



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 04:21 PM UTC

PDB ID : 8E6S / pdb_00008e6s
EMDB ID : EMD-27924
Title : Human TRPM2 ion channel in 1 mM dADPR and Ca²⁺
Authors : Wang, L.; Fu, T.M.; Xia, S.; Wu, H.
Deposited on : 2022-08-23
Resolution : 4.60 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

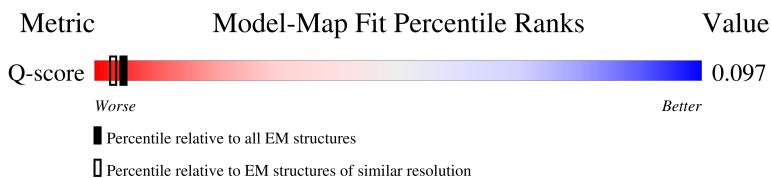
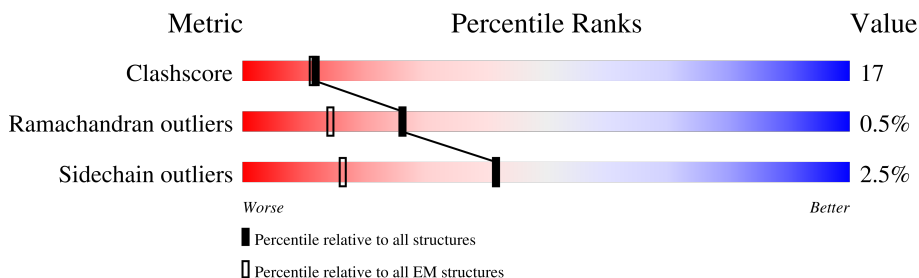
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2407 (4.10 - 5.10)

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	1503	39% 56% 31% 12%
1	B	1503	39% 56% 31% 12%
1	C	1503	40% 56% 30% 12%
1	D	1503	39% 56% 31% 12%

2 Entry composition [i](#)

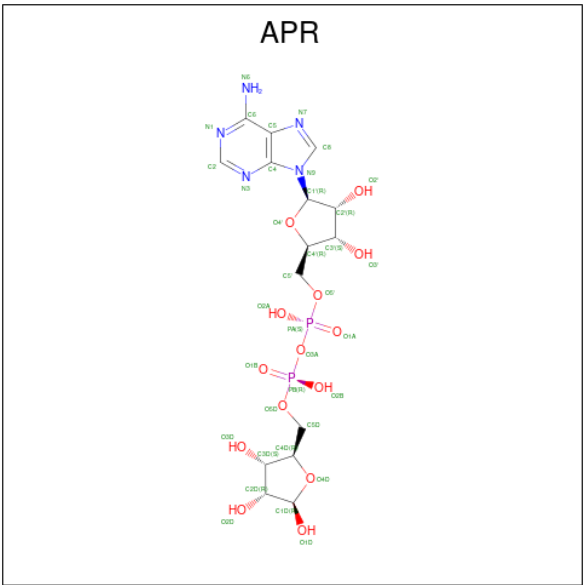
There are 5 unique types of molecules in this entry. The entry contains 42336 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Transient receptor potential cation channel subfamily M member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1330	Total 10521	6791	1829	1851	50	0	0
1	B	1330	Total 10521	6791	1829	1851	50	0	0
1	C	1330	Total 10521	6791	1829	1851	50	0	0
1	D	1330	Total 10521	6791	1829	1851	50	0	0

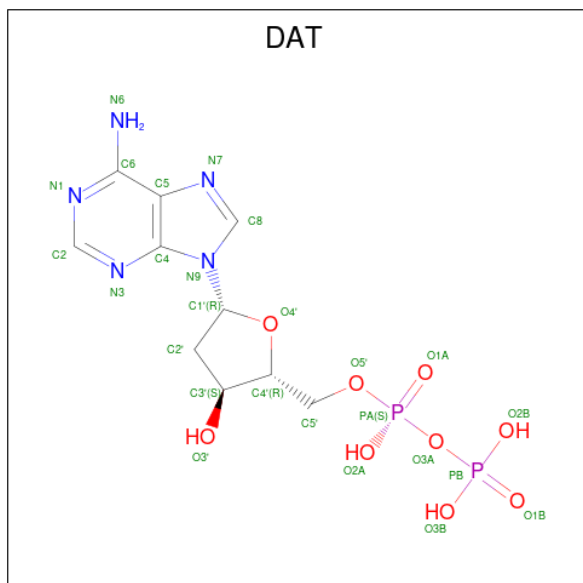
- Molecule 2 is ADENOSINE-5-DIPHOSPHORIBOSE (CCD ID: APR) (formula: C₁₅H₂₃N₅O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	N	O	P	0
			35	15	5	13	2	
2	D	1	Total	C	N	O	P	0
			35	15	5	13	2	

- Molecule 3 is 2'-DEOXYADENOSINE-5'-DIPHOSPHATE (CCD ID: DAT) (formula: $C_{10}H_{15}N_5O_9P_2$).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			26	10	5	9	2	
3	B	1	Total	C	N	O	P	0
			26	10	5	9	2	
3	C	1	Total	C	N	O	P	0
			26	10	5	9	2	
3	D	1	Total	C	N	O	P	0
			26	10	5	9	2	

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Zn	0
			1	1	
4	B	1	Total	Zn	0
			1	1	
4	C	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
4	D	1	Total	Zn	0
			1	1	

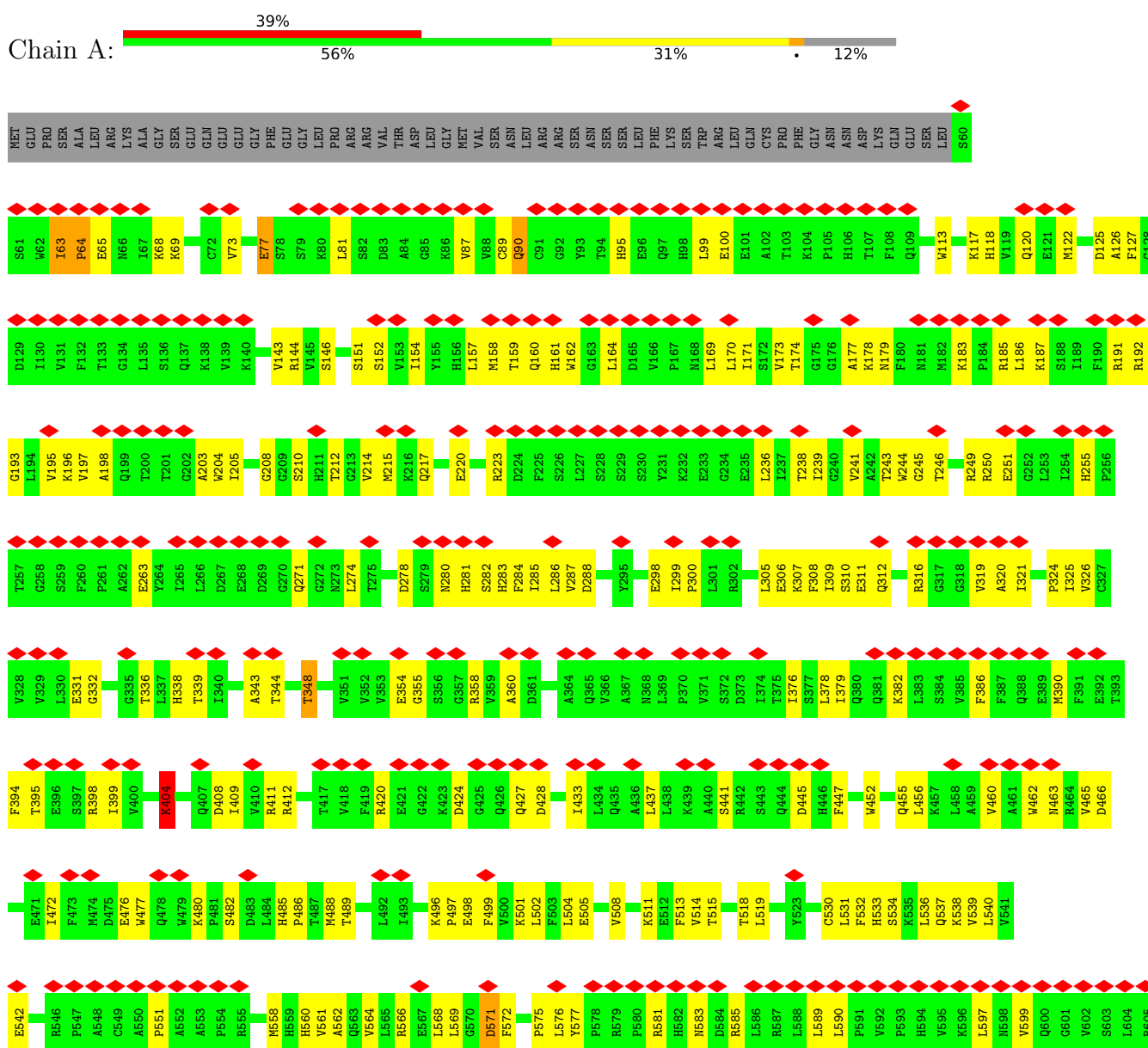
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ca	0
			1	1	
5	B	1	Total	Ca	0
			1	1	
5	C	1	Total	Ca	0
			1	1	
5	D	1	Total	Ca	0
			1	1	

3 Residue-property plots

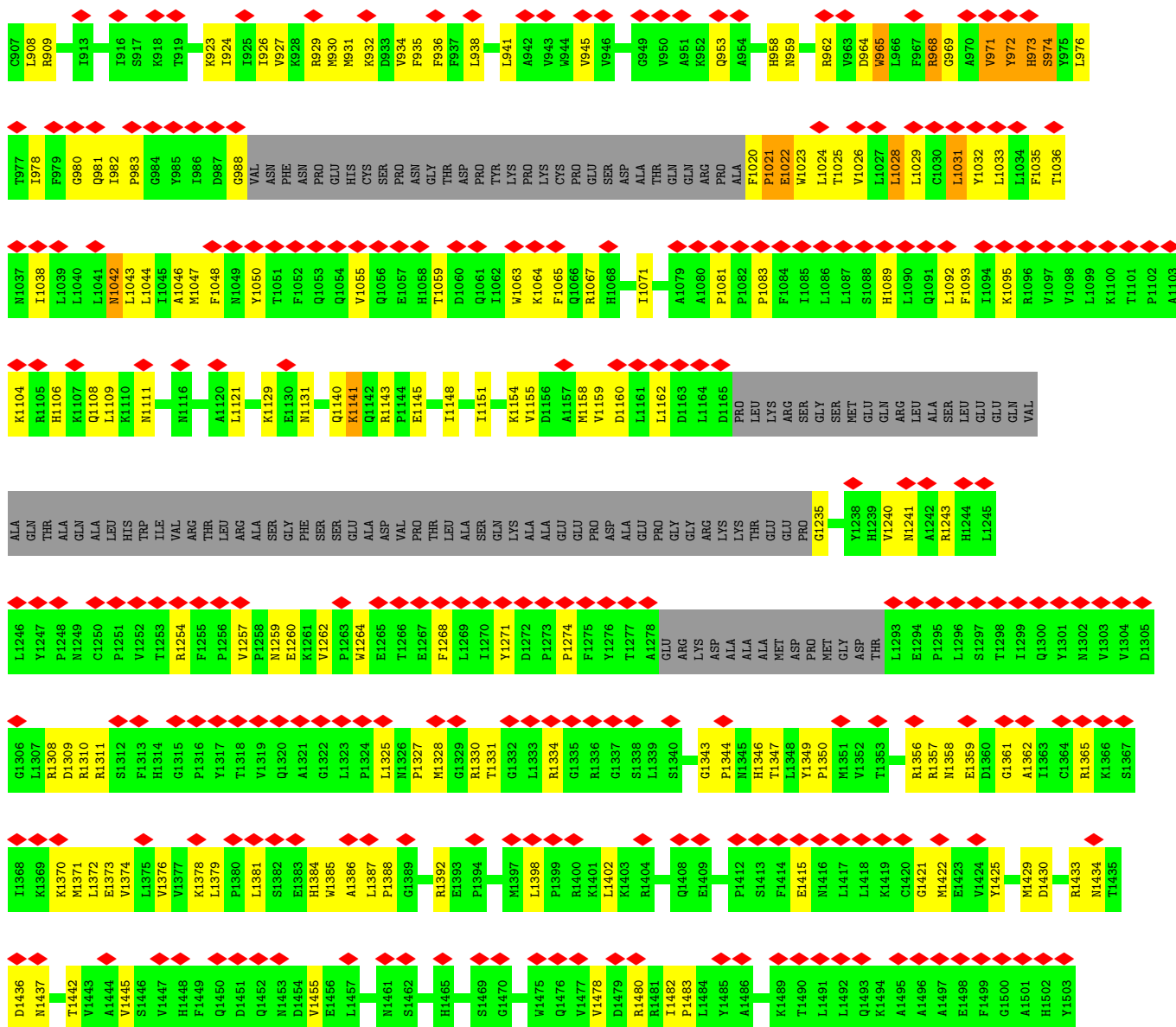
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Transient receptor potential cation channel subfamily M member 2

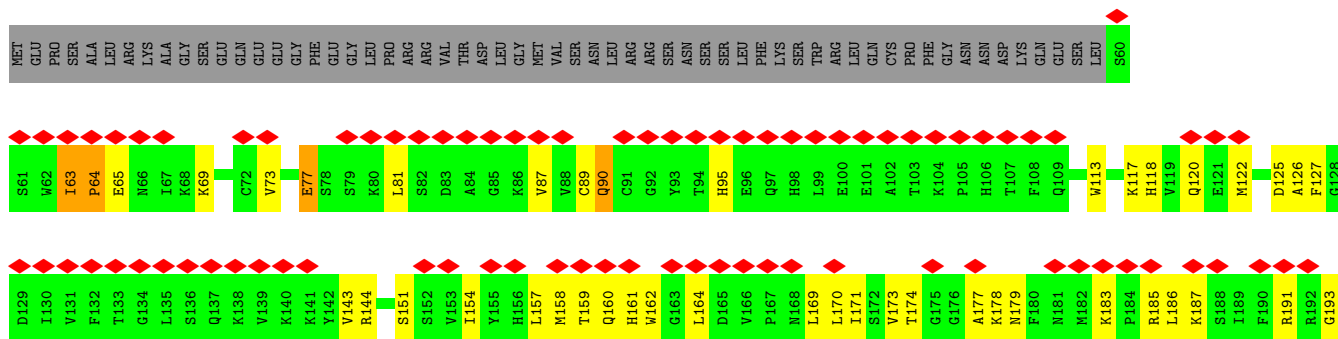




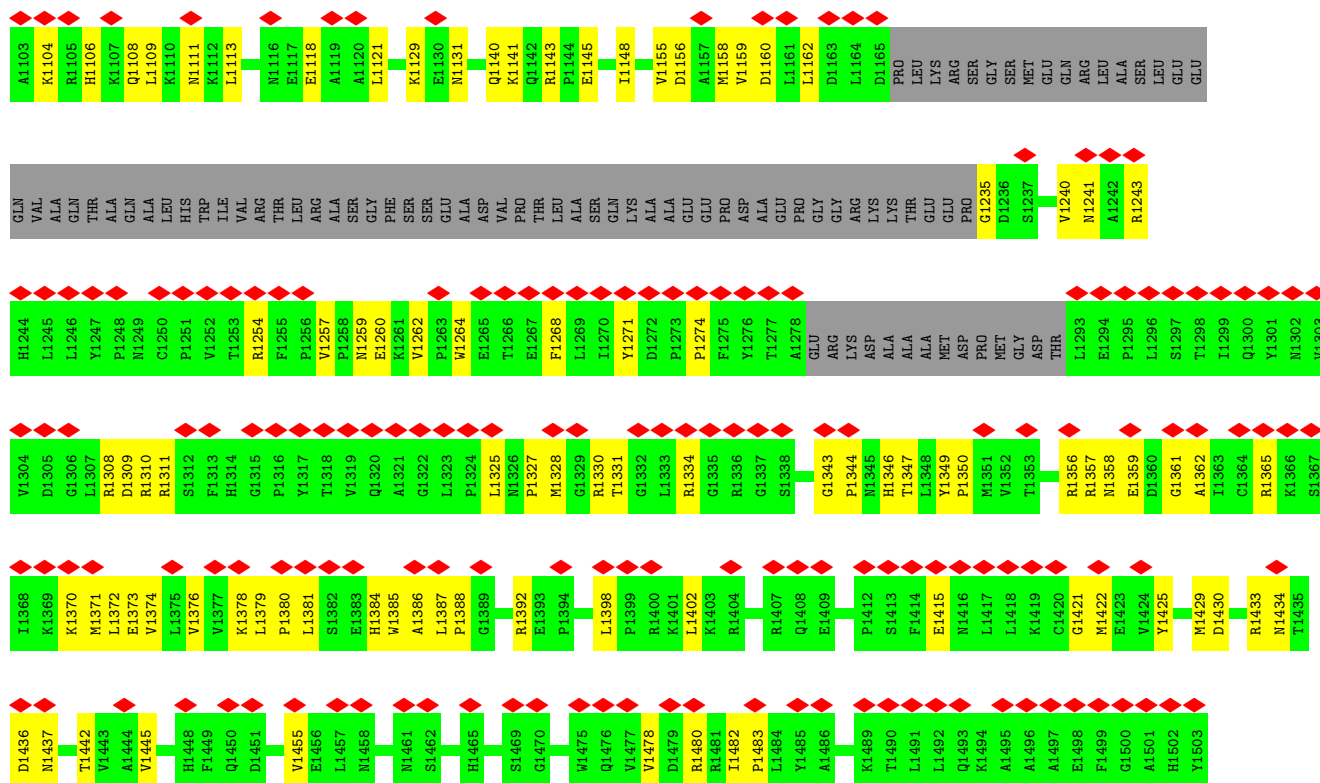




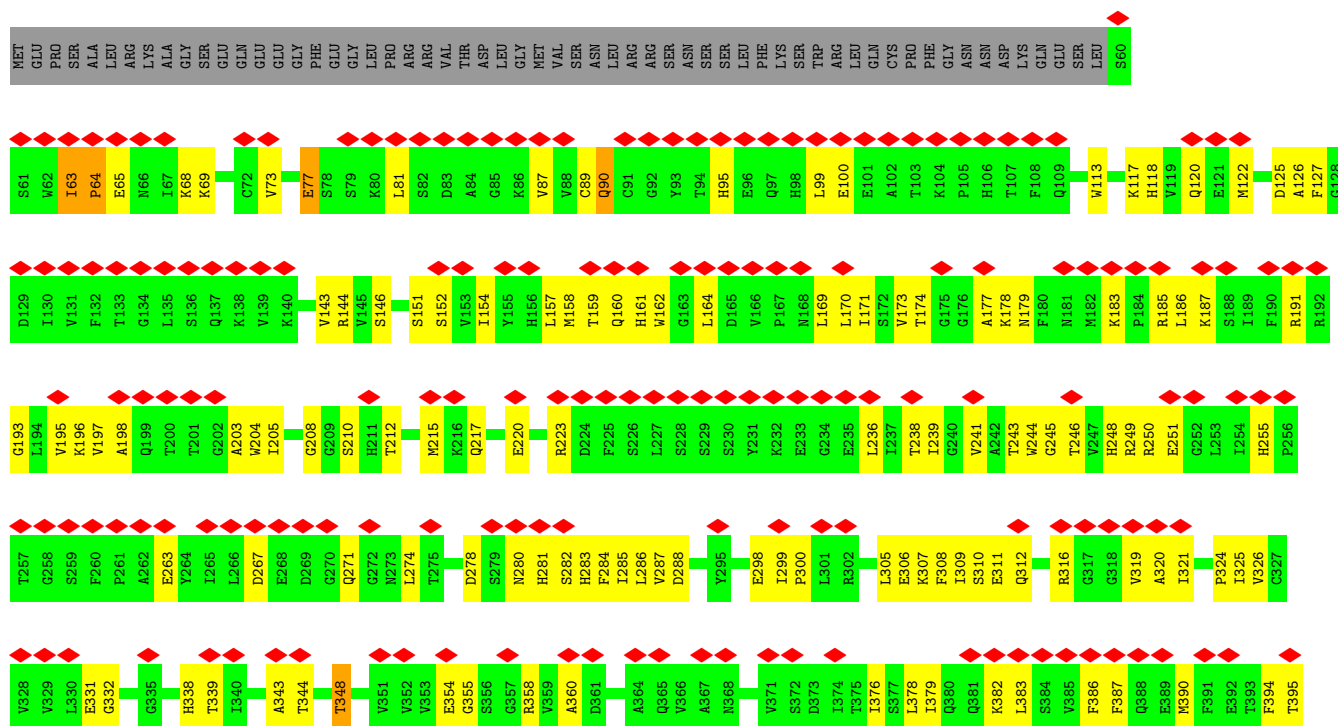
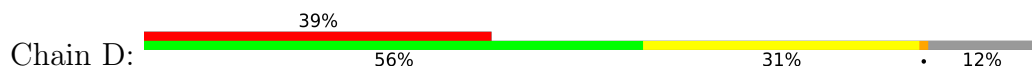
Chain C: 40% 56% 30% 12%



M1037	T977	C907	S826	S748	M675	L607	R546	D475	E331	L194
I1038	I978	L908	W827	V749	M676	Y608	P547	E476	F260	V195
L1039	F979	R909	C828	D750	L678	K609	A548	Q477	P261	K196
L1040	G980	I913	E829	W751	A679	R610	C549	Q478	A262	V197
M1041	Q981	I916	C830	G752	Y682	S611	A550	W479	E263	A198
L1042	I982	S917	A831	R755	E683	S612	P551	P481	Y264	Q199
L1044	P983	K918	I832	L758	E684	G613	A552	S482	I265	T200
	G984	R919	Y833		I687	H614	A553	D483	L266	T201
	Y985		L834		F690	V615	P554	L484	D267	G202
M1047	Y986				C693	T616	P555	H485	E268	A203
F1048	D987	K923	V840	F763	W694	F617	M558	T487	G270	W204
N1049	Y1050	I924	C841	L764	R695	T618	H559	V488	Q271	I205
T1051	T1051	I925	R844	L765	R696	M619	H560	F419	G272	G208
F1052	F1052	A927		T767	K696	D620	H561	N273	G273	G209
Q1053	Q1053	K928	F848	L768	D697	P621	V561	L274	N274	S210
Q1054	Q1054	R929	Y849	G769	E698	I622	A562	E421	T275	H011
V1055	V1055	M930	Y849	L770	E699	R623	O563	G422	D278	M215
Q1056	Q1056	M931	D850	L771	R700	L625	V564	K423	S279	K216
E1057	E1057	K932	P851	S772	A701		L565	S494	N280	Q217
H1058	H1058	D933	D852	F773	Q702		R566	G425	H281	E220
T1059	T1059	V934	E853	R774	K703		L567	Q426	H282	
D1060	D1060	F935	C854	E775	R707		E567	Q427	H283	
Q1061	Q1061	L938	C855	K776	E710		L568	D428	F284	R223
I1062	I1062	F939	L856	R777			L569		I285	D224
W1063	W1063	L940	M857	L778	G713		L570	I433	L286	F225
K1064	K1064	L941	M857	Q779	K714		L571	L434	L287	S226
F1065	F1065	A942	K859	D780	Q715		L572	Q435	D288	
Q1066	Q1066	Y943	A860	T715	P575		L573	A367	L227	
R1067	R1067	V944		T716	L576		L574	N368	Y295	
H1068	H1068	V945		C717	Y577		L575			
		V946	F864	G782	P578		L576	L437		
I1071	I1071	S947	N869	T783	E512		L577	L438	E298	
E1072	E1072	F948	N869	F784	R579		L578	K439	I299	
E1073	E1073	G949	D872	A785	P580		L579	A440	P300	
A1079	A1079	V950	D872	L786	R581		L580	S441	L301	
A1080	A1080	K951	G874	A786	H882		L581	R442	L302	
P1081	P1081	R952	A875	R787	N883		L582	S443		
P1082	P1082	Q953	L876	F795	H884		L583	Q444	L305	
P1083	P1083	A954	L877	Y796	D584		L584	D445	E306	
F1084	F1084	N959	V880	Y797	A650		L585	F447	K307	
L1085	L1085	R962	A881	W798	L653		L586	W452	I309	
L1086	L1086	Y963	C882	F799	A654		L587	Q380	F308	
L1087	L1087	D964	L883	H800	K657		L588	Q381	E311	
S1088	S1088	Y965	T894	L803	L658		L589	L382	Q312	
H1089	H1089	L966	I888	L804	L659		L590	L383		
L1090	L1090	F967	A890	L805	R660		L591	S384		
Q1091	Q1091	R968	A890	L810	E661		L592	V385	R316	
L1092	L1092	G969	R896	C811	L662		L593	F386	G317	
F1093	F1093	A970		W743	S663		L594	A459	G318	
I1094	I1094	Y971	L899	W744	K664		L595	V460	Q388	
K1095	K1095	Y972	D902	W745	E665		L596	A461	Q389	
R1096	R1096	H973	F903	G745	E666		L597	W462	A320	
V1097	V1097	S974	I904	W746	E667		L598	N463	I321	
V1098	V1098	Y975	L905	L747	D668		L599	F394	P324	
L1099	L1099	L976	F906		T669		L600	Y466	I325	
K1100	K1100				D670		L601	D466	I254	
T1101	T1101				S671		L602	E471	H255	
P1102	P1102						L603	I472	P256	
							L604	F473	V257	
							L605	M474	G258	
							S606		S259	



• Molecule 1: Transient receptor potential cation channel subfamily M member 2





SI312	F1313	HI314	GI315	PI316	VI317	TI318	VI319	QI320	AI321	GI322	L1323	PI324	L1325	NI326	PI327	MI328	GI329	RI330	TI331	GI332	L1333	RI334	GI335	RI336	GI337	SI338	GI343	PI344	NI345	HI346	TI347	L1348	Y1349	PI350	MI351	VI352	TI353	RI354	W1355	RI356	RI357	NI358	E1359	DI360	GI361	AI362	TI363	CI364	RI365	K1366	SI367	TI368	K1369	MI370	L1372	E1373	VI374
L1375	VI376	VI377	K1378	L1379	PI380	L1381	SI382	E1383	HI384	W1385	AI386	L1387	PI388	GI389	RI392	E1393	PI394	L1398	PI399	RI400	K1401	L1402	K1403	RI404	Q1408	E1409	PI412	SI413	F1414	E1415	N1416	L1417	L1418	K1419	C1420	GI421	M1422	E1423	VI424	Y1425	MI429	D1430	D1431	PI432	RI433	N1434	TI435	D1436	N1437	TI442	VI443	A1444					
HI448	F1449	Q1450	D1451	Q1452	NI453	D1454	VI455	E1456	L1457	NI458	MI461	SI462	HI465	SI469	GI470	W1475	Q1476	VI477	VI478	D1479	RI480	RI481	I1482	PI483	L1484	Y1485	A1486	K1489	TI490	L1491	L1492	Q1493	K1494	A1495	A1496	A1497	E1498	F1499	GI500	A1501	HI502	Y1503															

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	95674	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 ($e^-/\text{\AA}^2$)	49	Depositor
Minimum defocus (nm)	8000	Depositor
Maximum defocus (nm)	22000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.852	Depositor
Minimum map value	-0.361	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.169	Depositor
Map size (Å)	388.80002, 388.80002, 388.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CA, APR, DAT

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	0.18	0/10787	0.52	6/14658 (0.0%)
1	B	0.18	0/10787	0.52	6/14658 (0.0%)
1	C	0.18	0/10787	0.52	6/14658 (0.0%)
1	D	0.18	0/10787	0.52	6/14658 (0.0%)
All	All	0.18	0/43148	0.52	24/58632 (0.0%)

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	6
1	B	0	6
1	C	0	6
1	D	0	6
All	All	0	24

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	974	SER	N-CA-C	5.98	121.14	113.18
1	B	974	SER	N-CA-C	5.96	121.11	113.18
1	D	974	SER	N-CA-C	5.96	121.10	113.18
1	A	974	SER	N-CA-C	5.93	121.07	113.18
1	A	404	LYS	CB-CG-CD	5.82	124.69	111.30
1	D	404	LYS	CB-CG-CD	5.82	124.69	111.30
1	C	404	LYS	CB-CG-CD	5.81	124.67	111.30
1	B	404	LYS	CB-CG-CD	5.81	124.66	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	973	HIS	N-CA-C	5.69	122.93	110.80
1	D	973	HIS	N-CA-C	5.68	122.89	110.80
1	A	973	HIS	N-CA-C	5.67	122.89	110.80
1	B	973	HIS	N-CA-C	5.67	122.87	110.80
1	D	844	MET	CA-CB-CG	5.61	125.33	114.10
1	B	972	TYR	CA-C-N	-5.60	110.84	121.54
1	B	972	TYR	C-N-CA	-5.60	110.84	121.54
1	D	972	TYR	CA-C-N	-5.60	110.84	121.54
1	D	972	TYR	C-N-CA	-5.60	110.84	121.54
1	A	844	MET	CA-CB-CG	5.60	125.29	114.10
1	C	972	TYR	CA-C-N	-5.59	110.86	121.54
1	C	972	TYR	C-N-CA	-5.59	110.86	121.54
1	C	844	MET	CA-CB-CG	5.59	125.28	114.10
1	B	844	MET	CA-CB-CG	5.58	125.27	114.10
1	A	972	TYR	CA-C-N	-5.57	110.91	121.54
1	A	972	TYR	C-N-CA	-5.57	110.91	121.54

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1021	PRO	Peptide
1	A	63	ILE	Peptide
1	A	666	GLU	Peptide
1	A	965	TRP	Peptide
1	A	968	ARG	Peptide
1	A	971	VAL	Peptide
1	B	1021	PRO	Peptide
1	B	63	ILE	Peptide
1	B	666	GLU	Peptide
1	B	965	TRP	Peptide
1	B	968	ARG	Peptide
1	B	971	VAL	Peptide
1	C	1021	PRO	Peptide
1	C	63	ILE	Peptide
1	C	666	GLU	Peptide
1	C	965	TRP	Peptide
1	C	968	ARG	Peptide
1	C	971	VAL	Peptide
1	D	1021	PRO	Peptide
1	D	63	ILE	Peptide
1	D	666	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	D	965	TRP	Peptide
1	D	968	ARG	Peptide
1	D	971	VAL	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10521	0	10407	395	0
1	B	10521	0	10407	409	0
1	C	10521	0	10407	392	0
1	D	10521	0	10407	373	0
2	A	35	0	19	1	0
2	B	35	0	19	1	0
2	C	35	0	19	1	0
2	D	35	0	19	0	0
3	A	26	0	12	1	0
3	B	26	0	12	1	0
3	C	26	0	12	1	0
3	D	26	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	42336	0	41752	1451	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 17.

All (1451) 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:1022:GLU:HB3	1:D:975:TYR:N	1.66	1.09
1:A:1024:LEU:H	1:B:972:TYR:C	1.70	0.99
1:C:1022:GLU:HB3	1:D:975:TYR:H	0.84	0.99
1:C:1022:GLU:CB	1:D:975:TYR:H	1.78	0.95
1:B:981:GLN:NE2	1:C:981:GLN:OE1	1.99	0.95
1:A:1042:ASN:HD22	1:B:930:MET:HE3	1.30	0.93
1:A:1025:THR:H	1:B:973:HIS:HA	1.37	0.88
1:B:1021:PRO:HA	1:C:971:VAL:H	1.35	0.88
1:B:1020:PHE:N	1:C:964:ASP:OD2	2.07	0.88
1:A:1021:PRO:HD3	1:B:965:TRP:HD1	1.40	0.85
1:B:687:ILE:HD11	1:B:729:PHE:HA	1.59	0.84
1:A:700:ARG:HA	1:A:703:LYS:HG2	1.59	0.84
1:D:700:ARG:HA	1:D:703:LYS:HG2	1.59	0.84
1:C:687:ILE:HD11	1:C:729:PHE:HA	1.59	0.84
1:A:687:ILE:HD11	1:A:729:PHE:HA	1.59	0.83
1:D:687:ILE:HD11	1:D:729:PHE:HA	1.59	0.83
1:B:278:ASP:HB2	1:B:280:ASN:HD22	1.45	0.82
1:C:278:ASP:HB2	1:C:280:ASN:HD22	1.45	0.82
1:C:700:ARG:HA	1:C:703:LYS:HG2	1.59	0.82
1:B:700:ARG:HA	1:B:703:LYS:HG2	1.59	0.82
1:B:1021:PRO:HB3	1:C:972:TYR:HB2	1.61	0.81
1:D:278:ASP:HB2	1:D:280:ASN:HD22	1.45	0.81
1:A:223:ARG:NH2	1:A:280:ASN:OD1	2.14	0.81
1:A:278:ASP:HB2	1:A:280:ASN:HD22	1.45	0.81
1:C:223:ARG:NH2	1:C:280:ASN:OD1	2.14	0.81
1:B:223:ARG:NH2	1:B:280:ASN:OD1	2.14	0.80
1:B:1038:ILE:HG23	1:C:1044:LEU:HD13	1.64	0.80
1:D:223:ARG:NH2	1:D:280:ASN:OD1	2.14	0.80
1:A:404:LYS:HA	1:A:404:LYS:HE3	1.63	0.80
1:A:1025:THR:OG1	1:B:973:HIS:O	1.99	0.79
1:B:404:LYS:HE3	1:B:404:LYS:HA	1.63	0.79
1:D:404:LYS:HE3	1:D:404:LYS:HA	1.63	0.79
1:B:659:LEU:HD22	1:B:679:ALA:HB2	1.64	0.79
1:C:1021:PRO:HB3	1:D:972:TYR:HB3	1.64	0.78
1:C:659:LEU:HD22	1:C:679:ALA:HB2	1.64	0.78
1:A:1158:MET:HE1	1:B:1158:MET:HG3	1.65	0.77
1:C:404:LYS:HE3	1:C:404:LYS:HA	1.63	0.77
1:A:659:LEU:HD22	1:A:679:ALA:HB2	1.64	0.77
1:A:957:ILE:HG23	1:B:819:VAL:HG22	1.67	0.77
1:D:659:LEU:HD22	1:D:679:ALA:HB2	1.64	0.76
1:B:1022:GLU:N	1:C:971:VAL:N	2.33	0.76
1:B:1026:VAL:HG13	1:B:1029:LEU:HD12	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1026:VAL:HG13	1:D:1029:LEU:HD12	1.67	0.76
1:A:1024:LEU:HB3	1:B:972:TYR:O	1.86	0.76
1:C:1026:VAL:HG13	1:C:1029:LEU:HD12	1.67	0.76
1:D:589:LEU:HD12	1:D:590:LEU:HG	1.68	0.76
1:A:589:LEU:HD12	1:A:590:LEU:HG	1.68	0.75
1:A:1026:VAL:HG13	1:A:1029:LEU:HD12	1.67	0.75
1:A:923:LYS:HE3	1:D:1043:LEU:HA	1.69	0.74
1:C:589:LEU:HD12	1:C:590:LEU:HG	1.68	0.74
1:A:973:HIS:H	1:D:1022:GLU:HA	1.50	0.74
1:B:589:LEU:HD12	1:B:590:LEU:HG	1.68	0.74
1:A:1023:TRP:NE1	1:B:968:ARG:O	2.22	0.73
1:C:973:HIS:HD2	1:C:974:SER:HB3	1.53	0.73
1:B:1021:PRO:CA	1:C:971:VAL:H	2.00	0.73
1:B:973:HIS:HD2	1:B:974:SER:HB3	1.53	0.73
1:C:1376:VAL:HG22	1:C:1478:VAL:HG11	1.70	0.73
1:B:1358:ASN:HD21	1:B:1362:ALA:HB3	1.54	0.72
1:C:700:ARG:HH21	1:C:1121:LEU:HA	1.55	0.72
1:D:973:HIS:HD2	1:D:974:SER:HB3	1.53	0.72
1:D:1376:VAL:HG22	1:D:1478:VAL:HG11	1.70	0.72
1:A:1376:VAL:HG22	1:A:1478:VAL:HG11	1.70	0.72
1:A:700:ARG:HH21	1:A:1121:LEU:HA	1.55	0.72
1:A:1021:PRO:HD3	1:B:965:TRP:CD1	2.24	0.72
1:C:1358:ASN:HD21	1:C:1362:ALA:HB3	1.55	0.72
1:A:1156:ASP:OD1	1:B:1154:LYS:NZ	2.20	0.72
1:B:700:ARG:HH21	1:B:1121:LEU:HA	1.55	0.72
1:B:1376:VAL:HG22	1:B:1478:VAL:HG11	1.70	0.72
1:A:973:HIS:HD2	1:A:974:SER:HB3	1.53	0.72
1:D:700:ARG:HH21	1:D:1121:LEU:HA	1.55	0.72
1:A:1358:ASN:HD21	1:A:1362:ALA:HB3	1.55	0.71
1:B:1020:PHE:O	1:C:971:VAL:N	2.23	0.71
1:C:325:ILE:HD12	1:C:348:THR:HG22	1.73	0.71
1:C:1020:PHE:O	1:D:971:VAL:N	2.17	0.71
1:A:1152:SER:HA	1:B:1151:ILE:HD11	1.72	0.71
1:C:332:GLY:H	1:C:358:ARG:HH21	1.39	0.71
1:D:332:GLY:H	1:D:358:ARG:HH21	1.38	0.70
1:A:1024:LEU:N	1:B:971:VAL:O	2.24	0.70
1:D:325:ILE:HD12	1:D:348:THR:HG22	1.73	0.70
1:D:1358:ASN:HD21	1:D:1362:ALA:HB3	1.55	0.70
1:C:1158:MET:HE1	1:D:1158:MET:HG3	1.73	0.70
1:A:325:ILE:HD12	1:A:348:THR:HG22	1.73	0.70
1:B:325:ILE:HD12	1:B:348:THR:HG22	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:GLY:H	1:B:358:ARG:HH21	1.38	0.69
1:A:1024:LEU:HB2	1:B:971:VAL:O	1.92	0.69
1:C:249:ARG:NH1	1:C:251:GLU:O	2.26	0.69
1:A:1042:ASN:ND2	1:B:930:MET:HE3	2.08	0.69
1:A:1049:ASN:HD22	1:B:1048:PHE:HE2	1.41	0.68
1:B:249:ARG:NH1	1:B:251:GLU:O	2.26	0.68
1:D:159:THR:OG1	1:D:160:GLN:OE1	2.10	0.68
1:D:249:ARG:NH1	1:D:251:GLU:O	2.26	0.68
1:A:249:ARG:NH1	1:A:251:GLU:O	2.26	0.68
1:A:332:GLY:H	1:A:358:ARG:HH21	1.39	0.68
1:C:683:GLU:N	1:C:683:GLU:OE1	2.26	0.68
1:B:278:ASP:HB2	1:B:280:ASN:ND2	2.08	0.68
1:C:278:ASP:HB2	1:C:280:ASN:ND2	2.08	0.68
1:A:683:GLU:N	1:A:683:GLU:OE1	2.26	0.68
1:A:159:THR:OG1	1:A:160:GLN:OE1	2.10	0.68
1:D:1357:ARG:HH21	1:D:1361:GLY:HA3	1.59	0.68
1:B:683:GLU:OE1	1:B:683:GLU:N	2.26	0.68
1:B:1038:ILE:HA	1:C:1044:LEU:HD22	1.76	0.68
1:D:959:ASN:HB3	1:D:962:ARG:HB2	1.76	0.68
1:C:159:THR:OG1	1:C:160:GLN:OE1	2.10	0.68
1:C:571:ASP:OD1	1:C:571:ASP:N	2.27	0.68
1:D:625:LEU:HG	1:D:641:ILE:HD13	1.76	0.68
1:A:959:ASN:HB3	1:A:962:ARG:HB2	1.76	0.67
1:B:625:LEU:HG	1:B:641:ILE:HD13	1.76	0.67
1:A:583:ASN:OD1	1:A:585:ARG:NH1	2.28	0.67
1:B:583:ASN:OD1	1:B:585:ARG:NH1	2.28	0.67
1:B:159:THR:OG1	1:B:160:GLN:OE1	2.10	0.67
1:B:1357:ARG:HH21	1:B:1361:GLY:HA3	1.59	0.67
1:C:1357:ARG:HH21	1:C:1361:GLY:HA3	1.59	0.67
1:D:278:ASP:HB2	1:D:280:ASN:ND2	2.08	0.67
1:D:583:ASN:OD1	1:D:585:ARG:NH1	2.28	0.67
1:D:683:GLU:OE1	1:D:683:GLU:N	2.27	0.67
1:A:278:ASP:HB2	1:A:280:ASN:ND2	2.08	0.67
1:B:571:ASP:OD1	1:B:571:ASP:N	2.27	0.67
1:D:571:ASP:OD1	1:D:571:ASP:N	2.27	0.67
1:A:571:ASP:N	1:A:571:ASP:OD1	2.27	0.67
1:A:625:LEU:HG	1:A:641:ILE:HD13	1.76	0.67
1:A:1357:ARG:HH21	1:A:1361:GLY:HA3	1.59	0.67
1:C:583:ASN:OD1	1:C:585:ARG:NH1	2.28	0.67
1:C:625:LEU:HG	1:C:641:ILE:HD13	1.76	0.67
1:D:183:LYS:NZ	1:D:355:GLY:O	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1365:ARG:HH11	1:A:1370:LYS:HD3	1.60	0.67
1:B:183:LYS:NZ	1:B:355:GLY:O	2.27	0.67
1:A:621:PRO:HD2	1:A:622:ILE:H	1.60	0.66
1:A:472:ILE:HG23	1:A:477:TRP:HH2	1.61	0.66
1:B:472:ILE:HG23	1:B:477:TRP:HH2	1.61	0.66
1:C:472:ILE:HG23	1:C:477:TRP:HH2	1.61	0.66
1:D:1365:ARG:HH11	1:D:1370:LYS:HD3	1.60	0.66
1:C:533:HIS:O	1:C:537:GLN:NE2	2.29	0.66
1:C:1365:ARG:HH11	1:C:1370:LYS:HD3	1.60	0.66
1:B:1022:GLU:O	1:B:1023:TRP:HD1	1.78	0.66
1:B:959:ASN:HB3	1:B:962:ARG:HB2	1.76	0.66
1:C:183:LYS:NZ	1:C:355:GLY:O	2.27	0.66
1:C:959:ASN:HB3	1:C:962:ARG:HB2	1.76	0.66
1:D:533:HIS:O	1:D:537:GLN:NE2	2.29	0.66
1:D:621:PRO:HD2	1:D:622:ILE:H	1.60	0.66
1:B:621:PRO:HD2	1:B:622:ILE:H	1.60	0.66
1:B:1021:PRO:HA	1:C:971:VAL:N	2.10	0.66
1:C:707:ARG:HB3	1:C:717:CYS:HB2	1.78	0.66
1:B:480:LYS:HG3	1:B:482:SER:H	1.61	0.65
1:C:621:PRO:HD2	1:C:622:ILE:H	1.60	0.65
1:D:480:LYS:HG3	1:D:482:SER:H	1.62	0.65
1:D:1022:GLU:O	1:D:1023:TRP:HD1	1.78	0.65
1:A:480:LYS:HG3	1:A:482:SER:H	1.62	0.65
1:C:1022:GLU:O	1:C:1023:TRP:HD1	1.78	0.65
1:B:445:ASP:OD1	1:B:1480:ARG:NH2	2.29	0.65
1:B:1022:GLU:H	1:C:971:VAL:N	1.92	0.65
1:B:1031:LEU:HD11	1:C:945:VAL:HG11	1.77	0.65
1:A:445:ASP:OD1	1:A:1480:ARG:NH2	2.29	0.65
1:A:533:HIS:O	1:A:537:GLN:NE2	2.29	0.65
1:B:958:HIS:HB3	1:C:818:MET:SD	2.36	0.65
1:D:707:ARG:HB3	1:D:717:CYS:HB2	1.78	0.65
1:B:731:SER:HA	1:B:736:GLN:HE22	1.62	0.65
1:B:1022:GLU:N	1:C:971:VAL:H	1.93	0.65
1:B:1031:LEU:HD11	1:C:945:VAL:HG21	1.77	0.65
1:C:480:LYS:HG3	1:C:482:SER:H	1.62	0.65
1:D:445:ASP:OD1	1:D:1480:ARG:NH2	2.29	0.65
1:D:472:ILE:HG23	1:D:477:TRP:HH2	1.61	0.65
1:A:354:GLU:HA	1:A:360:ALA:HB1	1.79	0.65
1:B:1365:ARG:HH11	1:B:1370:LYS:HD3	1.60	0.65
1:A:179:ASN:HD22	1:A:390:MET:HE2	1.62	0.65
1:A:730:VAL:HA	1:A:735:ILE:HD13	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1022:GLU:O	1:A:1023:TRP:HD1	1.78	0.65
1:B:179:ASN:HD22	1:B:390:MET:HE2	1.62	0.65
1:C:445:ASP:OD1	1:C:1480:ARG:NH2	2.29	0.65
1:D:730:VAL:HA	1:D:735:ILE:HD13	1.79	0.65
1:B:354:GLU:HA	1:B:360:ALA:HB1	1.79	0.65
1:B:533:HIS:O	1:B:537:GLN:NE2	2.29	0.65
1:A:1020:PHE:HD1	1:B:965:TRP:NE1	1.96	0.64
1:B:707:ARG:HB3	1:B:717:CYS:HB2	1.78	0.64
1:C:354:GLU:HA	1:C:360:ALA:HB1	1.79	0.64
1:C:642:TRP:CD1	1:C:645:SER:HG	2.16	0.64
1:B:730:VAL:HA	1:B:735:ILE:HD13	1.79	0.64
1:C:731:SER:HA	1:C:736:GLN:HE22	1.62	0.64
1:C:179:ASN:HD22	1:C:390:MET:HE2	1.62	0.64
1:D:731:SER:HA	1:D:736:GLN:HE22	1.62	0.64
1:A:566:ARG:HD2	1:A:569:LEU:HD11	1.80	0.64
1:C:730:VAL:HA	1:C:735:ILE:HD13	1.79	0.64
1:C:1482:ILE:HD12	1:C:1483:PRO:HD2	1.80	0.64
1:B:1140:GLN:HA	1:B:1143:ARG:HH22	1.63	0.64
1:D:217:GLN:HA	1:D:220:GLU:HG2	1.80	0.64
1:A:707:ARG:HB3	1:A:717:CYS:HB2	1.78	0.64
1:D:354:GLU:HA	1:D:360:ALA:HB1	1.79	0.64
1:D:566:ARG:HD2	1:D:569:LEU:HD11	1.80	0.64
1:C:566:ARG:HD2	1:C:569:LEU:HD11	1.80	0.64
1:D:179:ASN:HD22	1:D:390:MET:HE2	1.61	0.64
1:A:1346:HIS:HB2	1:A:1392:ARG:H	1.63	0.64
1:C:1398:LEU:HD21	1:C:1415:GLU:HG2	1.80	0.64
1:A:632:GLN:HB3	1:A:634:ARG:NH1	2.13	0.63
1:B:1310:ARG:HH12	1:B:1344:PRO:HD3	1.64	0.63
1:B:1379:LEU:HD23	1:B:1381:LEU:H	1.63	0.63
1:A:731:SER:HA	1:A:736:GLN:HE22	1.62	0.63
1:A:1154:LYS:NZ	1:D:1156:ASP:OD1	2.29	0.63
1:B:1346:HIS:HB2	1:B:1392:ARG:H	1.63	0.63
1:D:1398:LEU:HD21	1:D:1415:GLU:HG2	1.80	0.63
1:A:183:LYS:NZ	1:A:355:GLY:O	2.27	0.63
1:B:358:ARG:HA	1:B:386:PHE:HB3	1.81	0.63
1:C:1310:ARG:HH12	1:C:1344:PRO:HD3	1.64	0.63
1:A:117:LYS:HE3	1:A:118:HIS:HD2	1.64	0.63
1:A:217:GLN:HA	1:A:220:GLU:HG2	1.80	0.63
1:A:1140:GLN:HA	1:A:1143:ARG:HH22	1.63	0.63
1:A:1379:LEU:HD23	1:A:1381:LEU:H	1.63	0.63
1:C:1140:GLN:HA	1:C:1143:ARG:HH22	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:LYS:HE3	1:D:217:GLN:HB3	1.80	0.63
1:D:1310:ARG:HH12	1:D:1344:PRO:HD3	1.64	0.63
1:A:1310:ARG:HH12	1:A:1344:PRO:HD3	1.64	0.63
1:C:358:ARG:HA	1:C:386:PHE:HB3	1.81	0.63
1:A:1028:LEU:HA	1:A:1031:LEU:HB2	1.81	0.63
1:A:1482:ILE:HD12	1:A:1483:PRO:HD2	1.80	0.63
1:B:187:LYS:HE3	1:B:217:GLN:HB3	1.80	0.63
1:B:1028:LEU:HA	1:B:1031:LEU:HB2	1.81	0.63
1:C:217:GLN:HA	1:C:220:GLU:HG2	1.80	0.63
1:A:77:GLU:HA	1:A:89:CYS:HA	1.81	0.63
1:A:144:ARG:NH2	1:A:288:ASP:OD2	2.28	0.63
1:B:117:LYS:HE3	1:B:118:HIS:HD2	1.64	0.63
1:B:566:ARG:HD2	1:B:569:LEU:HD11	1.80	0.63
1:B:632:GLN:HB3	1:B:634:ARG:NH1	2.14	0.63
1:C:1028:LEU:HA	1:C:1031:LEU:HB2	1.81	0.63
1:D:632:GLN:HB3	1:D:634:ARG:NH1	2.14	0.63
1:A:923:LYS:NZ	1:D:1042:ASN:OD1	2.28	0.62
1:B:1433:ARG:NH1	3:B:1602:DAT:N7	2.45	0.62
1:C:632:GLN:HB3	1:C:634:ARG:NH1	2.14	0.62
1:A:358:ARG:HA	1:A:386:PHE:HB3	1.81	0.62
1:D:1028:LEU:HA	1:D:1031:LEU:HB2	1.81	0.62
1:C:187:LYS:HE3	1:C:217:GLN:HB3	1.80	0.62
1:D:1140:GLN:HA	1:D:1143:ARG:HH22	1.63	0.62
1:D:1346:HIS:HB2	1:D:1392:ARG:H	1.63	0.62
1:A:1398:LEU:HD21	1:A:1415:GLU:HG2	1.80	0.62
1:B:193:GLY:HA2	1:B:196:LYS:HE3	1.81	0.62
1:B:217:GLN:HA	1:B:220:GLU:HG2	1.80	0.62
1:C:1021:PRO:HA	1:D:972:TYR:H	1.64	0.62
1:C:1379:LEU:HD23	1:C:1381:LEU:H	1.63	0.62
1:D:1433:ARG:NH1	3:D:1602:DAT:N7	2.45	0.62
1:A:193:GLY:HA2	1:A:196:LYS:HE3	1.81	0.62
1:A:1433:ARG:NH1	3:A:1602:DAT:N7	2.45	0.62
1:C:1350:PRO:HG2	1:C:1388:PRO:HG2	1.82	0.62
1:D:358:ARG:HA	1:D:386:PHE:HB3	1.81	0.62
1:D:642:TRP:CD1	1:D:645:SER:HG	2.17	0.62
1:D:1350:PRO:HG2	1:D:1388:PRO:HG2	1.82	0.62
1:C:77:GLU:HA	1:C:89:CYS:HA	1.81	0.62
1:C:1308:ARG:HH21	1:C:1343:GLY:HA3	1.65	0.62
1:C:1346:HIS:HB2	1:C:1392:ARG:H	1.63	0.62
1:D:1482:ILE:HD12	1:D:1483:PRO:HD2	1.80	0.62
1:A:187:LYS:HE3	1:A:217:GLN:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:LYS:HE3	1:D:118:HIS:HD2	1.64	0.62
1:A:1022:GLU:HG2	1:B:973:HIS:NE2	2.14	0.62
1:A:1350:PRO:HG2	1:A:1388:PRO:HG2	1.82	0.62
1:B:1350:PRO:HG2	1:B:1388:PRO:HG2	1.82	0.62
1:B:1482:ILE:HD12	1:B:1483:PRO:HD2	1.80	0.62
1:D:1308:ARG:HH21	1:D:1343:GLY:HA3	1.65	0.62
1:A:1308:ARG:HH21	1:A:1343:GLY:HA3	1.65	0.62
1:C:193:GLY:HA2	1:C:196:LYS:HE3	1.81	0.62
1:C:1023:TRP:CD2	1:D:976:LEU:HD13	2.34	0.62
1:D:710:GLU:HA	1:D:714:LYS:HE3	1.82	0.62
1:D:1379:LEU:HD23	1:D:1381:LEU:H	1.63	0.62
1:A:710:GLU:HA	1:A:714:LYS:HE3	1.82	0.61
1:B:1308:ARG:HH21	1:B:1343:GLY:HA3	1.65	0.61
1:C:117:LYS:HE3	1:C:118:HIS:HD2	1.64	0.61
1:D:193:GLY:HA2	1:D:196:LYS:HE3	1.81	0.61
1:A:763:PHE:HB3	1:A:764:PRO:HD3	1.83	0.61
1:B:77:GLU:HA	1:B:89:CYS:HA	1.81	0.61
1:B:287:VAL:HG21	1:B:298:GLU:HB3	1.82	0.61
1:B:710:GLU:HA	1:B:714:LYS:HE3	1.82	0.61
1:C:710:GLU:HA	1:C:714:LYS:HE3	1.82	0.61
1:A:642:TRP:CD1	1:A:645:SER:HG	2.18	0.61
1:B:144:ARG:NH2	1:B:288:ASP:OD2	2.28	0.61
1:B:1398:LEU:HD21	1:B:1415:GLU:HG2	1.80	0.61
1:C:763:PHE:HB3	1:C:764:PRO:HD3	1.83	0.61
1:D:763:PHE:HB3	1:D:764:PRO:HD3	1.83	0.61
1:A:1032:TYR:O	1:A:1036:THR:HG23	2.01	0.61
1:C:187:LYS:NZ	1:C:220:GLU:OE2	2.29	0.61
1:C:287:VAL:HG21	1:C:298:GLU:HB3	1.82	0.61
1:B:763:PHE:HB3	1:B:764:PRO:HD3	1.83	0.61
1:C:558:MET:HB2	1:C:577:TYR:CZ	2.36	0.61
1:C:1433:ARG:NH1	3:C:1602:DAT:N7	2.45	0.61
1:D:1310:ARG:NH1	1:D:1344:PRO:HD3	2.16	0.61
1:D:1032:TYR:O	1:D:1036:THR:HG23	2.01	0.61
1:B:1032:TYR:O	1:B:1036:THR:HG23	2.01	0.61
1:C:1349:TYR:HD2	1:C:1387:LEU:HD12	1.66	0.60
1:B:1349:TYR:HD2	1:B:1387:LEU:HD12	1.66	0.60
1:D:1349:TYR:HD2	1:D:1387:LEU:HD12	1.66	0.60
1:D:77:GLU:HA	1:D:89:CYS:HA	1.81	0.60
1:D:144:ARG:NH2	1:D:288:ASP:OD2	2.28	0.60
1:A:287:VAL:HG21	1:A:298:GLU:HB3	1.82	0.60
1:B:1310:ARG:NH1	1:B:1344:PRO:HD3	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:MET:HB2	1:A:577:TYR:CZ	2.36	0.60
1:B:404:LYS:HA	1:B:404:LYS:CE	2.32	0.60
1:B:1022:GLU:H	1:C:970:ALA:C	2.10	0.60
1:D:287:VAL:HG21	1:D:298:GLU:HB3	1.82	0.60
1:D:558:MET:HB2	1:D:577:TYR:CZ	2.36	0.60
1:C:1310:ARG:NH1	1:C:1344:PRO:HD3	2.16	0.60
1:B:519:LEU:HD21	1:B:618:THR:HG21	1.84	0.60
1:A:187:LYS:NZ	1:A:220:GLU:OE2	2.29	0.60
1:A:519:LEU:HD21	1:A:618:THR:HG21	1.84	0.59
1:A:1310:ARG:NH1	1:A:1344:PRO:HD3	2.16	0.59
1:C:144:ARG:NH2	1:C:288:ASP:OD2	2.28	0.59
1:C:514:VAL:HB	1:C:621:PRO:HB3	1.84	0.59
1:A:404:LYS:HA	1:A:404:LYS:CE	2.32	0.59
1:A:1021:PRO:CD	1:B:965:TRP:HD1	2.14	0.59
1:A:1349:TYR:HD2	1:A:1387:LEU:HD12	1.66	0.59
1:C:1032:TYR:O	1:C:1036:THR:HG23	2.01	0.59
1:D:519:LEU:HD21	1:D:618:THR:HG21	1.84	0.59
1:D:187:LYS:NZ	1:D:220:GLU:OE2	2.29	0.59
1:A:1022:GLU:HA	1:B:973:HIS:H	1.67	0.59
1:D:927:VAL:HA	1:D:930:MET:HG3	1.85	0.59
1:C:404:LYS:HA	1:C:404:LYS:CE	2.32	0.59
1:B:558:MET:HB2	1:B:577:TYR:CZ	2.36	0.59
1:D:514:VAL:HB	1:D:621:PRO:HB3	1.85	0.59
1:C:463:ASN:HB2	1:C:496:LYS:HE2	1.84	0.59
1:D:404:LYS:HA	1:D:404:LYS:CE	2.32	0.59
1:D:463:ASN:HB2	1:D:496:LYS:HE2	1.84	0.59
1:A:344:THR:HG22	1:A:412:ARG:HD2	1.84	0.59
1:A:1023:TRP:HB2	1:B:971:VAL:C	2.28	0.59
1:B:154:ILE:HG22	1:B:158:MET:HE2	1.85	0.59
1:C:927:VAL:HA	1:C:930:MET:HG3	1.85	0.59
1:A:463:ASN:HB2	1:A:496:LYS:HE2	1.84	0.59
1:A:927:VAL:HA	1:A:930:MET:HG3	1.85	0.58
1:B:642:TRP:CD1	1:B:645:SER:HG	2.20	0.58
1:A:514:VAL:HB	1:A:621:PRO:HB3	1.84	0.58
1:B:344:THR:HG22	1:B:412:ARG:HD2	1.84	0.58
1:B:1033:LEU:O	1:B:1036:THR:OG1	2.18	0.58
1:B:1268:PHE:HB3	1:B:1271:TYR:HB2	1.85	0.58
1:C:519:LEU:HD21	1:C:618:THR:HG21	1.84	0.58
1:B:463:ASN:HB2	1:B:496:LYS:HE2	1.84	0.58
1:B:927:VAL:HA	1:B:930:MET:HG3	1.85	0.58
1:C:73:VAL:HG11	1:C:120:GLN:HG3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:PHE:HA	1:A:398:ARG:HD3	1.86	0.58
1:C:154:ILE:HG22	1:C:158:MET:HE2	1.85	0.58
1:A:154:ILE:HG22	1:A:158:MET:HE2	1.85	0.58
1:A:1033:LEU:O	1:A:1036:THR:OG1	2.18	0.58
1:A:1081:PRO:HB2	1:A:1083:PRO:HD2	1.86	0.58
1:B:514:VAL:HB	1:B:621:PRO:HB3	1.84	0.58
1:C:344:THR:HG22	1:C:412:ARG:HD2	1.84	0.58
1:D:697:ASP:OD2	1:D:700:ARG:NH1	2.37	0.58
1:B:621:PRO:HD2	1:B:622:ILE:HD12	1.86	0.58
1:B:1081:PRO:HB2	1:B:1083:PRO:HD2	1.86	0.58
1:D:621:PRO:HD2	1:D:622:ILE:HD12	1.86	0.58
1:D:1268:PHE:HB3	1:D:1271:TYR:HB2	1.85	0.58
1:A:249:ARG:NH2	1:A:263:GLU:O	2.37	0.58
1:C:621:PRO:HD2	1:C:622:ILE:HD12	1.86	0.58
1:A:1309:ASP:HA	1:A:1311:ARG:HH11	1.69	0.58
1:D:73:VAL:HG11	1:D:120:GLN:HG3	1.86	0.58
1:D:496:LYS:HD2	1:D:497:PRO:HD2	1.86	0.58
1:D:394:PHE:HA	1:D:398:ARG:HD3	1.86	0.58
1:B:1309:ASP:HA	1:B:1311:ARG:HH11	1.69	0.57
1:C:496:LYS:HD2	1:C:497:PRO:HD2	1.86	0.57
1:C:1309:ASP:HA	1:C:1311:ARG:HH11	1.69	0.57
1:C:170:LEU:HB2	1:C:325:ILE:HG22	1.86	0.57
1:B:212:THR:O	1:B:215:MET:HB3	2.04	0.57
1:B:249:ARG:NH2	1:B:263:GLU:O	2.37	0.57
1:B:394:PHE:HA	1:B:398:ARG:HD3	1.86	0.57
1:C:1033:LEU:O	1:C:1036:THR:OG1	2.18	0.57
1:C:1268:PHE:HB3	1:C:1271:TYR:HB2	1.85	0.57
1:D:154:ILE:HG22	1:D:158:MET:HE2	1.85	0.57
1:D:212:THR:O	1:D:215:MET:HB3	2.05	0.57
1:D:636:GLU:O	1:D:640:ILE:HG12	2.04	0.57
1:D:1081:PRO:HB2	1:D:1083:PRO:HD2	1.86	0.57
1:D:1309:ASP:HA	1:D:1311:ARG:HH11	1.69	0.57
1:A:212:THR:O	1:A:215:MET:HB3	2.05	0.57
1:A:621:PRO:HD2	1:A:622:ILE:HD12	1.86	0.57
1:A:1268:PHE:HB3	1:A:1271:TYR:HB2	1.85	0.57
1:A:697:ASP:OD2	1:A:700:ARG:NH1	2.37	0.57
1:B:496:LYS:HD2	1:B:497:PRO:HD2	1.86	0.57
1:B:697:ASP:OD2	1:B:700:ARG:NH1	2.37	0.57
1:A:744:TRP:HB3	1:A:747:LEU:HB3	1.86	0.57
1:B:73:VAL:HG11	1:B:120:GLN:HG3	1.86	0.57
1:C:1081:PRO:HB2	1:C:1083:PRO:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:344:THR:HG22	1:D:412:ARG:HD2	1.84	0.57
1:D:654:ALA:HB2	1:D:720:LEU:HD21	1.87	0.57
1:A:1308:ARG:O	1:A:1310:ARG:NH1	2.38	0.57
1:A:73:VAL:HG11	1:A:120:GLN:HG3	1.86	0.57
1:B:170:LEU:HD23	1:B:204:TRP:HB2	1.87	0.57
1:B:636:GLU:O	1:B:640:ILE:HG12	2.04	0.57
1:C:636:GLU:O	1:C:640:ILE:HG12	2.04	0.57
1:C:654:ALA:HB2	1:C:720:LEU:HD21	1.87	0.57
1:A:1026:VAL:HG21	1:B:974:SER:O	2.05	0.57
1:A:1042:ASN:OD1	1:A:1042:ASN:C	2.48	0.57
1:B:1042:ASN:OD1	1:B:1042:ASN:C	2.48	0.57
1:C:394:PHE:HA	1:C:398:ARG:HD3	1.86	0.57
1:A:496:LYS:HD2	1:A:497:PRO:HD2	1.86	0.56
1:A:1032:TYR:HA	1:A:1035:PHE:HD2	1.70	0.56
1:B:744:TRP:HB3	1:B:747:LEU:HB3	1.86	0.56
1:C:249:ARG:NH2	1:C:263:GLU:O	2.37	0.56
1:C:697:ASP:OD2	1:C:700:ARG:NH1	2.37	0.56
1:D:170:LEU:HD23	1:D:204:TRP:HB2	1.87	0.56
1:A:1159:VAL:HG21	1:B:1154:LYS:HE2	1.87	0.56
1:B:170:LEU:HB2	1:B:325:ILE:HG22	1.86	0.56
1:C:744:TRP:HB3	1:C:747:LEU:HB3	1.86	0.56
1:D:170:LEU:HB2	1:D:325:ILE:HG22	1.86	0.56
1:C:1308:ARG:O	1:C:1310:ARG:NH1	2.38	0.56
1:D:538:LYS:O	1:D:542:GLU:HG2	2.06	0.56
1:D:744:TRP:HB3	1:D:747:LEU:HB3	1.86	0.56
1:A:636:GLU:O	1:A:640:ILE:HG12	2.04	0.56
1:C:1425:TYR:O	1:C:1442:THR:OG1	2.24	0.56
1:D:249:ARG:NH2	1:D:263:GLU:O	2.37	0.56
1:A:170:LEU:HB2	1:A:325:ILE:HG22	1.86	0.56
1:A:1425:TYR:O	1:A:1442:THR:OG1	2.24	0.56
1:B:1308:ARG:O	1:B:1310:ARG:NH1	2.38	0.56
1:C:212:THR:O	1:C:215:MET:HB3	2.04	0.56
1:D:568:LEU:O	1:D:657:LYS:NZ	2.39	0.56
1:A:538:LYS:O	1:A:542:GLU:HG2	2.06	0.56
1:A:1274:PRO:O	1:A:1334:ARG:NH1	2.39	0.56
1:C:170:LEU:HD23	1:C:204:TRP:HB2	1.87	0.56
1:C:568:LEU:O	1:C:657:LYS:NZ	2.39	0.56
1:A:654:ALA:HB2	1:A:720:LEU:HD21	1.87	0.56
1:D:1042:ASN:OD1	1:D:1042:ASN:C	2.48	0.56
1:D:1274:PRO:O	1:D:1334:ARG:NH1	2.39	0.56
1:A:1378:LYS:HG3	1:A:1385:TRP:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1331:THR:HG21	1:B:1434:ASN:HB2	1.88	0.56
1:D:1032:TYR:HA	1:D:1035:PHE:HD2	1.70	0.56
1:D:1378:LYS:HG3	1:D:1385:TRP:HA	1.88	0.56
1:C:1274:PRO:O	1:C:1334:ARG:NH1	2.39	0.56
1:D:1308:ARG:O	1:D:1310:ARG:NH1	2.38	0.56
1:A:727:MET:HB3	1:A:728:LYS:HZ2	1.72	0.55
1:B:187:LYS:NZ	1:B:220:GLU:OE2	2.29	0.55
1:B:515:THR:H	1:B:518:THR:HB	1.72	0.55
1:B:540:LEU:HA	1:B:560:HIS:CE1	2.42	0.55
1:B:1046:ALA:HA	1:C:1048:PHE:CZ	2.40	0.55
1:B:1274:PRO:O	1:B:1334:ARG:NH1	2.39	0.55
1:B:538:LYS:O	1:B:542:GLU:HG2	2.06	0.55
1:C:660:LYS:O	1:C:663:SER:OG	2.22	0.55
1:C:1032:TYR:HA	1:C:1035:PHE:HD2	1.70	0.55
1:C:1042:ASN:C	1:C:1042:ASN:OD1	2.48	0.55
1:C:1055:VAL:O	1:C:1059:THR:N	2.39	0.55
1:C:1437:ASN:ND2	1:C:1437:ASN:O	2.39	0.55
1:D:1331:THR:HG21	1:D:1434:ASN:HB2	1.88	0.55
1:A:965:TRP:HA	1:D:1020:PHE:N	2.22	0.55
1:A:1042:ASN:HB2	1:B:1044:LEU:HD11	1.89	0.55
1:B:654:ALA:HB2	1:B:720:LEU:HD21	1.87	0.55
1:D:1437:ASN:O	1:D:1437:ASN:ND2	2.39	0.55
1:A:515:THR:H	1:A:518:THR:HB	1.72	0.55
1:A:1023:TRP:H	1:B:972:TYR:N	2.04	0.55
1:A:1437:ASN:ND2	1:A:1437:ASN:O	2.39	0.55
1:B:568:LEU:O	1:B:657:LYS:NZ	2.39	0.55
1:C:540:LEU:HA	1:C:560:HIS:CE1	2.42	0.55
1:C:1022:GLU:HG2	1:D:974:SER:H	1.70	0.55
1:A:540:LEU:HA	1:A:560:HIS:CE1	2.42	0.55
1:A:568:LEU:O	1:A:657:LYS:NZ	2.39	0.55
1:A:1035:PHE:HE1	1:B:938:LEU:HD22	1.72	0.55
1:A:238:THR:HG22	1:A:281:HIS:CD2	2.42	0.55
1:B:238:THR:HG22	1:B:281:HIS:CD2	2.42	0.55
1:B:1437:ASN:O	1:B:1437:ASN:ND2	2.39	0.55
1:C:1331:THR:HG21	1:C:1434:ASN:HB2	1.88	0.55
1:C:1022:GLU:OE1	1:D:974:SER:OG	2.24	0.55
1:A:170:LEU:HD23	1:A:204:TRP:HB2	1.87	0.55
1:C:538:LYS:O	1:C:542:GLU:HG2	2.06	0.54
1:C:1023:TRP:CG	1:D:976:LEU:HD13	2.42	0.54
1:B:164:LEU:HB3	1:B:204:TRP:HH2	1.72	0.54
1:B:1032:TYR:HA	1:B:1035:PHE:HD2	1.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:515:THR:H	1:C:518:THR:HB	1.72	0.54
1:D:486:PRO:O	1:D:489:THR:OG1	2.23	0.54
1:B:1378:LYS:HG3	1:B:1385:TRP:HA	1.88	0.54
1:C:164:LEU:HB3	1:C:204:TRP:HH2	1.73	0.54
1:D:164:LEU:HB3	1:D:204:TRP:HH2	1.73	0.54
1:D:540:LEU:HA	1:D:560:HIS:CE1	2.41	0.54
1:D:1241:ASN:HB3	1:D:1430:ASP:HB3	1.90	0.54
1:B:1055:VAL:O	1:B:1059:THR:N	2.39	0.54
1:C:1378:LYS:HG3	1:C:1385:TRP:HA	1.88	0.54
1:B:427:GLN:HG2	1:B:428:ASP:H	1.71	0.54
1:B:1235:GLY:N	1:B:1260:GLU:OE1	2.41	0.54
1:C:1241:ASN:HB3	1:C:1430:ASP:HB3	1.90	0.54
1:A:427:GLN:HG2	1:A:428:ASP:H	1.71	0.54
1:C:427:GLN:HG2	1:C:428:ASP:H	1.72	0.54
1:C:973:HIS:CD2	1:C:974:SER:HB3	2.40	0.54
1:D:238:THR:HG22	1:D:281:HIS:CD2	2.42	0.54
1:D:278:ASP:OD2	1:D:281:HIS:ND1	2.40	0.54
1:D:515:THR:H	1:D:518:THR:HB	1.72	0.54
1:A:173:VAL:HG23	1:A:205:ILE:HD11	1.90	0.54
1:A:1043:LEU:HA	1:B:923:LYS:HE3	1.90	0.54
1:C:982:ILE:HD12	1:C:983:PRO:HD2	1.90	0.54
1:D:982:ILE:HD12	1:D:983:PRO:HD2	1.90	0.54
1:C:238:THR:HG22	1:C:281:HIS:CD2	2.42	0.53
1:B:1241:ASN:HB3	1:B:1430:ASP:HB3	1.90	0.53
1:C:486:PRO:O	1:C:489:THR:OG1	2.23	0.53
1:D:1425:TYR:O	1:D:1442:THR:OG1	2.24	0.53
1:A:486:PRO:O	1:A:489:THR:OG1	2.23	0.53
1:A:1331:THR:HG21	1:A:1434:ASN:HB2	1.88	0.53
1:B:973:HIS:CD2	1:B:974:SER:HB3	2.40	0.53
1:C:561:VAL:HA	1:C:564:VAL:HG12	1.90	0.53
1:A:657:LYS:NZ	1:A:661:GLU:OE2	2.40	0.53
1:A:1241:ASN:HB3	1:A:1430:ASP:HB3	1.90	0.53
1:B:173:VAL:HG23	1:B:205:ILE:HD11	1.90	0.53
1:C:278:ASP:OD2	1:C:281:HIS:ND1	2.40	0.53
1:D:660:LYS:O	1:D:663:SER:OG	2.22	0.53
1:C:566:ARG:HA	1:C:569:LEU:HG	1.90	0.53
1:A:663:SER:HB3	1:A:675:MET:SD	2.49	0.53
1:D:173:VAL:HG23	1:D:205:ILE:HD11	1.90	0.53
1:A:1254:ARG:NH2	1:A:1331:THR:O	2.42	0.53
1:B:1425:TYR:O	1:B:1442:THR:OG1	2.24	0.53
1:D:427:GLN:HG2	1:D:428:ASP:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:663:SER:HB3	1:B:675:MET:SD	2.49	0.53
1:B:1358:ASN:OD1	1:B:1359:GLU:N	2.38	0.53
1:C:1235:GLY:N	1:C:1260:GLU:OE1	2.41	0.53
1:A:775:GLU:O	1:A:780:ASP:N	2.38	0.53
1:C:1254:ARG:NH2	1:C:1331:THR:O	2.42	0.53
1:D:566:ARG:HA	1:D:569:LEU:HG	1.90	0.53
1:A:1022:GLU:HG2	1:B:973:HIS:CE1	2.44	0.53
1:B:739:LEU:HA	1:B:742:VAL:HG12	1.91	0.53
1:B:1254:ARG:NH2	1:B:1331:THR:O	2.42	0.53
1:A:566:ARG:HA	1:A:569:LEU:HG	1.90	0.52
1:B:1109:LEU:H	1:B:1109:LEU:HD23	1.75	0.52
1:C:1020:PHE:HA	1:D:970:ALA:H	1.74	0.52
1:D:727:MET:HB3	1:D:728:LYS:HZ2	1.75	0.52
1:D:840:VAL:O	1:D:844:MET:HB2	2.09	0.52
1:D:1235:GLY:N	1:D:1260:GLU:OE1	2.41	0.52
1:A:164:LEU:HB3	1:A:204:TRP:HH2	1.73	0.52
1:A:395:THR:O	1:A:399:ILE:N	2.42	0.52
1:A:725:LYS:HA	1:A:1065:PHE:CZ	2.45	0.52
1:A:840:VAL:O	1:A:844:MET:HB2	2.09	0.52
1:A:1235:GLY:N	1:A:1260:GLU:OE1	2.41	0.52
1:C:173:VAL:HG23	1:C:205:ILE:HD11	1.90	0.52
1:D:1254:ARG:NH2	1:D:1331:THR:O	2.42	0.52
1:B:278:ASP:OD2	1:B:281:HIS:ND1	2.40	0.52
1:B:671:SER:O	1:B:675:MET:HG3	2.10	0.52
1:B:936:PHE:HD2	1:C:919:THR:OG1	1.92	0.52
1:C:940:LEU:HD13	1:D:920:LEU:HD21	1.91	0.52
1:A:982:ILE:HD12	1:A:983:PRO:HD2	1.90	0.52
1:A:1109:LEU:HD23	1:A:1109:LEU:H	1.74	0.52
1:B:657:LYS:NZ	1:B:661:GLU:OE2	2.40	0.52
1:C:840:VAL:O	1:C:844:MET:HB2	2.09	0.52
1:D:618:THR:OG1	1:D:619:MET:N	2.43	0.52
1:D:1109:LEU:HD23	1:D:1109:LEU:H	1.75	0.52
1:B:395:THR:O	1:B:399:ILE:N	2.42	0.52
1:B:725:LYS:HA	1:B:1065:PHE:CZ	2.45	0.52
1:B:978:ILE:C	1:B:980:GLY:H	2.18	0.52
1:B:982:ILE:HD12	1:B:983:PRO:HD2	1.90	0.52
1:C:671:SER:O	1:C:675:MET:HG3	2.10	0.52
1:C:978:ILE:C	1:C:980:GLY:H	2.18	0.52
1:C:1109:LEU:HD23	1:C:1109:LEU:H	1.75	0.52
1:D:69:LYS:NZ	1:D:125:ASP:OD1	2.43	0.52
1:D:725:LYS:HA	1:D:1065:PHE:CZ	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1023:TRP:HB2	1:B:971:VAL:O	2.10	0.52
1:B:566:ARG:HA	1:B:569:LEU:HG	1.90	0.52
1:B:727:MET:HB3	1:B:728:LYS:HZ2	1.75	0.52
1:B:840:VAL:O	1:B:844:MET:HB2	2.09	0.52
1:C:725:LYS:HA	1:C:1065:PHE:CZ	2.45	0.52
1:D:973:HIS:CD2	1:D:974:SER:HB3	2.40	0.52
1:B:69:LYS:NZ	1:B:125:ASP:OD1	2.43	0.52
1:B:241:VAL:HG12	1:B:285:ILE:HB	1.91	0.52
1:B:485:HIS:HD2	1:B:513:PHE:HD1	1.58	0.52
1:D:561:VAL:HA	1:D:564:VAL:HG12	1.90	0.52
1:D:1033:LEU:O	1:D:1036:THR:OG1	2.18	0.52
1:A:485:HIS:HD2	1:A:513:PHE:HD1	1.58	0.52
1:A:561:VAL:HA	1:A:564:VAL:HG12	1.90	0.52
1:A:678:LEU:HG	1:A:682:TYR:CE2	2.45	0.52
1:C:69:LYS:NZ	1:C:125:ASP:OD1	2.43	0.52
1:C:739:LEU:HA	1:C:742:VAL:HG12	1.91	0.52
1:D:739:LEU:HA	1:D:742:VAL:HG12	1.91	0.52
1:D:1140:GLN:HA	1:D:1143:ARG:NH2	2.25	0.52
1:A:700:ARG:NH2	1:A:1121:LEU:HA	2.25	0.52
1:A:973:HIS:CD2	1:A:974:SER:HB3	2.40	0.52
1:A:343:ALA:O	1:A:348:THR:OG1	2.28	0.52
1:B:561:VAL:HA	1:B:564:VAL:HG12	1.90	0.52
1:D:205:ILE:HG23	1:D:238:THR:HG23	1.93	0.52
1:D:663:SER:HB3	1:D:675:MET:SD	2.49	0.52
1:A:472:ILE:HG23	1:A:477:TRP:CH2	2.45	0.51
1:A:671:SER:O	1:A:675:MET:HG3	2.10	0.51
1:A:1374:VAL:HG23	1:A:1478:VAL:HG23	1.92	0.51
1:B:486:PRO:O	1:B:489:THR:OG1	2.23	0.51
1:C:241:VAL:HG12	1:C:285:ILE:HB	1.91	0.51
1:D:657:LYS:NZ	1:D:661:GLU:OE2	2.40	0.51
1:D:1155:VAL:O	1:D:1159:VAL:HG23	2.11	0.51
1:A:1140:GLN:HA	1:A:1143:ARG:NH2	2.25	0.51
1:B:618:THR:OG1	1:B:619:MET:N	2.43	0.51
1:B:1374:VAL:HG23	1:B:1478:VAL:HG23	1.92	0.51
1:C:663:SER:HB3	1:C:675:MET:SD	2.49	0.51
1:D:671:SER:O	1:D:675:MET:HG3	2.10	0.51
1:D:678:LEU:HG	1:D:682:TYR:CE2	2.45	0.51
1:A:69:LYS:NZ	1:A:125:ASP:OD1	2.43	0.51
1:A:241:VAL:HG12	1:A:285:ILE:HB	1.91	0.51
1:A:437:LEU:O	1:A:441:SER:HB2	2.10	0.51
1:A:739:LEU:HA	1:A:742:VAL:HG12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:ILE:HG23	1:C:238:THR:HG23	1.93	0.51
1:C:343:ALA:O	1:C:348:THR:OG1	2.28	0.51
1:D:978:ILE:C	1:D:980:GLY:H	2.18	0.51
1:A:978:ILE:C	1:A:980:GLY:H	2.18	0.51
1:A:1055:VAL:O	1:A:1059:THR:N	2.39	0.51
1:A:1365:ARG:NH1	1:A:1370:LYS:HD3	2.26	0.51
1:B:982:ILE:HG23	1:C:981:GLN:HG2	1.92	0.51
1:B:1021:PRO:C	1:C:971:VAL:H	2.18	0.51
1:C:437:LEU:O	1:C:441:SER:HB2	2.10	0.51
1:C:1140:GLN:HA	1:C:1143:ARG:NH2	2.25	0.51
1:D:581:ARG:NH1	1:D:599:VAL:O	2.43	0.51
1:A:660:LYS:O	1:A:663:SER:OG	2.22	0.51
1:C:1020:PHE:N	1:D:969:GLY:HA3	2.25	0.51
1:C:1374:VAL:HG23	1:C:1478:VAL:HG23	1.92	0.51
1:D:1055:VAL:O	1:D:1059:THR:N	2.39	0.51
1:A:1155:VAL:O	1:A:1159:VAL:HG23	2.11	0.51
1:C:208:GLY:C	1:C:215:MET:HE1	2.36	0.51
1:B:1155:VAL:O	1:B:1159:VAL:HG23	2.11	0.51
1:D:934:VAL:HG13	1:D:1047:MET:HE3	1.92	0.51
1:A:205:ILE:HG23	1:A:238:THR:HG23	1.93	0.51
1:A:208:GLY:C	1:A:215:MET:HE1	2.36	0.51
1:A:278:ASP:OD2	1:A:281:HIS:ND1	2.40	0.51
1:A:581:ARG:NH1	1:A:599:VAL:O	2.43	0.51
1:A:1140:GLN:HG3	1:A:1143:ARG:HH22	1.76	0.51
1:B:1365:ARG:NH1	1:B:1370:LYS:HD3	2.26	0.51
1:C:1155:VAL:O	1:C:1159:VAL:HG23	2.11	0.51
1:A:926:ILE:O	1:A:929:ARG:HG3	2.11	0.51
1:A:1023:TRP:N	1:B:973:HIS:N	2.59	0.51
1:B:208:GLY:C	1:B:215:MET:HE1	2.36	0.51
1:B:581:ARG:NH1	1:B:599:VAL:O	2.43	0.51
1:B:1140:GLN:HA	1:B:1143:ARG:NH2	2.25	0.51
1:C:344:THR:HG21	1:C:409:ILE:HA	1.93	0.51
1:C:926:ILE:O	1:C:929:ARG:HG3	2.11	0.51
1:A:344:THR:HG21	1:A:409:ILE:HA	1.93	0.51
1:B:205:ILE:HG23	1:B:238:THR:HG23	1.93	0.51
1:B:343:ALA:O	1:B:348:THR:OG1	2.28	0.51
1:B:926:ILE:O	1:B:929:ARG:HG3	2.11	0.51
1:B:1020:PHE:O	1:C:970:ALA:HB3	2.10	0.51
1:B:1140:GLN:HG3	1:B:1143:ARG:HH22	1.76	0.51
1:C:452:TRP:CZ3	1:C:477:TRP:HB3	2.46	0.51
1:C:934:VAL:HG13	1:C:1047:MET:HE3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:660:LYS:O	1:B:663:SER:OG	2.23	0.50
1:C:581:ARG:NH1	1:C:599:VAL:O	2.43	0.50
1:C:1140:GLN:HG3	1:C:1143:ARG:HH22	1.76	0.50
1:D:727:MET:HB3	1:D:728:LYS:NZ	2.26	0.50
1:D:1140:GLN:HG3	1:D:1143:ARG:HH22	1.76	0.50
1:A:727:MET:HB3	1:A:728:LYS:NZ	2.26	0.50
1:A:820:ASP:OD2	1:A:826:SER:OG	2.30	0.50
1:B:678:LEU:HG	1:B:682:TYR:CE2	2.45	0.50
1:B:1095:LYS:HD2	1:B:1095:LYS:O	2.12	0.50
1:C:678:LEU:HG	1:C:682:TYR:CE2	2.45	0.50
1:D:299:ILE:HD13	1:D:338:HIS:HB3	1.93	0.50
1:D:926:ILE:O	1:D:929:ARG:HG3	2.11	0.50
1:A:669:THR:OG1	1:A:670:ASP:OD1	2.28	0.50
1:A:981:GLN:NE2	1:B:981:GLN:OE1	2.45	0.50
1:B:197:VAL:HG23	1:B:462:TRP:HZ2	1.77	0.50
1:B:437:LEU:O	1:B:441:SER:HB2	2.10	0.50
1:B:934:VAL:HG13	1:B:1047:MET:HE3	1.92	0.50
1:D:208:GLY:C	1:D:215:MET:HE1	2.36	0.50
1:D:241:VAL:HG12	1:D:285:ILE:HB	1.91	0.50
1:D:452:TRP:CZ3	1:D:477:TRP:HB3	2.46	0.50
1:D:820:ASP:OD2	1:D:826:SER:OG	2.30	0.50
1:D:1374:VAL:HG23	1:D:1478:VAL:HG23	1.92	0.50
1:A:197:VAL:HG23	1:A:462:TRP:HZ2	1.76	0.50
1:A:452:TRP:CZ3	1:A:477:TRP:HB3	2.46	0.50
1:B:230:SER:HA	1:C:696:LYS:HE2	1.93	0.50
1:B:852:ASP:H	1:B:859:LYS:HD3	1.77	0.50
1:C:727:MET:HB3	1:C:728:LYS:NZ	2.26	0.50
1:D:395:THR:O	1:D:399:ILE:N	2.42	0.50
1:D:485:HIS:HD2	1:D:513:PHE:HD1	1.58	0.50
1:A:924:ILE:HA	1:A:927:VAL:HG22	1.94	0.50
1:B:299:ILE:HD13	1:B:338:HIS:HB3	1.93	0.50
1:D:319:VAL:HG23	1:D:320:ALA:H	1.77	0.50
1:A:452:TRP:CH2	1:A:477:TRP:HB3	2.47	0.50
1:A:852:ASP:H	1:A:859:LYS:HD3	1.77	0.50
1:B:452:TRP:CH2	1:B:477:TRP:HB3	2.47	0.50
1:B:820:ASP:OD2	1:B:826:SER:OG	2.30	0.50
1:C:197:VAL:HG23	1:C:462:TRP:HZ2	1.76	0.50
1:D:437:LEU:O	1:D:441:SER:HB2	2.10	0.50
1:A:934:VAL:HG13	1:A:1047:MET:HE3	1.92	0.50
1:A:1043:LEU:O	1:A:1047:MET:HG3	2.12	0.50
1:B:924:ILE:HA	1:B:927:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1478:VAL:HG12	1:B:1482:ILE:HD13	1.94	0.50
1:C:485:HIS:HD2	1:C:513:PHE:HD1	1.58	0.50
1:C:1095:LYS:HD2	1:C:1095:LYS:O	2.12	0.50
1:D:852:ASP:H	1:D:859:LYS:HD3	1.77	0.50
1:D:1095:LYS:O	1:D:1095:LYS:HD2	2.12	0.50
1:A:299:ILE:HD13	1:A:338:HIS:HB3	1.93	0.50
1:A:1478:VAL:HG12	1:A:1482:ILE:HD13	1.94	0.50
1:B:452:TRP:CZ3	1:B:477:TRP:HB3	2.46	0.50
1:B:775:GLU:O	1:B:780:ASP:N	2.38	0.50
1:C:1384:HIS:CE1	1:C:1386:ALA:HB2	2.47	0.50
1:D:1243:ARG:NH1	1:D:1257:VAL:O	2.45	0.50
1:A:441:SER:HA	1:A:447:PHE:HD2	1.77	0.50
1:A:618:THR:OG1	1:A:619:MET:N	2.43	0.50
1:A:1095:LYS:HD2	1:A:1095:LYS:O	2.12	0.50
1:A:1384:HIS:CE1	1:A:1386:ALA:HB2	2.47	0.50
1:B:344:THR:HG21	1:B:409:ILE:HA	1.93	0.50
1:B:700:ARG:NH2	1:B:1121:LEU:HA	2.25	0.50
1:B:727:MET:HB3	1:B:728:LYS:NZ	2.26	0.50
1:C:1043:LEU:O	1:C:1047:MET:HG3	2.12	0.50
1:D:343:ALA:O	1:D:348:THR:OG1	2.28	0.50
1:D:441:SER:HA	1:D:447:PHE:HD2	1.77	0.50
1:D:775:GLU:O	1:D:780:ASP:N	2.38	0.50
1:B:1384:HIS:CE1	1:B:1386:ALA:HB2	2.47	0.49
1:C:284:PHE:CZ	1:C:286:LEU:HD13	2.47	0.49
1:C:452:TRP:CH2	1:C:477:TRP:HB3	2.47	0.49
1:C:924:ILE:HA	1:C:927:VAL:HG22	1.94	0.49
1:D:284:PHE:CZ	1:D:286:LEU:HD13	2.47	0.49
1:D:344:THR:HG21	1:D:409:ILE:HA	1.93	0.49
1:D:924:ILE:HA	1:D:927:VAL:HG22	1.94	0.49
1:A:284:PHE:CZ	1:A:286:LEU:HD13	2.47	0.49
1:B:669:THR:OG1	1:B:670:ASP:OD1	2.28	0.49
1:B:1043:LEU:O	1:B:1047:MET:HG3	2.12	0.49
1:D:197:VAL:HG23	1:D:462:TRP:HZ2	1.76	0.49
1:D:452:TRP:CH2	1:D:477:TRP:HB3	2.47	0.49
1:D:1384:HIS:CE1	1:D:1386:ALA:HB2	2.47	0.49
1:A:319:VAL:HG23	1:A:320:ALA:H	1.77	0.49
1:B:1243:ARG:NH1	1:B:1257:VAL:O	2.45	0.49
1:C:395:THR:O	1:C:399:ILE:N	2.42	0.49
1:C:1243:ARG:NH1	1:C:1257:VAL:O	2.45	0.49
1:B:284:PHE:CZ	1:B:286:LEU:HD13	2.47	0.49
1:B:1020:PHE:C	1:C:970:ALA:H	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:ILE:HD13	1:C:338:HIS:HB3	1.93	0.49
1:C:852:ASP:H	1:C:859:LYS:HD3	1.77	0.49
1:C:1022:GLU:CG	1:D:974:SER:H	2.25	0.49
1:A:127:PHE:O	1:A:255:HIS:NE2	2.46	0.49
1:A:245:GLY:O	1:A:250:ARG:NH1	2.46	0.49
1:B:1026:VAL:CG1	1:C:976:LEU:HD23	2.42	0.49
1:A:1243:ARG:NH1	1:A:1257:VAL:O	2.45	0.49
1:B:864:PHE:CD1	1:B:869:ASN:HB3	2.48	0.49
1:D:699:GLU:OE1	1:D:702:GLN:NE2	2.46	0.49
1:B:127:PHE:O	1:B:255:HIS:NE2	2.46	0.49
1:B:888:ILE:HG22	1:B:890:ALA:H	1.78	0.49
1:D:174:THR:HG21	1:D:339:THR:HG21	1.94	0.49
1:D:245:GLY:O	1:D:250:ARG:NH1	2.46	0.49
1:B:699:GLU:OE1	1:B:702:GLN:NE2	2.46	0.49
1:C:669:THR:OG1	1:C:670:ASP:OD1	2.28	0.49
1:C:699:GLU:OE1	1:C:702:GLN:NE2	2.46	0.49
1:C:820:ASP:OD2	1:C:826:SER:OG	2.30	0.49
1:C:864:PHE:CD1	1:C:869:ASN:HB3	2.48	0.49
1:D:906:PHE:HA	1:D:909:ARG:HD3	1.94	0.49
1:A:326:VAL:HG21	1:A:433:ILE:HG23	1.95	0.49
1:B:307:LYS:O	1:B:310:SER:HB3	2.13	0.49
1:B:319:VAL:HG23	1:B:320:ALA:H	1.77	0.49
1:B:326:VAL:HG21	1:B:433:ILE:HG23	1.95	0.49
1:D:1043:LEU:O	1:D:1047:MET:HG3	2.12	0.49
1:A:324:PRO:HB3	1:A:437:LEU:HD22	1.95	0.49
1:A:906:PHE:HA	1:A:909:ARG:HD3	1.95	0.49
1:C:245:GLY:O	1:C:250:ARG:NH1	2.46	0.49
1:C:307:LYS:O	1:C:310:SER:HB3	2.13	0.49
1:C:1022:GLU:HA	1:D:974:SER:H	1.76	0.49
1:C:1478:VAL:HG12	1:C:1482:ILE:HD13	1.94	0.49
1:D:324:PRO:HB3	1:D:437:LEU:HD22	1.95	0.49
1:D:669:THR:OG1	1:D:670:ASP:OD1	2.28	0.49
1:D:745:GLY:H	1:D:795:PRO:HD2	1.78	0.49
1:B:245:GLY:O	1:B:250:ARG:NH1	2.46	0.48
1:C:700:ARG:NH2	1:C:1121:LEU:HA	2.25	0.48
1:D:816:VAL:HG11	1:D:832:ILE:HG12	1.95	0.48
1:A:174:THR:HG21	1:A:339:THR:HG21	1.94	0.48
1:A:307:LYS:O	1:A:310:SER:HB3	2.13	0.48
1:A:679:ALA:HA	1:A:682:TYR:HD2	1.78	0.48
1:B:713:GLY:O	1:B:715:THR:HG23	2.14	0.48
1:C:127:PHE:O	1:C:255:HIS:NE2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:816:VAL:HG11	1:C:832:ILE:HG12	1.95	0.48
1:D:864:PHE:CD1	1:D:869:ASN:HB3	2.48	0.48
1:D:1330:ARG:NE	1:D:1436:ASP:OD2	2.40	0.48
1:D:1478:VAL:HG12	1:D:1482:ILE:HD13	1.94	0.48
1:A:699:GLU:OE1	1:A:702:GLN:NE2	2.46	0.48
1:A:816:VAL:HG11	1:A:832:ILE:HG12	1.95	0.48
1:B:690:PHE:HA	1:B:693:CYS:SG	2.54	0.48
1:C:906:PHE:HA	1:C:909:ARG:HD3	1.94	0.48
1:C:1022:GLU:HG2	1:D:974:SER:N	2.29	0.48
1:D:485:HIS:O	1:D:489:THR:HG23	2.14	0.48
1:B:1141:LYS:HE3	1:B:1141:LYS:HB3	1.70	0.48
1:C:319:VAL:HG23	1:C:320:ALA:H	1.77	0.48
1:D:888:ILE:HG22	1:D:890:ALA:H	1.78	0.48
1:A:223:ARG:HH12	1:A:280:ASN:HB3	1.78	0.48
1:A:690:PHE:HA	1:A:693:CYS:SG	2.54	0.48
1:B:177:ALA:O	1:B:178:LYS:HG2	2.14	0.48
1:B:324:PRO:HB3	1:B:437:LEU:HD22	1.95	0.48
1:B:679:ALA:HA	1:B:682:TYR:HD2	1.78	0.48
1:B:906:PHE:HA	1:B:909:ARG:HD3	1.94	0.48
1:C:679:ALA:HA	1:C:682:TYR:HD2	1.78	0.48
1:C:745:GLY:H	1:C:795:PRO:HD2	1.78	0.48
1:C:888:ILE:HG22	1:C:890:ALA:H	1.78	0.48
1:D:307:LYS:O	1:D:310:SER:HB3	2.13	0.48
1:D:326:VAL:HG21	1:D:433:ILE:HG23	1.95	0.48
1:D:472:ILE:HG23	1:D:477:TRP:CH2	2.45	0.48
1:A:177:ALA:O	1:A:178:LYS:HG2	2.14	0.48
1:A:713:GLY:O	1:A:715:THR:HG23	2.14	0.48
1:A:864:PHE:CD1	1:A:869:ASN:HB3	2.48	0.48
1:B:183:LYS:HE3	1:B:185:ARG:NH1	2.29	0.48
1:C:653:LEU:HD13	1:C:721:ALA:HB2	1.96	0.48
1:D:679:ALA:HA	1:D:682:TYR:HD2	1.78	0.48
1:D:690:PHE:HA	1:D:693:CYS:SG	2.54	0.48
1:D:700:ARG:NH2	1:D:1121:LEU:HA	2.25	0.48
1:A:745:GLY:H	1:A:795:PRO:HD2	1.78	0.48
1:A:1026:VAL:HG23	1:B:974:SER:HA	1.96	0.48
1:B:816:VAL:HG11	1:B:832:ILE:HG12	1.95	0.48
1:C:713:GLY:O	1:C:715:THR:HG23	2.14	0.48
1:D:223:ARG:HH12	1:D:280:ASN:HB3	1.78	0.48
1:D:941:LEU:O	1:D:945:VAL:HG23	2.14	0.48
1:A:420:ARG:HB2	1:A:424:ASP:HB3	1.95	0.48
1:A:888:ILE:HG22	1:A:890:ALA:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:ARG:HH12	1:B:280:ASN:HB3	1.78	0.48
1:B:653:LEU:HD13	1:B:721:ALA:HB2	1.96	0.48
1:B:941:LEU:O	1:B:945:VAL:HG23	2.14	0.48
1:C:326:VAL:HG21	1:C:433:ILE:HG23	1.95	0.48
1:C:441:SER:HA	1:C:447:PHE:HD2	1.77	0.48
1:C:727:MET:HB3	1:C:728:LYS:HZ2	1.78	0.48
1:D:183:LYS:HE3	1:D:185:ARG:NH1	2.29	0.48
1:A:208:GLY:O	1:A:215:MET:HE1	2.14	0.48
1:A:485:HIS:O	1:A:489:THR:HG23	2.14	0.48
1:B:420:ARG:HB2	1:B:424:ASP:HB3	1.95	0.48
1:D:713:GLY:O	1:D:715:THR:HG23	2.14	0.48
1:C:174:THR:HG21	1:C:339:THR:HG21	1.94	0.48
1:C:223:ARG:HH12	1:C:280:ASN:HB3	1.78	0.48
1:C:1365:ARG:NH1	1:C:1370:LYS:HD3	2.26	0.48
1:D:177:ALA:O	1:D:178:LYS:HG2	2.14	0.48
1:D:647:ASP:OD2	1:D:650:ALA:HB3	2.14	0.48
1:C:597:LEU:HB3	1:C:599:VAL:HG22	1.96	0.47
1:C:941:LEU:O	1:C:945:VAL:HG23	2.14	0.47
1:A:647:ASP:OD2	1:A:650:ALA:HB3	2.14	0.47
1:A:941:LEU:O	1:A:945:VAL:HG23	2.14	0.47
1:B:597:LEU:HB3	1:B:599:VAL:HG22	1.96	0.47
1:B:745:GLY:H	1:B:795:PRO:HD2	1.78	0.47
1:B:817:LEU:O	1:B:896:ARG:NH1	2.47	0.47
1:B:1330:ARG:NE	1:B:1436:ASP:OD2	2.40	0.47
1:A:576:LEU:HD11	1:A:619:MET:HE3	1.96	0.47
1:B:174:THR:HG21	1:B:339:THR:HG21	1.94	0.47
1:C:177:ALA:O	1:C:178:LYS:HG2	2.14	0.47
1:C:183:LYS:HE3	1:C:185:ARG:NH1	2.29	0.47
1:C:1089:HIS:HA	1:C:1093:PHE:HD2	1.80	0.47
1:D:208:GLY:O	1:D:215:MET:HE1	2.14	0.47
1:A:306:GLU:HA	1:A:309:ILE:HG12	1.97	0.47
1:A:597:LEU:HB3	1:A:599:VAL:HG22	1.96	0.47
1:B:187:LYS:HE2	1:B:191:ARG:HH21	1.80	0.47
1:C:81:LEU:H	1:C:81:LEU:HD23	1.79	0.47
1:C:208:GLY:O	1:C:215:MET:HE1	2.14	0.47
1:C:647:ASP:OD2	1:C:650:ALA:HB3	2.14	0.47
1:A:781:VAL:HG11	1:A:787:ARG:HH11	1.79	0.47
1:A:931:MET:HA	1:A:934:VAL:HG22	1.97	0.47
1:A:1023:TRP:H	1:B:973:HIS:N	2.12	0.47
1:B:441:SER:HA	1:B:447:PHE:HD2	1.77	0.47
1:B:936:PHE:HD2	1:C:919:THR:HG1	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:485:HIS:O	1:C:489:THR:HG23	2.14	0.47
1:C:690:PHE:HA	1:C:693:CYS:SG	2.54	0.47
1:C:781:VAL:HG11	1:C:787:ARG:HH11	1.79	0.47
1:D:781:VAL:HG11	1:D:787:ARG:HH11	1.79	0.47
1:A:973:HIS:CD2	1:D:1022:GLU:HG2	2.50	0.47
1:A:1063:TRP:NE1	1:A:1067:ARG:HD2	2.30	0.47
1:B:208:GLY:O	1:B:215:MET:HE1	2.14	0.47
1:B:485:HIS:O	1:B:489:THR:HG23	2.14	0.47
1:B:781:VAL:HG11	1:B:787:ARG:HH11	1.79	0.47
1:D:1089:HIS:HA	1:D:1093:PHE:HD2	1.80	0.47
1:A:183:LYS:HE3	1:A:185:ARG:NH1	2.29	0.47
1:A:653:LEU:HD13	1:A:721:ALA:HB2	1.96	0.47
1:A:817:LEU:O	1:A:896:ARG:NH1	2.47	0.47
1:B:81:LEU:HD23	1:B:81:LEU:H	1.79	0.47
1:B:1063:TRP:NE1	1:B:1067:ARG:HD2	2.30	0.47
1:C:324:PRO:HB3	1:C:437:LEU:HD22	1.95	0.47
1:C:657:LYS:NZ	1:C:661:GLU:OE2	2.40	0.47
1:C:1156:ASP:OD1	1:D:1154:LYS:NZ	2.31	0.47
1:C:1358:ASN:OD1	1:C:1359:GLU:N	2.38	0.47
1:D:597:LEU:HB3	1:D:599:VAL:HG22	1.96	0.47
1:C:775:GLU:O	1:C:780:ASP:N	2.38	0.47
1:D:187:LYS:HE2	1:D:191:ARG:HH21	1.80	0.47
1:D:306:GLU:HA	1:D:309:ILE:HG12	1.97	0.47
1:D:576:LEU:HD11	1:D:619:MET:HE3	1.96	0.47
1:A:187:LYS:HE2	1:A:191:ARG:HH21	1.80	0.47
1:A:749:VAL:HG22	1:A:750:ASP:H	1.80	0.47
1:B:647:ASP:OD2	1:B:650:ALA:HB3	2.14	0.47
1:B:1089:HIS:HA	1:B:1093:PHE:HD2	1.80	0.47
1:C:420:ARG:HB2	1:C:424:ASP:HB3	1.95	0.47
1:C:817:LEU:O	1:C:896:ARG:NH1	2.47	0.47
1:D:127:PHE:O	1:D:255:HIS:NE2	2.46	0.47
1:A:715:THR:HB	1:A:720:LEU:H	1.80	0.47
1:A:770:LEU:HG	1:A:771:ILE:H	1.80	0.47
1:B:931:MET:HA	1:B:934:VAL:HG22	1.97	0.47
1:C:310:SER:HB2	1:C:325:ILE:HG21	1.97	0.47
1:C:1063:TRP:NE1	1:C:1067:ARG:HD2	2.30	0.47
1:D:420:ARG:HB2	1:D:424:ASP:HB3	1.95	0.47
1:D:452:TRP:HA	1:D:455:GLN:OE1	2.15	0.47
1:D:653:LEU:HD13	1:D:721:ALA:HB2	1.96	0.47
1:D:1063:TRP:NE1	1:D:1067:ARG:HD2	2.30	0.47
1:D:1365:ARG:NH1	1:D:1370:LYS:HD3	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:732:HIS:O	1:A:734:GLY:N	2.48	0.46
1:A:1020:PHE:N	1:B:965:TRP:CD1	2.83	0.46
1:B:306:GLU:HA	1:B:309:ILE:HG12	1.97	0.46
1:B:310:SER:HB2	1:B:325:ILE:HG21	1.97	0.46
1:B:576:LEU:HD11	1:B:619:MET:HE3	1.96	0.46
1:B:732:HIS:O	1:B:734:GLY:N	2.48	0.46
1:B:749:VAL:HG22	1:B:750:ASP:H	1.80	0.46
1:C:940:LEU:HD22	1:D:920:LEU:HD11	1.97	0.46
1:D:817:LEU:O	1:D:896:ARG:NH1	2.47	0.46
1:B:311:GLU:HB2	1:B:312:GLN:OE1	2.15	0.46
1:B:619:MET:SD	1:B:623:ARG:HD3	2.54	0.46
1:B:715:THR:HB	1:B:720:LEU:H	1.81	0.46
1:C:452:TRP:HA	1:C:455:GLN:OE1	2.15	0.46
1:D:569:LEU:HD13	1:D:572:PHE:HB2	1.98	0.46
1:D:770:LEU:HG	1:D:771:ILE:H	1.80	0.46
1:A:619:MET:SD	1:A:623:ARG:HD3	2.55	0.46
1:A:800:HIS:HA	1:A:803:ILE:HD12	1.98	0.46
1:B:198:ALA:HB1	1:B:236:LEU:HD22	1.97	0.46
1:C:311:GLU:HB2	1:C:312:GLN:OE1	2.16	0.46
1:D:311:GLU:HB2	1:D:312:GLN:OE1	2.15	0.46
1:D:619:MET:SD	1:D:623:ARG:HD3	2.55	0.46
1:D:931:MET:HA	1:D:934:VAL:HG22	1.97	0.46
1:A:783:THR:HG22	1:A:785:ALA:H	1.80	0.46
1:A:1046:ALA:CB	1:B:923:LYS:HE2	2.45	0.46
1:A:1089:HIS:HA	1:A:1093:PHE:HD2	1.80	0.46
1:B:452:TRP:CD1	1:B:452:TRP:C	2.93	0.46
1:C:198:ALA:HB1	1:C:236:LEU:HD22	1.97	0.46
1:C:472:ILE:HG23	1:C:477:TRP:CH2	2.45	0.46
1:C:619:MET:SD	1:C:623:ARG:HD3	2.54	0.46
1:D:331:GLU:HB3	1:D:358:ARG:NH2	2.30	0.46
1:A:198:ALA:HB1	1:A:236:LEU:HD22	1.97	0.46
1:A:311:GLU:HB2	1:A:312:GLN:OE1	2.16	0.46
1:B:569:LEU:HD13	1:B:572:PHE:HB2	1.98	0.46
1:C:331:GLU:HB3	1:C:358:ARG:NH2	2.30	0.46
1:C:576:LEU:HD11	1:C:619:MET:HE3	1.96	0.46
1:D:646:GLN:HG2	1:D:647:ASP:N	2.30	0.46
1:A:378:LEU:HD21	1:A:382:LYS:HE2	1.97	0.46
1:A:437:LEU:O	1:A:441:SER:CB	2.64	0.46
1:A:569:LEU:HD13	1:A:572:PHE:HB2	1.98	0.46
1:A:920:LEU:HD11	1:D:940:LEU:HD22	1.97	0.46
1:B:331:GLU:HB3	1:B:358:ARG:NH2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:783:THR:HG22	1:B:785:ALA:H	1.80	0.46
1:B:800:HIS:HA	1:B:803:ILE:HD12	1.98	0.46
1:C:1022:GLU:HG2	1:D:974:SER:OG	2.15	0.46
1:D:63:ILE:HD13	1:D:127:PHE:CE2	2.51	0.46
1:D:800:HIS:HA	1:D:803:ILE:HD12	1.98	0.46
1:B:77:GLU:HB3	1:B:95:HIS:NE2	2.31	0.46
1:C:646:GLN:HG2	1:C:647:ASP:N	2.30	0.46
1:C:749:VAL:HG22	1:C:750:ASP:H	1.80	0.46
1:C:931:MET:HA	1:C:934:VAL:HG22	1.97	0.46
1:D:81:LEU:HD23	1:D:81:LEU:H	1.79	0.46
1:D:452:TRP:CD1	1:D:452:TRP:C	2.93	0.46
1:D:732:HIS:O	1:D:734:GLY:N	2.48	0.46
1:D:1358:ASN:OD1	1:D:1359:GLU:N	2.38	0.46
1:A:975:TYR:H	1:D:1022:GLU:HB3	1.81	0.46
1:B:770:LEU:HG	1:B:771:ILE:H	1.80	0.46
1:C:306:GLU:HA	1:C:309:ILE:HG12	1.97	0.46
1:D:715:THR:HB	1:D:720:LEU:H	1.81	0.46
1:D:783:THR:HG22	1:D:785:ALA:H	1.80	0.46
1:A:63:ILE:HD13	1:A:127:PHE:CE2	2.51	0.46
1:A:81:LEU:H	1:A:81:LEU:HD23	1.79	0.46
1:B:63:ILE:HD13	1:B:127:PHE:CE2	2.51	0.46
1:C:63:ILE:HD13	1:C:127:PHE:CE2	2.51	0.46
1:C:193:GLY:HA2	1:C:196:LYS:HG2	1.98	0.46
1:A:185:ARG:NH1	1:A:186:LEU:HB2	2.31	0.46
1:A:244:TRP:O	1:A:250:ARG:HD3	2.16	0.46
1:A:331:GLU:HB3	1:A:358:ARG:NH2	2.30	0.46
1:B:196:LYS:HG3	1:B:197:VAL:N	2.31	0.46
1:B:452:TRP:HA	1:B:455:GLN:OE1	2.15	0.46
1:B:558:MET:SD	1:B:575:PRO:HG2	2.57	0.46
1:B:646:GLN:HG2	1:B:647:ASP:N	2.30	0.46
1:B:1145:GLU:O	1:B:1148:ILE:HG22	2.16	0.46
1:C:196:LYS:HG3	1:C:197:VAL:N	2.31	0.46
1:C:378:LEU:HD21	1:C:382:LYS:HE2	1.97	0.46
1:C:796:VAL:HA	1:C:799:PHE:HD2	1.81	0.46
1:D:185:ARG:NH1	1:D:186:LEU:HB2	2.31	0.46
1:A:127:PHE:H	1:A:255:HIS:HE2	1.63	0.45
1:A:310:SER:HB2	1:A:325:ILE:HG21	1.97	0.45
1:B:755:ARG:HD3	1:B:771:ILE:HD11	1.99	0.45
1:C:77:GLU:HB3	1:C:95:HIS:NE2	2.31	0.45
1:C:127:PHE:H	1:C:255:HIS:HE2	1.63	0.45
1:C:187:LYS:HE2	1:C:191:ARG:HH21	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:569:LEU:HD13	1:C:572:PHE:HB2	1.98	0.45
1:C:1308:ARG:HB3	1:C:1310:ARG:HH11	1.81	0.45
1:D:77:GLU:HB3	1:D:95:HIS:NE2	2.31	0.45
1:D:198:ALA:HB1	1:D:236:LEU:HD22	1.97	0.45
1:D:310:SER:HB2	1:D:325:ILE:HG21	1.97	0.45
1:A:193:GLY:HA2	1:A:196:LYS:HG2	1.98	0.45
1:B:623:ARG:HG3	1:B:624:ASP:N	2.32	0.45
1:C:618:THR:OG1	1:C:619:MET:N	2.43	0.45
1:D:244:TRP:O	1:D:250:ARG:HD3	2.16	0.45
1:D:437:LEU:O	1:D:441:SER:CB	2.64	0.45
1:A:810:LEU:HG	1:A:903:PHE:CE1	2.52	0.45
1:B:437:LEU:O	1:B:441:SER:CB	2.64	0.45
1:B:1308:ARG:HB3	1:B:1310:ARG:HH11	1.81	0.45
1:C:336:THR:OG1	2:C:1601:APR:O2B	2.33	0.45
1:C:697:ASP:OD2	1:C:700:ARG:HD3	2.17	0.45
1:C:715:THR:HB	1:C:720:LEU:H	1.81	0.45
1:C:755:ARG:HD3	1:C:771:ILE:HD11	1.99	0.45
1:D:127:PHE:H	1:D:255:HIS:HE2	1.63	0.45
1:D:796:VAL:HA	1:D:799:PHE:HD2	1.82	0.45
1:A:452:TRP:HA	1:A:455:GLN:OE1	2.15	0.45
1:A:558:MET:SD	1:A:575:PRO:HG2	2.56	0.45
1:A:623:ARG:HG3	1:A:624:ASP:N	2.32	0.45
1:A:646:GLN:HG2	1:A:647:ASP:N	2.30	0.45
1:B:697:ASP:OD2	1:B:700:ARG:HD3	2.17	0.45
1:C:534:SER:O	1:C:538:LYS:HG2	2.17	0.45
1:C:690:PHE:HD2	1:C:732:HIS:CD2	2.34	0.45
1:C:800:HIS:HA	1:C:803:ILE:HD12	1.98	0.45
1:A:1145:GLU:O	1:A:1148:ILE:HG22	2.16	0.45
1:B:244:TRP:O	1:B:250:ARG:HD3	2.16	0.45
1:B:864:PHE:HA	1:B:869:ASN:HB2	1.99	0.45
1:C:185:ARG:NH1	1:C:186:LEU:HB2	2.31	0.45
1:C:437:LEU:O	1:C:441:SER:CB	2.64	0.45
1:C:770:LEU:HG	1:C:771:ILE:H	1.80	0.45
1:C:864:PHE:HA	1:C:869:ASN:HB2	1.99	0.45
1:D:378:LEU:HD21	1:D:382:LYS:HE2	1.97	0.45
1:A:1330:ARG:NE	1:A:1436:ASP:OD2	2.40	0.45
1:B:127:PHE:H	1:B:255:HIS:HE2	1.63	0.45
1:B:810:LEU:HG	1:B:903:PHE:CE1	2.52	0.45
1:C:558:MET:SD	1:C:575:PRO:HG2	2.56	0.45
1:D:558:MET:SD	1:D:575:PRO:HG2	2.56	0.45
1:D:810:LEU:HG	1:D:903:PHE:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1145:GLU:O	1:D:1148:ILE:HG22	2.16	0.45
1:A:77:GLU:HB3	1:A:95:HIS:NE2	2.31	0.45
1:A:196:LYS:HG3	1:A:197:VAL:N	2.31	0.45
1:B:185:ARG:NH1	1:B:186:LEU:HB2	2.32	0.45
1:B:193:GLY:HA2	1:B:196:LYS:HG2	1.98	0.45
1:C:783:THR:HG22	1:C:785:ALA:H	1.80	0.45
1:D:238:THR:N	1:D:282:SER:OG	2.49	0.45
1:D:697:ASP:OD2	1:D:700:ARG:HD3	2.17	0.45
1:B:378:LEU:HD21	1:B:382:LYS:HE2	1.97	0.45
1:B:642:TRP:HA	1:B:645:SER:HG	1.82	0.45
1:C:609:LYS:O	1:C:610:ARG:HG2	2.17	0.45
1:A:923:LYS:HZ1	1:D:1042:ASN:CG	2.20	0.45
1:A:1358:ASN:OD1	1:A:1359:GLU:N	2.38	0.45
1:B:246:THR:HA	1:B:274:LEU:HD23	1.99	0.45
1:B:472:ILE:HG23	1:B:477:TRP:CH2	2.45	0.45
1:B:796:VAL:HA	1:B:799:PHE:HD2	1.82	0.45
1:D:749:VAL:HG22	1:D:750:ASP:H	1.80	0.45
1:A:697:ASP:OD2	1:A:700:ARG:HD3	2.17	0.45
1:A:864:PHE:HA	1:A:869:ASN:HB2	1.99	0.45
1:B:534:SER:O	1:B:538:LYS:HG2	2.17	0.45
1:D:623:ARG:HG3	1:D:624:ASP:N	2.32	0.45
1:A:246:THR:HA	1:A:274:LEU:HD23	1.99	0.44
1:A:452:TRP:CD1	1:A:452:TRP:C	2.93	0.44
1:A:1308:ARG:HB3	1:A:1310:ARG:HH11	1.81	0.44
1:B:857:MET:SD	1:B:858:LYS:NZ	2.86	0.44
1:B:1043:LEU:HD12	1:C:923:LYS:HE3	1.99	0.44
1:C:244:TRP:O	1:C:250:ARG:HD3	2.16	0.44
1:C:810:LEU:HG	1:C:903:PHE:CE1	2.52	0.44
1:C:1067:ARG:O	1:C:1071:ILE:HG12	2.17	0.44
1:C:1370:LYS:HE3	1:C:1372:LEU:HA	1.99	0.44
1:D:193:GLY:HA2	1:D:196:LYS:HG2	1.98	0.44
1:A:796:VAL:HA	1:A:799:PHE:HD2	1.82	0.44
1:A:923:LYS:HG2	1:D:1043:LEU:HD12	1.99	0.44
1:B:169:LEU:HG	1:B:171:ILE:HG12	1.98	0.44
1:C:1145:GLU:O	1:C:1148:ILE:HG22	2.16	0.44
1:D:169:LEU:HG	1:D:171:ILE:HG12	1.98	0.44
1:D:196:LYS:HG3	1:D:197:VAL:N	2.31	0.44
1:D:534:SER:O	1:D:538:LYS:HG2	2.17	0.44
1:D:755:ARG:HD3	1:D:771:ILE:HD11	1.99	0.44
1:A:731:SER:HA	1:A:736:GLN:NE2	2.31	0.44
1:A:744:TRP:CD1	1:A:747:LEU:HD23	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1370:LYS:HE3	1:A:1372:LEU:HA	1.99	0.44
1:B:562:ALA:O	1:B:566:ARG:HG2	2.18	0.44
1:C:732:HIS:O	1:C:734:GLY:N	2.48	0.44
1:C:744:TRP:CD1	1:C:747:LEU:HD23	2.53	0.44
1:D:731:SER:HA	1:D:736:GLN:NE2	2.31	0.44
1:D:744:TRP:CD1	1:D:747:LEU:HD23	2.53	0.44
1:A:169:LEU:HG	1:A:171:ILE:HG12	1.99	0.44
1:A:1067:ARG:O	1:A:1071:ILE:HG12	2.17	0.44
1:B:1025:THR:OG1	1:C:973:HIS:O	2.30	0.44
1:D:864:PHE:HA	1:D:869:ASN:HB2	1.99	0.44
1:A:766:LEU:HD11	1:A:773:PHE:CZ	2.53	0.44
1:A:795:PRO:O	1:A:798:VAL:HG22	2.18	0.44
1:B:609:LYS:O	1:B:610:ARG:HG2	2.17	0.44
1:B:1106:HIS:CE1	1:B:1108:GLN:HG2	2.53	0.44
1:B:1370:LYS:HE3	1:B:1372:LEU:HA	1.99	0.44
1:C:452:TRP:CD1	1:C:452:TRP:C	2.93	0.44
1:C:466:ASP:OD1	1:C:466:ASP:N	2.50	0.44
1:C:623:ARG:HG3	1:C:624:ASP:N	2.31	0.44
1:D:151:SER:HA	1:D:154:ILE:HD12	1.99	0.44
1:D:795:PRO:O	1:D:798:VAL:HG22	2.18	0.44
1:A:1024:LEU:CB	1:B:971:VAL:O	2.62	0.44
1:B:336:THR:OG1	2:B:1601:APR:O2B	2.33	0.44
1:D:246:THR:HA	1:D:274:LEU:HD23	1.99	0.44
1:D:1067:ARG:O	1:D:1071:ILE:HG12	2.17	0.44
1:B:463:ASN:HA	1:B:499:PHE:HE2	1.83	0.44
1:B:744:TRP:CD1	1:B:747:LEU:HD23	2.53	0.44
1:C:238:THR:N	1:C:282:SER:OG	2.49	0.44
1:C:730:VAL:O	1:C:1064:LYS:NZ	2.51	0.44
1:C:1022:GLU:O	1:C:1023:TRP:CD1	2.66	0.44
1:D:1370:LYS:HE3	1:D:1372:LEU:HA	1.99	0.44
1:A:534:SER:O	1:A:538:LYS:HG2	2.17	0.44
1:A:1035:PHE:HE1	1:B:938:LEU:CD2	2.31	0.44
1:B:766:LEU:HD11	1:B:773:PHE:CZ	2.53	0.44
1:B:850:ASP:O	1:B:859:LYS:NZ	2.51	0.44
1:C:562:ALA:O	1:C:566:ARG:HG2	2.18	0.44
1:C:971:VAL:HG12	1:C:972:TYR:HA	2.00	0.44
1:D:562:ALA:O	1:D:566:ARG:HG2	2.18	0.44
1:A:536:LEU:HA	1:A:539:VAL:HG22	2.00	0.44
1:A:562:ALA:O	1:A:566:ARG:HG2	2.17	0.44
1:A:755:ARG:HD3	1:A:771:ILE:HD11	1.99	0.44
1:A:850:ASP:O	1:A:859:LYS:NZ	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1067:ARG:O	1:B:1071:ILE:HG12	2.17	0.44
1:D:766:LEU:HD11	1:D:773:PHE:CZ	2.53	0.44
1:D:971:VAL:HG12	1:D:972:TYR:HA	2.00	0.44
1:A:532:PHE:O	1:A:536:LEU:HD23	2.18	0.43
1:A:1106:HIS:CE1	1:A:1108:GLN:HG2	2.53	0.43
1:B:725:LYS:HG2	1:B:727:MET:HE3	2.00	0.43
1:B:795:PRO:O	1:B:798:VAL:HG22	2.18	0.43
1:B:958:HIS:ND1	1:C:818:MET:SD	2.91	0.43
1:C:169:LEU:HG	1:C:171:ILE:HG12	1.99	0.43
1:C:850:ASP:O	1:C:859:LYS:NZ	2.51	0.43
1:C:1022:GLU:CA	1:D:974:SER:H	2.31	0.43
1:C:1330:ARG:NE	1:C:1436:ASP:OD2	2.40	0.43
1:D:536:LEU:HA	1:D:539:VAL:HG22	2.00	0.43
1:D:850:ASP:O	1:D:859:LYS:NZ	2.51	0.43
1:A:463:ASN:HA	1:A:499:PHE:HE2	1.83	0.43
1:A:932:LYS:HA	1:A:932:LYS:HD2	1.86	0.43
1:B:89:CYS:O	1:B:90:GLN:HB2	2.18	0.43
1:C:463:ASN:HA	1:C:499:PHE:HE2	1.83	0.43
1:D:63:ILE:C	1:D:65:GLU:H	2.26	0.43
1:D:609:LYS:O	1:D:610:ARG:HG2	2.17	0.43
1:D:1308:ARG:HB3	1:D:1310:ARG:HH11	1.81	0.43
1:A:157:LEU:O	1:A:161:HIS:HB2	2.18	0.43
1:A:609:LYS:O	1:A:610:ARG:HG2	2.17	0.43
1:A:1151:ILE:HG22	1:B:1151:ILE:HD12	2.00	0.43
1:B:63:ILE:C	1:B:65:GLU:H	2.26	0.43
1:B:151:SER:HA	1:B:154:ILE:HD12	1.99	0.43
1:B:485:HIS:HD2	1:B:513:PHE:CD1	2.37	0.43
1:B:953:GLN:NE2	1:B:968:ARG:HH12	2.16	0.43
1:B:1031:LEU:HD21	1:C:945:VAL:HG21	2.00	0.43
1:C:151:SER:HA	1:C:154:ILE:HD12	1.99	0.43
1:C:246:THR:HA	1:C:274:LEU:HD23	1.99	0.43
1:C:725:LYS:HG2	1:C:727:MET:HE3	2.00	0.43
1:C:766:LEU:HD11	1:C:773:PHE:CZ	2.53	0.43
1:C:795:PRO:O	1:C:798:VAL:HG22	2.18	0.43
1:C:935:PHE:HA	1:C:938:LEU:HD12	2.00	0.43
1:D:157:LEU:O	1:D:161:HIS:HB2	2.18	0.43
1:A:238:THR:N	1:A:282:SER:OG	2.49	0.43
1:A:725:LYS:NZ	1:A:727:MET:HE3	2.34	0.43
1:B:628:TRP:O	1:B:632:GLN:HG3	2.19	0.43
1:B:731:SER:HA	1:B:736:GLN:NE2	2.31	0.43
1:C:511:LYS:HA	1:C:621:PRO:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:466:ASP:N	1:D:466:ASP:OD1	2.50	0.43
1:A:63:ILE:C	1:A:65:GLU:H	2.26	0.43
1:A:89:CYS:O	1:A:90:GLN:HB2	2.18	0.43
1:A:120:GLN:NE2	1:A:122:MET:SD	2.92	0.43
1:A:628:TRP:O	1:A:632:GLN:HG3	2.19	0.43
1:A:1056:GLN:HB2	1:D:1050:TYR:HB3	1.99	0.43
1:B:408:ASP:OD1	1:B:411:ARG:NH1	2.51	0.43
1:C:157:LEU:O	1:C:161:HIS:HB2	2.18	0.43
1:C:316:ARG:HB3	1:C:321:ILE:HG13	2.01	0.43
1:D:89:CYS:O	1:D:90:GLN:HB2	2.18	0.43
1:D:316:ARG:HB3	1:D:321:ILE:HG13	2.01	0.43
1:A:441:SER:HA	1:A:447:PHE:CD2	2.54	0.43
1:B:1023:TRP:H	1:C:971:VAL:C	2.26	0.43
1:C:532:PHE:O	1:C:536:LEU:HD23	2.18	0.43
1:C:731:SER:HA	1:C:736:GLN:NE2	2.31	0.43
1:C:953:GLN:NE2	1:C:968:ARG:HH12	2.16	0.43
1:D:120:GLN:NE2	1:D:122:MET:SD	2.92	0.43
1:A:151:SER:HA	1:A:154:ILE:HD12	1.99	0.43
1:A:336:THR:OG1	2:A:1601:APR:O2B	2.33	0.43
1:A:485:HIS:HD2	1:A:513:PHE:CD1	2.36	0.43
1:B:120:GLN:NE2	1:B:122:MET:SD	2.92	0.43
1:B:532:PHE:O	1:B:536:LEU:HD23	2.18	0.43
1:B:1347:THR:HB	1:B:1349:TYR:HE1	1.83	0.43
1:C:530:CYS:SG	1:C:531:LEU:N	2.92	0.43
1:C:725:LYS:NZ	1:C:727:MET:HE3	2.33	0.43
1:D:725:LYS:HG2	1:D:727:MET:HE3	2.00	0.43
1:A:376:ILE:O	1:A:379:ILE:HB	2.19	0.43
1:A:953:GLN:NE2	1:A:968:ARG:HH12	2.16	0.43
1:B:157:LEU:O	1:B:161:HIS:HB2	2.18	0.43
1:C:63:ILE:C	1:C:65:GLU:H	2.26	0.43
1:C:657:LYS:HG2	1:C:661:GLU:OE2	2.19	0.43
1:D:441:SER:HA	1:D:447:PHE:CD2	2.54	0.43
1:D:530:CYS:SG	1:D:531:LEU:N	2.92	0.43
1:D:1141:LYS:HB3	1:D:1141:LYS:HE3	1.70	0.43
1:A:1024:LEU:N	1:B:972:TYR:O	2.48	0.43
1:C:120:GLN:NE2	1:C:122:MET:SD	2.92	0.43
1:C:932:LYS:HA	1:C:932:LYS:HD2	1.86	0.43
1:C:1106:HIS:CE1	1:C:1108:GLN:HG2	2.53	0.43
1:D:463:ASN:HA	1:D:499:PHE:HE2	1.83	0.43
1:D:657:LYS:HG2	1:D:661:GLU:OE2	2.19	0.43
1:D:730:VAL:O	1:D:1064:LYS:NZ	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:953:GLN:NE2	1:D:968:ARG:HH12	2.16	0.43
1:D:1106:HIS:CE1	1:D:1108:GLN:HG2	2.53	0.43
1:A:857:MET:SD	1:A:858:LYS:NZ	2.86	0.43
1:C:1384:HIS:HE1	1:C:1386:ALA:HB2	1.84	0.43
1:D:408:ASP:OD1	1:D:411:ARG:NH1	2.51	0.43
1:D:725:LYS:NZ	1:D:727:MET:HE3	2.34	0.43
1:D:854:CYS:SG	1:D:855:GLY:N	2.92	0.43
1:D:1347:THR:HB	1:D:1349:TYR:HE1	1.83	0.43
1:A:725:LYS:HG2	1:A:727:MET:HE3	2.00	0.42
1:A:1347:THR:HB	1:A:1349:TYR:HE1	1.83	0.42
1:B:99:LEU:HB3	1:B:100:GLU:H	1.66	0.42
1:B:501:LYS:O	1:B:504:LEU:HG	2.19	0.42
1:B:1063:TRP:CE2	1:B:1067:ARG:HD2	2.54	0.42
1:B:1356:ARG:HH12	1:B:1358:ASN:HD22	1.67	0.42
1:C:63:ILE:C	1:C:65:GLU:N	2.77	0.42
1:C:89:CYS:O	1:C:90:GLN:HB2	2.18	0.42
1:C:1347:THR:HB	1:C:1349:TYR:HE1	1.83	0.42
1:A:99:LEU:HB3	1:A:100:GLU:H	1.66	0.42
1:B:90:GLN:HG2	1:B:113:TRP:CG	2.54	0.42
1:B:982:ILE:CG2	1:C:981:GLN:HG2	2.50	0.42
1:C:501:LYS:O	1:C:504:LEU:HG	2.19	0.42
1:C:959:ASN:HB2	1:C:964:ASP:HB2	2.01	0.42
1:C:1259:ASN:HA	1:C:1262:VAL:HG13	2.01	0.42
1:D:511:LYS:HA	1:D:621:PRO:HG2	2.00	0.42
1:D:532:PHE:O	1:D:536:LEU:HD23	2.18	0.42
1:D:533:HIS:CD2	1:D:537:GLN:HE22	2.38	0.42
1:D:935:PHE:HA	1:D:938:LEU:HD12	2.00	0.42
1:A:63:ILE:C	1:A:65:GLU:N	2.77	0.42
1:A:730:VAL:O	1:A:1064:LYS:NZ	2.51	0.42
1:B:725:LYS:NZ	1:B:727:MET:HE3	2.33	0.42
1:D:63:ILE:C	1:D:65:GLU:N	2.77	0.42
1:D:485:HIS:HD2	1:D:513:PHE:CD1	2.36	0.42
1:D:959:ASN:HB2	1:D:964:ASP:HB2	2.01	0.42
1:D:1063:TRP:CE2	1:D:1067:ARG:HD2	2.55	0.42
1:D:1398:LEU:HD12	1:D:1402:LEU:HB3	2.01	0.42
1:A:530:CYS:SG	1:A:531:LEU:N	2.92	0.42
1:A:959:ASN:HB2	1:A:964:ASP:HB2	2.01	0.42
1:A:1022:GLU:O	1:A:1023:TRP:CD1	2.66	0.42
1:A:1154:LYS:HE2	1:D:1159:VAL:HG21	2.02	0.42
1:B:63:ILE:C	1:B:65:GLU:N	2.77	0.42
1:B:316:ARG:HB3	1:B:321:ILE:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1022:GLU:HA	1:C:972:TYR:N	2.34	0.42
1:B:1259:ASN:HA	1:B:1262:VAL:HG13	2.02	0.42
1:C:376:ILE:O	1:C:379:ILE:HB	2.19	0.42
1:C:408:ASP:OD1	1:C:411:ARG:NH1	2.51	0.42
1:C:628:TRP:O	1:C:632:GLN:HG3	2.19	0.42
1:D:1356:ARG:HH12	1:D:1358:ASN:HD22	1.67	0.42
1:D:1373:GLU:CD	1:D:1373:GLU:H	2.28	0.42
1:A:169:LEU:HB3	1:A:203:ALA:HA	2.02	0.42
1:A:657:LYS:HG2	1:A:661:GLU:OE2	2.19	0.42
1:A:935:PHE:HA	1:A:938:LEU:HD12	2.00	0.42
1:A:971:VAL:HG12	1:A:972:TYR:HA	2.00	0.42
1:A:1063:TRP:CE2	1:A:1067:ARG:HD2	2.55	0.42
1:A:1356:ARG:HH12	1:A:1358:ASN:HD22	1.67	0.42
1:B:376:ILE:O	1:B:379:ILE:HB	2.19	0.42
1:B:530:CYS:SG	1:B:531:LEU:N	2.92	0.42
1:B:959:ASN:HB2	1:B:964:ASP:HB2	2.01	0.42
1:B:971:VAL:HG12	1:B:972:TYR:HA	2.00	0.42
1:B:1022:GLU:O	1:B:1023:TRP:CD1	2.66	0.42
1:B:1024:LEU:O	1:B:1028:LEU:HD23	2.20	0.42
1:C:90:GLN:HG2	1:C:113:TRP:CG	2.54	0.42
1:C:536:LEU:HA	1:C:539:VAL:HG22	2.00	0.42
1:D:63:ILE:HG22	1:D:64:PRO:HD3	2.02	0.42
1:D:126:ALA:HB3	1:D:144:ARG:HB2	2.02	0.42
1:D:1384:HIS:HE1	1:D:1386:ALA:HB2	1.84	0.42
1:A:316:ARG:HB3	1:A:321:ILE:HG13	2.00	0.42
1:A:854:CYS:SG	1:A:855:GLY:N	2.93	0.42
1:A:972:TYR:HB3	1:D:1021:PRO:HB3	2.01	0.42
1:B:536:LEU:HA	1:B:539:VAL:HG22	2.00	0.42
1:C:63:ILE:HG22	1:C:64:PRO:HD3	2.02	0.42
1:C:1373:GLU:H	1:C:1373:GLU:CD	2.28	0.42
1:D:99:LEU:HB3	1:D:100:GLU:H	1.66	0.42
1:D:501:LYS:O	1:D:504:LEU:HG	2.19	0.42
1:A:637:LEU:O	1:A:641:ILE:HG13	2.20	0.42
1:A:642:TRP:HA	1:A:645:SER:HG	1.84	0.42
1:A:648:CYS:SG	1:A:1129:LYS:HD3	2.59	0.42
1:A:973:HIS:N	1:D:1022:GLU:HA	2.28	0.42
1:A:1373:GLU:CD	1:A:1373:GLU:H	2.28	0.42
1:B:657:LYS:HG2	1:B:661:GLU:OE2	2.19	0.42
1:B:1373:GLU:CD	1:B:1373:GLU:H	2.28	0.42
1:C:465:VAL:HG11	1:C:498:GLU:HB3	2.02	0.42
1:C:533:HIS:CD2	1:C:537:GLN:HE22	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1158:MET:SD	1:C:1162:LEU:HD21	2.60	0.42
1:D:143:VAL:HB	1:D:162:TRP:HZ2	1.85	0.42
1:D:485:HIS:HA	1:D:488:MET:HG2	2.01	0.42
1:A:408:ASP:OD1	1:A:411:ARG:NH1	2.51	0.42
1:A:1024:LEU:O	1:A:1028:LEU:HD23	2.20	0.42
1:B:271:GLN:HB2	1:B:274:LEU:O	2.20	0.42
1:B:730:VAL:O	1:B:1064:LYS:NZ	2.51	0.42
1:C:854:CYS:SG	1:C:855:GLY:N	2.92	0.42
1:C:1024:LEU:O	1:C:1028:LEU:HD23	2.20	0.42
1:C:1356:ARG:HH12	1:C:1358:ASN:HD22	1.67	0.42
1:D:642:TRP:HA	1:D:645:SER:HG	1.85	0.42
1:D:1259:ASN:HA	1:D:1262:VAL:HG13	2.02	0.42
1:A:533:HIS:CD2	1:A:537:GLN:HE22	2.38	0.42
1:A:1259:ASN:HA	1:A:1262:VAL:HG13	2.02	0.42
1:B:485:HIS:HA	1:B:488:MET:HG2	2.01	0.42
1:B:533:HIS:CD2	1:B:537:GLN:HE22	2.38	0.42
1:B:854:CYS:SG	1:B:855:GLY:N	2.92	0.42
1:C:126:ALA:HB3	1:C:144:ARG:HB2	2.02	0.42
1:C:284:PHE:HZ	1:C:286:LEU:HD13	1.85	0.42
1:C:637:LEU:O	1:C:641:ILE:HG13	2.20	0.42
1:D:90:GLN:HG2	1:D:113:TRP:CG	2.54	0.42
1:A:973:HIS:O	1:D:1025:THR:OG1	2.35	0.42
1:B:284:PHE:HZ	1:B:286:LEU:HD13	1.85	0.42
1:B:511:LYS:HA	1:B:621:PRO:HG2	2.00	0.42
1:B:935:PHE:HA	1:B:938:LEU:HD12	2.00	0.42
1:B:1021:PRO:CA	1:C:972:TYR:H	2.32	0.42
1:B:1046:ALA:HA	1:C:1048:PHE:CE2	2.55	0.42
1:B:1140:GLN:HA	1:B:1143:ARG:HH12	1.85	0.42
1:C:485:HIS:HA	1:C:488:MET:HG2	2.01	0.42
1:C:976:LEU:HD11	1:C:978:ILE:HB	2.02	0.42
1:D:376:ILE:O	1:D:379:ILE:HB	2.19	0.42
1:D:628:TRP:O	1:D:632:GLN:HG3	2.19	0.42
1:D:1024:LEU:O	1:D:1028:LEU:HD23	2.20	0.42
1:D:1429:MET:HG3	1:D:1430:ASP:N	2.35	0.42
1:A:502:LEU:O	1:A:505:GLU:HG3	2.20	0.41
1:B:930:MET:HB2	1:B:1047:MET:HE1	2.02	0.41
1:B:1347:THR:HB	1:B:1349:TYR:CE1	2.55	0.41
1:C:169:LEU:HB3	1:C:203:ALA:HA	2.02	0.41
1:C:1398:LEU:HD12	1:C:1402:LEU:HB3	2.02	0.41
1:D:657:LYS:O	1:D:661:GLU:HG3	2.20	0.41
1:D:930:MET:HB2	1:D:1047:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1022:GLU:O	1:D:1023:TRP:CD1	2.66	0.41
1:D:1158:MET:SD	1:D:1162:LEU:HD21	2.60	0.41
1:D:1431:ASP:HA	1:D:1432:PRO:HD3	1.94	0.41
1:A:90:GLN:HG2	1:A:113:TRP:CG	2.55	0.41
1:A:465:VAL:HG11	1:A:498:GLU:HB3	2.02	0.41
1:A:920:LEU:HD21	1:D:940:LEU:HD22	2.01	0.41
1:B:243:THR:HG22	1:B:245:GLY:H	1.85	0.41
1:B:558:MET:O	1:B:562:ALA:HB2	2.20	0.41
1:B:731:SER:CA	1:B:736:GLN:HE22	2.31	0.41
1:B:1092:LEU:HD11	1:B:1104:LYS:HD2	2.02	0.41
1:C:143:VAL:HB	1:C:162:TRP:HZ2	1.85	0.41
1:C:558:MET:O	1:C:562:ALA:HB2	2.20	0.41
1:C:1063:TRP:CE2	1:C:1067:ARG:HD2	2.55	0.41
1:D:169:LEU:HB3	1:D:203:ALA:HA	2.02	0.41
1:D:271:GLN:HB2	1:D:274:LEU:O	2.20	0.41
1:D:465:VAL:HG11	1:D:498:GLU:HB3	2.02	0.41
1:D:806:TYR:OH	1:D:909:ARG:HB2	2.20	0.41
1:A:63:ILE:HG22	1:A:64:PRO:HD3	2.02	0.41
1:A:143:VAL:HB	1:A:162:TRP:HZ2	1.85	0.41
1:A:192:ARG:HA	1:A:192:ARG:HD3	1.91	0.41
1:A:411:ARG:CZ	1:A:1240:VAL:HG11	2.51	0.41
1:A:466:ASP:OD1	1:A:466:ASP:N	2.50	0.41
1:A:1092:LEU:HD11	1:A:1104:LYS:HD2	2.02	0.41
1:A:1347:THR:HB	1:A:1349:TYR:CE1	2.55	0.41
1:B:143:VAL:HB	1:B:162:TRP:HZ2	1.85	0.41
1:B:465:VAL:HG11	1:B:498:GLU:HB3	2.02	0.41
1:B:637:LEU:O	1:B:641:ILE:HG13	2.20	0.41
1:B:648:CYS:SG	1:B:1129:LYS:HD3	2.59	0.41
1:C:151:SER:OG	1:C:305:LEU:HD12	2.20	0.41
1:C:441:SER:HA	1:C:447:PHE:CD2	2.54	0.41
1:C:502:LEU:O	1:C:505:GLU:HG3	2.20	0.41
1:C:648:CYS:SG	1:C:1129:LYS:HD3	2.59	0.41
1:C:1023:TRP:HA	1:D:976:LEU:HB2	2.02	0.41
1:C:1347:THR:HB	1:C:1349:TYR:CE1	2.55	0.41
1:A:126:ALA:HB3	1:A:144:ARG:HB2	2.02	0.41
1:A:271:GLN:HB2	1:A:274:LEU:O	2.20	0.41
1:A:501:LYS:O	1:A:504:LEU:HG	2.19	0.41
1:A:511:LYS:HA	1:A:621:PRO:HG2	2.00	0.41
1:A:558:MET:O	1:A:562:ALA:HB2	2.21	0.41
1:A:657:LYS:O	1:A:661:GLU:HG3	2.20	0.41
1:A:726:ASP:HB2	1:A:1065:PHE:HE1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:SER:CA	1:A:736:GLN:HE22	2.31	0.41
1:A:806:TYR:OH	1:A:909:ARG:HB2	2.20	0.41
1:A:1429:MET:HG3	1:A:1430:ASP:N	2.35	0.41
1:B:117:LYS:HE3	1:B:118:HIS:CD2	2.50	0.41
1:B:411:ARG:CZ	1:B:1240:VAL:HG11	2.51	0.41
1:B:466:ASP:OD1	1:B:466:ASP:N	2.50	0.41
1:B:502:LEU:O	1:B:505:GLU:HG3	2.20	0.41
1:B:657:LYS:O	1:B:661:GLU:HG3	2.20	0.41
1:B:806:TYR:OH	1:B:909:ARG:HB2	2.20	0.41
1:C:243:THR:HG22	1:C:245:GLY:H	1.85	0.41
1:D:117:LYS:HE3	1:D:118:HIS:CD2	2.50	0.41
1:D:932:LYS:HA	1:D:932:LYS:HD2	1.86	0.41
1:A:918:LYS:HZ3	1:D:936:PHE:HE2	1.67	0.41
1:A:1140:GLN:HA	1:A:1143:ARG:HH12	1.85	0.41
1:A:1398:LEU:HD12	1:A:1402:LEU:HB3	2.02	0.41
1:B:441:SER:HA	1:B:447:PHE:CD2	2.54	0.41
1:B:893:TYR:HB3	1:B:894:PRO:HD3	2.03	0.41
1:C:1140:GLN:HA	1:C:1143:ARG:HH12	1.85	0.41
1:D:637:LEU:O	1:D:641:ILE:HG13	2.20	0.41
1:D:648:CYS:SG	1:D:1129:LYS:HD3	2.59	0.41
1:A:243:THR:HG22	1:A:245:GLY:H	1.85	0.41
1:A:331:GLU:HB3	1:A:358:ARG:HH21	1.86	0.41
1:A:1384:HIS:HE1	1:A:1386:ALA:HB2	1.84	0.41
1:B:239:ILE:HG13	1:B:283:HIS:HB2	2.02	0.41
1:B:932:LYS:HD2	1:B:932:LYS:HA	1.86	0.41
1:B:1042:ASN:HB3	1:C:1044:LEU:HD21	2.03	0.41
1:B:1264:TRP:CE2	1:B:1325:LEU:HD13	2.56	0.41
1:C:731:SER:CA	1:C:736:GLN:HE22	2.31	0.41
1:D:502:LEU:O	1:D:505:GLU:HG3	2.20	0.41
1:A:485:HIS:HA	1:A:488:MET:HG2	2.01	0.41
1:B:63:ILE:HG22	1:B:64:PRO:HD3	2.02	0.41
1:B:126:ALA:HB3	1:B:144:ARG:HB2	2.02	0.41
1:B:1021:PRO:HA	1:C:972:TYR:H	1.86	0.41
1:C:411:ARG:CZ	1:C:1240:VAL:HG11	2.51	0.41
1:C:1429:MET:HG3	1:C:1430:ASP:N	2.35	0.41
1:D:243:THR:HG22	1:D:245:GLY:H	1.85	0.41
1:D:411:ARG:CZ	1:D:1240:VAL:HG11	2.51	0.41
1:D:1347:THR:HB	1:D:1349:TYR:CE1	2.55	0.41
1:A:299:ILE:HB	1:A:300:PRO:HD3	2.03	0.41
1:C:379:ILE:HD13	1:C:379:ILE:HA	1.93	0.41
1:C:930:MET:HB2	1:C:1047:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1092:LEU:HD11	1:C:1104:LYS:HD2	2.02	0.41
1:D:151:SER:OG	1:D:305:LEU:HD12	2.20	0.41
1:D:299:ILE:HB	1:D:300:PRO:HD3	2.03	0.41
1:D:331:GLU:HB3	1:D:358:ARG:HH21	1.86	0.41
1:D:731:SER:CA	1:D:736:GLN:HE22	2.31	0.41
1:D:1264:TRP:CE2	1:D:1325:LEU:HD13	2.56	0.41
1:A:151:SER:OG	1:A:305:LEU:HD12	2.20	0.41
1:A:875:ALA:HB1	1:A:906:PHE:HE1	1.86	0.41
1:A:927:VAL:HA	1:A:930:MET:CG	2.50	0.41
1:A:1024:LEU:CB	1:B:972:TYR:O	2.64	0.41
1:A:1264:TRP:CE2	1:A:1325:LEU:HD13	2.56	0.41
1:B:151:SER:OG	1:B:305:LEU:HD12	2.20	0.41
1:B:238:THR:N	1:B:282:SER:OG	2.49	0.41
1:B:299:ILE:HB	1:B:300:PRO:HD3	2.03	0.41
1:B:976:LEU:HD11	1:B:978:ILE:HB	2.02	0.41
1:B:1042:ASN:CB	1:C:1044:LEU:HD21	2.51	0.41
1:B:1158:MET:SD	1:B:1162:LEU:HD21	2.60	0.41
1:B:1398:LEU:HD12	1:B:1402:LEU:HB3	2.02	0.41
1:B:1429:MET:HG3	1:B:1430:ASP:N	2.36	0.41
1:C:271:GLN:HB2	1:C:274:LEU:O	2.20	0.41
1:C:632:GLN:HB3	1:C:634:ARG:HH12	1.86	0.41
1:C:657:LYS:O	1:C:661:GLU:HG3	2.20	0.41
1:C:928:LYS:HB2	1:C:928:LYS:HE2	1.95	0.41
1:D:1327:PRO:O	1:D:1328:MET:HB3	2.21	0.41
1:A:214:VAL:HA	1:A:217:GLN:HB2	2.03	0.41
1:A:239:ILE:HG13	1:A:283:HIS:HB2	2.02	0.41
1:A:538:LYS:HA	1:A:538:LYS:HD3	1.82	0.41
1:A:893:TYR:HB3	1:A:894:PRO:HD3	2.03	0.41
1:A:1158:MET:SD	1:A:1162:LEU:HD21	2.60	0.41
1:B:586:LEU:HB3	1:B:587:ARG:HE	1.86	0.41
1:B:690:PHE:HD2	1:B:732:HIS:ND1	2.19	0.41
1:C:1379:LEU:HG	1:C:1380:PRO:HD2	2.03	0.41
1:D:210:SER:C	1:D:278:ASP:HB3	2.46	0.41
1:D:284:PHE:HZ	1:D:286:LEU:HD13	1.85	0.41
1:D:976:LEU:HD11	1:D:978:ILE:HB	2.03	0.41
1:D:1089:HIS:HA	1:D:1093:PHE:CD2	2.56	0.41
1:D:1355:TRP:HE1	1:D:1450:GLN:C	2.30	0.41
1:A:569:LEU:HD13	1:A:572:PHE:CG	2.56	0.40
1:A:930:MET:HB2	1:A:1047:MET:HE1	2.02	0.40
1:A:1113:LEU:HB3	1:A:1118:GLU:HG3	2.03	0.40
1:A:1379:LEU:HG	1:A:1380:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:726:ASP:HB2	1:B:1065:PHE:HE1	1.85	0.40
1:B:875:ALA:HB1	1:B:906:PHE:HE1	1.86	0.40
1:B:1327:PRO:O	1:B:1328:MET:HB3	2.21	0.40
1:C:299:ILE:HB	1:C:300:PRO:HD3	2.03	0.40
1:C:383:LEU:HA	1:C:387:PHE:HD2	1.86	0.40
1:C:806:TYR:OH	1:C:909:ARG:HB2	2.20	0.40
1:C:844:MET:HE1	1:C:848:PHE:CE2	2.56	0.40
1:D:68:LYS:O	1:D:146:SER:HB3	2.21	0.40
1:D:239:ILE:HG13	1:D:283:HIS:HB2	2.02	0.40
1:D:726:ASP:HB2	1:D:1065:PHE:HE1	1.86	0.40
1:D:893:TYR:HB3	1:D:894:PRO:HD3	2.03	0.40
1:D:907:CYS:HA	1:D:910:LEU:HD12	2.03	0.40
1:D:1092:LEU:HD11	1:D:1104:LYS:HD2	2.02	0.40
1:A:210:SER:C	1:A:278:ASP:HB3	2.47	0.40
1:A:456:LEU:O	1:A:460:VAL:HG13	2.22	0.40
1:B:1047:MET:HA	1:B:1050:TYR:CE2	2.56	0.40
1:C:1089:HIS:HA	1:C:1093:PHE:CD2	2.56	0.40
1:D:569:LEU:HD13	1:D:572:PHE:CG	2.56	0.40
1:D:1140:GLN:HA	1:D:1143:ARG:HH12	1.85	0.40
1:A:152:SER:HA	1:A:308:PHE:CE2	2.57	0.40
1:A:476:GLU:O	1:A:476:GLU:HG2	2.21	0.40
1:A:928:LYS:HB2	1:A:928:LYS:HE2	1.95	0.40
1:B:169:LEU:HB3	1:B:203:ALA:HA	2.02	0.40
1:B:569:LEU:HD13	1:B:572:PHE:CG	2.56	0.40
1:B:1421:GLY:HA3	1:B:1445:VAL:HG22	2.04	0.40
1:C:117:LYS:HE3	1:C:118:HIS:CD2	2.50	0.40
1:C:210:SER:C	1:C:278:ASP:HB3	2.47	0.40
1:C:331:GLU:HB3	1:C:358:ARG:HH21	1.86	0.40
1:C:1113:LEU:HB3	1:C:1118:GLU:HG3	2.03	0.40
1:C:1264:TRP:CE2	1:C:1325:LEU:HD13	2.56	0.40
1:C:1327:PRO:O	1:C:1328:MET:HB3	2.21	0.40
1:D:152:SER:HA	1:D:308:PHE:CE2	2.57	0.40
1:D:248:HIS:NE2	1:D:267:ASP:OD2	2.52	0.40
1:D:558:MET:O	1:D:562:ALA:HB2	2.20	0.40
1:D:1064:LYS:HE2	1:D:1064:LYS:HB3	1.93	0.40
1:A:68:LYS:O	1:A:146:SER:HB3	2.21	0.40
1:A:690:PHE:HD2	1:A:732:HIS:ND1	2.19	0.40
1:A:1355:TRP:HE1	1:A:1450:GLN:C	2.30	0.40
1:B:210:SER:C	1:B:278:ASP:HB3	2.47	0.40
1:B:988:GLY:C	1:C:985:TYR:HB2	2.46	0.40
1:C:460:VAL:HG12	1:C:499:PHE:CD1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:476:GLU:O	1:C:476:GLU:HG2	2.22	0.40
1:C:696:LYS:HD2	1:C:696:LYS:HA	1.82	0.40
1:C:875:ALA:HB1	1:C:906:PHE:HE1	1.86	0.40
1:D:690:PHE:HD2	1:D:732:HIS:ND1	2.19	0.40
1:A:976:LEU:HD11	1:A:978:ILE:HB	2.02	0.40
1:A:1043:LEU:HA	1:B:923:LYS:CE	2.52	0.40
1:A:1047:MET:HA	1:A:1050:TYR:CE2	2.56	0.40
1:A:1421:GLY:HA3	1:A:1445:VAL:HG22	2.04	0.40
1:B:68:LYS:O	1:B:146:SER:HB3	2.21	0.40
1:B:844:MET:HE1	1:B:848:PHE:CE2	2.56	0.40
1:C:456:LEU:O	1:C:460:VAL:HG13	2.22	0.40
1:C:1309:ASP:HA	1:C:1311:ARG:NH1	2.36	0.40
1:C:1421:GLY:HA3	1:C:1445:VAL:HG22	2.04	0.40
1:D:383:LEU:HA	1:D:387:PHE:HD2	1.87	0.40
1:D:844:MET:HE1	1:D:848:PHE:CE2	2.56	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	1322/1503 (88%)	1169 (88%)	147 (11%)	6 (0%)	24	63
1	B	1322/1503 (88%)	1170 (88%)	145 (11%)	7 (0%)	24	63
1	C	1322/1503 (88%)	1171 (89%)	144 (11%)	7 (0%)	24	63
1	D	1322/1503 (88%)	1171 (89%)	145 (11%)	6 (0%)	24	63
All	All	5288/6012 (88%)	4681 (88%)	581 (11%)	26 (0%)	26	63

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	PRO
1	A	87	VAL
1	B	64	PRO
1	B	87	VAL
1	C	64	PRO
1	C	87	VAL
1	D	64	PRO
1	D	87	VAL
1	A	90	GLN
1	A	1022	GLU
1	B	90	GLN
1	B	1022	GLU
1	C	90	GLN
1	C	1022	GLU
1	D	90	GLN
1	D	1022	GLU
1	A	1455	VAL
1	B	1455	VAL
1	C	1455	VAL
1	D	1455	VAL
1	A	551	PRO
1	B	551	PRO
1	C	551	PRO
1	D	551	PRO
1	B	969	GLY
1	C	969	GLY

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	1109/1318 (84%)	1081 (98%)	28 (2%)	42	62
1	B	1109/1318 (84%)	1081 (98%)	28 (2%)	42	62
1	C	1109/1318 (84%)	1081 (98%)	28 (2%)	42	62
1	D	1109/1318 (84%)	1081 (98%)	28 (2%)	42	62
All	All	4436/5272 (84%)	4324 (98%)	112 (2%)	42	62

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	GLU
1	A	195	VAL
1	A	348	THR
1	A	404	LYS
1	A	508	VAL
1	A	571	ASP
1	A	635	ARG
1	A	636	GLU
1	A	666	GLU
1	A	667	GLU
1	A	670	ASP
1	A	683	GLU
1	A	699	GLU
1	A	716	THR
1	A	804	LEU
1	A	834	LEU
1	A	844	MET
1	A	857	MET
1	A	908	LEU
1	A	1028	LEU
1	A	1031	LEU
1	A	1042	ASN
1	A	1111	ASN
1	A	1131	ASN
1	A	1141	LYS
1	A	1160	ASP
1	A	1371	MET
1	A	1422	MET
1	B	77	GLU
1	B	195	VAL
1	B	348	THR
1	B	404	LYS
1	B	508	VAL
1	B	571	ASP
1	B	635	ARG
1	B	636	GLU
1	B	666	GLU
1	B	667	GLU
1	B	670	ASP
1	B	683	GLU
1	B	699	GLU
1	B	716	THR

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Mol	Chain	Res	Type
1	B	804	LEU
1	B	834	LEU
1	B	844	MET
1	B	857	MET
1	B	908	LEU
1	B	1028	LEU
1	B	1031	LEU
1	B	1042	ASN
1	B	1111	ASN
1	B	1131	ASN
1	B	1141	LYS
1	B	1160	ASP
1	B	1371	MET
1	B	1422	MET
1	C	77	GLU
1	C	195	VAL
1	C	348	THR
1	C	404	LYS
1	C	508	VAL
1	C	571	ASP
1	C	635	ARG
1	C	636	GLU
1	C	666	GLU
1	C	667	GLU
1	C	670	ASP
1	C	683	GLU
1	C	699	GLU
1	C	716	THR
1	C	804	LEU
1	C	834	LEU
1	C	844	MET
1	C	857	MET
1	C	908	LEU
1	C	1028	LEU
1	C	1031	LEU
1	C	1042	ASN
1	C	1111	ASN
1	C	1131	ASN
1	C	1141	LYS
1	C	1160	ASP
1	C	1371	MET
1	C	1422	MET

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Mol	Chain	Res	Type
1	D	77	GLU
1	D	195	VAL
1	D	348	THR
1	D	404	LYS
1	D	508	VAL
1	D	571	ASP
1	D	635	ARG
1	D	636	GLU
1	D	666	GLU
1	D	667	GLU
1	D	670	ASP
1	D	683	GLU
1	D	699	GLU
1	D	716	THR
1	D	804	LEU
1	D	834	LEU
1	D	844	MET
1	D	857	MET
1	D	908	LEU
1	D	1028	LEU
1	D	1031	LEU
1	D	1042	ASN
1	D	1111	ASN
1	D	1131	ASN
1	D	1141	LYS
1	D	1160	ASP
1	D	1371	MET
1	D	1422	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	118	HIS
1	A	156	HIS
1	A	179	ASN
1	A	211	HIS
1	A	294	GLN
1	A	451	ASN
1	A	454	HIS
1	A	537	GLN
1	A	632	GLN

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Mol	Chain	Res	Type
1	A	684	HIS
1	A	732	HIS
1	A	869	ASN
1	A	981	GLN
1	A	1061	GLN
1	A	1384	HIS
1	A	1437	ASN
1	A	1448	HIS
1	B	66	ASN
1	B	118	HIS
1	B	156	HIS
1	B	179	ASN
1	B	211	HIS
1	B	451	ASN
1	B	454	HIS
1	B	537	GLN
1	B	632	GLN
1	B	684	HIS
1	B	732	HIS
1	B	869	ASN
1	B	1061	GLN
1	B	1384	HIS
1	B	1437	ASN
1	B	1448	HIS
1	C	66	ASN
1	C	118	HIS
1	C	156	HIS
1	C	179	ASN
1	C	451	ASN
1	C	454	HIS
1	C	537	GLN
1	C	632	GLN
1	C	684	HIS
1	C	869	ASN
1	C	1384	HIS
1	C	1437	ASN
1	C	1448	HIS
1	D	66	ASN
1	D	118	HIS
1	D	156	HIS
1	D	179	ASN
1	D	454	HIS

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Mol	Chain	Res	Type
1	D	537	GLN
1	D	632	GLN
1	D	684	HIS
1	D	732	HIS
1	D	869	ASN
1	D	1061	GLN
1	D	1384	HIS
1	D	1437	ASN
1	D	1448	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	$\# Z > 2$
2	APR	D	1601	-	38,38,39	0.48	0	54,58,60	0.68	1 (1%)
3	DAT	D	1602	-	27,28,28	0.59	0	41,43,43	0.66	0
3	DAT	B	1602	-	27,28,28	0.58	0	41,43,43	0.66	0
2	APR	A	1601	-	38,38,39	0.48	0	54,58,60	0.68	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	APR	C	1601	-	38,38,39	0.47	0	54,58,60	0.68	1 (1%)
2	APR	B	1601	-	38,38,39	0.48	0	54,58,60	0.68	1 (1%)
3	DAT	A	1602	-	27,28,28	0.59	0	41,43,43	0.66	0
3	DAT	C	1602	-	27,28,28	0.59	0	41,43,43	0.65	0

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
2	APR	D	1601	-	-	0/22/50/54	0/4/4/4
3	DAT	D	1602	-	-	2/16/28/28	0/3/3/3
3	DAT	B	1602	-	-	2/16/28/28	0/3/3/3
2	APR	A	1601	-	-	0/22/50/54	0/4/4/4
2	APR	C	1601	-	-	0/22/50/54	0/4/4/4
2	APR	B	1601	-	-	0/22/50/54	0/4/4/4
3	DAT	A	1602	-	-	2/16/28/28	0/3/3/3
3	DAT	C	1602	-	-	2/16/28/28	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1601	APR	C1D-C2D-C3D	-3.04	98.54	102.29
2	A	1601	APR	C1D-C2D-C3D	-3.04	98.55	102.29
2	B	1601	APR	C1D-C2D-C3D	-3.02	98.57	102.29
2	C	1601	APR	C1D-C2D-C3D	-3.01	98.59	102.29

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1602	DAT	PB-O3A-PA-O5'
3	B	1602	DAT	PB-O3A-PA-O5'
3	C	1602	DAT	PB-O3A-PA-O5'
3	D	1602	DAT	PB-O3A-PA-O5'
3	A	1602	DAT	C2'-C1'-N9-C4
3	B	1602	DAT	C2'-C1'-N9-C4
3	C	1602	DAT	C2'-C1'-N9-C4

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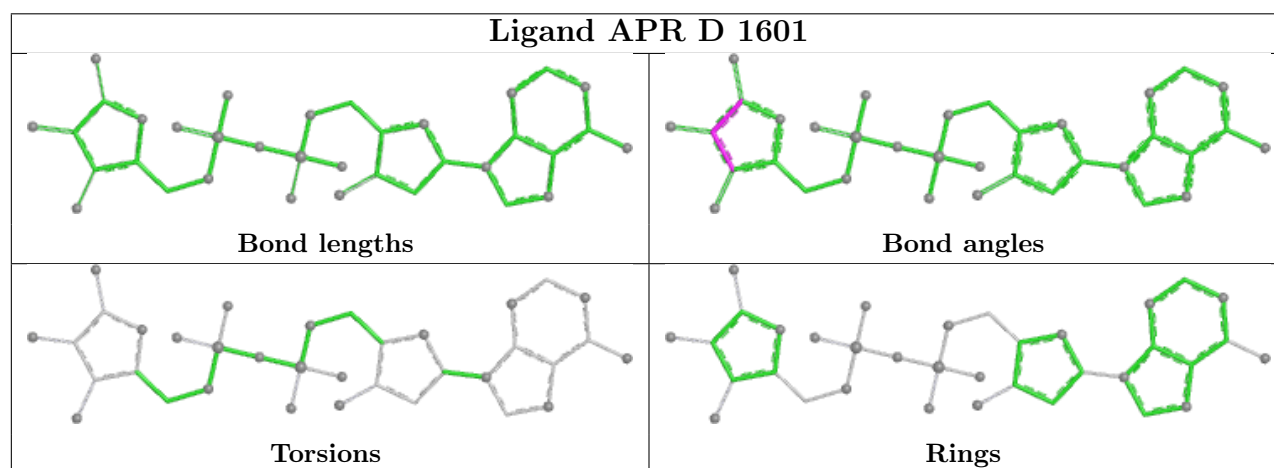
Mol	Chain	Res	Type	Atoms
3	D	1602	DAT	C2'-C1'-N9-C4

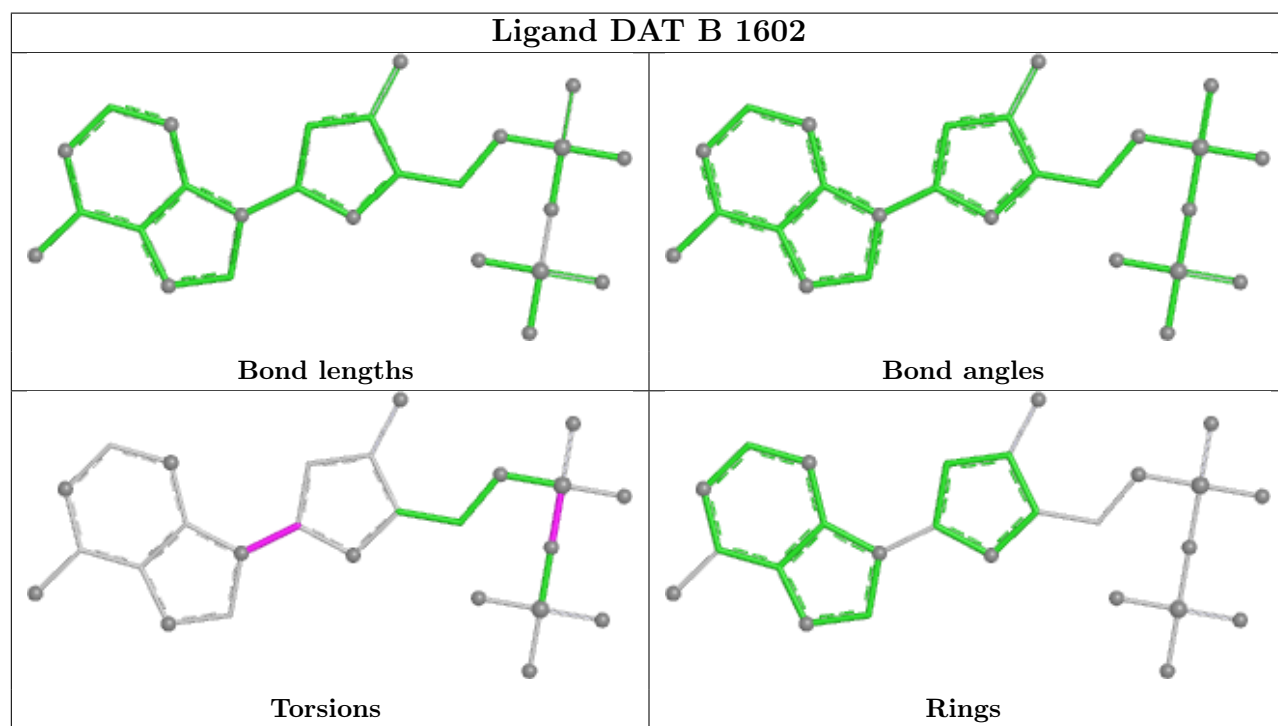
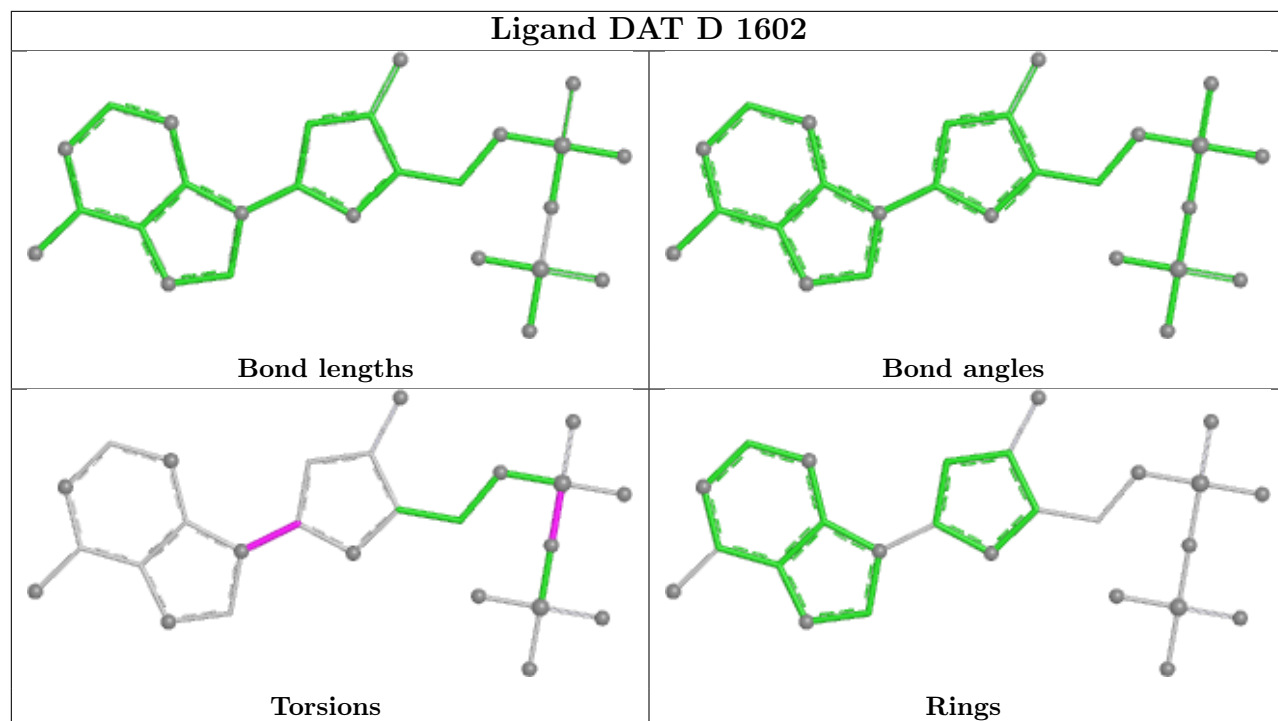
There are no ring outliers.

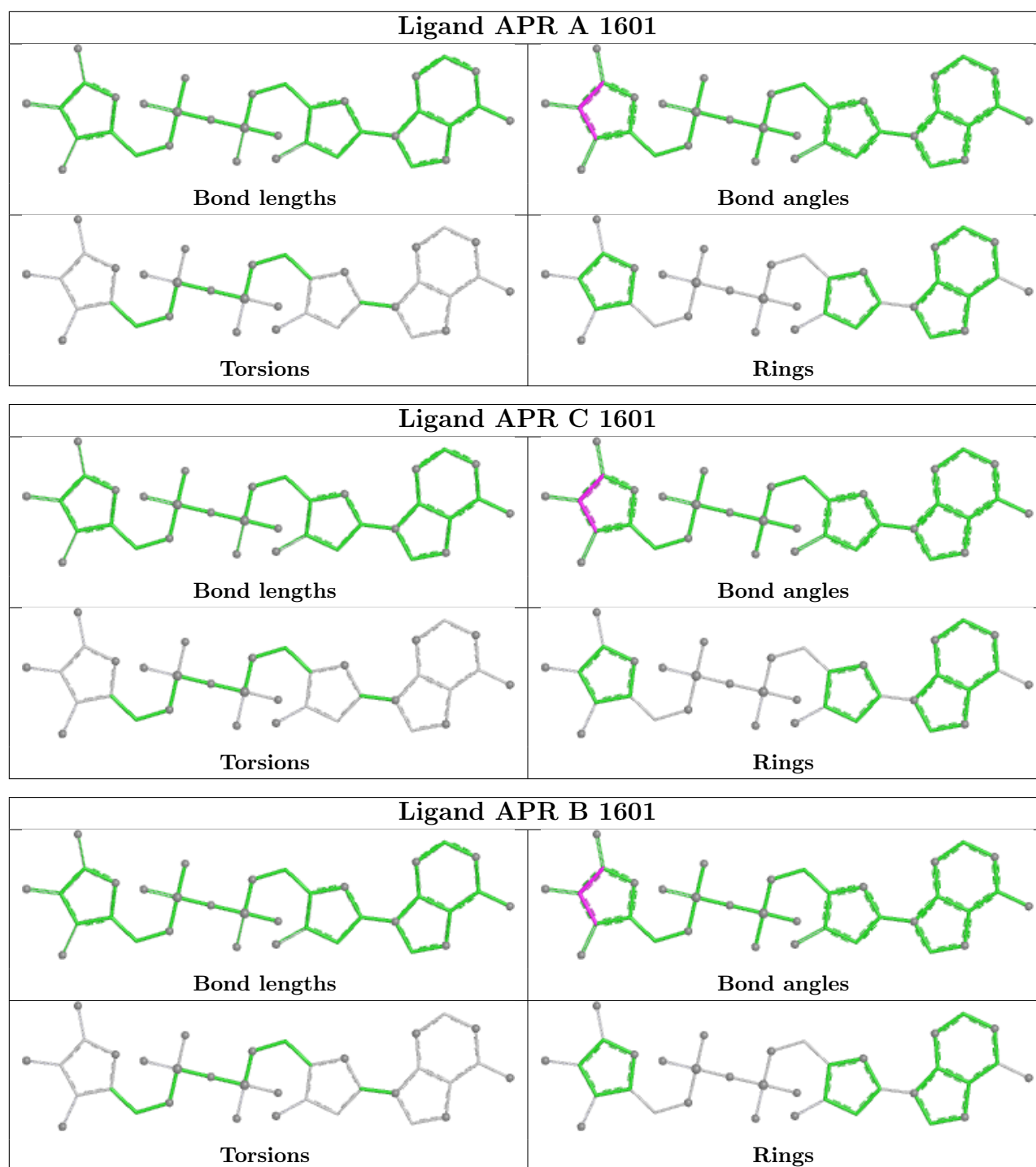
7 monomers are involved in 7 short contacts:

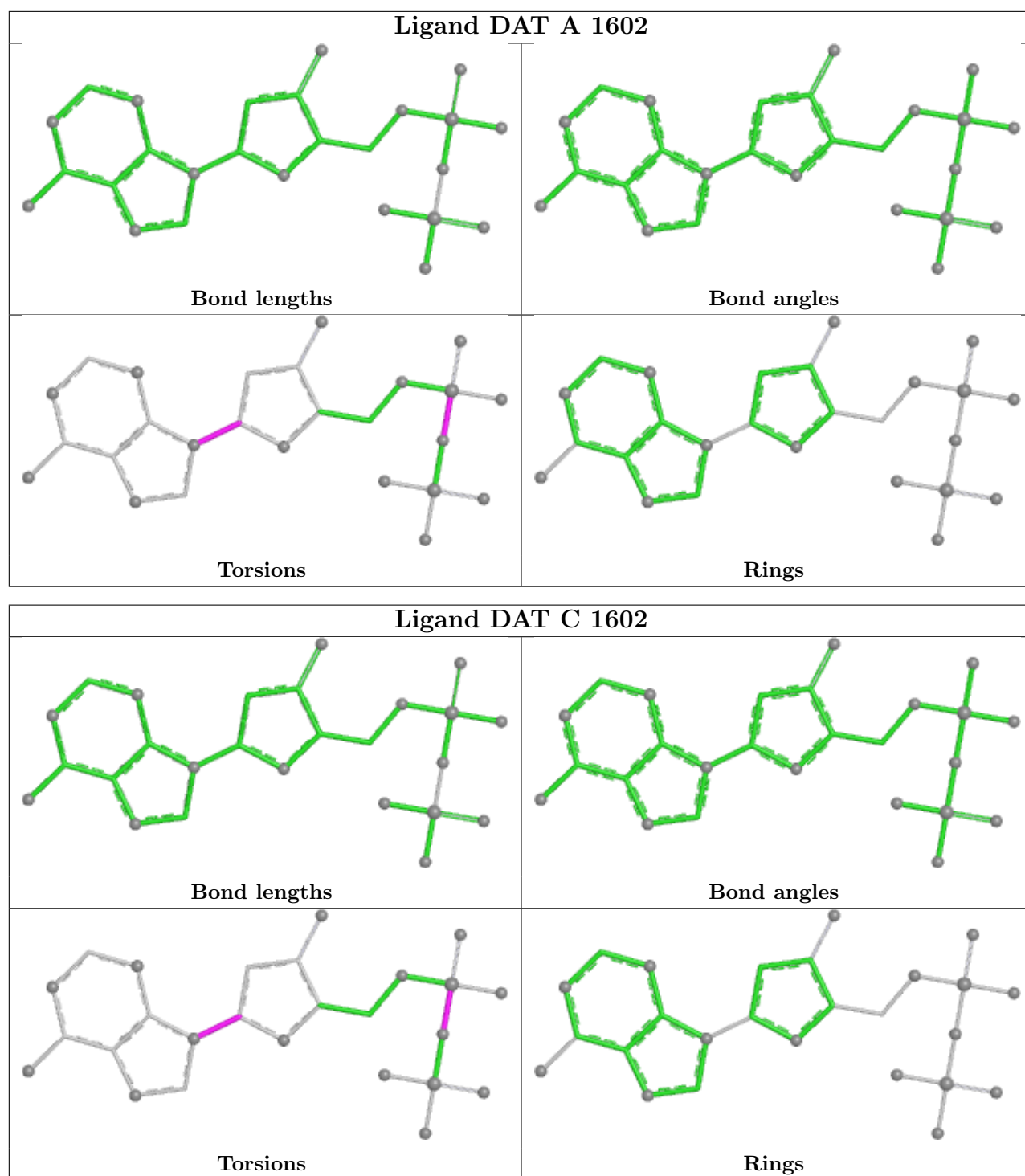
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1602	DAT	1	0
3	B	1602	DAT	1	0
2	A	1601	APR	1	0
2	C	1601	APR	1	0
2	B	1601	APR	1	0
3	A	1602	DAT	1	0
3	C	1602	DAT	1	0

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 ⓘ

There are no chain breaks in this entry.

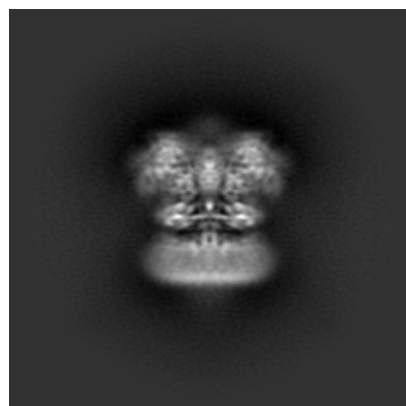
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27924. These allow visual inspection of the internal detail of the map and identification of artifacts.

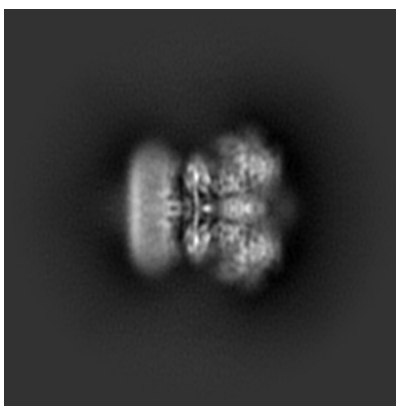
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

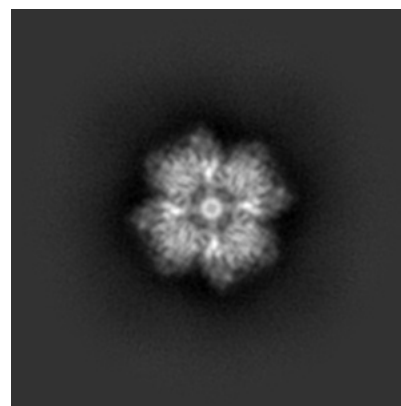
6.1.1 Primary map



X

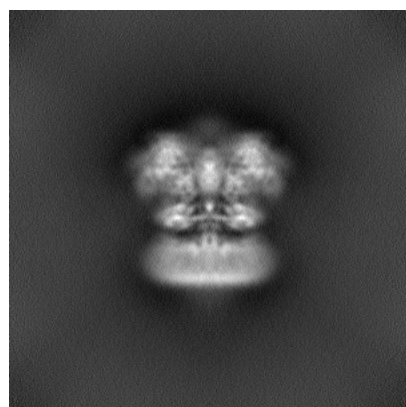


Y

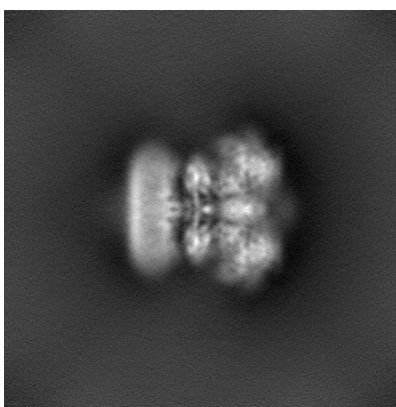


Z

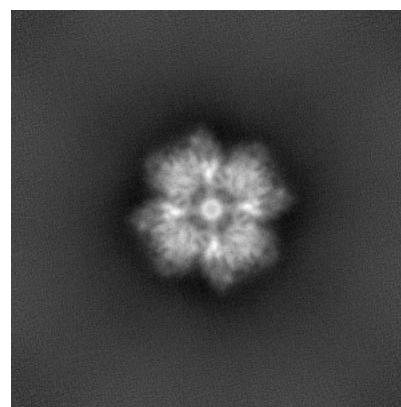
6.1.2 Raw map



X



Y

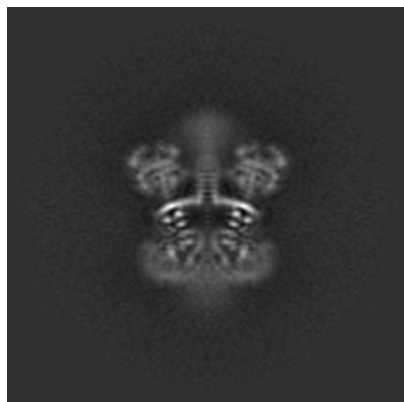


Z

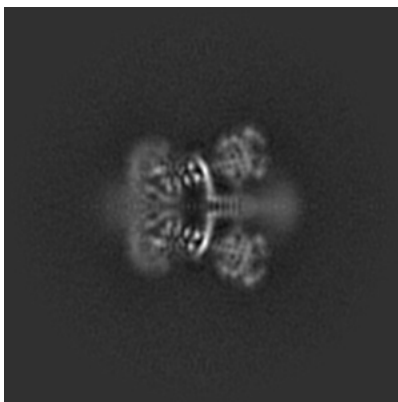
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

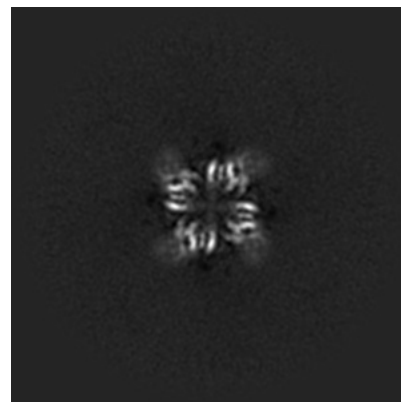
6.2.1 Primary map



X Index: 180

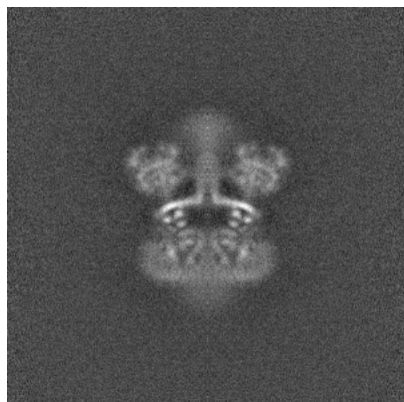


Y Index: 180

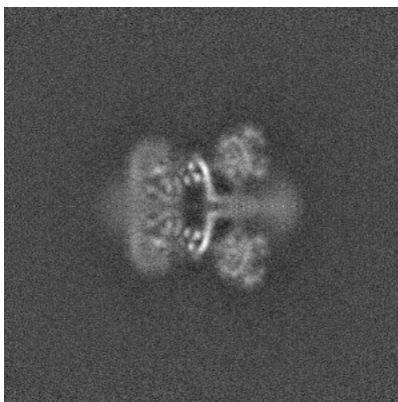


Z Index: 180

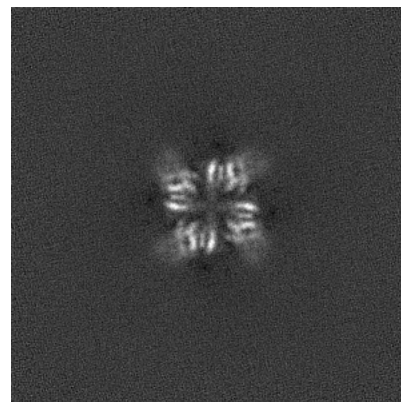
6.2.2 Raw map



X Index: 180



Y Index: 180

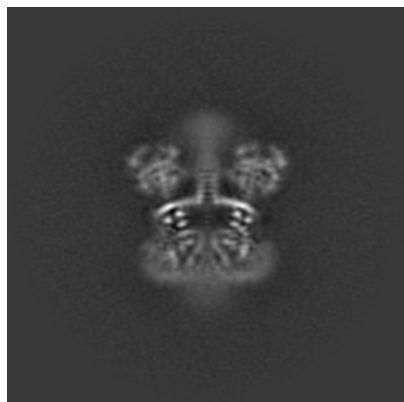


Z Index: 180

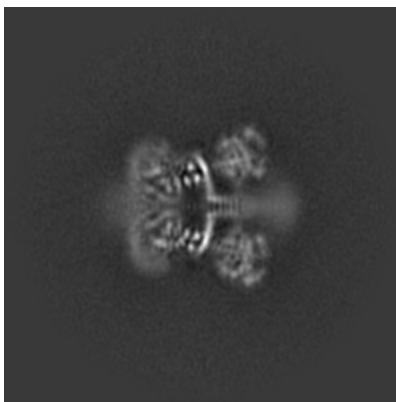
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

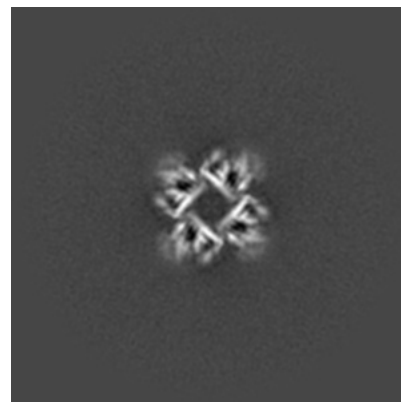
6.3.1 Primary map



X Index: 179

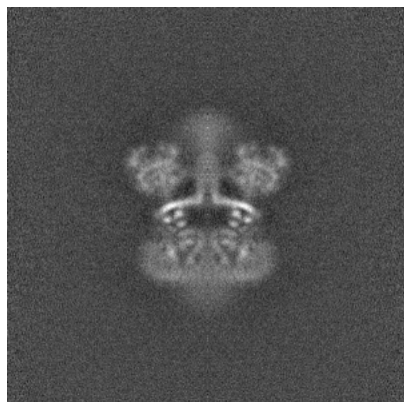


Y Index: 179

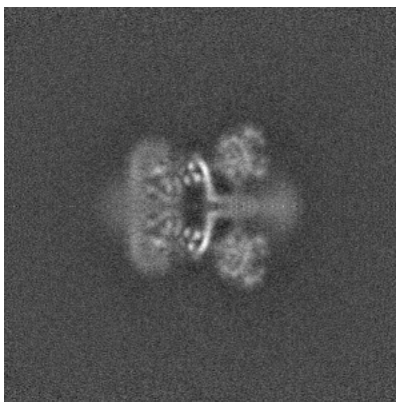


Z Index: 173

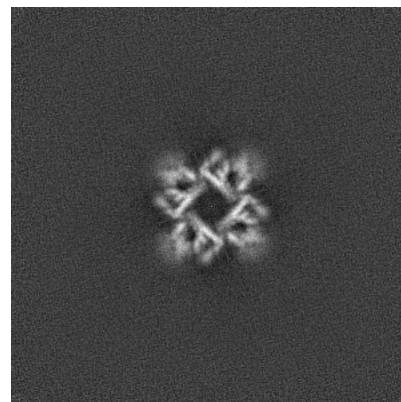
6.3.2 Raw map



X Index: 180



Y Index: 180

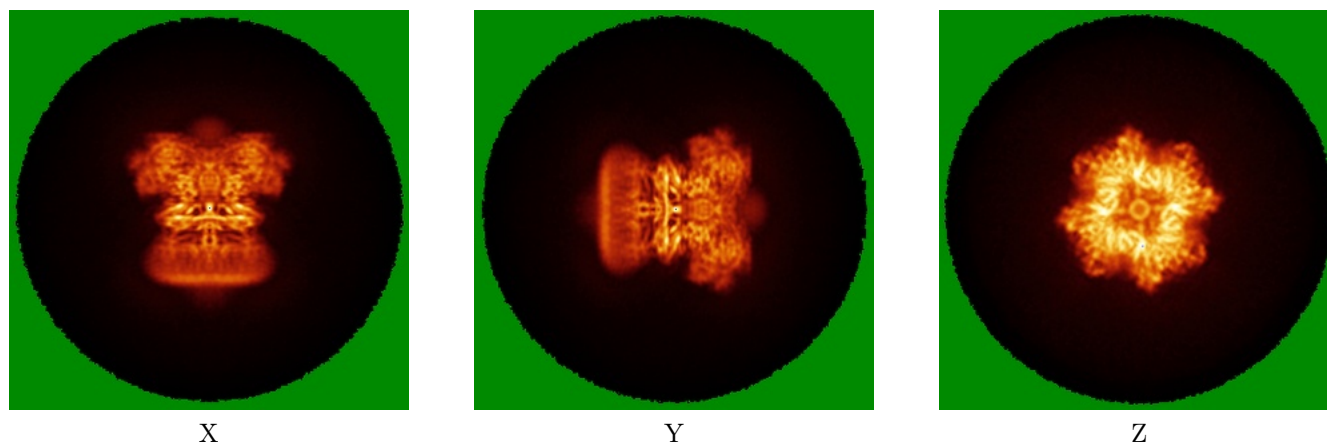


Z Index: 173

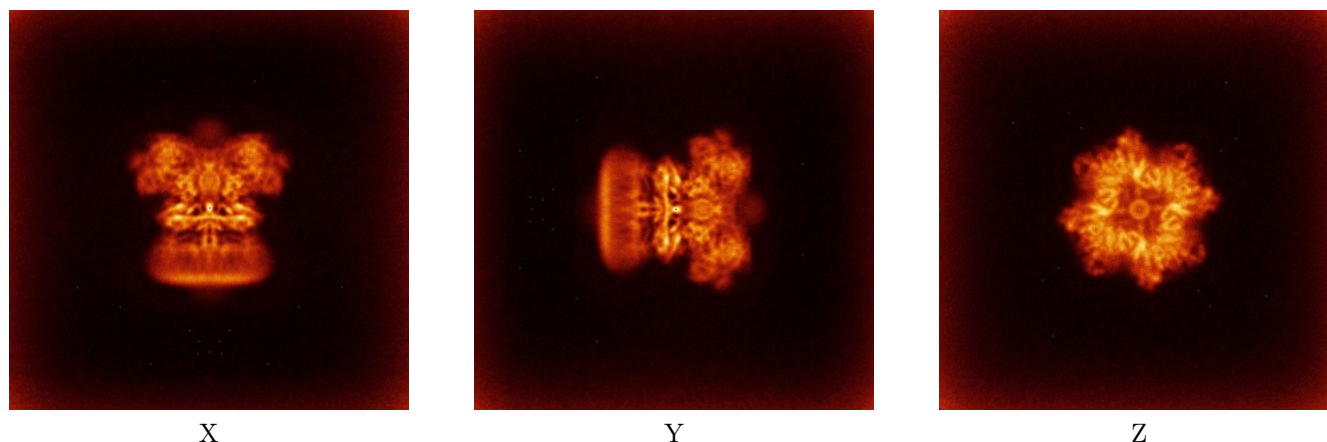
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

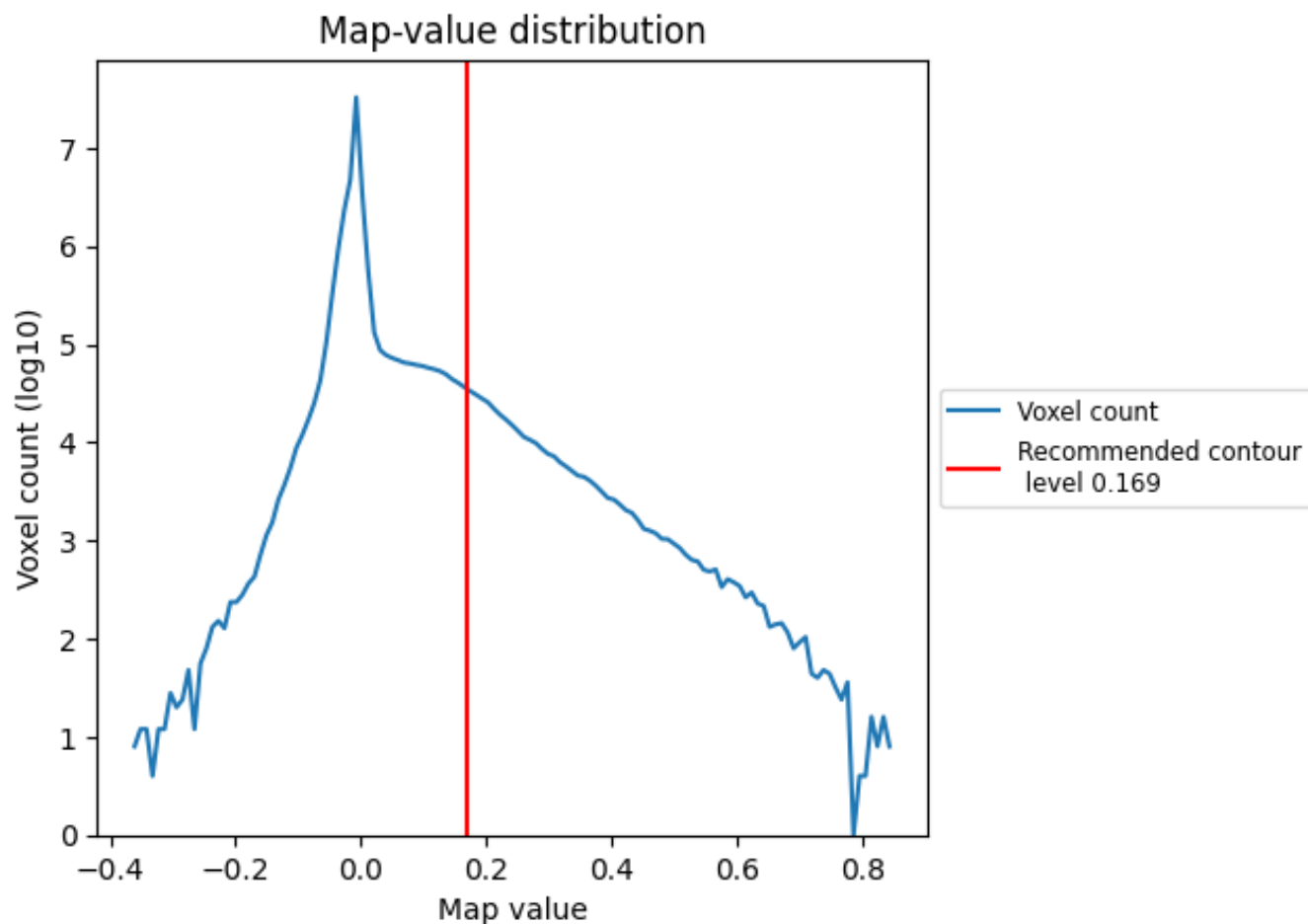
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

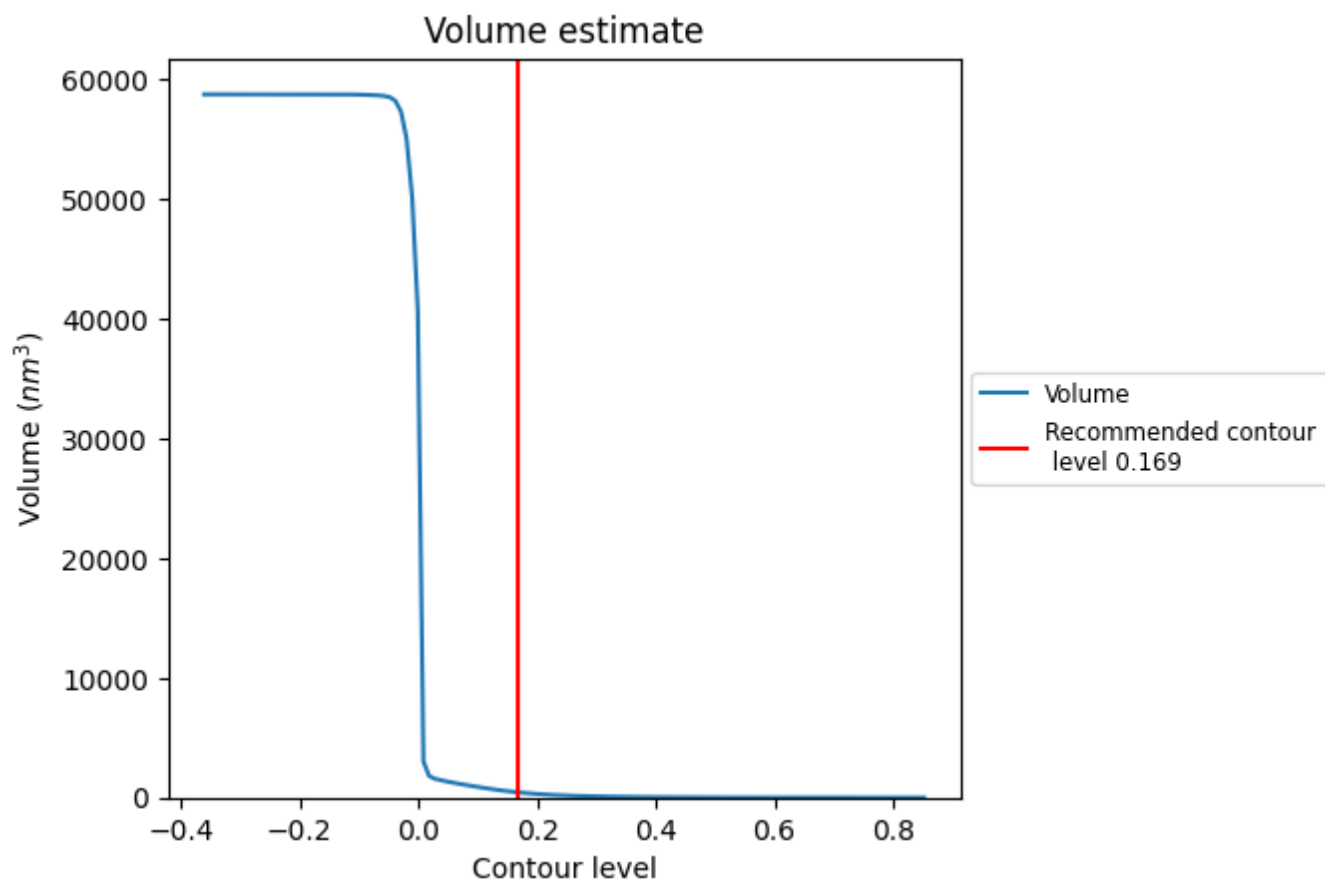
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

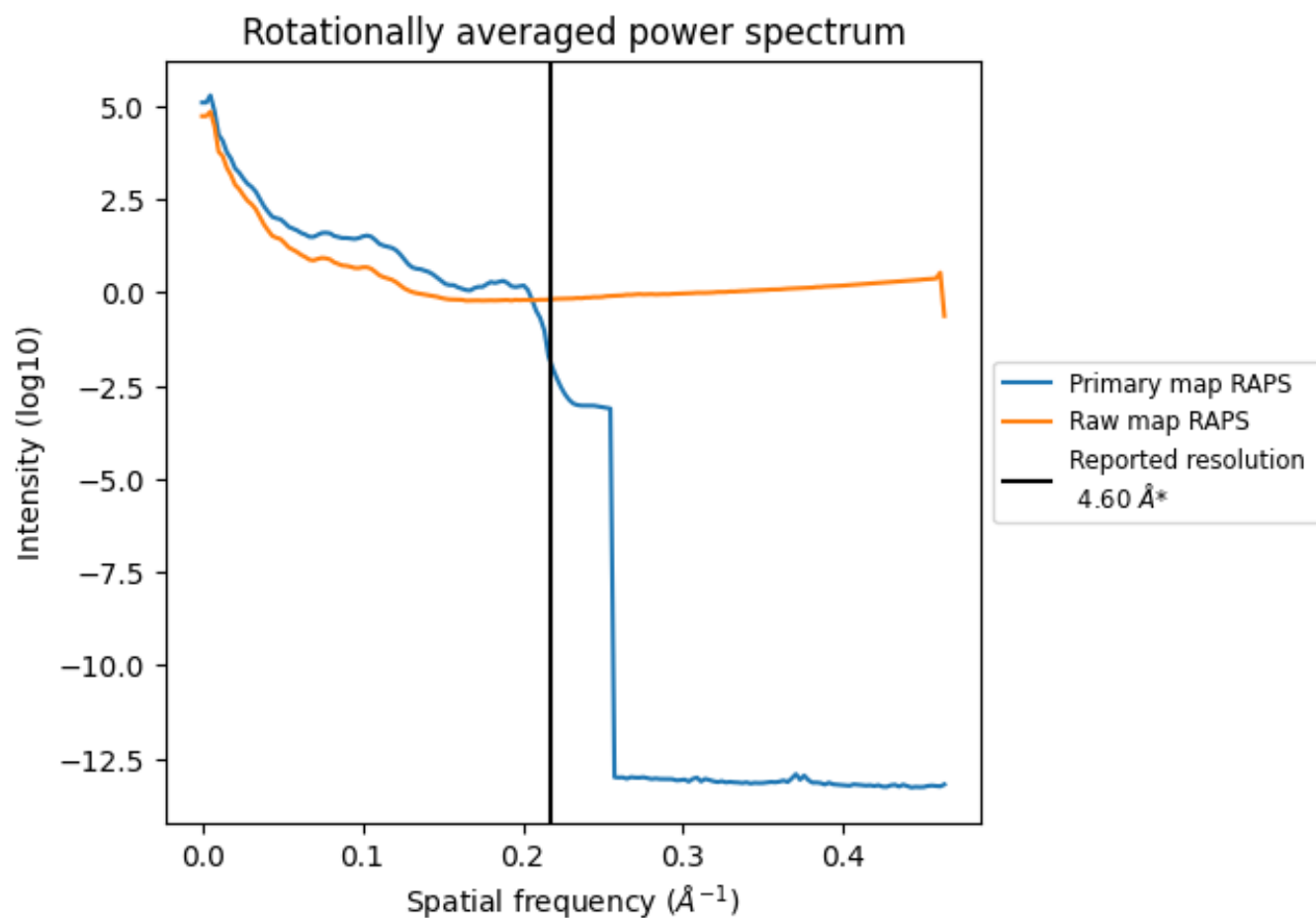
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 431 nm³; this corresponds to an approximate mass of 390 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

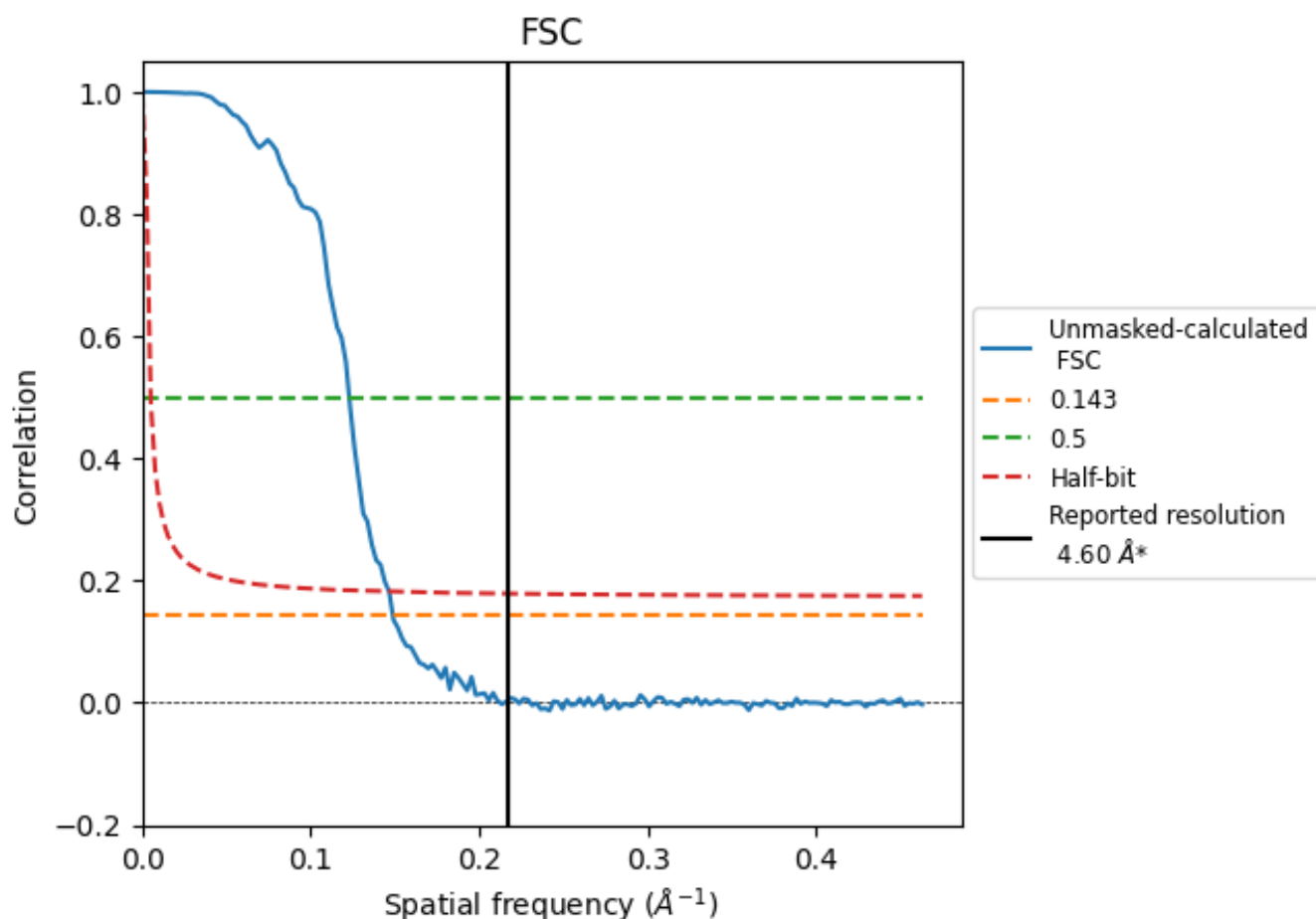


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

8.2 Resolution estimates [i](#)

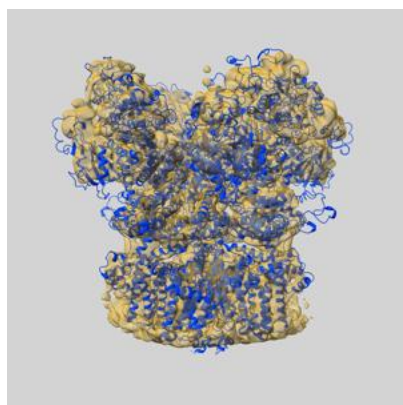
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.72	8.14	6.82

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.72 differs from the reported value 4.6 by more than 10 %

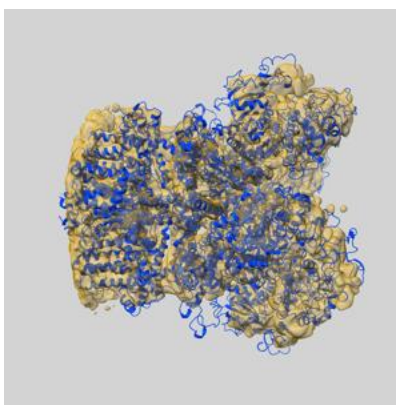
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27924 and PDB model 8E6S. Per-residue inclusion information can be found in section [3](#) on page [6](#).

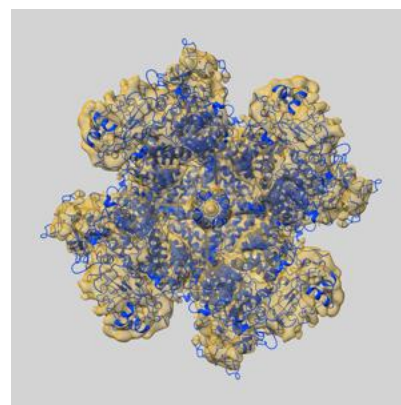
9.1 Map-model overlay [i](#)



X



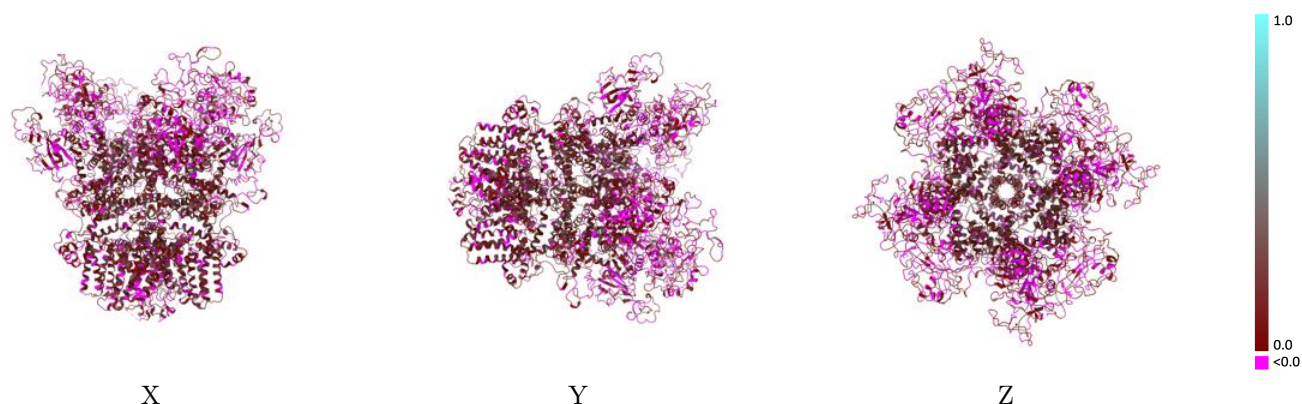
Y



Z

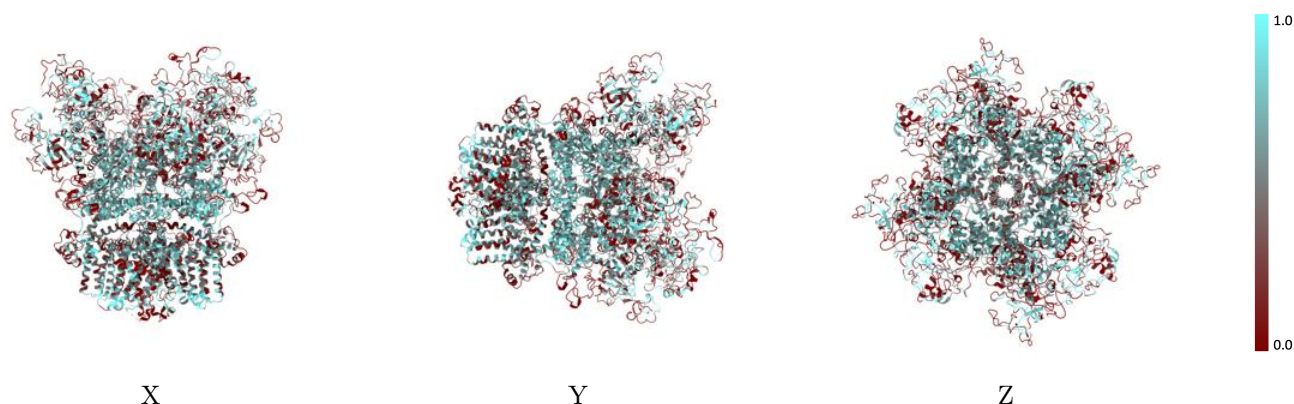
The images above show the 3D surface view of the map at the recommended contour level 0.169 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



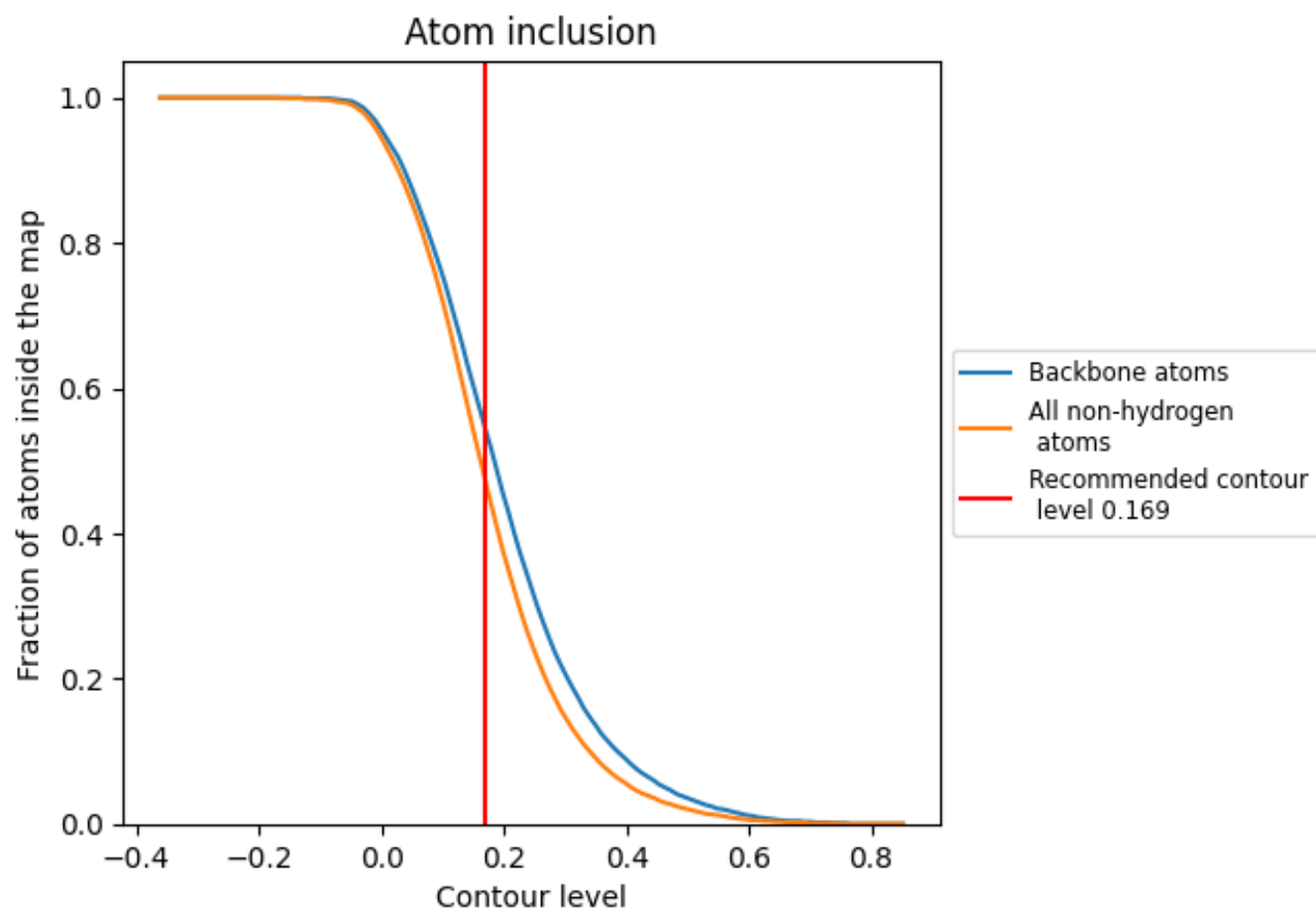
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.169).

9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 48% 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 (0.169) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4750	0.0970
A	0.4750	0.0990
B	0.4760	0.0970
C	0.4710	0.0940
D	0.4760	0.0970

