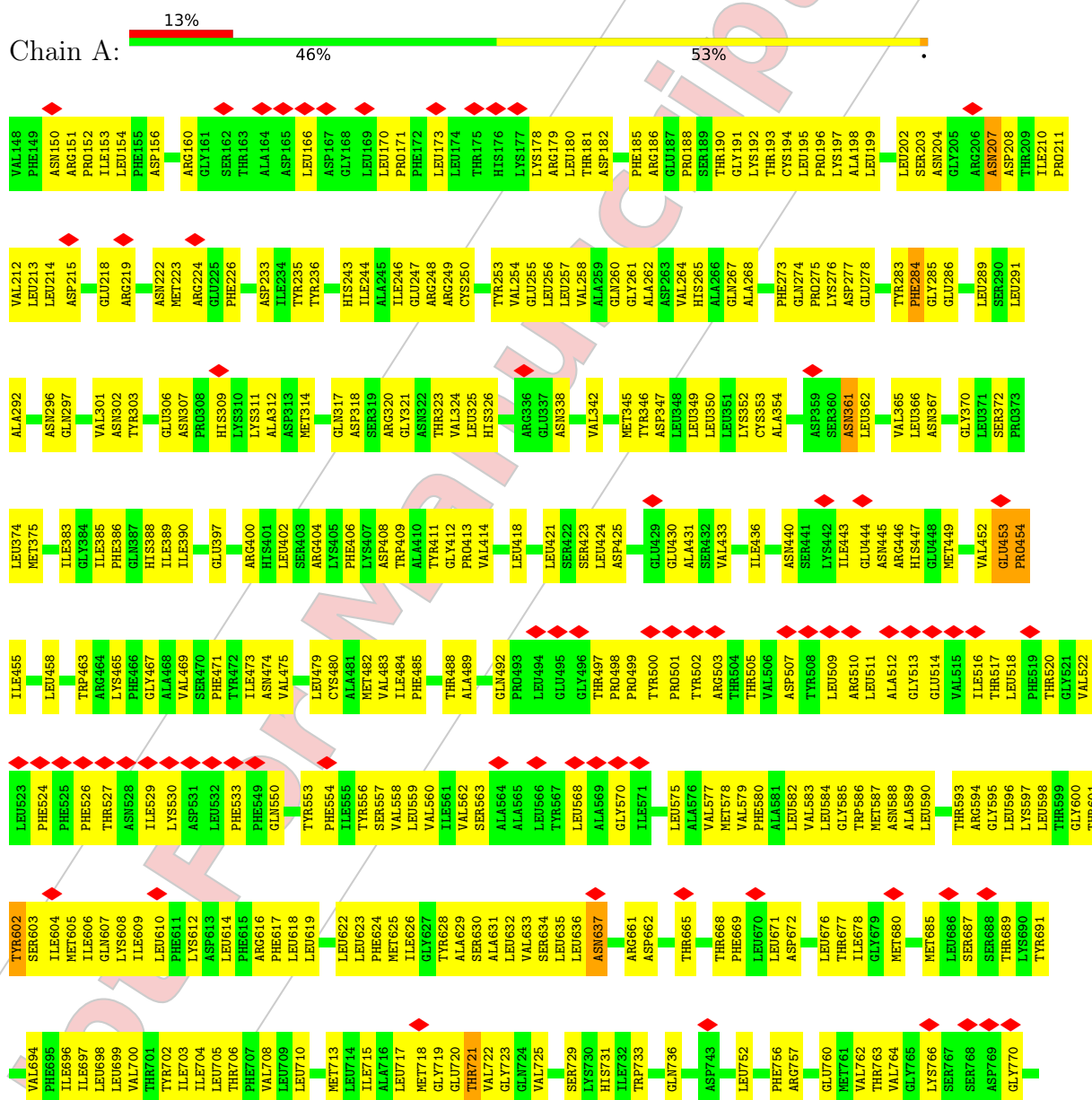
- Molecule 4 is a ligand with the chemical component id HCO but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for HCO. Consequently no firm identification of ligand chemistry can be made. Once the structure is annotated then an identification and diagram will be given here.

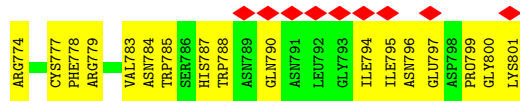
Mol	Chain	Residues	Atoms						AltConf
4	B	1	Total	C	F	H	N	O	0
			63	26	3	29	3	2	
4	D	1	Total	C	F	H	N	O	0
			63	26	3	29	3	2	

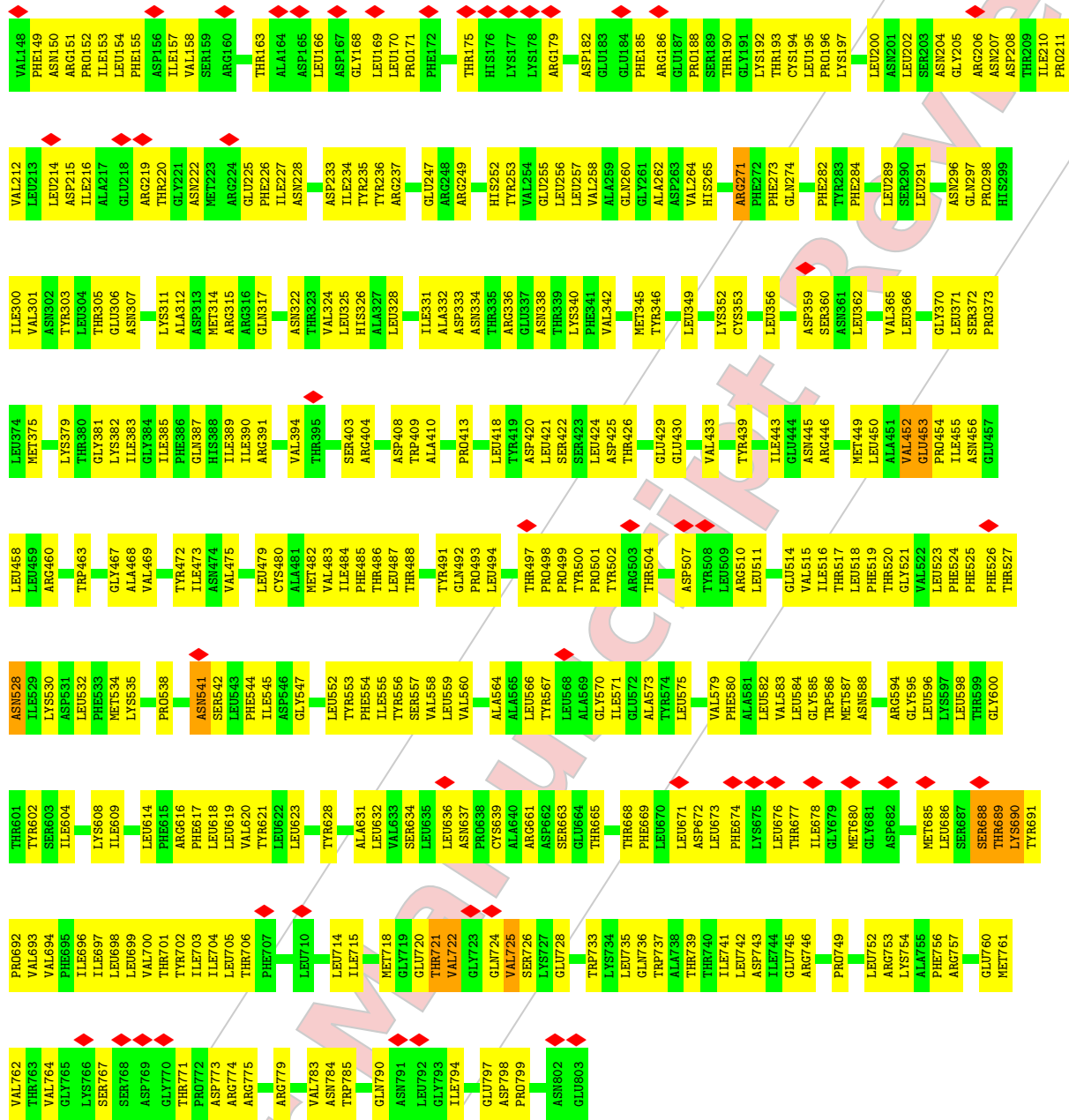
3 Residue-property plots

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.

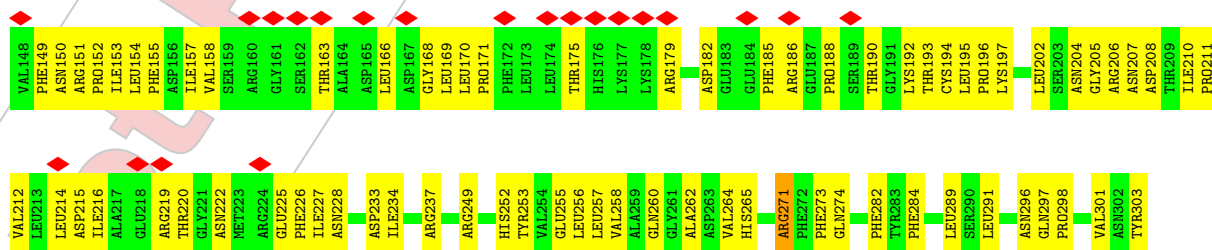
• Molecule 1:







• Molecule 2:



GLY770	THR771	PRO772	ASP773	ARG774	ARG775	ARG779	VAL783	ASN784	TRP785	GLN790	ASN791	LEU792	GLY793	ILE794	GLU797	ASP798	PRO799	ASN802	GLU803	LEU304	THR305	GLY381	LYS382	GLY384	ILE385	PHE386	GLN387	HIS388	ILE389	ILE390	ARG391	VAL394	THR395	ASP398	SER403	ARG404	ASP408	TRP409	ALA410	TYR411	GLY412	PRO413	GLU418	TYR419	ASP420	LEU421	SER422	SER423	LEU424	ASP425	THR426	GLU429	GLU430	VAL433	TYR439	ILE443	GLU444	ASN445	ARG446	MET449	LEU450	ALA451	VAL452	GLU453	PRO454	ILE455	ASN456	GLU457	LEU458	LYS379
LEU696	ILE697	LEU698	LEU699	VAL700	THR701	TYR702	ILE703	ILE704	LEU705	THR706	PHE707	LEU714	ILE715	MET718	GLY719	THR721	VAL722	GLY723	GLN724	VAL725	SER726	LYS727	GLU728	TRP733	LYS734	LEU735	GLN736	TRP737	ALA738	THR739	THR740	ILE741	LEU742	ASP743	ARG746	PRO749	LEU752	ARG753	LYS754	ALA755	PHE756	ARG757	GLU760	MET761	VAL762	THR763	VAL764	SER767	SER768	ASP769																				
ASN528	ILE529	ASP531	LEU532	PHE533	MET534	LYS535	PRO538	ASN541	SER542	LEU543	PHE544	ILE545	ASP546	GLY547	LEU552	TYR553	PHE554	ILE555	TYR556	SER557	VAL558	LEU559	VAL560	ALA564	ALA565	LEU566	TYR567	LEU568	ILE571	GLU572	ALA573	TYR574	LEU575	ALA576	VAL579	PHE580	ALA581	LEU582	VAL583	LEU584	GLY585	TRP586	MET587	ASN588	ARG594	GLY595	LEU596	GLY600	ILE604																					
LEU459	ARG460	TRP463	GLY467	ALA468	VAL469	TYR472	ILE473	ILE474	ASN474	VAL475	TYR478	LEU479	CYS480	ALA481	MET482	VAL483	ILE484	PHE485	THR486	LEU487	THR488	GLN492	PRO493	LEU494	THR497	PRO498	PRO499	TYR500	PRO501	TYR502	ARG503	THR504	THR505	VAL506	ASP507	TYR508	LEU509	ARG510	LEU511	GLU514	VAL515	ILE516	THR517	LEU518	PHE519	THR520	GLY521	VAL522	LEU523	PHE524	PHE525	PHE526	THR527																	
THR390	GLY381	LYS382	GLY384	ILE385	PHE386	GLN387	HIS388	ILE389	ILE390	ARG391	VAL394	THR395	ASP398	SER403	ARG404	ASP408	TRP409	ALA410	TYR411	GLY412	PRO413	LEU418	TYR419	ASP420	LEU421	SER422	SER423	LEU424	ASP425	THR426	GLU429	GLU430	VAL433	TYR439	ILE443	GLU444	ASN445	ARG446	MET449	LEU450	ALA451	VAL452	GLU453	PRO454	ILE455	ASN456	GLU457	LEU458																						
LEU304	THR305	GLY381	LYS382	GLY384	ILE385	PHE386	GLN387	HIS388	ILE389	ILE390	ARG391	VAL394	THR395	ASP398	SER403	ARG404	ASP408	TRP409	ALA410	TYR411	GLY412	PRO413	LEU418	TYR419	ASP420	LEU421	SER422	SER423	LEU424	ASP425	THR426	GLU429	GLU430	VAL433	TYR439	ILE443	GLU444	ASN445	ARG446	MET449	LEU450	ALA451	VAL452	GLU453	PRO454	ILE455	ASN456	GLU457	LEU458																					
LYS311	ALA312	ASP313	MET314	ARG315	ARG316	GLN317	ASN322	THR323	VAL324	LEU325	HIS326	ALA327	LEU328	ILE331	ALA332	ASP333	ASN334	THR335	ARG336	GLU337	ASN338	THR339	LYS340	PHE341	VAL342	MET345	TYR346	LEU349	LYS352	CYS353	LEU356	ASP359	SER360	ASN361	LEU362	VAL365	LEU366	GLY370	LEU371	SER372	PRO373	LEU374	MET375	LYS379																										

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	Not provided	
Voltage (kV)	Not provided	
Electron dose ($e^-/\text{\AA}^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	Not provided	
Maximum map value	0.877	Depositor
Minimum map value	-0.547	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.114	Depositor
Map size (Å)	265.6, 265.6, 265.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83000004, 0.83000004, 0.83000004	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: HCO, POV

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	0.28	0/5105	0.43	0/6921
1	C	0.28	0/5105	0.43	0/6921
2	B	0.29	0/5234	0.45	0/7095
2	D	0.29	0/5234	0.45	0/7095
All	All	0.29	0/20678	0.44	0/28032

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	2
1	C	0	2
2	B	0	3
2	D	0	3
All	All	0	10

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	284	PHE	Peptide
1	A	453	GLU	Peptide
2	B	688	SER	Peptide
2	B	689	THR	Peptide
2	B	721	THR	Peptide

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Mol	Chain	Res	Type	Group
1	C	284	PHE	Peptide
1	C	453	GLU	Peptide
2	D	688	SER	Peptide
2	D	689	THR	Peptide
2	D	721	THR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4990	0	5056	317	0
1	C	4990	0	5056	303	0
2	B	5116	0	5182	329	0
2	D	5116	0	5182	323	0
3	A	28	34	30	2	0
3	B	52	82	82	4	0
3	C	28	34	30	3	0
3	D	52	82	82	4	0
4	B	34	29	0	1	0
4	D	34	29	0	1	0
All	All	20440	290	20700	1200	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 29.

All (1200) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:LEU:HG	2:B:205:GLY:HA2	1.48	0.96
1:C:661:ARG:HG2	1:C:687:SER:HB2	1.49	0.94
2:D:202:LEU:HG	2:D:205:GLY:HA2	1.48	0.94
1:A:661:ARG:HG2	1:A:687:SER:HB2	1.49	0.92
2:D:524:PHE:HA	3:D:902:POV:H13B	1.54	0.89
2:B:408:ASP:HB2	2:B:418:LEU:HD13	1.55	0.89
2:D:408:ASP:HB2	2:D:418:LEU:HD13	1.55	0.86
1:A:800:GLY:HA3	2:B:235:TYR:HE2	1.40	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:766:LYS:HD2	1:A:770:GLY:HA2	1.57	0.86
1:C:766:LYS:HD2	1:C:770:GLY:HA2	1.57	0.85
2:B:443:ILE:HD11	2:B:541:ASN:HB3	1.58	0.84
2:D:443:ILE:HD11	2:D:541:ASN:HB3	1.58	0.84
1:A:719:GLY:HA2	2:D:722:VAL:HG13	1.61	0.82
2:B:494:LEU:HD21	2:B:575:LEU:HD22	1.60	0.82
2:D:494:LEU:HD21	2:D:575:LEU:HD22	1.60	0.82
1:C:583:VAL:HG21	2:D:698:LEU:HD11	1.63	0.79
2:B:676:LEU:HD11	2:B:699:LEU:HD21	1.66	0.78
1:A:628:TYR:HE1	2:D:583:VAL:HB	1.46	0.78
2:D:390:ILE:HD11	2:D:424:LEU:HD21	1.65	0.77
1:A:800:GLY:N	2:B:236:TYR:OH	2.17	0.77
2:B:524:PHE:HA	3:B:902:POV:H13B	1.67	0.77
2:B:390:ILE:HD11	2:B:424:LEU:HD21	1.65	0.77
2:D:249:ARG:HG2	2:D:297:GLN:HE21	1.51	0.76
1:A:192:LYS:HD3	1:A:197:LYS:HE3	1.68	0.76
2:B:249:ARG:HG2	2:B:297:GLN:HE21	1.51	0.76
1:C:440:ASN:O	1:C:446:ARG:NH2	2.19	0.76
1:C:685:MET:HA	1:C:689:THR:HG21	1.67	0.76
1:C:722:VAL:HG12	2:D:715:ILE:HG23	1.67	0.76
2:D:190:THR:HG23	2:D:192:LYS:H	1.51	0.76
2:D:676:LEU:HD11	2:D:699:LEU:HD21	1.66	0.76
1:A:440:ASN:O	1:A:446:ARG:NH2	2.19	0.75
1:A:685:MET:HA	1:A:689:THR:HG21	1.67	0.75
1:C:192:LYS:HD3	1:C:197:LYS:HE3	1.68	0.75
2:B:190:THR:HG23	2:B:192:LYS:H	1.51	0.75
2:D:527:THR:HG22	2:D:530:LYS:HD2	1.68	0.75
2:D:472:TYR:HA	2:D:475:VAL:HG12	1.68	0.75
2:D:552:LEU:HB3	2:D:588:ASN:HD21	1.51	0.75
2:D:661:ARG:HG3	2:D:665:THR:HG21	1.69	0.74
1:A:637:ASN:HB3	2:D:494:LEU:HD12	1.69	0.74
2:B:206:ARG:O	2:B:253:TYR:OH	2.04	0.74
2:B:552:LEU:HB3	2:B:588:ASN:HD21	1.51	0.74
2:D:206:ARG:O	2:D:253:TYR:OH	2.04	0.74
2:B:527:THR:HG22	2:B:530:LYS:HD2	1.68	0.74
2:B:661:ARG:HG3	2:B:665:THR:HG21	1.69	0.74
2:D:463:TRP:HA	2:D:467:GLY:HA3	1.70	0.74
2:B:472:TYR:HA	2:B:475:VAL:HG12	1.68	0.73
2:B:544:PHE:O	2:B:736:GLN:NE2	2.20	0.73
1:A:800:GLY:HA3	2:B:235:TYR:CE2	2.23	0.73
1:A:630:SER:OG	2:D:486:THR:HG23	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:544:PHE:O	2:D:736:GLN:NE2	2.20	0.72
1:C:665:THR:OG1	1:C:668:THR:OG1	2.08	0.71
2:B:761:MET:HE2	2:B:774:ARG:HE	1.55	0.71
1:A:582:LEU:HD23	2:B:631:ALA:HB2	1.71	0.71
1:A:665:THR:OG1	1:A:668:THR:OG1	2.08	0.71
2:B:463:TRP:HA	2:B:467:GLY:HA3	1.70	0.71
1:C:256:LEU:O	1:C:260:GLN:NE2	2.23	0.71
1:A:412:GLY:N	2:B:247:GLU:OE2	2.24	0.70
1:A:256:LEU:O	1:A:260:GLN:NE2	2.23	0.70
1:C:193:THR:HG22	1:C:194:CYS:H	1.57	0.70
1:A:193:THR:HG22	1:A:194:CYS:H	1.57	0.69
2:D:761:MET:HE2	2:D:774:ARG:HE	1.55	0.69
2:D:154:LEU:HA	2:D:157:ILE:HD12	1.74	0.69
1:A:418:LEU:HD21	1:A:762:VAL:HG11	1.74	0.69
2:D:628:TYR:OH	2:D:698:LEU:O	2.11	0.69
2:D:493:PRO:HB2	2:D:499:PRO:HB3	1.75	0.69
1:A:278:GLU:OE1	1:A:320:ARG:NH2	2.27	0.68
2:B:628:TYR:OH	2:B:698:LEU:O	2.11	0.68
2:D:394:VAL:N	2:D:403:SER:OG	2.27	0.68
1:A:408:ASP:OD2	1:A:779:ARG:NH1	2.26	0.68
1:C:151:ARG:HB3	1:C:152:PRO:HD3	1.76	0.68
1:C:278:GLU:OE1	1:C:320:ARG:NH2	2.27	0.68
1:C:408:ASP:OD2	1:C:779:ARG:NH1	2.26	0.68
2:B:686:LEU:HD13	2:B:688:SER:H	1.59	0.67
1:C:418:LEU:HD21	1:C:762:VAL:HG11	1.74	0.67
1:C:453:GLU:O	1:C:455:ILE:N	2.28	0.67
2:B:394:VAL:N	2:B:403:SER:OG	2.27	0.67
1:A:603:SER:O	1:A:606:ILE:HG22	1.95	0.67
1:A:453:GLU:O	1:A:455:ILE:N	2.28	0.67
2:B:154:LEU:HA	2:B:157:ILE:HD12	1.74	0.67
1:C:550:GLN:HA	1:C:553:TYR:HD2	1.60	0.67
2:D:686:LEU:HD13	2:D:688:SER:H	1.59	0.67
1:A:151:ARG:HB3	1:A:152:PRO:HD3	1.75	0.67
2:B:493:PRO:HB2	2:B:499:PRO:HB3	1.75	0.67
1:A:584:LEU:HA	1:A:587:MET:HE3	1.76	0.66
1:A:785:TRP:CZ3	2:B:333:ASP:HB2	2.30	0.66
2:B:665:THR:HB	2:B:668:THR:OG1	1.95	0.66
2:D:151:ARG:HB3	2:D:152:PRO:HD3	1.77	0.66
1:A:719:GLY:CA	2:D:722:VAL:HG13	2.24	0.66
1:C:665:THR:HG1	1:C:668:THR:HG1	1.43	0.66
1:A:550:GLN:HA	1:A:553:TYR:HD2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:170:LEU:HB3	2:D:171:PRO:HD3	1.78	0.66
2:B:151:ARG:HB3	2:B:152:PRO:HD3	1.77	0.66
2:B:721:THR:HB	1:C:715:ILE:HG23	1.78	0.66
2:D:665:THR:HB	2:D:668:THR:OG1	1.95	0.66
1:C:583:VAL:HG11	2:D:698:LEU:HD12	1.77	0.66
1:A:179:ARG:N	1:A:182:ASP:OD2	2.28	0.65
2:B:170:LEU:HB3	2:B:171:PRO:HD3	1.77	0.65
1:C:603:SER:O	1:C:606:ILE:HG22	1.95	0.65
2:B:767:SER:OG	2:B:771:THR:OG1	2.12	0.65
1:C:179:ARG:N	1:C:182:ASP:OD2	2.28	0.65
2:B:264:VAL:CG1	2:B:312:ALA:HB2	2.27	0.65
1:A:414:VAL:HG11	2:B:282:PHE:HB2	1.79	0.65
1:A:425:ASP:HB2	1:A:458:LEU:HD21	1.79	0.65
2:B:179:ARG:HG3	2:B:220:THR:HB	1.78	0.65
2:D:264:VAL:CG1	2:D:312:ALA:HB2	2.27	0.65
1:A:170:LEU:HB3	1:A:171:PRO:HD3	1.78	0.64
2:D:208:ASP:O	2:D:211:PRO:HD2	1.98	0.64
1:A:482:MET:HE1	1:A:585:GLY:HA3	1.78	0.64
2:D:720:GLU:HA	2:D:724:GLN:OE1	1.98	0.64
2:B:208:ASP:O	2:B:211:PRO:HD2	1.98	0.64
2:B:720:GLU:HA	2:B:724:GLN:OE1	1.98	0.64
1:C:170:LEU:HB3	1:C:171:PRO:HD3	1.79	0.64
2:D:525:PHE:HB2	2:D:557:SER:OG	1.97	0.64
1:C:296:ASN:HA	1:C:345:MET:HE1	1.78	0.64
1:C:425:ASP:HB2	1:C:458:LEU:HD21	1.79	0.64
1:C:498:PRO:HG2	1:C:570:GLY:HA2	1.80	0.64
1:A:498:PRO:HG2	1:A:570:GLY:HA2	1.80	0.64
2:B:193:THR:HG22	2:B:194:CYS:H	1.63	0.64
2:B:525:PHE:HB2	2:B:557:SER:OG	1.97	0.64
2:B:661:ARG:CG	2:B:665:THR:HG21	2.28	0.64
2:D:289:LEU:HD21	2:D:314:MET:HG2	1.80	0.64
2:B:210:ILE:HB	2:B:211:PRO:HD3	1.81	0.63
2:D:678:ILE:HG13	2:D:680:MET:HG3	1.80	0.63
2:B:678:ILE:HG13	2:B:680:MET:HG3	1.80	0.63
2:B:420:ASP:OD2	2:B:775:ARG:NH1	2.31	0.63
2:B:760:GLU:HG3	2:B:762:VAL:HG23	1.80	0.63
2:D:179:ARG:HG3	2:D:220:THR:HB	1.78	0.63
2:D:420:ASP:OD2	2:D:775:ARG:NH1	2.31	0.63
2:D:760:GLU:HG3	2:D:762:VAL:HG23	1.80	0.63
2:B:289:LEU:HD21	2:B:314:MET:HG2	1.80	0.63
2:D:661:ARG:CG	2:D:665:THR:HG21	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:LEU:O	2:B:260:GLN:NE2	2.32	0.63
2:B:689:THR:HG23	2:B:692:PRO:HA	1.80	0.63
1:A:507:ASP:OD1	1:A:510:ARG:NH1	2.30	0.63
1:A:556:TYR:HB2	1:A:584:LEU:HD12	1.81	0.63
2:D:256:LEU:O	2:D:260:GLN:NE2	2.32	0.63
2:D:693:VAL:HA	2:D:696:ILE:HG22	1.81	0.63
2:B:677:THR:HA	2:B:703:ILE:HD12	1.79	0.62
2:B:693:VAL:HA	2:B:696:ILE:HG22	1.81	0.62
1:C:507:ASP:OD1	1:C:510:ARG:NH1	2.30	0.62
2:D:677:THR:HA	2:D:703:ILE:HD12	1.79	0.62
1:A:296:ASN:HA	1:A:345:MET:HE1	1.82	0.62
2:B:408:ASP:HB2	2:B:418:LEU:CD1	2.29	0.62
1:C:556:TYR:HB2	1:C:584:LEU:HD12	1.81	0.62
2:D:193:THR:HG22	2:D:194:CYS:H	1.63	0.62
2:D:689:THR:HG23	2:D:692:PRO:HA	1.81	0.62
1:A:760:GLU:OE2	1:A:779:ARG:NE	2.32	0.62
2:B:443:ILE:HD11	2:B:541:ASN:CB	2.30	0.62
2:B:452:VAL:HG23	2:B:453:GLU:H	1.64	0.62
2:B:790:GLN:O	2:B:794:ILE:HD11	1.99	0.62
1:C:474:ASN:HB3	3:C:902:POV:P	2.40	0.62
1:C:760:GLU:OE2	1:C:779:ARG:NE	2.32	0.62
2:D:790:GLN:O	2:D:794:ILE:HD11	1.99	0.62
2:D:210:ILE:HB	2:D:211:PRO:HD3	1.81	0.62
1:A:696:ILE:O	1:A:700:VAL:HG23	2.00	0.61
1:A:801:LYS:N	2:B:235:TYR:OH	2.24	0.61
2:B:521:GLY:O	2:B:557:SER:OG	2.09	0.61
2:D:452:VAL:HG23	2:D:453:GLU:H	1.64	0.61
2:D:305:THR:OG1	2:D:306:GLU:OE1	2.17	0.61
2:B:725:VAL:O	2:B:728:GLU:N	2.34	0.61
1:C:600:GLY:HA3	1:C:602:TYR:CE2	2.35	0.61
1:C:696:ILE:O	1:C:700:VAL:HG23	2.00	0.61
1:A:302:ASN:O	1:A:306:GLU:HG2	2.01	0.61
1:C:302:ASN:O	1:C:306:GLU:HG2	2.01	0.61
1:C:717:LEU:O	1:C:722:VAL:HG22	2.01	0.61
2:D:504:THR:HG23	2:D:507:ASP:H	1.65	0.61
1:A:383:ILE:HD11	1:A:445:ASN:CB	2.31	0.61
1:A:600:GLY:HA3	1:A:602:TYR:CE2	2.36	0.61
1:A:717:LEU:O	1:A:722:VAL:HG22	2.01	0.61
2:B:504:THR:HG23	2:B:507:ASP:H	1.65	0.61
1:A:631:ALA:HB1	2:D:579:VAL:HG13	1.83	0.60
1:C:383:ILE:HD11	1:C:445:ASN:CB	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:454:PRO:O	1:C:458:LEU:N	2.19	0.60
1:A:154:LEU:HD11	1:A:194:CYS:SG	2.42	0.60
2:B:298:PRO:HG3	2:B:345:MET:HE2	1.81	0.60
2:D:524:PHE:HA	3:D:902:POV:C13	2.30	0.60
2:D:725:VAL:O	2:D:728:GLU:N	2.34	0.60
1:A:763:THR:OG1	1:A:774:ARG:NH1	2.29	0.60
1:A:634:SER:O	2:D:494:LEU:HD11	2.01	0.60
2:B:583:VAL:HG11	1:C:698:LEU:HD11	1.82	0.60
1:C:421:LEU:HD21	1:C:778:PHE:HB2	1.83	0.60
2:B:617:PHE:HD2	2:B:618:LEU:HD22	1.66	0.60
1:A:408:ASP:OD1	1:A:796:ASN:ND2	2.35	0.60
1:C:482:MET:HE1	1:C:585:GLY:HA3	1.82	0.60
1:C:584:LEU:HA	1:C:587:MET:HE3	1.84	0.60
2:D:767:SER:OG	2:D:771:THR:OG1	2.12	0.60
2:B:632:LEU:HD21	2:B:698:LEU:HB3	1.84	0.60
1:C:685:MET:O	1:C:689:THR:OG1	2.08	0.60
2:D:222:ASN:O	2:D:225:GLU:N	2.31	0.60
2:D:469:VAL:O	2:D:473:ILE:HG12	2.02	0.60
1:A:222:ASN:O	1:A:226:PHE:N	2.35	0.60
1:A:421:LEU:HD21	1:A:778:PHE:HB2	1.83	0.60
1:A:579:VAL:HG13	2:B:631:ALA:HB1	1.84	0.60
1:A:715:ILE:HG23	2:D:721:THR:HB	1.84	0.60
1:C:154:LEU:HD11	1:C:194:CYS:SG	2.42	0.60
2:B:215:ASP:O	2:B:219:ARG:HG2	2.02	0.59
1:A:181:THR:HG22	1:A:222:ASN:HD22	1.67	0.59
1:C:258:VAL:HG11	1:C:303:TYR:HE2	1.66	0.59
2:D:500:TYR:HB2	2:D:501:PRO:HD3	1.84	0.59
2:B:222:ASN:HB3	2:B:225:GLU:HB3	1.84	0.59
1:C:274:GLN:OE1	1:C:320:ARG:NH2	2.35	0.59
2:D:410:ALA:HB1	2:D:790:GLN:HG2	1.84	0.59
2:D:521:GLY:O	2:D:557:SER:OG	2.09	0.59
2:D:617:PHE:HD2	2:D:618:LEU:HD22	1.66	0.59
2:D:298:PRO:HG3	2:D:345:MET:HE2	1.84	0.59
2:D:632:LEU:HD21	2:D:698:LEU:HB3	1.84	0.59
1:A:258:VAL:HG11	1:A:303:TYR:HE2	1.66	0.59
2:B:469:VAL:O	2:B:473:ILE:HG12	2.02	0.59
1:C:181:THR:HG22	1:C:222:ASN:HD22	1.67	0.59
2:B:410:ALA:HB1	2:B:790:GLN:HG2	1.83	0.59
2:D:542:SER:O	2:D:547:GLY:HA3	2.03	0.59
1:A:502:TYR:HE2	1:A:511:LEU:HD12	1.67	0.59
1:A:274:GLN:OE1	1:A:320:ARG:NH2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:408:ASP:OD1	1:C:796:ASN:ND2	2.35	0.59
1:C:502:TYR:HE2	1:C:511:LEU:HD12	1.67	0.59
1:C:763:THR:OG1	1:C:774:ARG:NH1	2.29	0.59
2:D:584:LEU:HD23	2:D:587:MET:HE3	1.86	0.58
1:C:474:ASN:HB3	3:C:902:POV:O13	2.03	0.58
2:B:542:SER:O	2:B:547:GLY:HA3	2.03	0.58
2:D:494:LEU:CD2	2:D:575:LEU:HD22	2.32	0.58
2:D:215:ASP:O	2:D:219:ARG:HG2	2.03	0.58
2:D:222:ASN:HB3	2:D:225:GLU:HB3	1.84	0.58
2:D:676:LEU:HD13	2:D:699:LEU:HD11	1.86	0.58
2:B:669:PHE:HA	2:B:672:ASP:HB2	1.86	0.58
2:D:443:ILE:HD11	2:D:541:ASN:CB	2.30	0.58
2:B:482:MET:CE	2:B:585:GLY:HA3	2.34	0.58
2:B:673:LEU:O	2:B:677:THR:HG23	2.03	0.58
1:C:524:PHE:HB2	1:C:557:SER:HB3	1.86	0.58
2:D:482:MET:CE	2:D:585:GLY:HA3	2.34	0.58
1:A:389:ILE:O	1:A:404:ARG:HD3	2.03	0.58
2:B:500:TYR:HB2	2:B:501:PRO:HD3	1.84	0.58
1:C:389:ILE:O	1:C:404:ARG:HD3	2.04	0.58
2:D:526:PHE:HB3	2:D:530:LYS:NZ	2.18	0.58
1:A:617:PHE:HB2	1:A:713:MET:SD	2.44	0.58
2:B:257:LEU:O	2:B:262:ALA:HB2	2.04	0.58
1:C:222:ASN:O	1:C:226:PHE:N	2.35	0.58
1:A:524:PHE:HB2	1:A:557:SER:HB3	1.86	0.58
1:A:636:LEU:HB3	1:A:689:THR:HG22	1.86	0.58
2:B:186:ARG:HG3	2:B:192:LYS:O	2.05	0.57
2:B:475:VAL:O	2:B:479:LEU:HD23	2.04	0.57
2:D:257:LEU:O	2:D:262:ALA:HB2	2.04	0.57
2:D:725:VAL:HG13	2:D:728:GLU:HB3	1.86	0.57
1:A:501:PRO:HB3	1:A:503:ARG:NH1	2.19	0.57
2:B:494:LEU:CD2	2:B:575:LEU:HD22	2.32	0.57
1:C:471:PHE:CE2	1:C:595:GLY:HA3	2.40	0.57
2:D:408:ASP:HB2	2:D:418:LEU:CD1	2.29	0.57
1:A:474:ASN:HB3	3:A:902:POV:P	2.45	0.57
2:B:305:THR:OG1	2:B:306:GLU:OE1	2.17	0.57
2:D:331:ILE:O	2:D:331:ILE:HD12	2.05	0.57
2:D:673:LEU:O	2:D:677:THR:HG23	2.03	0.57
2:B:222:ASN:O	2:B:225:GLU:N	2.31	0.57
1:C:501:PRO:HB3	1:C:503:ARG:NH1	2.19	0.57
1:C:617:PHE:HB2	1:C:713:MET:SD	2.44	0.57
1:A:207:ASN:HB3	1:A:210:ILE:CD1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:PHE:CE2	1:A:595:GLY:HA3	2.40	0.57
2:B:331:ILE:HD12	2:B:331:ILE:O	2.04	0.57
2:B:389:ILE:O	2:B:404:ARG:HD3	2.04	0.57
1:C:530:LYS:HA	1:C:533:PHE:HB3	1.86	0.57
1:A:628:TYR:CE1	2:D:583:VAL:HB	2.36	0.57
2:D:475:VAL:O	2:D:479:LEU:HD23	2.04	0.57
1:A:530:LYS:HA	1:A:533:PHE:HB3	1.86	0.57
2:B:179:ARG:N	2:B:182:ASP:OD2	2.29	0.57
1:C:582:LEU:HD23	2:D:631:ALA:HB2	1.86	0.57
1:C:760:GLU:HG3	1:C:762:VAL:HG23	1.87	0.57
2:D:418:LEU:HD21	2:D:762:VAL:HG21	1.87	0.57
1:A:582:LEU:HD23	2:B:631:ALA:CB	2.34	0.56
1:A:760:GLU:HG3	1:A:762:VAL:HG23	1.87	0.56
2:B:676:LEU:HD13	2:B:699:LEU:HD11	1.86	0.56
2:B:725:VAL:HG13	2:B:728:GLU:HB3	1.86	0.56
2:D:484:ILE:O	2:D:488:THR:HG23	2.05	0.56
2:D:676:LEU:CD1	2:D:699:LEU:HD21	2.35	0.56
2:B:609:ILE:O	2:B:614:LEU:HD23	2.05	0.56
2:D:342:VAL:HG12	2:D:385:ILE:HD12	1.87	0.56
1:A:489:ALA:O	2:B:634:SER:OG	2.19	0.56
1:A:785:TRP:CH2	2:B:333:ASP:HB2	2.40	0.56
2:B:366:LEU:HD22	2:B:370:GLY:O	2.05	0.56
2:B:526:PHE:HB3	2:B:530:LYS:NZ	2.18	0.56
1:C:636:LEU:HB3	1:C:689:THR:HG22	1.86	0.56
2:D:186:ARG:HG3	2:D:192:LYS:O	2.04	0.56
2:D:366:LEU:HD22	2:D:370:GLY:O	2.05	0.56
2:D:609:ILE:O	2:D:614:LEU:HD23	2.05	0.56
1:A:463:TRP:HA	1:A:467:GLY:HA3	1.88	0.56
1:A:631:ALA:HB1	2:D:579:VAL:CG1	2.35	0.56
2:B:166:LEU:HD11	2:B:212:VAL:HG11	1.86	0.56
2:B:524:PHE:HA	3:B:902:POV:C13	2.35	0.56
2:B:628:TYR:CE2	2:B:702:TYR:HB2	2.41	0.56
1:C:721:THR:O	1:C:725:VAL:HG22	2.05	0.56
2:D:600:GLY:O	2:D:604:ILE:HG12	2.06	0.56
2:D:669:PHE:HA	2:D:672:ASP:HB2	1.86	0.56
1:A:517:THR:HG22	1:A:560:VAL:HG11	1.88	0.56
1:C:207:ASN:HB3	1:C:210:ILE:CD1	2.35	0.56
1:C:418:LEU:HG	1:C:777:CYS:HB3	1.88	0.56
1:A:418:LEU:HG	1:A:777:CYS:HB3	1.88	0.56
1:A:601:THR:CG2	1:A:605:MET:HB2	2.36	0.56
2:B:600:GLY:O	2:B:604:ILE:HG12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:517:THR:HG22	1:C:560:VAL:HG11	1.88	0.56
2:D:389:ILE:O	2:D:404:ARG:HD3	2.04	0.56
1:A:383:ILE:HD11	1:A:445:ASN:HB3	1.87	0.56
2:B:325:LEU:HD22	2:B:346:TYR:CD1	2.41	0.56
2:B:484:ILE:O	2:B:488:THR:HG23	2.05	0.56
1:C:463:TRP:HA	1:C:467:GLY:HA3	1.88	0.56
1:A:443:ILE:HG22	1:A:449:MET:HE1	1.88	0.56
1:A:721:THR:O	1:A:725:VAL:HG22	2.05	0.56
2:B:151:ARG:NH1	2:B:188:PRO:HD3	2.21	0.56
2:D:166:LEU:HD11	2:D:212:VAL:HG11	1.86	0.56
2:D:760:GLU:HG3	2:D:762:VAL:CG2	2.35	0.56
2:B:342:VAL:HG12	2:B:385:ILE:HD12	1.87	0.56
2:B:383:ILE:HD11	2:B:445:ASN:HD21	1.71	0.56
2:B:418:LEU:HD21	2:B:762:VAL:HG21	1.87	0.56
1:C:443:ILE:HG22	1:C:449:MET:HE1	1.88	0.56
1:A:517:THR:O	1:A:520:THR:OG1	2.21	0.55
2:B:154:LEU:HD13	2:B:185:PHE:HZ	1.71	0.55
2:B:519:PHE:CE2	2:B:523:LEU:HD11	2.41	0.55
2:D:151:ARG:NH1	2:D:188:PRO:HD3	2.21	0.55
1:A:255:GLU:HG2	1:A:303:TYR:CZ	2.41	0.55
2:B:760:GLU:HG3	2:B:762:VAL:CG2	2.36	0.55
2:D:154:LEU:HD13	2:D:185:PHE:HZ	1.71	0.55
2:D:383:ILE:HD11	2:D:445:ASN:HD21	1.71	0.55
2:D:553:TYR:CZ	2:D:588:ASN:HB3	2.41	0.55
2:B:195:LEU:HB3	2:B:196:PRO:HD3	1.87	0.55
1:A:218:GLU:HB3	1:A:223:MET:CE	2.37	0.55
1:C:323:THR:H	1:C:326:HIS:HD2	1.54	0.55
2:D:519:PHE:CE2	2:D:523:LEU:HD11	2.41	0.55
2:D:284:PHE:CZ	2:D:291:LEU:HD12	2.42	0.55
1:A:480:CYS:O	1:A:484:ILE:HG12	2.06	0.55
2:B:284:PHE:CZ	2:B:291:LEU:HD12	2.42	0.55
2:B:482:MET:HE2	2:B:585:GLY:HA3	1.89	0.55
1:C:480:CYS:O	1:C:484:ILE:HG12	2.06	0.55
1:C:637:ASN:ND2	1:C:662:ASP:OD2	2.40	0.55
2:B:154:LEU:HD13	2:B:185:PHE:CZ	2.42	0.55
2:B:154:LEU:HD23	2:B:158:VAL:HG23	1.89	0.55
2:B:553:TYR:CZ	2:B:588:ASN:HB3	2.41	0.55
1:C:297:GLN:O	1:C:301:VAL:HG23	2.07	0.55
1:C:590:LEU:HD11	1:C:602:TYR:OH	2.07	0.55
2:D:594:ARG:HG2	2:D:736:GLN:HB3	1.89	0.55
2:D:628:TYR:CE2	2:D:702:TYR:HB2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:LEU:O	1:A:262:ALA:HB2	2.07	0.55
1:C:255:GLU:HG2	1:C:303:TYR:CZ	2.41	0.55
1:C:601:THR:CG2	1:C:605:MET:HB2	2.36	0.55
2:D:325:LEU:HD22	2:D:346:TYR:CD1	2.41	0.55
1:A:323:THR:H	1:A:326:HIS:HD2	1.54	0.55
1:A:465:LYS:NZ	1:A:757:ARG:O	2.40	0.55
2:B:381:GLY:HA2	2:B:449:MET:CE	2.37	0.55
1:C:267:GLN:HA	1:C:286:GLU:O	2.07	0.55
1:C:489:ALA:O	2:D:634:SER:OG	2.22	0.55
1:C:618:LEU:O	1:C:622:LEU:HD13	2.06	0.55
2:D:179:ARG:N	2:D:182:ASP:OD2	2.29	0.55
1:A:267:GLN:HA	1:A:286:GLU:O	2.07	0.55
2:B:722:VAL:HG13	1:C:719:GLY:CA	2.37	0.55
1:A:199:LEU:O	1:A:202:LEU:HD22	2.07	0.54
1:A:637:ASN:ND2	1:A:662:ASP:OD2	2.40	0.54
2:B:202:LEU:HD11	2:B:253:TYR:HE2	1.72	0.54
2:B:764:VAL:HG12	2:B:773:ASP:O	2.07	0.54
1:C:257:LEU:O	1:C:262:ALA:HB2	2.07	0.54
1:C:383:ILE:HD11	1:C:445:ASN:HB3	1.87	0.54
1:C:583:VAL:HG21	2:D:698:LEU:CD1	2.36	0.54
1:A:685:MET:O	1:A:689:THR:OG1	2.08	0.54
1:C:199:LEU:O	1:C:202:LEU:HD22	2.07	0.54
2:D:202:LEU:HD11	2:D:253:TYR:HE2	1.72	0.54
1:C:218:GLU:HB3	1:C:223:MET:CE	2.37	0.54
1:C:475:VAL:O	1:C:479:LEU:HD23	2.07	0.54
2:D:154:LEU:HD23	2:D:158:VAL:HG23	1.89	0.54
1:C:582:LEU:HD23	2:D:631:ALA:CB	2.37	0.54
2:D:195:LEU:HB3	2:D:196:PRO:HD3	1.87	0.54
2:B:421:LEU:HD21	2:B:458:LEU:HD13	1.89	0.54
2:B:494:LEU:HD12	1:C:637:ASN:HB3	1.89	0.54
2:D:381:GLY:HA2	2:D:449:MET:CE	2.37	0.54
1:A:475:VAL:O	1:A:479:LEU:HD23	2.07	0.54
2:D:336:ARG:O	2:D:340:LYS:HG2	2.07	0.54
1:A:618:LEU:O	1:A:622:LEU:HD13	2.06	0.54
1:A:454:PRO:O	1:A:458:LEU:N	2.19	0.54
1:A:474:ASN:OD1	1:A:475:VAL:N	2.41	0.54
1:A:637:ASN:O	1:A:662:ASP:HB3	2.08	0.54
1:A:700:VAL:O	1:A:704:ILE:HG12	2.08	0.54
1:C:409:TRP:HB2	1:C:799:PRO:HA	1.90	0.54
2:B:532:LEU:HG	2:B:538:PRO:HG3	1.90	0.54
2:B:721:THR:HG21	1:C:715:ILE:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:582:LEU:HD23	2:D:631:ALA:HA	1.90	0.54
2:D:154:LEU:HD13	2:D:185:PHE:CZ	2.42	0.54
2:D:764:VAL:HG12	2:D:773:ASP:O	2.07	0.54
1:A:590:LEU:HD11	1:A:602:TYR:OH	2.07	0.53
2:B:168:GLY:C	2:B:171:PRO:HD2	2.29	0.53
2:B:265:HIS:NE2	2:B:312:ALA:HA	2.23	0.53
2:D:421:LEU:HD21	2:D:458:LEU:HD13	1.89	0.53
1:A:297:GLN:O	1:A:301:VAL:HG23	2.07	0.53
2:D:516:ILE:O	2:D:520:THR:HG23	2.08	0.53
2:B:671:LEU:O	2:B:674:PHE:HB2	2.09	0.53
2:B:676:LEU:CD1	2:B:699:LEU:HD21	2.35	0.53
2:D:485:PHE:CE2	2:D:582:LEU:HD22	2.44	0.53
1:A:623:LEU:HD12	2:D:586:TRP:O	2.09	0.53
2:B:594:ARG:HG2	2:B:736:GLN:HB3	1.89	0.53
1:C:474:ASN:OD1	1:C:475:VAL:N	2.41	0.53
1:C:700:VAL:O	1:C:704:ILE:HG12	2.08	0.53
2:D:170:LEU:CD2	2:D:219:ARG:HG3	2.38	0.53
1:A:186:ARG:NH2	1:A:191:GLY:O	2.42	0.53
1:A:409:TRP:HB2	1:A:799:PRO:HA	1.90	0.53
1:A:697:ILE:HD11	2:D:580:PHE:HZ	1.73	0.53
2:B:418:LEU:CD2	2:B:762:VAL:HG21	2.39	0.53
2:D:258:VAL:HA	2:D:262:ALA:CB	2.38	0.53
2:D:332:ALA:O	2:D:382:LYS:HD2	2.09	0.53
2:B:258:VAL:HA	2:B:262:ALA:CB	2.38	0.53
1:C:180:LEU:HD21	1:C:213:LEU:HD12	1.91	0.53
1:C:249:ARG:HD2	1:C:297:GLN:HE21	1.74	0.53
2:D:413:PRO:O	2:D:783:VAL:HG13	2.09	0.53
2:D:443:ILE:HG22	2:D:446:ARG:NE	2.24	0.53
2:D:532:LEU:HG	2:D:538:PRO:HG3	1.90	0.53
2:D:671:LEU:O	2:D:674:PHE:HB2	2.09	0.53
1:A:166:LEU:HD13	1:A:212:VAL:HG11	1.91	0.53
1:A:386:PHE:CZ	1:A:390:ILE:HD11	2.44	0.53
2:B:332:ALA:O	2:B:382:LYS:HD2	2.09	0.53
2:B:336:ARG:O	2:B:340:LYS:HG2	2.07	0.53
2:B:383:ILE:HD11	2:B:445:ASN:OD1	2.08	0.53
2:B:485:PHE:CE2	2:B:582:LEU:HD22	2.43	0.53
2:B:486:THR:HG23	1:C:630:SER:OG	2.08	0.53
1:C:342:VAL:HG12	1:C:385:ILE:HD12	1.90	0.53
1:C:465:LYS:NZ	1:C:757:ARG:O	2.40	0.53
2:D:375:MET:HG2	2:D:433:VAL:HG22	1.89	0.53
2:B:677:THR:HA	2:B:703:ILE:CD1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:693:VAL:O	2:D:697:ILE:HG12	2.09	0.53
1:A:342:VAL:HG12	1:A:385:ILE:HD12	1.90	0.53
1:A:502:TYR:CE2	1:A:511:LEU:HB2	2.44	0.53
1:C:471:PHE:HE2	1:C:595:GLY:HA3	1.74	0.53
1:C:637:ASN:O	1:C:662:ASP:HB3	2.08	0.53
2:D:383:ILE:HD11	2:D:445:ASN:OD1	2.08	0.53
1:A:253:TYR:HB3	1:A:257:LEU:HD13	1.91	0.53
1:A:421:LEU:CD2	1:A:778:PHE:HB2	2.39	0.53
1:A:698:LEU:CD1	2:D:583:VAL:HG11	2.39	0.53
2:B:265:HIS:HE2	2:B:312:ALA:HA	1.74	0.53
2:B:413:PRO:O	2:B:783:VAL:HG13	2.09	0.53
2:B:516:ILE:O	2:B:520:THR:HG23	2.08	0.53
4:B:901:HCO:C27	3:B:902:POV:H15B	2.39	0.53
1:C:151:ARG:NH1	1:C:188:PRO:HD3	2.24	0.53
1:C:386:PHE:CZ	1:C:390:ILE:HD11	2.44	0.53
1:A:418:LEU:CD2	1:A:762:VAL:HG11	2.39	0.52
1:C:198:ALA:HB1	1:C:210:ILE:HD11	1.90	0.52
1:C:418:LEU:CD2	1:C:762:VAL:HG11	2.39	0.52
2:D:265:HIS:NE2	2:D:312:ALA:HA	2.23	0.52
2:D:418:LEU:CD2	2:D:762:VAL:HG21	2.39	0.52
1:A:608:LYS:O	1:A:612:LYS:HB2	2.09	0.52
2:B:443:ILE:HG22	2:B:446:ARG:NE	2.24	0.52
2:D:168:GLY:C	2:D:171:PRO:HD2	2.29	0.52
2:B:375:MET:HG2	2:B:433:VAL:HG22	1.89	0.52
2:B:584:LEU:HD23	2:B:587:MET:CE	2.39	0.52
1:C:180:LEU:HD11	1:C:194:CYS:SG	2.50	0.52
2:D:265:HIS:HE2	2:D:312:ALA:HA	1.74	0.52
1:C:502:TYR:CE2	1:C:511:LEU:HB2	2.44	0.52
1:A:249:ARG:HD2	1:A:297:GLN:HE21	1.74	0.52
2:D:453:GLU:HB2	2:D:454:PRO:HD3	1.92	0.52
2:B:721:THR:HB	1:C:715:ILE:CG2	2.39	0.52
1:C:253:TYR:HB3	1:C:257:LEU:HD13	1.91	0.52
2:D:450:LEU:HD12	2:D:735:LEU:HD23	1.92	0.52
1:A:505:THR:O	1:A:509:LEU:HG	2.10	0.52
2:B:170:LEU:CD2	2:B:219:ARG:HG3	2.38	0.52
1:A:198:ALA:HB1	1:A:210:ILE:HD11	1.90	0.52
2:B:453:GLU:HB2	2:B:454:PRO:HD3	1.92	0.52
1:C:186:ARG:NH2	1:C:191:GLY:O	2.42	0.52
1:C:694:VAL:O	1:C:698:LEU:HD23	2.10	0.52
2:D:227:ILE:HG23	2:D:257:LEU:HD22	1.92	0.52
2:D:296:ASN:HA	2:D:345:MET:HE3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:584:LEU:HD23	2:D:587:MET:CE	2.39	0.52
2:D:677:THR:HA	2:D:703:ILE:CD1	2.39	0.52
1:A:151:ARG:NH1	1:A:188:PRO:HD3	2.24	0.52
1:A:180:LEU:HD11	1:A:194:CYS:SG	2.50	0.52
2:B:689:THR:O	2:B:691:TYR:N	2.42	0.52
1:C:218:GLU:HB3	1:C:223:MET:HE3	1.92	0.52
1:C:563:SER:OG	1:C:577:VAL:HG12	2.10	0.52
2:D:527:THR:HA	2:D:530:LYS:CG	2.40	0.52
4:D:901:HCO:C27	3:D:902:POV:H15B	2.40	0.52
1:A:518:LEU:O	1:A:522:VAL:HG23	2.10	0.52
2:B:450:LEU:HD12	2:B:735:LEU:HD23	1.92	0.52
2:B:604:ILE:HD11	2:B:736:GLN:OE1	2.10	0.52
2:B:737:TRP:CZ2	2:B:741:ILE:HD11	2.45	0.52
1:C:383:ILE:HD12	1:C:383:ILE:H	1.75	0.52
1:C:517:THR:O	1:C:520:THR:OG1	2.21	0.52
1:A:180:LEU:HD21	1:A:213:LEU:HD12	1.91	0.51
1:A:563:SER:OG	1:A:577:VAL:HG12	2.10	0.51
1:A:601:THR:HG22	1:A:605:MET:HB2	1.91	0.51
2:B:163:THR:O	2:B:166:LEU:HG	2.10	0.51
2:B:507:ASP:OD1	2:B:510:ARG:NH1	2.41	0.51
2:B:583:VAL:HG11	1:C:698:LEU:CD1	2.39	0.51
1:C:421:LEU:CD2	1:C:778:PHE:HB2	2.40	0.51
1:C:518:LEU:O	1:C:522:VAL:HG23	2.10	0.51
2:B:598:LEU:HD12	1:C:616:ARG:HE	1.74	0.51
1:C:505:THR:O	1:C:509:LEU:HG	2.10	0.51
2:D:163:THR:O	2:D:166:LEU:HG	2.10	0.51
2:D:233:ASP:O	2:D:237:ARG:HG2	2.11	0.51
1:A:383:ILE:HD12	1:A:383:ILE:H	1.75	0.51
1:A:471:PHE:HE2	1:A:595:GLY:HA3	1.74	0.51
2:B:693:VAL:O	2:B:697:ILE:HG12	2.09	0.51
2:B:233:ASP:OD1	2:B:234:ILE:N	2.44	0.51
1:C:166:LEU:HD13	1:C:212:VAL:HG11	1.91	0.51
1:C:610:LEU:O	1:C:614:LEU:HB2	2.11	0.51
2:D:604:ILE:HD11	2:D:736:GLN:OE1	2.10	0.51
2:D:689:THR:O	2:D:691:TYR:N	2.42	0.51
1:A:307:ASN:OD1	1:A:311:LYS:HG2	2.10	0.51
1:A:694:VAL:O	1:A:698:LEU:HD23	2.10	0.51
2:D:443:ILE:HG22	2:D:446:ARG:CZ	2.41	0.51
2:B:722:VAL:HG13	1:C:719:GLY:HA2	1.93	0.51
1:C:608:LYS:O	1:C:612:LYS:HB2	2.09	0.51
1:C:699:LEU:O	1:C:703:ILE:HG12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:214:LEU:CD1	2:D:227:ILE:HD11	2.40	0.51
2:D:507:ASP:OD1	2:D:510:ARG:NH1	2.41	0.51
1:A:610:LEU:O	1:A:614:LEU:HB2	2.11	0.51
1:A:720:GLU:O	1:A:723:GLY:N	2.28	0.51
2:B:249:ARG:HG2	2:B:297:GLN:NE2	2.24	0.51
2:B:724:GLN:O	2:B:726:SER:N	2.44	0.51
2:D:425:ASP:HB2	2:D:458:LEU:HD21	1.93	0.51
2:D:499:PRO:HD2	2:D:567:TYR:CE1	2.46	0.51
1:A:474:ASN:HB3	3:A:902:POV:O13	2.10	0.51
2:B:227:ILE:HG23	2:B:257:LEU:HD22	1.92	0.51
2:B:425:ASP:HB2	2:B:458:LEU:HD21	1.93	0.51
2:B:499:PRO:HD2	2:B:567:TYR:CE1	2.46	0.51
2:B:527:THR:HA	2:B:530:LYS:CG	2.40	0.51
2:D:409:TRP:HA	2:D:794:ILE:HG23	1.93	0.51
2:D:671:LEU:HA	2:D:674:PHE:CD2	2.46	0.51
1:A:413:PRO:O	1:A:783:VAL:HG13	2.11	0.51
1:C:697:ILE:HD12	1:C:698:LEU:HD22	1.92	0.51
2:D:724:GLN:O	2:D:726:SER:N	2.44	0.51
2:B:694:VAL:O	2:B:698:LEU:HD23	2.11	0.51
2:D:153:ILE:O	2:D:157:ILE:HG13	2.11	0.51
2:D:694:VAL:O	2:D:698:LEU:HD23	2.11	0.51
2:D:737:TRP:CZ2	2:D:741:ILE:HD11	2.45	0.51
1:A:697:ILE:HD12	1:A:698:LEU:HD22	1.92	0.50
1:C:582:LEU:HD23	2:D:631:ALA:CA	2.41	0.50
2:D:502:TYR:HB3	2:D:507:ASP:HB3	1.93	0.50
1:A:633:VAL:HA	1:A:636:LEU:CD2	2.42	0.50
1:A:698:LEU:HD11	2:D:583:VAL:HG11	1.93	0.50
1:A:718:MET:HA	1:A:722:VAL:HG21	1.93	0.50
1:A:718:MET:HA	1:A:722:VAL:CG2	2.41	0.50
1:C:601:THR:HG22	1:C:605:MET:HB2	1.91	0.50
2:D:150:ASN:H	2:D:153:ILE:HB	1.76	0.50
2:D:233:ASP:OD1	2:D:234:ILE:N	2.44	0.50
2:D:439:TYR:O	2:D:446:ARG:NH2	2.45	0.50
1:A:699:LEU:O	1:A:703:ILE:HG12	2.11	0.50
2:B:179:ARG:HG3	2:B:220:THR:CB	2.42	0.50
2:B:714:LEU:O	2:B:718:MET:HG2	2.12	0.50
2:B:733:TRP:O	2:B:736:GLN:N	2.44	0.50
1:C:307:ASN:OD1	1:C:311:LYS:HG2	2.10	0.50
1:C:718:MET:HA	1:C:722:VAL:CG2	2.41	0.50
2:D:760:GLU:OE2	2:D:779:ARG:NH1	2.45	0.50
1:A:527:THR:HA	1:A:530:LYS:HE3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:214:LEU:CD1	2:B:227:ILE:HD11	2.40	0.50
2:B:233:ASP:O	2:B:237:ARG:HG2	2.11	0.50
2:B:443:ILE:HG22	2:B:446:ARG:CZ	2.41	0.50
2:B:671:LEU:HA	2:B:674:PHE:CD2	2.46	0.50
1:C:413:PRO:O	1:C:783:VAL:HG13	2.11	0.50
2:D:222:ASN:O	2:D:226:PHE:N	2.42	0.50
2:B:346:TYR:CG	2:B:385:ILE:HD11	2.46	0.50
2:B:760:GLU:OE2	2:B:779:ARG:NH1	2.44	0.50
1:C:514:GLU:O	1:C:518:LEU:HG	2.11	0.50
2:B:153:ILE:O	2:B:157:ILE:HG13	2.11	0.50
1:C:250:CYS:O	1:C:254:VAL:HG23	2.12	0.50
1:C:787:HIS:O	1:C:790:GLN:HG3	2.12	0.50
2:D:714:LEU:O	2:D:718:MET:HG2	2.12	0.50
1:A:413:PRO:HG3	1:A:788:TRP:CH2	2.47	0.50
1:A:583:VAL:HG21	2:B:698:LEU:HD11	1.94	0.50
1:A:787:HIS:O	1:A:790:GLN:HG3	2.12	0.50
1:C:720:GLU:O	1:C:723:GLY:N	2.28	0.50
1:A:514:GLU:O	1:A:518:LEU:HG	2.11	0.50
2:B:502:TYR:HB3	2:B:507:ASP:HB3	1.93	0.50
1:C:633:VAL:HA	1:C:636:LEU:CD2	2.42	0.50
2:B:409:TRP:HA	2:B:794:ILE:HG23	1.93	0.49
2:B:485:PHE:CD1	2:B:517:THR:HG21	2.47	0.49
2:B:583:VAL:HB	1:C:628:TYR:HE1	1.77	0.49
2:D:346:TYR:CG	2:D:385:ILE:HD11	2.46	0.49
1:C:192:LYS:HD3	1:C:197:LYS:CE	2.41	0.49
2:B:439:TYR:O	2:B:446:ARG:NH2	2.45	0.49
2:B:661:ARG:CB	2:B:665:THR:HG21	2.42	0.49
2:D:170:LEU:HD22	2:D:219:ARG:HG3	1.94	0.49
2:D:502:TYR:HD1	2:D:507:ASP:HB3	1.77	0.49
2:D:701:THR:O	2:D:705:LEU:HD23	2.12	0.49
2:B:222:ASN:O	2:B:226:PHE:N	2.42	0.49
2:B:639:CYS:HB2	2:B:663:SER:HB3	1.95	0.49
2:B:701:THR:O	2:B:705:LEU:HD23	2.12	0.49
1:C:413:PRO:HG3	1:C:788:TRP:CH2	2.47	0.49
2:B:150:ASN:H	2:B:153:ILE:HB	1.76	0.49
1:C:275:PRO:CG	1:C:320:ARG:HH12	2.24	0.49
1:C:474:ASN:HD22	3:C:902:POV:H12A	1.76	0.49
1:C:685:MET:HA	1:C:689:THR:CG2	2.41	0.49
1:C:717:LEU:HD11	2:D:715:ILE:HD12	1.94	0.49
1:A:275:PRO:CG	1:A:320:ARG:HH12	2.24	0.49
2:B:297:GLN:O	2:B:301:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:559:LEU:HD11	1:C:577:VAL:HG13	1.94	0.49
1:C:718:MET:HA	1:C:722:VAL:HG21	1.93	0.49
1:C:366:LEU:HD22	1:C:370:GLY:O	2.13	0.49
2:D:179:ARG:HG3	2:D:220:THR:CB	2.42	0.49
2:D:284:PHE:CE2	2:D:291:LEU:HD12	2.48	0.49
2:D:297:GLN:O	2:D:301:VAL:HG23	2.12	0.49
2:D:639:CYS:HB2	2:D:663:SER:HB3	1.95	0.49
1:A:559:LEU:HD11	1:A:577:VAL:HG13	1.94	0.49
2:D:359:ASP:OD1	2:D:360:SER:N	2.46	0.49
2:D:733:TRP:O	2:D:736:GLN:N	2.44	0.49
1:A:250:CYS:O	1:A:254:VAL:HG23	2.12	0.49
2:B:264:VAL:HG12	2:B:312:ALA:HB2	1.94	0.49
2:B:485:PHE:CE1	2:B:517:THR:HG21	2.48	0.49
2:D:249:ARG:HG2	2:D:297:GLN:NE2	2.24	0.49
2:D:314:MET:HE1	2:D:353:CYS:N	2.28	0.49
1:A:317:GLN:HE21	1:A:365:VAL:CG1	2.26	0.48
1:C:488:THR:CG2	1:C:513:GLY:HA3	2.42	0.48
2:D:202:LEU:CG	2:D:205:GLY:HA2	2.33	0.48
2:D:485:PHE:CD1	2:D:517:THR:HG21	2.48	0.48
1:A:366:LEU:HD22	1:A:370:GLY:O	2.13	0.48
2:B:170:LEU:HD22	2:B:219:ARG:HG3	1.95	0.48
1:C:527:THR:HA	1:C:530:LYS:HE3	1.94	0.48
2:D:511:LEU:O	2:D:515:VAL:HG23	2.13	0.48
2:D:595:GLY:C	2:D:596:LEU:HD12	2.34	0.48
2:D:661:ARG:CB	2:D:665:THR:HG21	2.42	0.48
1:A:413:PRO:HG3	1:A:788:TRP:CZ3	2.49	0.48
2:B:179:ARG:HG2	2:B:222:ASN:OD1	2.13	0.48
1:A:619:LEU:O	1:A:623:LEU:HD23	2.13	0.48
2:B:284:PHE:CE2	2:B:291:LEU:HD12	2.48	0.48
1:C:482:MET:CE	1:C:585:GLY:HA3	2.43	0.48
2:D:535:LYS:HD2	2:D:746:ARG:NH2	2.28	0.48
1:A:488:THR:CG2	1:A:513:GLY:HA3	2.42	0.48
1:A:510:ARG:O	1:A:514:GLU:HG2	2.14	0.48
2:B:359:ASP:OD1	2:B:360:SER:N	2.46	0.48
2:B:511:LEU:O	2:B:515:VAL:HG23	2.13	0.48
2:B:535:LYS:HD2	2:B:746:ARG:NH2	2.28	0.48
1:C:258:VAL:HG13	1:C:309:HIS:CE1	2.49	0.48
1:C:406:PHE:CG	1:C:764:VAL:HG21	2.49	0.48
1:C:413:PRO:HG3	1:C:788:TRP:CZ3	2.48	0.48
2:D:636:LEU:HD23	2:D:637:ASN:O	2.14	0.48
1:A:258:VAL:HG13	1:A:309:HIS:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:510:ARG:O	1:C:514:GLU:HG2	2.14	0.48
2:D:324:VAL:HG11	2:D:349:LEU:HD23	1.96	0.48
2:D:482:MET:HE1	2:D:585:GLY:HA3	1.95	0.48
1:A:314:MET:HE1	1:A:352:LYS:C	2.34	0.48
1:C:156:ASP:OD2	1:C:160:ARG:NH2	2.46	0.48
1:C:317:GLN:HE21	1:C:365:VAL:CG1	2.26	0.48
2:D:264:VAL:HG12	2:D:312:ALA:HB2	1.94	0.48
1:A:156:ASP:OD2	1:A:160:ARG:NH2	2.46	0.48
1:A:218:GLU:HB3	1:A:223:MET:HE3	1.95	0.48
1:A:556:TYR:HB2	1:A:584:LEU:CD1	2.44	0.48
2:B:499:PRO:HD2	2:B:567:TYR:HE1	1.79	0.48
2:B:584:LEU:HD23	2:B:587:MET:HE3	1.94	0.48
1:A:676:LEU:HD23	1:A:676:LEU:O	2.14	0.48
2:B:595:GLY:C	2:B:596:LEU:HD12	2.34	0.48
1:C:593:THR:HB	1:C:598:LEU:O	2.14	0.48
2:D:171:PRO:O	2:D:175:THR:HG22	2.14	0.48
1:C:604:ILE:O	1:C:607:GLN:HB3	2.14	0.48
1:C:764:VAL:HG23	1:C:795:ILE:HD13	1.96	0.48
2:D:179:ARG:HG2	2:D:222:ASN:OD1	2.13	0.48
1:A:284:PHE:CE2	1:A:291:LEU:HB2	2.49	0.47
2:B:255:GLU:HA	2:B:303:TYR:CE2	2.49	0.47
2:B:324:VAL:HG11	2:B:349:LEU:HD23	1.96	0.47
1:A:150:ASN:OD1	1:A:153:ILE:HG22	2.14	0.47
1:A:301:VAL:HG11	1:A:349:LEU:HD11	1.96	0.47
1:A:406:PHE:CG	1:A:764:VAL:HG21	2.49	0.47
1:A:764:VAL:HG23	1:A:795:ILE:HD13	1.96	0.47
2:B:383:ILE:CD1	2:B:445:ASN:HD21	2.27	0.47
2:B:502:TYR:HD1	2:B:507:ASP:HB3	1.78	0.47
2:B:676:LEU:HD23	2:B:676:LEU:O	2.14	0.47
2:B:700:VAL:O	2:B:704:ILE:HG12	2.14	0.47
2:D:169:LEU:HD23	2:D:216:ILE:HD13	1.97	0.47
2:D:676:LEU:HD23	2:D:676:LEU:O	2.13	0.47
1:A:254:VAL:O	1:A:258:VAL:HG12	2.15	0.47
1:A:604:ILE:O	1:A:607:GLN:HB3	2.14	0.47
1:A:624:PHE:CE1	2:D:587:MET:HG2	2.49	0.47
2:B:163:THR:HA	2:B:166:LEU:CD2	2.44	0.47
2:B:571:ILE:HG22	2:B:573:ALA:H	1.79	0.47
2:B:575:LEU:O	2:B:579:VAL:HG23	2.14	0.47
1:C:706:THR:O	1:C:710:LEU:HD13	2.14	0.47
2:D:210:ILE:O	2:D:214:LEU:HD23	2.14	0.47
2:D:255:GLU:HA	2:D:303:TYR:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:420:ASP:O	2:D:422:SER:N	2.48	0.47
2:D:485:PHE:CE1	2:D:517:THR:HG21	2.48	0.47
1:A:706:THR:O	1:A:710:LEU:HD13	2.14	0.47
1:A:760:GLU:HG3	1:A:762:VAL:CG2	2.44	0.47
2:B:154:LEU:HD11	2:B:169:LEU:HD22	1.96	0.47
2:B:686:LEU:O	2:B:689:THR:HB	2.14	0.47
1:C:619:LEU:O	1:C:623:LEU:HD23	2.13	0.47
1:C:676:LEU:O	1:C:676:LEU:HD23	2.14	0.47
2:D:264:VAL:HG11	2:D:312:ALA:HB2	1.96	0.47
2:D:575:LEU:O	2:D:579:VAL:HG23	2.14	0.47
2:B:252:HIS:O	2:B:255:GLU:HB2	2.15	0.47
2:B:497:THR:HB	2:B:498:PRO:CD	2.44	0.47
1:C:265:HIS:CE1	1:C:312:ALA:HA	2.49	0.47
1:C:636:LEU:CB	1:C:689:THR:HG22	2.45	0.47
2:D:571:ILE:HG22	2:D:573:ALA:H	1.79	0.47
1:A:593:THR:HB	1:A:598:LEU:O	2.14	0.47
2:B:169:LEU:HD23	2:B:216:ILE:HD13	1.97	0.47
2:B:573:ALA:HA	1:C:691:TYR:OH	2.13	0.47
1:C:794:ILE:HG22	1:C:796:ASN:H	1.80	0.47
2:D:252:HIS:O	2:D:255:GLU:HB2	2.15	0.47
2:D:761:MET:HA	2:D:775:ARG:O	2.15	0.47
1:A:192:LYS:HD3	1:A:197:LYS:CE	2.41	0.47
2:B:210:ILE:O	2:B:214:LEU:HD23	2.14	0.47
2:B:315:ARG:HG2	2:B:362:LEU:HD23	1.96	0.47
2:B:718:MET:HA	2:B:721:THR:OG1	2.15	0.47
2:B:720:GLU:O	2:B:724:GLN:HB2	2.15	0.47
2:B:754:LYS:O	2:B:757:ARG:HG3	2.15	0.47
2:B:761:MET:HA	2:B:775:ARG:O	2.15	0.47
1:C:150:ASN:OD1	1:C:153:ILE:HG22	2.14	0.47
1:C:284:PHE:CE2	1:C:291:LEU:HB2	2.49	0.47
1:C:314:MET:HE1	1:C:352:LYS:C	2.35	0.47
1:C:705:LEU:O	1:C:708:VAL:HG22	2.15	0.47
2:D:322:ASN:HA	2:D:326:HIS:ND1	2.30	0.47
2:D:686:LEU:O	2:D:689:THR:HB	2.14	0.47
2:D:700:VAL:O	2:D:704:ILE:HG12	2.14	0.47
2:D:720:GLU:O	2:D:724:GLN:HB2	2.15	0.47
1:A:479:LEU:O	1:A:483:VAL:HG23	2.15	0.47
1:A:685:MET:HA	1:A:689:THR:CG2	2.41	0.47
2:B:636:LEU:HD23	2:B:637:ASN:O	2.14	0.47
1:C:301:VAL:HG11	1:C:349:LEU:HD11	1.97	0.47
1:C:498:PRO:O	1:C:500:TYR:N	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:760:GLU:HG3	1:C:762:VAL:CG2	2.44	0.47
1:A:210:ILE:HB	1:A:211:PRO:HD3	1.97	0.47
1:A:554:PHE:O	1:A:558:VAL:HG23	2.15	0.47
1:A:677:THR:HA	1:A:703:ILE:HD12	1.97	0.47
1:A:794:ILE:HG22	1:A:796:ASN:H	1.80	0.47
1:C:244:ILE:O	1:C:248:ARG:HG2	2.15	0.47
1:C:424:LEU:HD23	1:C:455:ILE:CD1	2.45	0.47
2:D:497:THR:HB	2:D:498:PRO:CD	2.44	0.47
2:B:163:THR:OG1	2:B:212:VAL:HG11	2.15	0.47
2:B:413:PRO:HG3	2:B:785:TRP:CZ3	2.50	0.47
2:D:413:PRO:HG3	2:D:785:TRP:CZ3	2.50	0.47
2:D:532:LEU:HG	2:D:538:PRO:CG	2.45	0.47
1:A:195:LEU:HB3	1:A:196:PRO:HD3	1.97	0.46
1:A:636:LEU:CB	1:A:689:THR:HG22	2.45	0.46
2:B:149:PHE:CD1	2:B:169:LEU:HD13	2.51	0.46
2:B:420:ASP:O	2:B:422:SER:N	2.48	0.46
2:D:150:ASN:N	2:D:153:ILE:HD12	2.31	0.46
2:D:163:THR:HA	2:D:166:LEU:CD2	2.44	0.46
1:A:258:VAL:HG22	1:A:309:HIS:HE1	1.81	0.46
1:A:265:HIS:CE1	1:A:312:ALA:HA	2.49	0.46
2:B:296:ASN:O	2:B:298:PRO:HD3	2.16	0.46
2:B:322:ASN:HA	2:B:326:HIS:ND1	2.30	0.46
2:B:527:THR:HA	2:B:530:LYS:HG3	1.97	0.46
2:B:532:LEU:HG	2:B:538:PRO:CG	2.45	0.46
1:C:275:PRO:HG2	1:C:320:ARG:HH12	1.79	0.46
1:C:575:LEU:O	1:C:579:VAL:HG23	2.15	0.46
2:D:163:THR:OG1	2:D:212:VAL:HG11	2.15	0.46
2:D:326:HIS:CD2	2:D:373:PRO:HG3	2.50	0.46
2:D:383:ILE:HD11	2:D:445:ASN:ND2	2.30	0.46
2:D:383:ILE:CD1	2:D:445:ASN:HD21	2.28	0.46
2:D:480:CYS:O	2:D:484:ILE:HG12	2.15	0.46
2:D:524:PHE:O	2:D:528:ASN:HB2	2.16	0.46
2:D:754:LYS:O	2:D:757:ARG:HG3	2.15	0.46
1:A:275:PRO:HG2	1:A:320:ARG:HH12	1.79	0.46
1:A:575:LEU:O	1:A:579:VAL:HG23	2.15	0.46
1:A:752:LEU:HD11	1:A:756:PHE:HE2	1.81	0.46
2:B:171:PRO:O	2:B:175:THR:HG22	2.14	0.46
2:B:527:THR:HG22	2:B:530:LYS:CD	2.43	0.46
1:C:210:ILE:HB	1:C:211:PRO:HD3	1.97	0.46
1:C:254:VAL:O	1:C:258:VAL:HG12	2.15	0.46
1:C:258:VAL:HA	1:C:262:ALA:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:479:LEU:O	1:C:483:VAL:HG23	2.15	0.46
2:D:737:TRP:CE2	2:D:741:ILE:HD11	2.50	0.46
1:A:694:VAL:HG11	2:D:576:ALA:HB1	1.97	0.46
2:B:314:MET:HE1	2:B:353:CYS:N	2.30	0.46
2:B:480:CYS:O	2:B:484:ILE:HG12	2.15	0.46
2:B:737:TRP:CE2	2:B:741:ILE:HD11	2.50	0.46
1:C:247:GLU:HB3	1:C:291:LEU:HD11	1.98	0.46
1:C:354:ALA:HB2	1:C:402:LEU:HD11	1.98	0.46
1:C:554:PHE:O	1:C:558:VAL:HG23	2.15	0.46
2:D:154:LEU:HD11	2:D:169:LEU:HD22	1.96	0.46
2:D:555:ILE:O	2:D:559:LEU:HD13	2.15	0.46
2:D:718:MET:HA	2:D:721:THR:OG1	2.15	0.46
1:A:447:HIS:NE2	1:A:731:HIS:HB3	2.31	0.46
1:A:453:GLU:HB3	1:A:454:PRO:CD	2.46	0.46
1:A:482:MET:CE	1:A:585:GLY:HA3	2.43	0.46
1:A:691:TYR:OH	2:D:572:GLU:HG3	2.16	0.46
2:B:383:ILE:HD11	2:B:445:ASN:ND2	2.30	0.46
1:C:556:TYR:HB2	1:C:584:LEU:CD1	2.44	0.46
1:C:559:LEU:HD21	1:C:580:PHE:CB	2.46	0.46
2:D:371:LEU:HD11	2:D:379:LYS:HD2	1.97	0.46
1:A:424:LEU:HD23	1:A:455:ILE:CD1	2.45	0.46
2:B:271:ARG:HA	2:B:274:GLN:HG2	1.97	0.46
2:B:326:HIS:CD2	2:B:373:PRO:HG3	2.50	0.46
2:B:602:TYR:HE2	1:C:620:VAL:HG21	1.80	0.46
1:C:453:GLU:HB3	1:C:454:PRO:CD	2.46	0.46
1:C:585:GLY:O	1:C:589:ALA:N	2.49	0.46
2:D:271:ARG:HA	2:D:274:GLN:HG2	1.97	0.46
2:D:671:LEU:HD13	2:D:674:PHE:HD2	1.80	0.46
1:A:629:ALA:O	1:A:633:VAL:HG13	2.16	0.46
1:C:677:THR:HA	1:C:703:ILE:HD12	1.97	0.46
2:D:149:PHE:CD1	2:D:169:LEU:HD13	2.51	0.46
2:D:157:ILE:HG21	2:D:166:LEU:HB3	1.98	0.46
2:D:296:ASN:O	2:D:298:PRO:HD3	2.16	0.46
1:A:705:LEU:O	1:A:708:VAL:HG22	2.15	0.46
1:C:202:LEU:HD23	1:C:202:LEU:H	1.80	0.46
1:C:215:ASP:O	1:C:219:ARG:HG2	2.16	0.46
1:C:296:ASN:CA	1:C:345:MET:HE1	2.46	0.46
1:C:447:HIS:NE2	1:C:731:HIS:HB3	2.31	0.46
1:C:573:ALA:HA	2:D:691:TYR:OH	2.16	0.46
2:D:498:PRO:HA	2:D:499:PRO:HD3	1.69	0.46
2:D:499:PRO:HD2	2:D:567:TYR:HE1	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:LEU:HD22	1:A:346:TYR:CD1	2.51	0.46
1:A:583:VAL:HG11	2:B:698:LEU:HD12	1.96	0.46
1:C:616:ARG:NH2	1:C:720:GLU:OE1	2.43	0.46
1:C:629:ALA:O	1:C:633:VAL:HG13	2.16	0.46
2:D:315:ARG:HG2	2:D:362:LEU:HD23	1.96	0.46
1:A:397:GLU:HA	1:A:400:ARG:HD2	1.98	0.45
1:A:492:GLN:OE1	1:A:510:ARG:HD2	2.17	0.45
1:A:559:LEU:HD21	1:A:580:PHE:CB	2.46	0.45
1:A:697:ILE:HD11	2:D:580:PHE:CZ	2.51	0.45
2:B:264:VAL:HG11	2:B:312:ALA:HB2	1.96	0.45
2:B:371:LEU:HD11	2:B:379:LYS:HD2	1.97	0.45
2:B:555:ILE:O	2:B:559:LEU:HD13	2.15	0.45
2:B:671:LEU:HD13	2:B:674:PHE:HD2	1.80	0.45
1:C:277:ASP:OD1	1:C:278:GLU:N	2.49	0.45
1:C:492:GLN:OE1	1:C:510:ARG:HD2	2.17	0.45
1:A:628:TYR:O	1:A:632:LEU:HD13	2.17	0.45
1:A:633:VAL:HA	1:A:636:LEU:HD23	1.99	0.45
2:B:524:PHE:O	2:B:528:ASN:HB2	2.16	0.45
1:C:195:LEU:HB3	1:C:196:PRO:HD3	1.97	0.45
2:D:671:LEU:O	2:D:671:LEU:HD12	2.16	0.45
2:D:743:ASP:OD1	2:D:746:ARG:NH1	2.34	0.45
1:A:509:LEU:O	1:A:512:ALA:HB3	2.16	0.45
1:A:597:LYS:HA	1:A:733:TRP:CZ3	2.52	0.45
1:A:628:TYR:CD2	1:A:702:TYR:HB2	2.51	0.45
2:B:150:ASN:N	2:B:153:ILE:HD12	2.31	0.45
2:B:202:LEU:CG	2:B:205:GLY:HA2	2.33	0.45
2:B:258:VAL:HA	2:B:262:ALA:HB2	1.98	0.45
1:C:752:LEU:HD11	1:C:756:PHE:HE2	1.81	0.45
2:D:494:LEU:HD21	2:D:575:LEU:CD2	2.41	0.45
1:A:582:LEU:HD23	2:B:631:ALA:CA	2.46	0.45
2:B:493:PRO:CB	2:B:499:PRO:HB3	2.45	0.45
1:C:325:LEU:HD22	1:C:346:TYR:CD1	2.51	0.45
1:C:509:LEU:O	1:C:512:ALA:HB3	2.16	0.45
1:C:628:TYR:CD2	1:C:702:TYR:HB2	2.52	0.45
2:D:479:LEU:O	2:D:483:VAL:HG23	2.16	0.45
2:D:554:PHE:O	2:D:558:VAL:HG23	2.17	0.45
1:A:244:ILE:O	1:A:248:ARG:HG2	2.15	0.45
1:A:247:GLU:HB3	1:A:291:LEU:HD11	1.98	0.45
2:B:492:GLN:NE2	2:B:493:PRO:HD2	2.32	0.45
2:B:554:PHE:O	2:B:558:VAL:HG23	2.17	0.45
2:B:580:PHE:O	2:B:583:VAL:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:671:LEU:O	2:B:671:LEU:HD12	2.16	0.45
1:A:202:LEU:HD23	1:A:202:LEU:H	1.80	0.45
1:A:277:ASP:OD1	1:A:278:GLU:N	2.49	0.45
1:A:354:ALA:HB2	1:A:402:LEU:HD11	1.98	0.45
1:C:258:VAL:HG22	1:C:309:HIS:HE1	1.80	0.45
1:C:527:THR:O	1:C:530:LYS:HG2	2.16	0.45
1:C:717:LEU:HD11	2:D:715:ILE:CD1	2.47	0.45
2:D:527:THR:HA	2:D:530:LYS:HG3	1.97	0.45
2:D:580:PHE:O	2:D:583:VAL:HG22	2.17	0.45
1:A:604:ILE:HG13	1:A:605:MET:HE2	1.99	0.45
1:C:372:SER:H	1:C:375:MET:HE3	1.81	0.45
2:B:439:TYR:HE1	2:B:739:THR:HG23	1.82	0.45
2:B:502:TYR:CD1	2:B:507:ASP:HB3	2.52	0.45
2:D:381:GLY:HA2	2:D:449:MET:HE1	1.97	0.45
2:D:439:TYR:HE1	2:D:739:THR:HG23	1.82	0.45
1:A:527:THR:O	1:A:530:LYS:HG2	2.16	0.45
2:B:479:LEU:O	2:B:483:VAL:HG23	2.16	0.45
1:A:215:ASP:O	1:A:219:ARG:HG2	2.16	0.44
1:A:324:VAL:HG11	1:A:349:LEU:HD23	1.99	0.44
1:A:616:ARG:NH2	1:A:720:GLU:OE1	2.43	0.44
1:C:324:VAL:HG11	1:C:349:LEU:HD23	1.99	0.44
1:C:397:GLU:HA	1:C:400:ARG:HD2	1.98	0.44
1:C:622:LEU:O	1:C:626:ILE:HG12	2.18	0.44
2:D:163:THR:OG1	2:D:166:LEU:HD11	2.17	0.44
2:D:566:LEU:HD22	2:D:571:ILE:HG21	1.99	0.44
1:A:208:ASP:O	1:A:211:PRO:HD2	2.17	0.44
1:A:622:LEU:O	1:A:626:ILE:HG12	2.18	0.44
1:A:797:GLU:O	1:A:799:PRO:HD3	2.18	0.44
2:B:157:ILE:HG21	2:B:166:LEU:HB3	1.98	0.44
1:C:323:THR:H	1:C:326:HIS:CD2	2.35	0.44
1:C:579:VAL:HG21	2:D:635:LEU:HB2	1.99	0.44
2:D:258:VAL:HA	2:D:262:ALA:HB2	1.98	0.44
1:A:264:VAL:HG23	1:A:265:HIS:CD2	2.53	0.44
1:A:413:PRO:HD2	2:B:282:PHE:CE1	2.52	0.44
2:B:566:LEU:HD22	2:B:571:ILE:HG21	1.99	0.44
1:C:633:VAL:HA	1:C:636:LEU:HD23	1.99	0.44
1:C:795:ILE:HG22	1:C:795:ILE:O	2.18	0.44
2:D:371:LEU:HD11	2:D:379:LYS:NZ	2.33	0.44
2:D:492:GLN:NE2	2:D:493:PRO:HD2	2.32	0.44
2:D:580:PHE:HA	2:D:583:VAL:HG22	2.00	0.44
1:A:207:ASN:HB3	1:A:210:ILE:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:VAL:HA	1:A:262:ALA:HB3	1.97	0.44
1:A:452:VAL:HG23	1:A:453:GLU:N	2.33	0.44
1:C:208:ASP:O	1:C:211:PRO:HD2	2.17	0.44
1:C:597:LYS:HA	1:C:733:TRP:CZ3	2.52	0.44
1:A:372:SER:H	1:A:375:MET:HE3	1.82	0.44
1:C:173:LEU:HD13	1:C:178:LYS:HB2	1.99	0.44
2:D:616:ARG:O	2:D:620:VAL:HG22	2.17	0.44
2:D:742:LEU:O	2:D:746:ARG:HG3	2.18	0.44
1:A:423:SER:O	1:A:433:VAL:HG23	2.18	0.44
1:A:452:VAL:HG23	1:A:453:GLU:H	1.83	0.44
1:A:498:PRO:O	1:A:500:TYR:N	2.43	0.44
1:A:500:TYR:OH	1:A:568:LEU:HA	2.18	0.44
2:B:371:LEU:HD11	2:B:379:LYS:NZ	2.33	0.44
2:B:616:ARG:O	2:B:620:VAL:HG22	2.17	0.44
1:C:452:VAL:HG23	1:C:453:GLU:N	2.33	0.44
1:C:485:PHE:CD2	1:C:582:LEU:HD13	2.53	0.44
1:C:500:TYR:OH	1:C:568:LEU:HA	2.18	0.44
1:C:797:GLU:O	1:C:799:PRO:HD3	2.18	0.44
1:A:424:LEU:HD23	1:A:455:ILE:HD11	2.00	0.44
1:A:785:TRP:HZ3	2:B:333:ASP:HB2	1.79	0.44
2:B:154:LEU:HD11	2:B:169:LEU:CD2	2.48	0.44
2:B:163:THR:OG1	2:B:166:LEU:HD11	2.17	0.44
1:A:236:TYR:OH	2:D:799:PRO:O	2.30	0.44
1:A:292:ALA:O	1:A:297:GLN:HB2	2.18	0.44
1:A:725:VAL:HG21	2:B:715:ILE:CG2	2.48	0.44
2:B:193:THR:HG22	2:B:194:CYS:N	2.32	0.44
2:D:456:ASN:OD1	2:D:460:ARG:NH1	2.51	0.44
2:D:502:TYR:CD1	2:D:507:ASP:HB3	2.52	0.44
2:B:472:TYR:CA	2:B:475:VAL:HG12	2.42	0.43
2:B:498:PRO:HA	2:B:499:PRO:HD3	1.69	0.43
2:B:686:LEU:CD1	2:B:688:SER:H	2.29	0.43
1:C:264:VAL:HG23	1:C:265:HIS:CD2	2.53	0.43
1:C:350:LEU:HD11	1:C:361:ASN:HD21	1.83	0.43
1:C:628:TYR:O	1:C:632:LEU:HD13	2.17	0.43
1:A:582:LEU:HD11	1:A:586:TRP:HE1	1.83	0.43
2:B:192:LYS:HD3	2:B:197:LYS:HE3	2.00	0.43
1:C:610:LEU:HA	1:C:614:LEU:HD23	2.01	0.43
1:C:632:LEU:HD11	1:C:698:LEU:HB3	1.99	0.43
1:C:764:VAL:CG2	1:C:795:ILE:HD13	2.48	0.43
1:A:485:PHE:HE2	1:A:582:LEU:HB2	1.83	0.43
1:A:498:PRO:HA	1:A:499:PRO:HD3	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:ARG:HG3	2:B:155:PHE:CE2	2.53	0.43
1:C:325:LEU:HD12	1:C:362:LEU:HB3	2.00	0.43
1:C:616:ARG:NH1	1:C:720:GLU:OE2	2.51	0.43
1:A:173:LEU:HD13	1:A:178:LYS:HB2	1.99	0.43
1:A:485:PHE:CD2	1:A:582:LEU:HD13	2.53	0.43
1:A:526:PHE:O	1:A:529:ILE:HG22	2.19	0.43
1:A:603:SER:OG	1:A:604:ILE:N	2.51	0.43
1:A:624:PHE:CE1	1:A:705:LEU:HD23	2.53	0.43
2:B:797:GLU:HG2	2:B:798:ASP:N	2.33	0.43
1:C:292:ALA:O	1:C:297:GLN:HB2	2.18	0.43
1:C:485:PHE:HE2	1:C:582:LEU:HB2	1.84	0.43
1:C:624:PHE:CE1	1:C:705:LEU:HD23	2.53	0.43
1:A:243:HIS:ND1	1:A:268:ALA:HB2	2.33	0.43
1:A:325:LEU:HD12	1:A:362:LEU:HB3	2.00	0.43
1:A:797:GLU:OE1	2:B:200:LEU:HB3	2.19	0.43
2:B:334:ASN:ND2	2:B:383:ILE:HD12	2.33	0.43
1:C:207:ASN:HB3	1:C:210:ILE:HD13	2.00	0.43
1:C:423:SER:O	1:C:433:VAL:HG23	2.18	0.43
1:C:582:LEU:HD11	1:C:586:TRP:HE1	1.83	0.43
2:D:258:VAL:HA	2:D:262:ALA:HB3	2.00	0.43
1:A:210:ILE:O	1:A:214:LEU:HD23	2.19	0.43
1:A:764:VAL:CG2	1:A:795:ILE:HD13	2.48	0.43
1:A:795:ILE:O	1:A:795:ILE:HG22	2.17	0.43
2:B:502:TYR:CB	2:B:507:ASP:HB3	2.48	0.43
1:C:452:VAL:HG23	1:C:453:GLU:H	1.82	0.43
2:D:154:LEU:HD11	2:D:169:LEU:CD2	2.48	0.43
2:D:331:ILE:H	2:D:331:ILE:HG13	1.70	0.43
2:D:366:LEU:CD2	2:D:372:SER:HB3	2.49	0.43
2:B:424:LEU:HD23	2:B:455:ILE:CD1	2.48	0.43
2:B:510:ARG:O	2:B:514:GLU:HG3	2.18	0.43
2:B:580:PHE:HA	2:B:583:VAL:HG22	2.00	0.43
2:B:583:VAL:O	2:B:587:MET:HG3	2.19	0.43
2:D:192:LYS:HD3	2:D:197:LYS:HE3	2.00	0.43
2:D:334:ASN:ND2	2:D:383:ILE:HD12	2.33	0.43
1:A:447:HIS:CE1	1:A:731:HIS:HB3	2.54	0.43
1:A:585:GLY:O	1:A:589:ALA:N	2.49	0.43
2:B:252:HIS:O	2:B:256:LEU:HD13	2.19	0.43
2:B:608:LYS:HZ3	2:B:725:VAL:HG11	1.82	0.43
2:B:743:ASP:OD1	2:B:746:ARG:NH1	2.34	0.43
2:B:752:LEU:HD11	2:B:756:PHE:HE2	1.83	0.43
1:C:233:ASP:OD2	1:C:235:TYR:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:HIS:ND1	1:C:268:ALA:HB2	2.33	0.43
1:C:594:ARG:NH2	1:C:736:GLN:HG2	2.34	0.43
2:D:752:LEU:HD11	2:D:756:PHE:HE2	1.83	0.43
2:D:760:GLU:O	2:D:762:VAL:HG23	2.19	0.43
1:A:243:HIS:CE1	1:A:268:ALA:HB2	2.54	0.43
1:A:632:LEU:HD11	1:A:698:LEU:HB3	1.99	0.43
2:B:307:ASN:OD1	2:B:311:LYS:HB3	2.19	0.43
2:B:672:ASP:HB3	2:B:685:MET:CE	2.49	0.43
2:B:742:LEU:O	2:B:746:ARG:HG3	2.18	0.43
1:C:243:HIS:CE1	1:C:268:ALA:HB2	2.54	0.43
1:C:526:PHE:O	1:C:529:ILE:HG22	2.19	0.43
1:C:558:VAL:O	1:C:562:VAL:HG23	2.19	0.43
1:C:603:SER:OG	1:C:604:ILE:N	2.51	0.43
2:D:493:PRO:CB	2:D:499:PRO:HB3	2.45	0.43
2:D:583:VAL:O	2:D:587:MET:HG3	2.19	0.43
1:A:233:ASP:OD2	1:A:235:TYR:HB3	2.19	0.43
1:A:414:VAL:HG13	1:A:414:VAL:O	2.19	0.43
1:A:661:ARG:CG	1:A:687:SER:HB2	2.35	0.43
2:B:456:ASN:OD1	2:B:460:ARG:NH1	2.51	0.43
2:D:151:ARG:HG3	2:D:155:PHE:CE2	2.53	0.43
2:D:426:THR:HG23	2:D:426:THR:O	2.19	0.43
2:D:510:ARG:O	2:D:514:GLU:HG3	2.18	0.43
1:A:321:GLY:HA3	1:A:367:ASN:HA	2.00	0.42
1:A:411:TYR:OH	2:B:291:LEU:HD11	2.18	0.42
1:C:215:ASP:O	1:C:218:GLU:HG2	2.19	0.42
2:D:298:PRO:HG3	2:D:345:MET:CE	2.49	0.42
2:D:387:GLN:O	2:D:391:ARG:HG2	2.19	0.42
2:D:502:TYR:CB	2:D:507:ASP:HB3	2.48	0.42
2:D:672:ASP:HB3	2:D:685:MET:CE	2.49	0.42
2:D:797:GLU:HG2	2:D:798:ASP:N	2.33	0.42
1:A:198:ALA:HB1	1:A:210:ILE:CD1	2.49	0.42
1:A:215:ASP:O	1:A:218:GLU:HG2	2.19	0.42
1:A:558:VAL:O	1:A:562:VAL:HG23	2.19	0.42
1:A:590:LEU:HD21	1:A:602:TYR:CZ	2.54	0.42
1:A:594:ARG:NH2	1:A:736:GLN:HG2	2.34	0.42
2:B:342:VAL:CG1	2:B:385:ILE:HD12	2.49	0.42
1:C:414:VAL:HG13	1:C:414:VAL:O	2.19	0.42
1:C:424:LEU:HD23	1:C:455:ILE:HD11	2.00	0.42
1:A:610:LEU:HA	1:A:614:LEU:HD23	2.01	0.42
2:B:326:HIS:HE2	2:B:373:PRO:HD3	1.84	0.42
2:B:494:LEU:HD21	2:B:575:LEU:CD2	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:586:TRP:O	1:C:623:LEU:HD12	2.20	0.42
2:B:760:GLU:O	2:B:762:VAL:HG23	2.19	0.42
1:C:198:ALA:HB1	1:C:210:ILE:CD1	2.49	0.42
1:C:253:TYR:O	1:C:257:LEU:HD13	2.20	0.42
1:C:447:HIS:CE1	1:C:731:HIS:HB3	2.54	0.42
1:C:590:LEU:HD21	1:C:602:TYR:CZ	2.54	0.42
2:D:424:LEU:HD23	2:D:455:ILE:CD1	2.48	0.42
2:D:474:ASN:O	2:D:478:TYR:N	2.46	0.42
1:A:559:LEU:HD21	1:A:580:PHE:HB2	2.02	0.42
1:A:719:GLY:N	2:D:722:VAL:HG22	2.33	0.42
2:B:556:TYR:O	2:B:560:VAL:HG23	2.20	0.42
2:B:690:LYS:O	2:B:692:PRO:HD3	2.19	0.42
1:C:436:ILE:HG23	1:C:440:ASN:OD1	2.19	0.42
1:C:511:LEU:O	1:C:514:GLU:HB2	2.19	0.42
1:C:563:SER:HB3	1:C:578:MET:SD	2.59	0.42
1:C:590:LEU:HD21	1:C:602:TYR:CE2	2.54	0.42
2:D:192:LYS:CD	2:D:197:LYS:HE3	2.49	0.42
1:A:253:TYR:O	1:A:257:LEU:HD13	2.20	0.42
2:B:282:PHE:CE2	2:B:284:PHE:HB3	2.54	0.42
2:B:324:VAL:O	2:B:328:LEU:HD13	2.20	0.42
2:B:527:THR:CG2	2:B:530:LYS:HD2	2.45	0.42
2:B:545:ILE:O	2:B:545:ILE:HG22	2.20	0.42
2:B:621:TYR:HE1	2:B:706:THR:HG22	1.84	0.42
1:C:289:LEU:HD21	1:C:314:MET:HG2	2.02	0.42
1:C:530:LYS:HA	1:C:533:PHE:CB	2.49	0.42
1:C:609:ILE:HG13	1:C:725:VAL:HG11	2.02	0.42
2:D:264:VAL:O	2:D:265:HIS:HB2	2.20	0.42
1:A:273:PHE:HE1	2:D:411:TYR:CZ	2.36	0.42
1:A:616:ARG:NH1	1:A:720:GLU:OE2	2.51	0.42
2:B:258:VAL:HA	2:B:262:ALA:HB3	2.00	0.42
2:B:366:LEU:CD2	2:B:372:SER:HB3	2.49	0.42
1:C:321:GLY:HA3	1:C:367:ASN:HA	2.00	0.42
1:C:498:PRO:HA	1:C:499:PRO:HD3	1.86	0.42
2:D:282:PHE:CE2	2:D:284:PHE:HB3	2.54	0.42
2:D:307:ASN:OD1	2:D:311:LYS:HB3	2.19	0.42
2:D:317:GLN:HE21	2:D:365:VAL:CG1	2.32	0.42
2:D:472:TYR:CA	2:D:475:VAL:HG12	2.42	0.42
2:D:749:PRO:O	2:D:753:ARG:HG3	2.20	0.42
1:A:530:LYS:HA	1:A:533:PHE:CB	2.49	0.42
2:B:192:LYS:CD	2:B:197:LYS:HE3	2.49	0.42
2:B:298:PRO:HG3	2:B:345:MET:CE	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:GLU:HB2	1:C:318:ASP:HB2	2.01	0.42
1:C:469:VAL:O	1:C:473:ILE:HD12	2.20	0.42
1:C:671:LEU:O	1:C:671:LEU:HD12	2.20	0.42
2:D:483:VAL:O	2:D:487:LEU:HD13	2.20	0.42
1:A:150:ASN:H	1:A:153:ILE:HG22	1.85	0.42
1:A:255:GLU:HA	1:A:258:VAL:HG12	2.01	0.42
1:A:350:LEU:HD11	1:A:361:ASN:HD21	1.83	0.42
1:A:436:ILE:HG23	1:A:440:ASN:OD1	2.19	0.42
1:A:469:VAL:O	1:A:473:ILE:HD12	2.20	0.42
1:A:609:ILE:HG13	1:A:725:VAL:HG11	2.02	0.42
1:C:258:VAL:HG22	1:C:309:HIS:CE1	2.55	0.42
1:C:559:LEU:HD21	1:C:580:PHE:HB2	2.02	0.42
1:A:286:GLU:HB2	1:A:318:ASP:HB2	2.01	0.42
1:A:511:LEU:O	1:A:514:GLU:HB2	2.19	0.42
1:A:559:LEU:CD1	1:A:577:VAL:HG13	2.50	0.42
1:A:718:MET:HG2	1:C:718:MET:HG2	2.02	0.42
2:B:305:THR:HG1	2:B:306:GLU:CD	2.20	0.42
2:B:387:GLN:O	2:B:391:ARG:HG2	2.19	0.42
2:B:485:PHE:CD2	2:B:582:LEU:HD13	2.55	0.42
2:B:524:PHE:HD1	3:B:902:POV:H13B	1.85	0.42
1:C:255:GLU:HA	1:C:258:VAL:HG12	2.02	0.42
2:D:342:VAL:CG1	2:D:385:ILE:HD12	2.49	0.42
2:D:485:PHE:CD2	2:D:582:LEU:HD13	2.55	0.42
2:D:527:THR:HG22	2:D:530:LYS:CD	2.43	0.42
1:A:296:ASN:CA	1:A:345:MET:HE1	2.49	0.42
1:A:671:LEU:HD12	1:A:671:LEU:O	2.20	0.42
1:A:678:ILE:HG13	1:A:680:MET:SD	2.60	0.42
1:A:725:VAL:O	1:A:729:SER:HB3	2.20	0.42
2:B:426:THR:HG23	2:B:426:THR:O	2.19	0.42
1:C:374:LEU:HD13	1:C:389:ILE:CG2	2.50	0.42
2:D:252:HIS:O	2:D:256:LEU:HD13	2.19	0.42
2:D:326:HIS:HE2	2:D:373:PRO:HD3	1.84	0.42
2:D:519:PHE:O	2:D:523:LEU:HG	2.20	0.42
2:D:608:LYS:HZ3	2:D:725:VAL:HG11	1.85	0.42
1:A:374:LEU:HD13	1:A:389:ILE:CG2	2.50	0.41
1:A:590:LEU:HD21	1:A:602:TYR:CE2	2.54	0.41
2:B:317:GLN:HE21	2:B:365:VAL:CG1	2.32	0.41
2:B:352:LYS:O	2:B:356:LEU:HD13	2.20	0.41
2:B:483:VAL:O	2:B:487:LEU:HD13	2.20	0.41
2:B:718:MET:HA	2:B:721:THR:HG1	1.85	0.41
1:C:425:ASP:OD2	1:C:462:LYS:NZ	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:596:LEU:O	1:C:597:LYS:HB2	2.20	0.41
2:D:324:VAL:O	2:D:328:LEU:HD13	2.20	0.41
1:A:276:LYS:HG3	1:A:276:LYS:O	2.20	0.41
1:A:669:PHE:HA	1:A:672:ASP:HB2	2.02	0.41
2:B:305:THR:O	2:B:311:LYS:HD3	2.20	0.41
1:C:443:ILE:HG22	1:C:449:MET:CE	2.51	0.41
1:C:445:ASN:O	1:C:449:MET:HG3	2.20	0.41
2:D:556:TYR:O	2:D:560:VAL:HG23	2.20	0.41
1:A:203:SER:OG	1:A:204:ASN:N	2.54	0.41
1:A:443:ILE:HG22	1:A:449:MET:CE	2.51	0.41
1:A:445:ASN:O	1:A:449:MET:HG3	2.20	0.41
1:A:563:SER:HB3	1:A:578:MET:SD	2.59	0.41
1:C:210:ILE:O	1:C:214:LEU:HD23	2.19	0.41
2:D:553:TYR:OH	2:D:588:ASN:O	2.28	0.41
2:D:621:TYR:HE1	2:D:706:THR:HG22	1.84	0.41
2:D:690:LYS:O	2:D:692:PRO:HD3	2.19	0.41
1:A:347:ASP:CG	1:A:388:HIS:HE2	2.24	0.41
1:A:516:ILE:O	1:A:520:THR:HG23	2.20	0.41
1:A:601:THR:HG21	1:A:605:MET:HB2	2.03	0.41
1:A:760:GLU:O	1:A:762:VAL:HG23	2.20	0.41
2:B:264:VAL:O	2:B:265:HIS:HB2	2.20	0.41
1:C:258:VAL:HG13	1:C:309:HIS:HE1	1.85	0.41
1:C:347:ASP:CG	1:C:388:HIS:HE2	2.24	0.41
1:C:559:LEU:CD1	1:C:577:VAL:HG13	2.50	0.41
2:D:429:GLU:O	2:D:430:GLU:HB2	2.20	0.41
1:A:722:VAL:HG12	2:B:715:ILE:HG23	2.02	0.41
2:B:273:PHE:CD1	2:B:284:PHE:HE1	2.38	0.41
1:C:265:HIS:NE2	1:C:312:ALA:HA	2.36	0.41
1:C:609:ILE:CG1	1:C:725:VAL:HG11	2.51	0.41
1:C:678:ILE:HG13	1:C:680:MET:SD	2.60	0.41
1:C:694:VAL:O	1:C:697:ILE:HG13	2.21	0.41
2:D:518:LEU:HD23	2:D:564:ALA:HB2	2.01	0.41
2:D:530:LYS:HD3	3:D:902:POV:H38A	2.02	0.41
2:D:545:ILE:HG22	2:D:545:ILE:O	2.20	0.41
1:A:314:MET:HE1	1:A:353:CYS:N	2.36	0.41
1:A:497:THR:OG1	1:A:498:PRO:HD2	2.21	0.41
2:B:383:ILE:HD12	2:B:383:ILE:H	1.86	0.41
2:B:518:LEU:HD13	2:B:518:LEU:O	2.21	0.41
1:C:246:ILE:HB	1:C:291:LEU:HD12	2.03	0.41
1:C:625:MET:HG2	1:C:702:TYR:OH	2.21	0.41
2:D:284:PHE:CE2	2:D:291:LEU:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:VAL:HG22	1:A:309:HIS:CE1	2.55	0.41
1:A:676:LEU:CD2	1:A:699:LEU:HD21	2.51	0.41
1:A:788:TRP:CZ2	2:B:296:ASN:HB2	2.56	0.41
2:B:346:TYR:CE2	2:B:389:ILE:HG12	2.56	0.41
2:B:452:VAL:HG23	2:B:453:GLU:N	2.34	0.41
2:B:518:LEU:HD23	2:B:564:ALA:HB2	2.01	0.41
2:B:619:LEU:O	2:B:623:LEU:HD23	2.21	0.41
1:C:276:LYS:HG3	1:C:276:LYS:O	2.20	0.41
1:C:447:HIS:CD2	1:C:731:HIS:HB3	2.56	0.41
1:C:669:PHE:HA	1:C:672:ASP:HB2	2.02	0.41
1:C:676:LEU:CD2	1:C:699:LEU:HD21	2.51	0.41
2:D:352:LYS:O	2:D:356:LEU:HD13	2.20	0.41
2:D:518:LEU:HD13	2:D:518:LEU:O	2.21	0.41
2:D:686:LEU:CD1	2:D:688:SER:H	2.29	0.41
1:A:224:ARG:NE	1:A:261:GLY:HA3	2.36	0.41
1:A:274:GLN:C	1:A:283:TYR:HB2	2.41	0.41
1:A:430:GLU:HG2	1:A:431:ALA:O	2.21	0.41
1:A:628:TYR:HD2	1:A:702:TYR:CD1	2.39	0.41
2:B:297:GLN:OE1	2:B:300:ILE:HD12	2.21	0.41
2:B:429:GLU:O	2:B:430:GLU:HB2	2.20	0.41
1:C:173:LEU:HD11	1:C:185:PHE:CE2	2.56	0.41
1:C:502:TYR:HE2	1:C:511:LEU:HB2	1.86	0.41
1:C:725:VAL:O	1:C:729:SER:HB3	2.20	0.41
1:C:787:HIS:HD2	1:C:790:GLN:HG2	1.86	0.41
2:D:273:PHE:CD1	2:D:284:PHE:HE1	2.38	0.41
1:A:265:HIS:NE2	1:A:312:ALA:HA	2.36	0.41
1:A:289:LEU:HD21	1:A:314:MET:HG2	2.01	0.41
1:A:383:ILE:HD11	1:A:445:ASN:CG	2.41	0.41
1:A:596:LEU:O	1:A:597:LYS:HB2	2.20	0.41
2:B:749:PRO:O	2:B:753:ARG:HG3	2.20	0.41
1:C:332:ALA:O	1:C:382:LYS:HD2	2.21	0.41
1:C:391:ARG:HB2	1:C:405:LYS:HD2	2.03	0.41
1:C:584:LEU:HA	1:C:587:MET:CE	2.50	0.41
1:C:608:LYS:HD3	1:C:724:GLN:OE1	2.21	0.41
1:C:628:TYR:HD2	1:C:702:TYR:CD1	2.39	0.41
2:D:720:GLU:OE2	2:D:721:THR:HG23	2.21	0.41
1:A:190:THR:HG22	1:A:233:ASP:HB2	2.03	0.41
1:A:210:ILE:H	1:A:210:ILE:HD12	1.86	0.41
1:A:246:ILE:HB	1:A:291:LEU:HD12	2.03	0.41
1:A:484:ILE:O	1:A:488:THR:HG23	2.21	0.41
1:C:500:TYR:HB2	1:C:501:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:760:GLU:O	1:C:762:VAL:HG23	2.20	0.41
2:D:305:THR:O	2:D:311:LYS:HD3	2.21	0.41
1:A:625:MET:HG2	1:A:702:TYR:OH	2.21	0.40
1:A:635:LEU:HD23	2:D:575:LEU:CD2	2.51	0.40
2:B:519:PHE:O	2:B:523:LEU:HG	2.20	0.40
1:C:274:GLN:C	1:C:283:TYR:HB2	2.41	0.40
1:C:516:ILE:O	1:C:520:THR:HG23	2.20	0.40
2:D:346:TYR:CE2	2:D:389:ILE:HG12	2.56	0.40
2:D:619:LEU:O	2:D:623:LEU:HD23	2.21	0.40
1:A:694:VAL:O	1:A:697:ILE:HG13	2.20	0.40
2:B:331:ILE:H	2:B:331:ILE:HG13	1.70	0.40
2:B:381:GLY:HA2	2:B:449:MET:HE1	2.02	0.40
2:B:570:GLY:H	2:B:571:ILE:HD12	1.86	0.40
2:B:785:TRP:HB2	1:C:337:GLU:HG2	2.02	0.40
1:C:383:ILE:HD11	1:C:445:ASN:CG	2.42	0.40
1:C:497:THR:OG1	1:C:498:PRO:HD2	2.21	0.40
1:A:260:GLN:O	1:A:262:ALA:N	2.53	0.40
1:A:720:GLU:O	1:A:722:VAL:N	2.54	0.40
2:B:284:PHE:CE2	2:B:291:LEU:HB2	2.56	0.40
2:D:170:LEU:HD21	2:D:219:ARG:HG3	2.03	0.40
2:D:443:ILE:HA	2:D:446:ARG:HG3	2.03	0.40
2:D:694:VAL:HA	2:D:697:ILE:HG12	2.04	0.40
1:A:366:LEU:CD2	1:A:372:SER:HB3	2.52	0.40
1:A:488:THR:HG21	1:A:513:GLY:HA3	2.03	0.40
2:B:271:ARG:HA	2:B:274:GLN:CG	2.52	0.40
2:B:463:TRP:O	2:B:468:ALA:N	2.50	0.40
2:B:797:GLU:O	2:B:799:PRO:HD3	2.21	0.40
1:C:210:ILE:HD12	1:C:210:ILE:H	1.86	0.40
1:C:224:ARG:NE	1:C:261:GLY:HA3	2.36	0.40
1:C:484:ILE:O	1:C:488:THR:HG23	2.21	0.40
2:D:366:LEU:HD23	2:D:372:SER:HB3	2.04	0.40
2:D:718:MET:HA	2:D:721:THR:HG1	1.86	0.40
2:D:797:GLU:O	2:D:799:PRO:HD3	2.21	0.40
1:A:173:LEU:HD11	1:A:185:PHE:CE2	2.56	0.40
1:A:193:THR:HG22	1:A:194:CYS:N	2.32	0.40
1:A:609:ILE:CG1	1:A:725:VAL:HG11	2.51	0.40
1:A:720:GLU:HG2	1:A:721:THR:H	1.86	0.40
1:A:725:VAL:HG21	2:B:715:ILE:HG22	2.02	0.40
2:B:491:TYR:O	2:B:510:ARG:HD3	2.22	0.40
2:B:745:GLU:HG2	2:B:753:ARG:NE	2.36	0.40
1:C:150:ASN:H	1:C:153:ILE:HG22	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:GLY:C	1:C:171:PRO:HD2	2.42	0.40
1:C:484:ILE:HG21	1:C:516:ILE:HD12	2.04	0.40
1:C:506:VAL:O	1:C:509:LEU:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	613/619 (99%)	532 (87%)	76 (12%)	5 (1%)	19	19
1	C	613/619 (99%)	532 (87%)	76 (12%)	5 (1%)	19	19
2	B	632/636 (99%)	539 (85%)	88 (14%)	5 (1%)	19	19
2	D	632/636 (99%)	539 (85%)	88 (14%)	5 (1%)	19	19
All	All	2490/2510 (99%)	2142 (86%)	328 (13%)	20 (1%)	24	19

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	725	VAL
2	D	725	VAL
1	A	602	TYR
1	A	721	THR
2	B	690	LYS
1	C	602	TYR
1	C	721	THR
2	D	690	LYS
2	B	722	VAL
2	D	722	VAL
1	A	444	GLU
2	B	453	GLU

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Mol	Chain	Res	Type
1	C	444	GLU
2	D	453	GLU
1	A	285	GLY
1	C	285	GLY
2	B	452	VAL
2	D	452	VAL
1	A	454	PRO
1	C	454	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	545/545 (100%)	539 (99%)	6 (1%)	73	73
1	C	545/545 (100%)	539 (99%)	6 (1%)	73	73
2	B	560/560 (100%)	551 (98%)	9 (2%)	62	62
2	D	560/560 (100%)	551 (98%)	9 (2%)	62	62
All	All	2210/2210 (100%)	2180 (99%)	30 (1%)	68	67

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	207	ASN
1	A	338	ASN
1	A	361	ASN
1	A	588	ASN
1	A	637	ASN
1	A	784	ASN
2	B	204	ASN
2	B	207	ASN
2	B	228	ASN
2	B	271	ARG
2	B	338	ASN
2	B	528	ASN
2	B	534	MET

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Mol	Chain	Res	Type
2	B	541	ASN
2	B	784	ASN
1	C	207	ASN
1	C	338	ASN
1	C	361	ASN
1	C	588	ASN
1	C	637	ASN
1	C	784	ASN
2	D	204	ASN
2	D	207	ASN
2	D	228	ASN
2	D	271	ARG
2	D	338	ASN
2	D	528	ASN
2	D	534	MET
2	D	541	ASN
2	D	784	ASN

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

Mol	Chain	Res	Type
1	A	201	ASN
1	A	207	ASN
1	A	228	ASN
1	A	260	GLN
1	A	309	HIS
1	A	317	GLN
1	A	326	HIS
1	A	361	ASN
1	A	588	ASN
1	A	637	ASN
1	A	712	ASN
1	A	784	ASN
1	A	787	HIS
2	B	176	HIS
2	B	204	ASN
2	B	207	ASN
2	B	260	GLN
2	B	317	GLN
2	B	492	GLN
2	B	528	ASN
2	B	541	ASN

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Mol	Chain	Res	Type
2	B	588	ASN
2	B	784	ASN
1	C	201	ASN
1	C	207	ASN
1	C	228	ASN
1	C	260	GLN
1	C	309	HIS
1	C	317	GLN
1	C	326	HIS
1	C	361	ASN
1	C	588	ASN
1	C	637	ASN
1	C	784	ASN
1	C	787	HIS
2	D	176	HIS
2	D	204	ASN
2	D	207	ASN
2	D	260	GLN
2	D	317	GLN
2	D	338	ASN
2	D	492	GLN
2	D	528	ASN
2	D	541	ASN
2	D	588	ASN
2	D	784	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	POV	A	902	-	27,27,51	0.39	0	33,35,59	0.37	0
3	POV	C	902	-	27,27,51	0.41	0	33,35,59	0.41	0
3	POV	B	902	-	51,51,51	0.35	0	57,59,59	0.75	1 (1%)
3	POV	D	902	-	51,51,51	0.35	0	57,59,59	0.76	1 (1%)

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	POV	A	902	-	-	9/31/31/55	-
3	POV	C	902	-	-	10/31/31/55	-
3	POV	B	902	-	-	29/55/55/55	-
3	POV	D	902	-	-	29/55/55/55	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	902	POV	O31-C3-C2	2.95	117.03	108.43
3	B	902	POV	O31-C3-C2	2.80	116.57	108.43

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	902	POV	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
3	A	902	POV	C1-O11-P-O14
3	A	902	POV	C11-O12-P-O11
3	A	902	POV	O12-C11-C12-N
3	B	902	POV	C1-O11-P-O13
3	B	902	POV	C1-O11-P-O14
3	B	902	POV	C11-O12-P-O11
3	B	902	POV	C11-O12-P-O13
3	B	902	POV	C11-O12-P-O14
3	B	902	POV	C32-C31-O31-C3
3	B	902	POV	O32-C31-O31-C3
3	C	902	POV	C1-O11-P-O12
3	C	902	POV	C1-O11-P-O13
3	C	902	POV	C1-O11-P-O14
3	C	902	POV	C11-O12-P-O11
3	C	902	POV	C11-O12-P-O14
3	C	902	POV	O12-C11-C12-N
3	D	902	POV	C11-O12-P-O11
3	D	902	POV	C11-O12-P-O13
3	D	902	POV	C11-O12-P-O14
3	D	902	POV	C32-C31-O31-C3
3	D	902	POV	O32-C31-O31-C3
3	A	902	POV	C1-O11-P-O12
3	B	902	POV	C1-O11-P-O12
3	D	902	POV	C1-O11-P-O12
3	B	902	POV	O21-C2-C3-O31
3	B	902	POV	C213-C214-C215-C216
3	D	902	POV	C213-C214-C215-C216
3	D	902	POV	C34-C35-C36-C37
3	D	902	POV	C1-C2-C3-O31
3	B	902	POV	C34-C35-C36-C37
3	B	902	POV	C311-C310-C39-C38
3	D	902	POV	O21-C2-C3-O31
3	D	902	POV	C311-C310-C39-C38
3	A	902	POV	C1-C2-C3-O31
3	B	902	POV	C1-C2-C3-O31
3	C	902	POV	C1-C2-C3-O31
3	B	902	POV	C32-C33-C34-C35
3	B	902	POV	O11-C1-C2-O21
3	C	902	POV	O21-C2-C3-O31
3	D	902	POV	C2-C1-O11-P
3	B	902	POV	C2-C1-O11-P
3	D	902	POV	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
3	D	902	POV	C212-C213-C214-C215
3	D	902	POV	C32-C33-C34-C35
3	B	902	POV	C214-C215-C216-C217
3	A	902	POV	C11-O12-P-O14
3	D	902	POV	C1-O11-P-O13
3	D	902	POV	C1-O11-P-O14
3	B	902	POV	O11-C1-C2-C3
3	D	902	POV	O11-C1-C2-C3
3	D	902	POV	C214-C215-C216-C217
3	B	902	POV	C212-C213-C214-C215
3	B	902	POV	O12-C11-C12-N
3	D	902	POV	O12-C11-C12-N
3	D	902	POV	C37-C38-C39-C310
3	A	902	POV	O21-C2-C3-O31
3	B	902	POV	C36-C37-C38-C39
3	D	902	POV	C310-C311-C312-C313
3	D	902	POV	C36-C37-C38-C39
3	D	902	POV	C39-C310-C311-C312
3	B	902	POV	C29-C210-C211-C212
3	D	902	POV	C29-C210-C211-C212
3	B	902	POV	C37-C38-C39-C310
3	B	902	POV	C310-C311-C312-C313
3	B	902	POV	O31-C31-C32-C33
3	D	902	POV	O31-C31-C32-C33
3	B	902	POV	C3-C2-O21-C21
3	D	902	POV	C3-C2-O21-C21
3	B	902	POV	C39-C310-C311-C312
3	C	902	POV	O31-C31-C32-C33
3	D	902	POV	O32-C31-C32-C33
3	B	902	POV	O32-C31-C32-C33
3	B	902	POV	O22-C21-O21-C2
3	D	902	POV	O22-C21-O21-C2
3	C	902	POV	O32-C31-C32-C33
3	A	902	POV	O31-C31-C32-C33

There are no ring outliers.

4 monomers are involved in 13 short contacts:

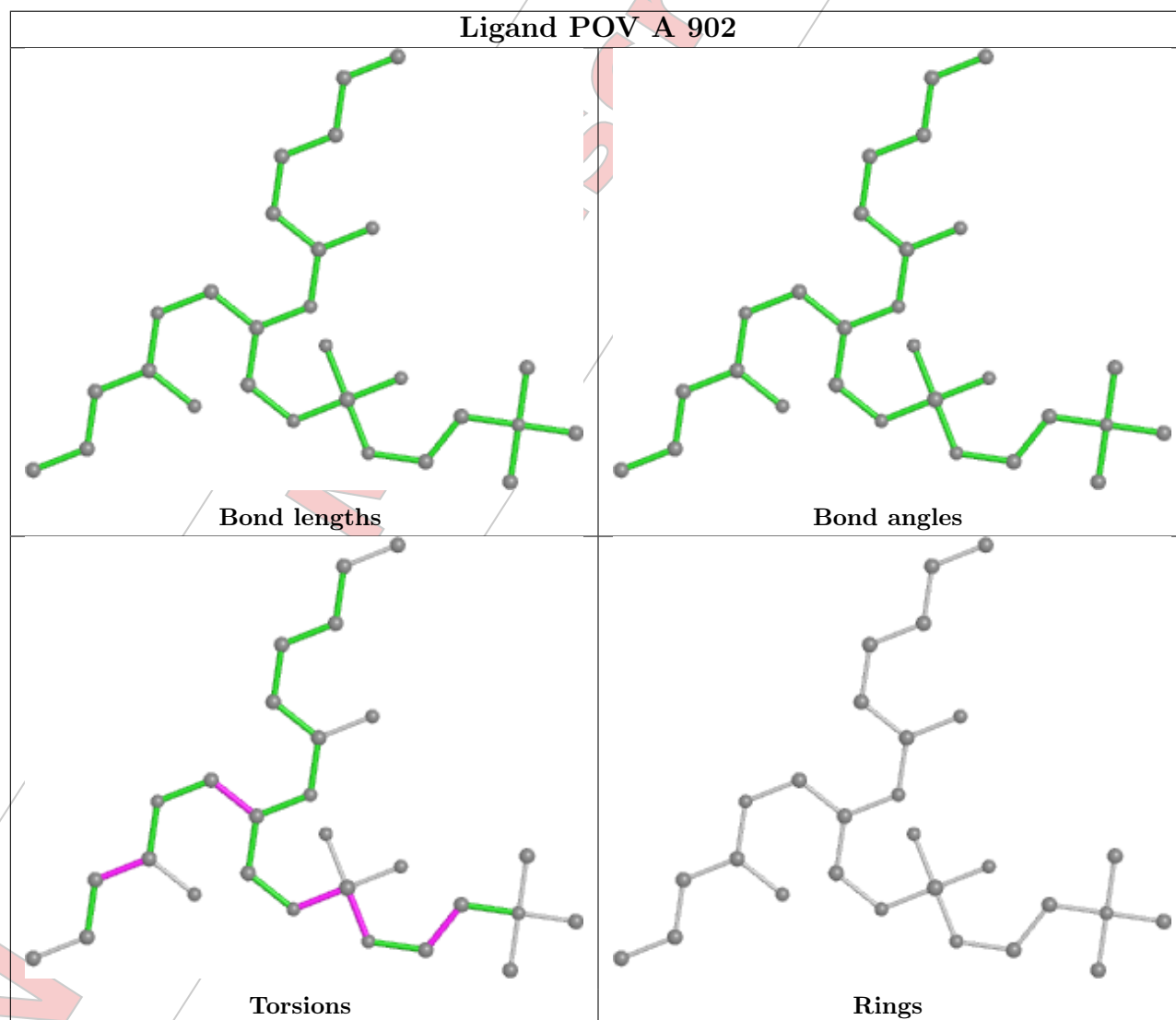
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	POV	2	0
3	C	902	POV	3	0
3	B	902	POV	4	0

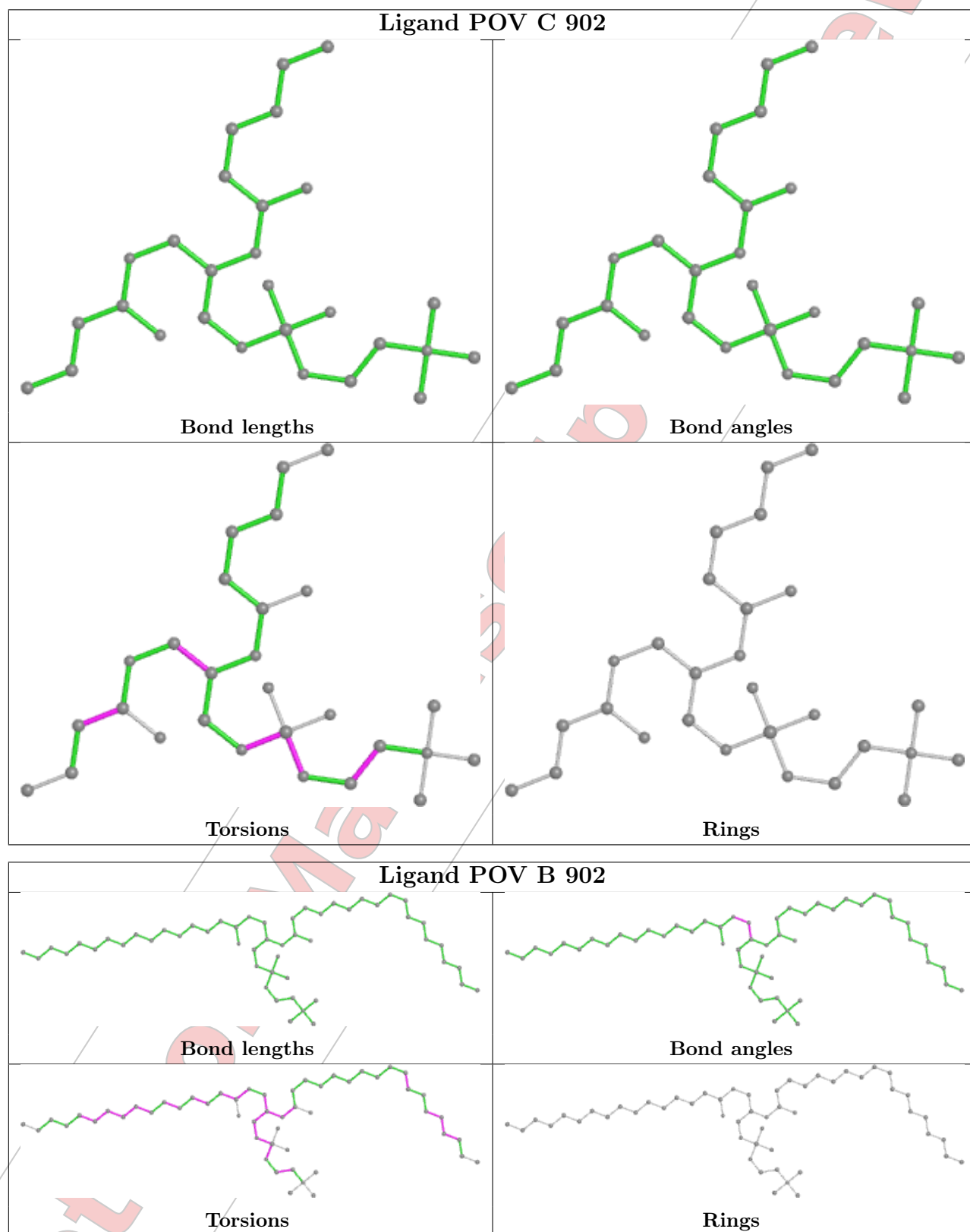
Continued on next page...

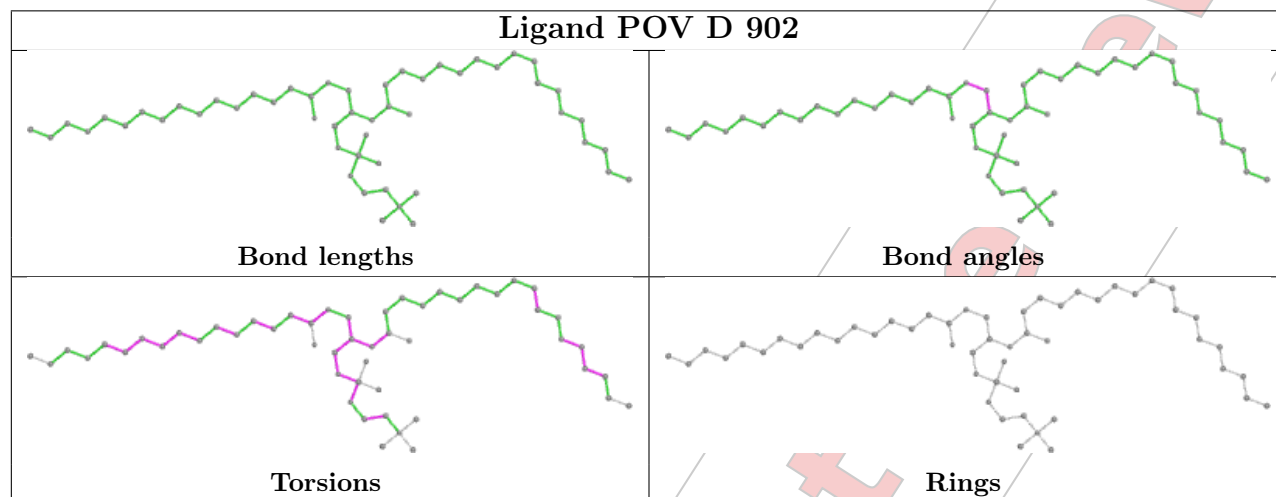
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	902	POV	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
1	C	2
2	B	1
2	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	533:PHE	C	549:PHE	N	17.07
1	C	533:PHE	C	549:PHE	N	17.07
1	B	640:ALA	C	661:ARG	N	12.07
1	D	640:ALA	C	661:ARG	N	12.07
1	A	640:ALA	C	661:ARG	N	6.64
1	C	640:ALA	C	661:ARG	N	6.64

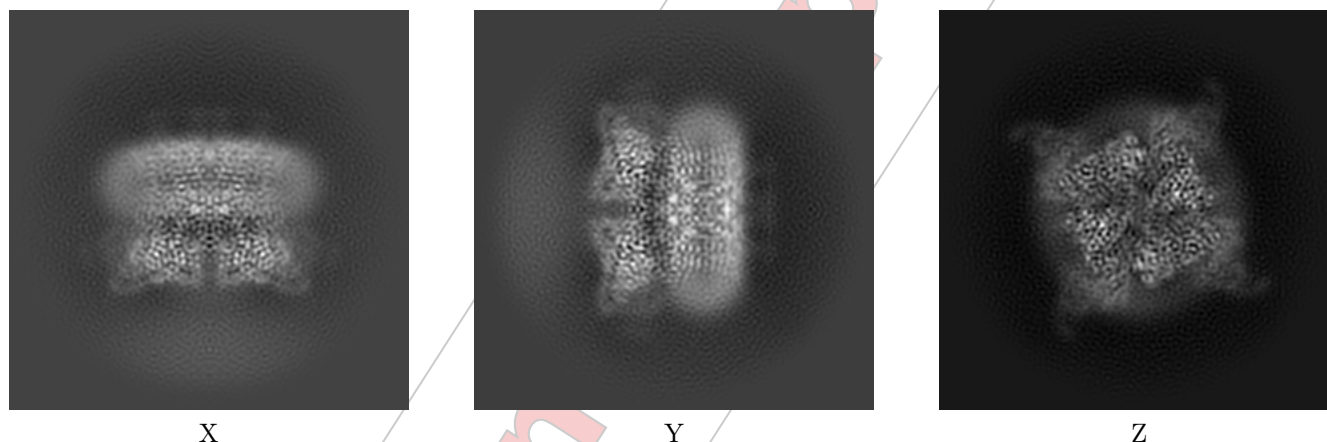
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry D_9100078168. 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](#)

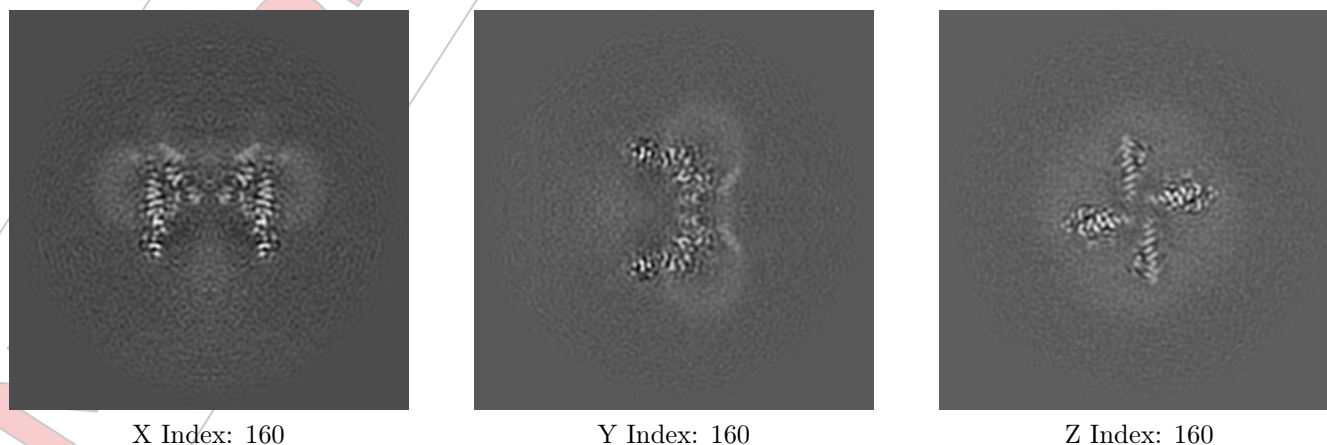
6.1.1 Primary map



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

6.2 Central slices [i](#)

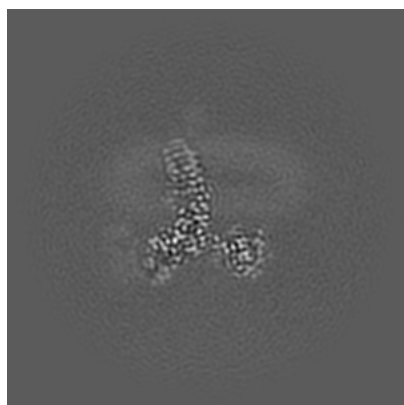
6.2.1 Primary map



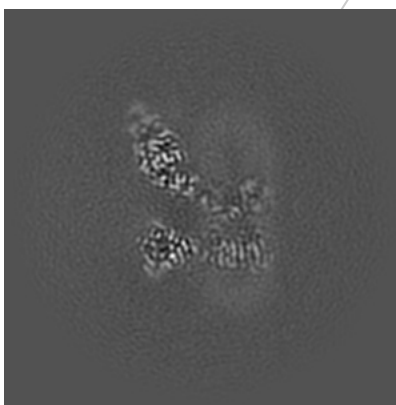
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

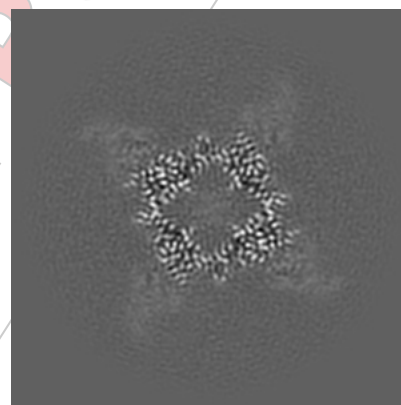
6.3.1 Primary map



X Index: 122



Y Index: 134

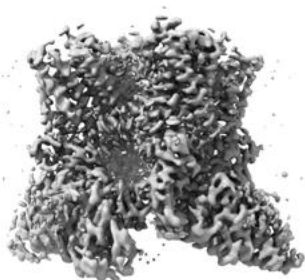


Z Index: 129

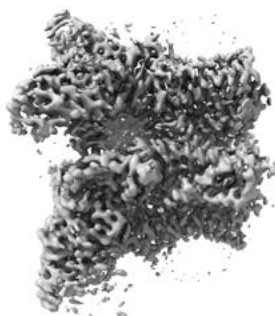
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

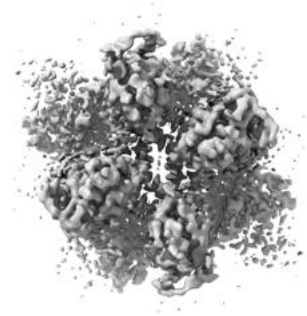
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.114. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5 Mask visualisation

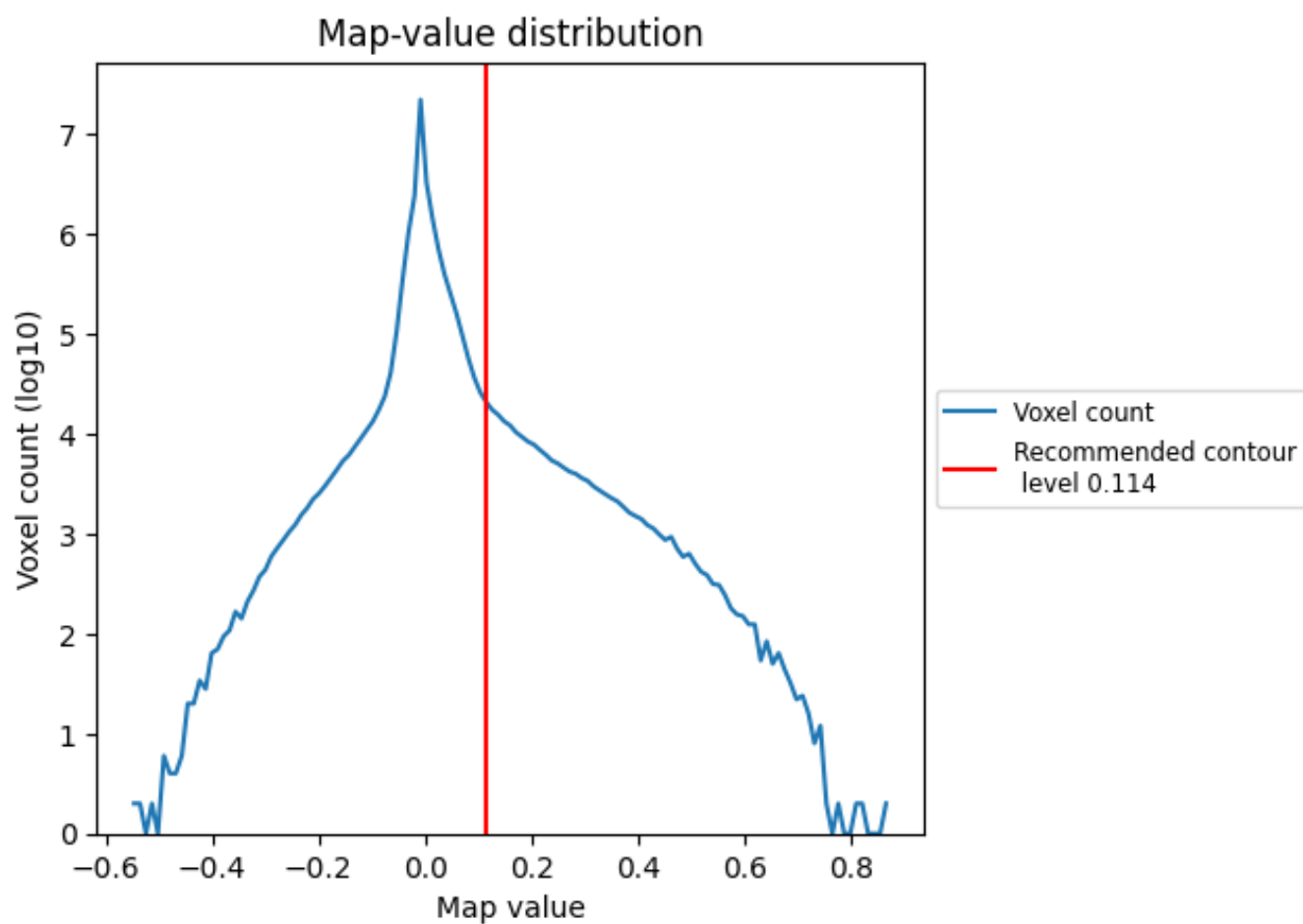
This section was not generated. No masks/segmentation were deposited.

Not For Manuscript Review

7 Map analysis ⓘ

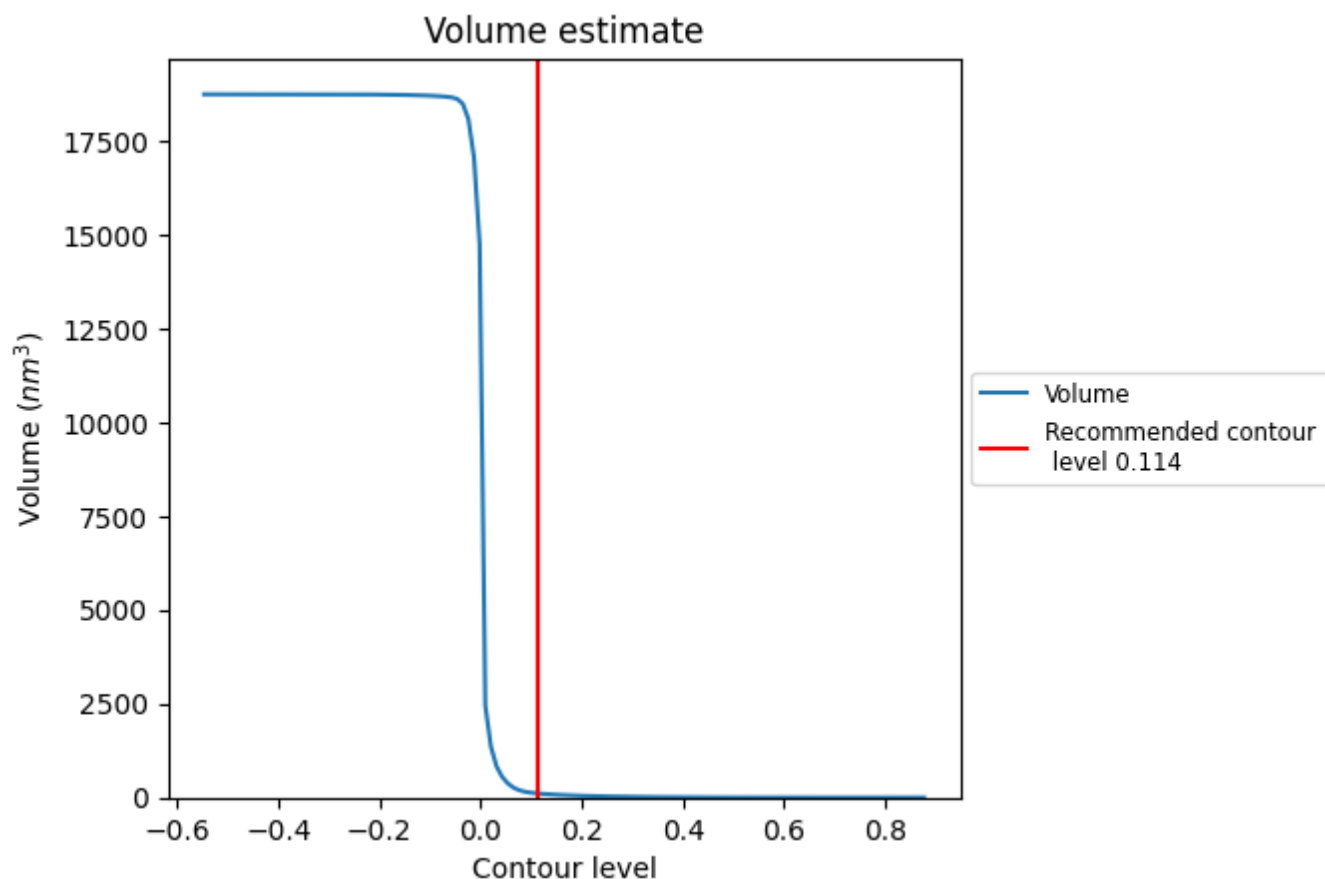
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

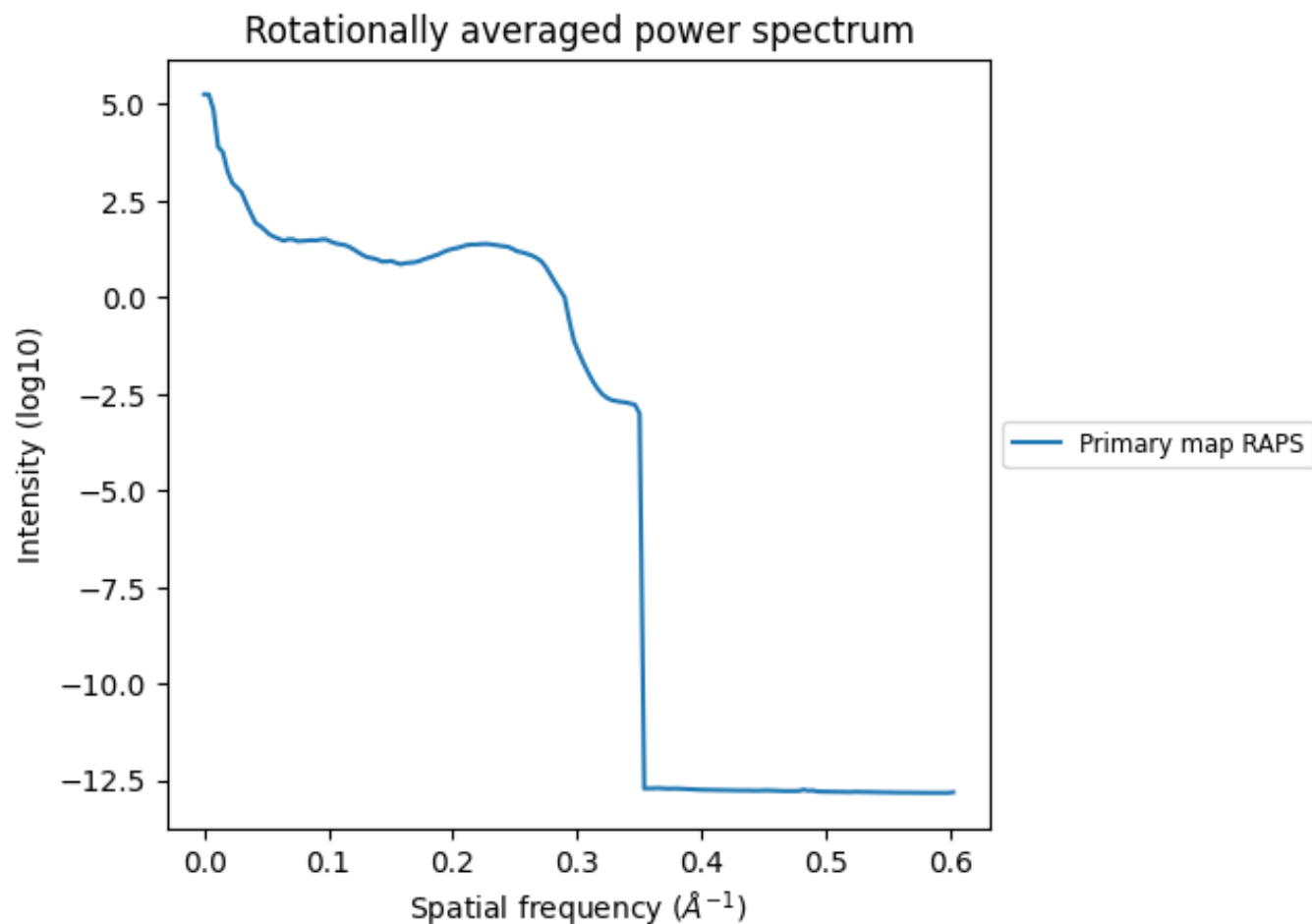
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 109 nm³; this corresponds to an approximate mass of 98 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 ⓘ



8 Fourier-Shell correlation ⓘ

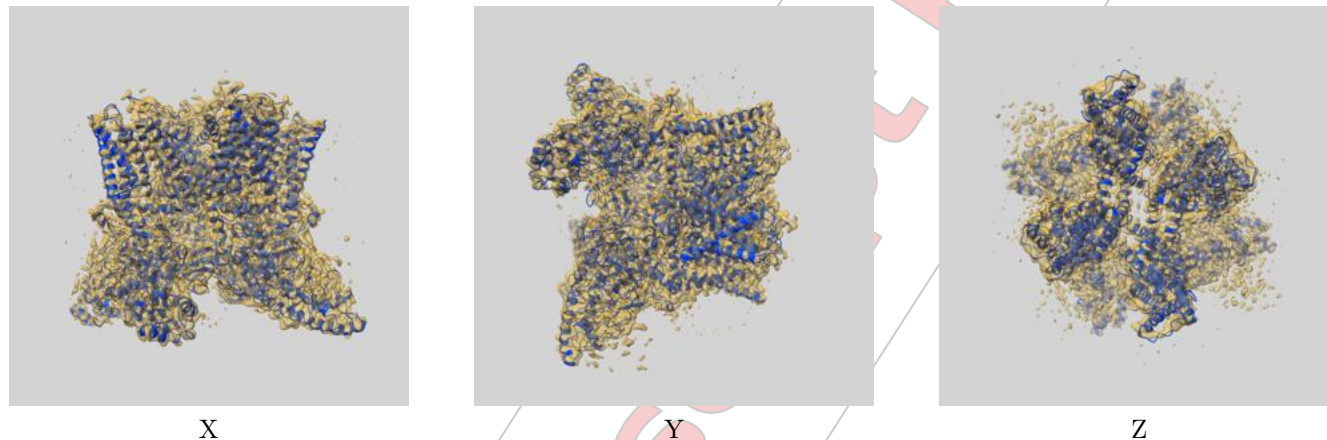
This section was not generated. No FSC curve or half-maps provided.

Not For Manuscript Review

9 Map-model fit ⓘ

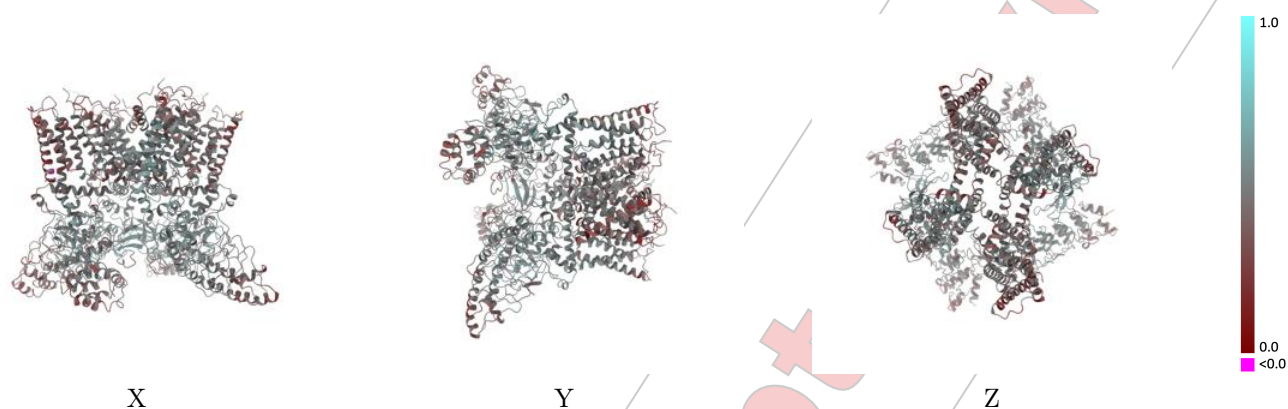
This section contains information regarding the fit between EMDB map D_9100078168 and PDB model D_9100078168. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay ⓘ



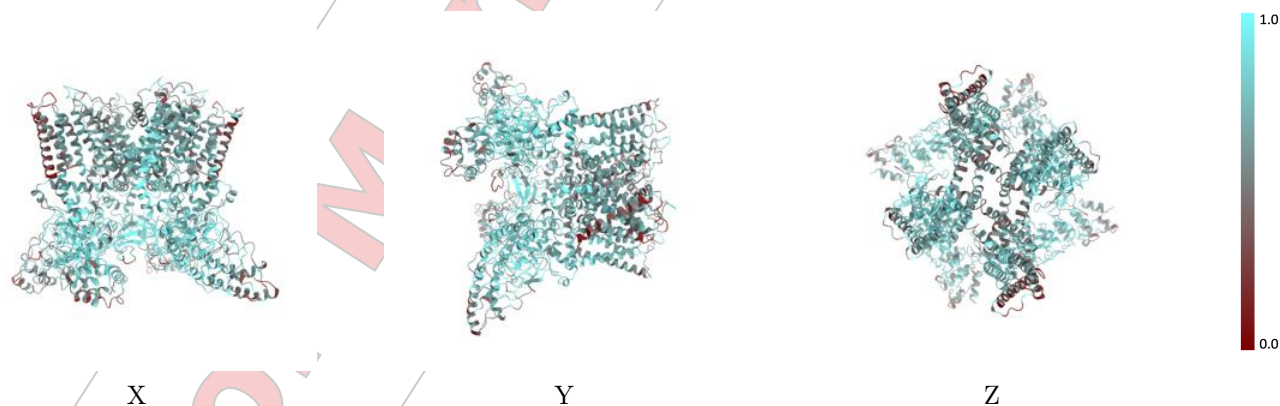
The images above show the 3D surface view of the map at the recommended contour level 0.114 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



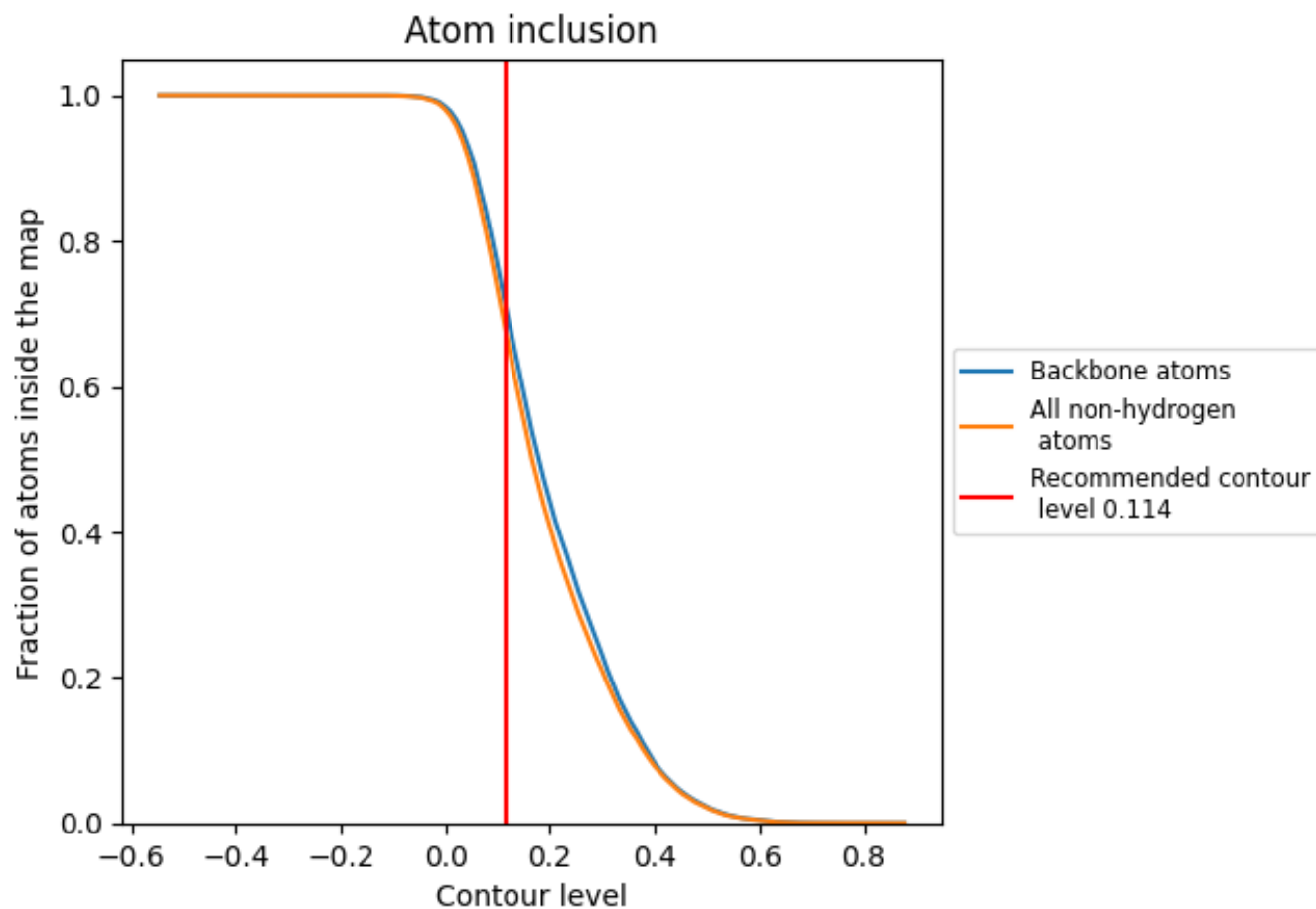
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.114).





9.4 Atom inclusion ⓘ



At the recommended contour level, 71% of all backbone atoms, 68% 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 (0.114) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6802	 0.4550
A	 0.6662	 0.4480
B	 0.7034	 0.4700
C	 0.6623	 0.4340
D	 0.7073	 0.4670

