



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 8, 2017 – 02:05 PM EST

PDB ID : 5MKF
EMDB ID: : EMD-3524
Title : cryoEM Structure of Polycystin-2 in complex with calcium and lipids
Authors : Wilkes, M.; Madej, M.G.; Ziegler, C.
Deposited on : 2016-12-04
Resolution : 4.20 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

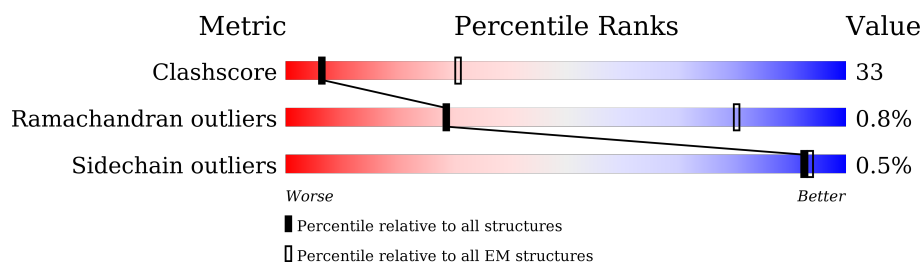
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	968	<div> <div>20%</div> <div>30%</div> <div>50%</div> </div>
1	B	968	<div> <div>20%</div> <div>29%</div> <div>50%</div> </div>
1	C	968	<div> <div>20%</div> <div>29%</div> <div>50%</div> </div>
1	D	968	<div> <div>19%</div> <div>30%</div> <div>50%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	1002	-	-	X	-
2	NAG	B	1002	-	-	X	-
2	NAG	C	1002	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	D	1002	-	-	X	-

2 Entry composition [i](#)

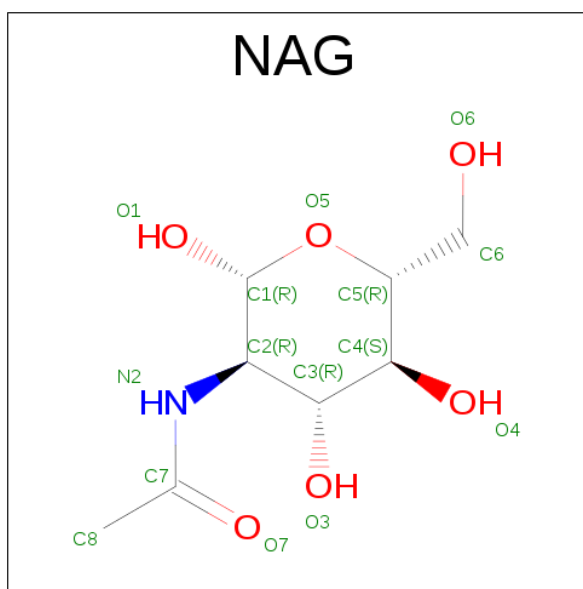
There are 6 unique types of molecules in this entry. The entry contains 16620 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Polycystin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	481	Total	C	N	O	S	0	0
			3962	2612	629	702	19		
1	B	481	Total	C	N	O	S	0	0
			3959	2610	629	702	18		
1	C	481	Total	C	N	O	S	0	0
			3959	2610	629	702	18		
1	D	481	Total	C	N	O	S	0	0
			3959	2610	629	702	18		

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



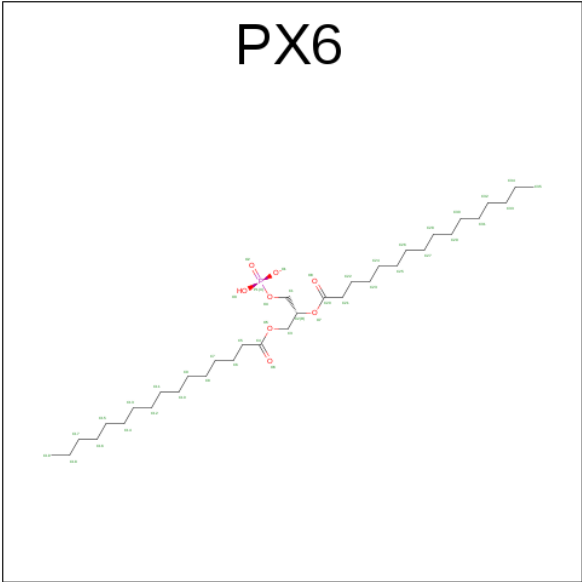
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			70	40	5	25	
2	A	1	Total	C	N	O	0
			70	40	5	25	
2	A	1	Total	C	N	O	0
			70	40	5	25	

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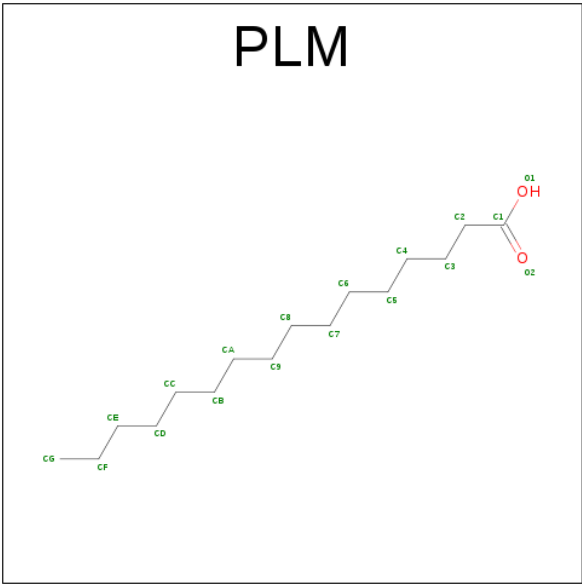
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			70	40	5	25	
2	A	1	Total	C	N	O	0
			70	40	5	25	
2	B	1	Total	C	N	O	0
			70	40	5	25	
2	B	1	Total	C	N	O	0
			70	40	5	25	
2	B	1	Total	C	N	O	0
			70	40	5	25	
2	B	1	Total	C	N	O	0
			70	40	5	25	
2	B	1	Total	C	N	O	0
			70	40	5	25	
2	C	1	Total	C	N	O	0
			70	40	5	25	
2	C	1	Total	C	N	O	0
			70	40	5	25	
2	C	1	Total	C	N	O	0
			70	40	5	25	
2	C	1	Total	C	N	O	0
			70	40	5	25	
2	C	1	Total	C	N	O	0
			70	40	5	25	
2	D	1	Total	C	N	O	0
			70	40	5	25	
2	D	1	Total	C	N	O	0
			70	40	5	25	
2	D	1	Total	C	N	O	0
			70	40	5	25	
2	D	1	Total	C	N	O	0
			70	40	5	25	
2	D	1	Total	C	N	O	0
			70	40	5	25	

- Molecule 3 is 1,2-DIPALMITOYL-SN-GLYCERO-3-PHOSPHATE (three-letter code: PX6) (formula: C₃₅H₆₈O₈P).



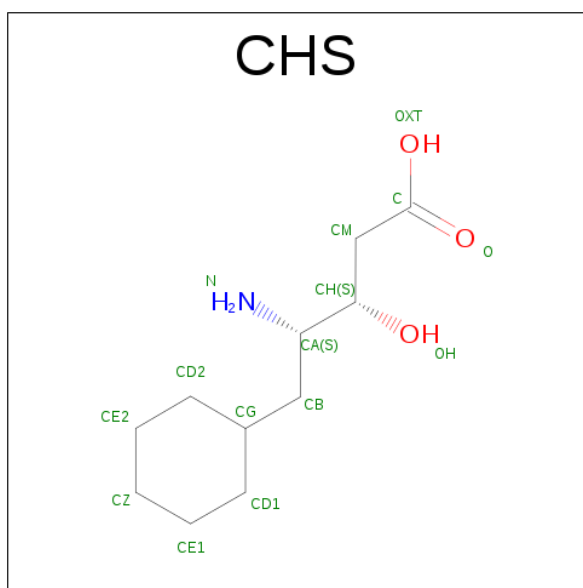
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			40	31	8	1	
3	B	1	Total	C	O	P	0
			40	31	8	1	
3	C	1	Total	C	O	P	0
			40	31	8	1	
3	D	1	Total	C	O	P	0
			40	31	8	1	

- Molecule 4 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			54	48	6	
4	A	1	Total	C	O	0
			54	48	6	
4	A	1	Total	C	O	0
			54	48	6	
4	B	1	Total	C	O	0
			54	48	6	
4	B	1	Total	C	O	0
			54	48	6	
4	B	1	Total	C	O	0
			54	48	6	
4	C	1	Total	C	O	0
			54	48	6	
4	C	1	Total	C	O	0
			54	48	6	
4	C	1	Total	C	O	0
			54	48	6	
4	D	1	Total	C	O	0
			54	48	6	
4	D	1	Total	C	O	0
			54	48	6	
4	D	1	Total	C	O	0
			54	48	6	

- Molecule 5 is 4-AMINO-5-CYCLOHEXYL-3-HYDROXY-PENTANOIC ACID (three-letter code: CHS) (formula: $C_{11}H_{21}NO_3$).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			30	22	2	6	
5	A	1	Total	C	N	O	0
			30	22	2	6	
5	B	1	Total	C	N	O	0
			30	22	2	6	
5	B	1	Total	C	N	O	0
			30	22	2	6	
5	C	1	Total	C	N	O	0
			30	22	2	6	
5	C	1	Total	C	N	O	0
			30	22	2	6	
5	D	1	Total	C	N	O	0
			30	22	2	6	
5	D	1	Total	C	N	O	0
			30	22	2	6	

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	B	1	Total	Ca	0
			1	1	
6	A	4	Total	Ca	0
			4	4	


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

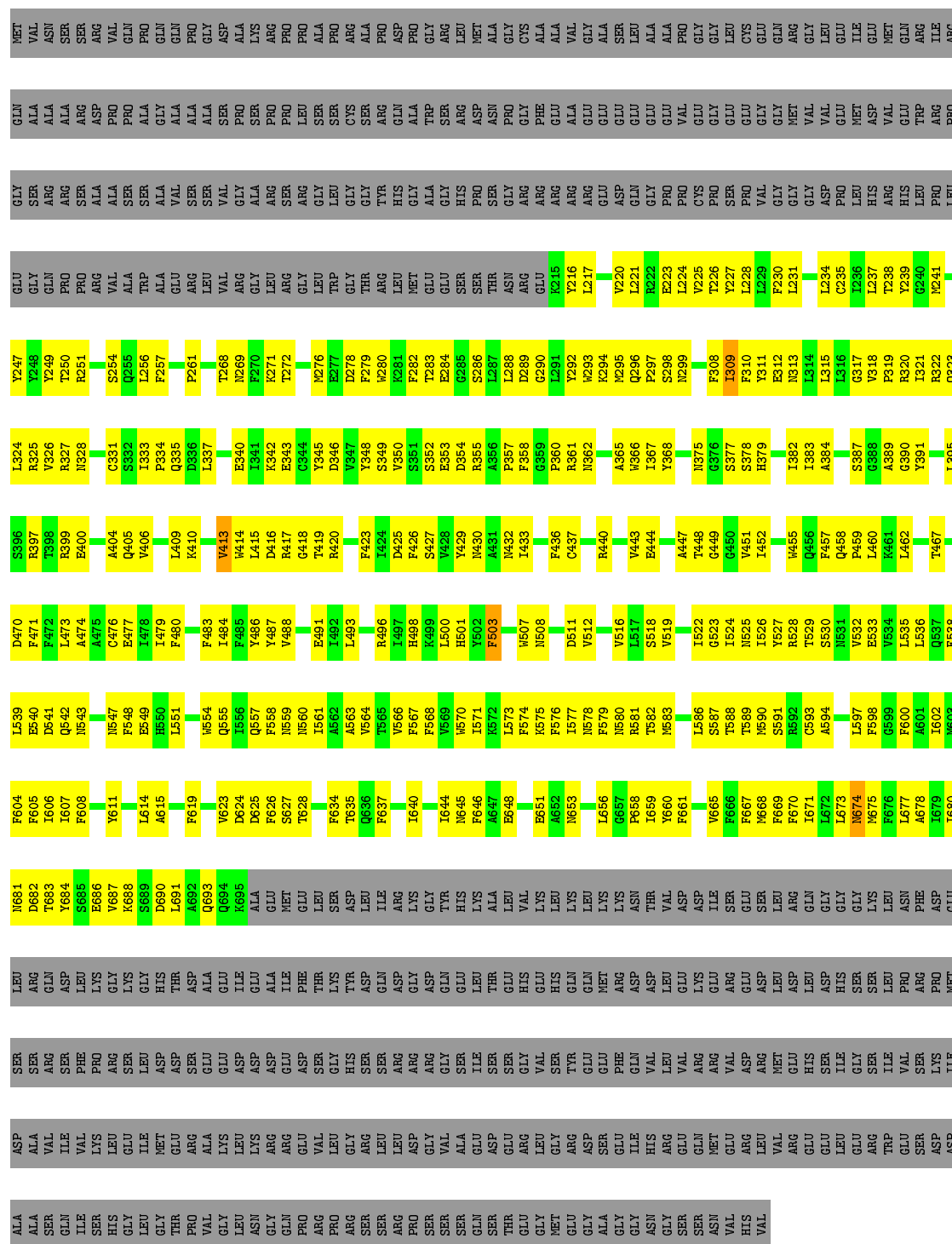
● Molecule 1: Polycystin-2



MET	GLN	GLY	GLU	Y247	R325	T398	A474		Y611	E886	PRO	LYS
VAL	ALA	SER	GLY	T246	V326	R399	A475	N647	L614	V687	ARG	GLY
ASN	ALA	ARG	GLN	T249	R327	E400	E476	F548	A615	K688	SER	LYS
SER	ALA	ARG	PRO	T250	N328		E477	E549		G689	LEU	GLY
ARG	ASP	SER	ARG	R251		A404	I478	H550	F619	D690	ASP	HIS
VAL	PRO	ALA	ALA		C331	Q405	I479	L551		L691	SER	THR
GLN	PRO	ALA	VAL	S254	S332	V406	F480		V623	A692	ASP	ASP
ILE	PRO	SER	ALA	Q256	I333	L409	F483	M554	D625	Q693	GLU	ALA
VAL	ALA	ILE	TRP	L256	P334	K410	I484	Q555	D626	Q694	GLU	ILE
GLN	GLY	ALA	ALA	F257	Q335	K413	F485	I556	F626	K695	ASP	GLY
VAL	ALA	VAL	GLU		D336	V414	Y486	Q557	S627		ASP	GLY
GLY	ALA	SER	ARG	P261	L337	H414	Y487	F558	T628		ASP	ALA
ILE	ALA	SER	LEU		E340	L415	V488	N559			GLU	ILE
GLY	SER	VAL	VAL	T268		D416		N560	F634		ASP	PHE
ASP	PRO	GLY	ARG	I269	E343	R417	E491	A563	T635		SER	THR
GLY	ALA	ALA	GLY	F270	C344	G418	I492	V564	Q636		GLY	LYS
PRO	PRO	ARG	LEU	K271	G345	T419	L493	T565	F637		GLY	THR
ARG	PRO	SER	ARG	T272	D346	R420	L496	V566	Q638		SER	GLN
LEU	LEU	ARG	GLY		V347		R496	F567	I639		ARG	ASP
ASN	SER	GLY	LEU	P276	Y348	F423	I497	F568	I640		ASP	GLY
ALA	PRO	TRP	TRP	E277	S349	I424	K498	N569	D643		ARG	GLY
PRO	CYS	GLY	GLY	D278	V350	D425	K499	V570	I644		GLY	VAL
ARG	ALA	SER	THR	F279		F426	L500	I571	M645		ALA	ALA
PRO	ARG	TYR	ARG	K280	S351	S427	H501	K572	M646		ILE	LYS
ASP	GLN	HIS	LEU	K281	S352	V428	F502	L573	P646		SER	THR
PRO	ALA	GLY	MET	F282	E353	Y429	F503	K574	A647		ASP	GLU
GLY	TRP	ALA	GLU	T283	D354	M430	L507	K575	B648		GLY	SER
ARG	ALA	GLY	GLU	E284	R355	M432	V507	F576			VAL	HIS
LEU	ARG	HIS	SER	K285	A356	A431	M508	N577	E651		GLY	LYS
LEU	ASP	PRO	ASN	S286	P357	I433		N578	A652		THR	HIS
ASP	ALA	ALA	SER		F358		D511	N579	M653		GLU	GLN
GLY	PRO	GLY	PRO		G359		V512	N580	L656		GLU	GLN
SER	GLY	ANG	ANG	D289	P360	F436	V516	R581	L657		GLU	MET
ALA	CYS	ARG	GLY	G290	R361	C437		T582	L658		GLU	ARG
SER	ALA	ALA	PHE	L291	N362		V516	T583	G657		GLU	ASP
GLN	ALA	ALA	ALA	Y292			L517	N583			VAL	ASP
ASP	GLY	VAL	VAL	K293		R440	L517		P658		VAL	THR
THR	GLY	ALA	ALA	L216	A365	V443	S518	L586	I659		LEU	LEU
GLY	GLY	GLY	GLY	L217	V366		V519		V660		VAL	GLU
LEU	GLY	GLY	ALA		I367	E444		S587			GLN	GLY
GLY	SER	GLY	SER	V220	Y368		T522	T588	V665		ARG	LYS
MET	GLY	GLY	ALA	L221		A447	G523	T589	F666		ARG	ILE
GLY	ALA	GLY	ALA	R222	N375	T448	I524	M590	F667		VAL	ARG
LEU	ALA	PRO	VAL	E223	G376	T449	M525	S591	M668		ASP	ARG
ALA	PRO	GLY	VAL	L224	S377	G449	I526	R592	M669		ARG	ASP
SER	GLY	GLY	GLY	V225	S378	G450	Y527	C593	F670		MET	LEU
ASP	GLY	GLY	GLY	T226	H379	V451	R528	A594			GLU	ASP
ILE	GLY	LEU	LEU	F310		I452	T529		L671		HIS	LEU
HIS	ASN	CYS	VAL	Y227			S530		L672		ASP	ASP
GLY	GLY	GLY	GLY	L228	I382	M455	S531	L597	L673		GLY	GLY
GLY	GLY	GLY	GLY	F230	E312	Q456	M531	F598	M674		HIS	GLY
SER	GLY	GLY	GLY	L231	N313	F457	V532	G599	M675		SER	SER
MET	ASN	GLY	GLY		A384	Q458		F600	F676		SER	LYS
GLY	VAL	MET	VAL				L535	F601	L677		ILE	LEU
ARG	HIS	GLY	VAL	L234	S387	P459	L536	A601	L677		VAL	PRO
LEU	LEU	GLY	VAL	C235	G388	L460	Q537	I602	A678		VAL	ASN
VAL	GLY	PRO	GLY	I236	A389		F538	M603	I679		SER	ARG
ARG	ILE	ASP	ILE	T237	G390	T467	F539	F604			LYS	PRO
GLY	VAL	ARG	VAL	K238	P319		L539	F605	I680		ILE	MET
LEU	GLY	MET	VAL	Y239	Y391	D470	E540	I606	M681		ASP	LEU
GLY	GLN	ARG	GLY			F471	D541	F607	D682		ALA	SER
LEU	TRP	TRP	TRP		L395	F472	Q542	L608	T683		ALA	ARG
GLY	ARG	ILE	ARG	M241	S396		F608		Y684		VAL	GLN
TRP	PRO		PRO		R397	L473	N543		S685		VAL	ILE

- Molecule 1: Polycystin-2

Chain C:  20% 29% 50%



- Molecule 1: Polycystin-2

[illegible]

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	35318	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLM, CHS, CA, PX6, NAG

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.52	0/4068	0.57	0/5521
1	B	0.52	0/4065	0.57	0/5518
1	C	0.52	0/4065	0.57	0/5518
1	D	0.52	0/4065	0.57	0/5518
All	All	0.52	0/16263	0.57	0/22075

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	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	579	PHE	Peptide
1	B	579	PHE	Peptide
1	C	579	PHE	Peptide
1	D	579	PHE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3962	0	3898	287	0
1	B	3959	0	3891	278	0
1	C	3959	0	3891	275	0
1	D	3959	0	3891	277	0
2	A	70	0	64	15	0
2	B	70	0	64	18	0
2	C	70	0	64	18	0
2	D	70	0	64	16	0
3	A	40	0	56	2	0
3	B	40	0	56	4	0
3	C	40	0	56	5	0
3	D	40	0	56	4	0
4	A	54	0	93	5	0
4	B	54	0	93	5	0
4	C	54	0	93	4	0
4	D	54	0	93	4	0
5	A	30	0	40	2	0
5	B	30	0	40	2	0
5	C	30	0	40	1	0
5	D	30	0	40	2	0
6	A	4	0	0	0	0
6	B	1	0	0	0	0
All	All	16620	0	16583	1082	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 33.

All (1082) 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:D:299:ASN:HD22	2:D:1005:NAG:C1	1.10	1.59
1:C:299:ASN:HD22	2:C:1005:NAG:C1	1.17	1.58
1:C:375:ASN:ND2	2:C:1003:NAG:C1	1.68	1.56
1:B:299:ASN:HD22	2:B:1005:NAG:C1	1.17	1.55
1:B:375:ASN:ND2	2:B:1003:NAG:C1	1.68	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ASN:HD22	2:A:1005:NAG:C1	1.17	1.52
1:B:360:PRO:HB2	2:B:1002:NAG:C8	1.51	1.39
1:A:360:PRO:HB2	2:A:1002:NAG:C8	1.51	1.37
1:D:299:ASN:ND2	2:D:1005:NAG:C1	1.86	1.37
1:D:360:PRO:HB2	2:D:1002:NAG:C8	1.53	1.36
1:C:360:PRO:HB2	2:C:1002:NAG:C8	1.51	1.36
1:B:299:ASN:ND2	2:B:1005:NAG:C1	1.92	1.32
1:A:299:ASN:ND2	2:A:1005:NAG:C1	1.92	1.32
1:C:299:ASN:ND2	2:C:1005:NAG:C1	1.92	1.29
1:B:360:PRO:CB	2:B:1002:NAG:H81	1.72	1.20
1:A:360:PRO:CB	2:A:1002:NAG:H81	1.72	1.19
1:C:360:PRO:CB	2:C:1002:NAG:H81	1.72	1.19
1:D:360:PRO:CB	2:D:1002:NAG:H81	1.75	1.14
1:A:581:ARG:HB2	1:A:583:MET:HG2	1.18	1.14
1:B:590:MET:SD	1:C:674:ASN:ND2	2.42	0.92
1:C:645:ASN:HB3	1:C:648:GLU:OE2	1.71	0.90
1:B:645:ASN:HB3	1:B:648:GLU:OE2	1.72	0.89
1:A:645:ASN:HB3	1:A:648:GLU:OE2	1.72	0.88
1:D:645:ASN:HB3	1:D:648:GLU:OE2	1.75	0.86
1:A:458:GLN:NE2	1:A:459:PRO:O	2.08	0.86
1:C:458:GLN:NE2	1:C:459:PRO:O	2.09	0.86
1:B:309:ILE:HG13	1:B:310:PHE:H	1.40	0.85
1:C:309:ILE:HG13	1:C:310:PHE:H	1.40	0.85
1:A:309:ILE:HG13	1:A:310:PHE:H	1.40	0.85
1:B:458:GLN:NE2	1:B:459:PRO:O	2.09	0.85
1:D:458:GLN:NE2	1:D:459:PRO:O	2.08	0.85
1:C:590:MET:SD	1:D:674:ASN:ND2	2.50	0.85
1:A:674:ASN:ND2	1:D:590:MET:SD	2.50	0.84
1:A:590:MET:SD	1:B:674:ASN:ND2	2.51	0.84
1:D:309:ILE:HG13	1:D:310:PHE:H	1.41	0.84
1:D:343:GLU:HA	2:D:1001:NAG:H62	1.60	0.84
1:A:581:ARG:HB2	1:A:583:MET:CG	2.07	0.82
1:B:343:GLU:HA	2:B:1001:NAG:H62	1.62	0.81
1:A:343:GLU:HA	2:A:1001:NAG:H62	1.62	0.81
2:B:1002:NAG:O3	2:B:1002:NAG:O7	1.99	0.81
1:D:360:PRO:HB2	2:D:1002:NAG:H81	0.82	0.81
2:A:1002:NAG:O3	2:A:1002:NAG:O7	1.99	0.81
1:C:525:ASN:OD1	1:C:526:ILE:N	2.14	0.81
1:B:525:ASN:OD1	1:B:526:ILE:N	2.14	0.80
1:D:525:ASN:OD1	1:D:526:ILE:N	2.14	0.80
1:A:323:GLN:HE22	1:A:414:TRP:HD1	1.30	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:ASN:OD1	1:A:526:ILE:N	2.14	0.79
1:A:360:PRO:CB	2:A:1002:NAG:C8	2.47	0.79
2:D:1002:NAG:O7	2:D:1002:NAG:O3	1.99	0.79
1:C:343:GLU:HA	2:C:1001:NAG:H62	1.62	0.79
1:B:323:GLN:HE22	1:B:414:TRP:HD1	1.30	0.79
2:C:1002:NAG:O3	2:C:1002:NAG:O7	1.99	0.79
1:B:397:ARG:HH11	1:B:543:ASN:HA	1.48	0.79
1:A:674:ASN:HA	1:D:680:ILE:HG21	1.65	0.78
1:D:397:ARG:HH11	1:D:543:ASN:HA	1.48	0.78
1:C:397:ARG:HH11	1:C:543:ASN:HA	1.48	0.78
1:D:323:GLN:HE22	1:D:414:TRP:HD1	1.30	0.78
1:C:680:ILE:HG21	1:D:674:ASN:HA	1.64	0.78
1:A:360:PRO:HB2	2:A:1002:NAG:H81	0.79	0.77
1:C:323:GLN:HE22	1:C:414:TRP:HD1	1.30	0.77
1:A:397:ARG:HH11	1:A:543:ASN:HA	1.48	0.77
1:A:680:ILE:HG21	1:B:674:ASN:HA	1.67	0.77
1:D:360:PRO:CB	2:D:1002:NAG:C8	2.49	0.77
1:C:360:PRO:CB	2:C:1002:NAG:C8	2.47	0.77
1:C:360:PRO:HB2	2:C:1002:NAG:H81	0.79	0.77
1:B:677:LEU:HD21	1:C:673:LEU:HD22	1.66	0.76
1:B:362:ASN:CB	2:B:1002:NAG:HN2	1.99	0.76
1:B:360:PRO:HB2	2:B:1002:NAG:H81	0.79	0.76
1:A:362:ASN:CB	2:A:1002:NAG:HN2	1.99	0.75
1:B:375:ASN:CG	2:B:1003:NAG:C1	2.54	0.75
1:A:268:THR:OG1	1:A:272:THR:O	2.05	0.75
1:C:328:ASN:OD1	2:C:1001:NAG:O5	2.04	0.75
1:B:328:ASN:OD1	2:B:1001:NAG:O5	2.04	0.75
1:C:362:ASN:CB	2:C:1002:NAG:HN2	1.99	0.75
1:C:677:LEU:HD21	1:D:673:LEU:HD22	1.69	0.75
1:C:268:THR:OG1	1:C:272:THR:O	2.05	0.74
1:C:375:ASN:CG	2:C:1003:NAG:C1	2.54	0.74
1:A:328:ASN:OD1	2:A:1001:NAG:O5	2.04	0.74
1:A:580:ASN:OD1	1:A:581:ARG:N	2.20	0.74
1:D:268:THR:OG1	1:D:272:THR:O	2.05	0.74
1:B:268:THR:OG1	1:B:272:THR:O	2.05	0.74
1:D:362:ASN:CB	2:D:1002:NAG:HN2	2.00	0.74
1:D:580:ASN:OD1	1:D:581:ARG:N	2.20	0.73
1:B:690:ASP:OD1	1:B:693:GLN:NE2	2.22	0.73
1:A:673:LEU:HD22	1:D:677:LEU:HD21	1.69	0.73
1:B:680:ILE:HG21	1:C:674:ASN:HA	1.69	0.73
1:A:690:ASP:OD1	1:A:693:GLN:NE2	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:690:ASP:OD1	1:D:693:GLN:NE2	2.22	0.73
1:B:360:PRO:CB	2:B:1002:NAG:C8	2.47	0.73
1:A:323:GLN:OE1	1:A:414:TRP:NE1	2.22	0.72
1:B:667:PHE:O	1:B:671:ILE:N	2.22	0.72
1:D:328:ASN:OD1	2:D:1001:NAG:O5	2.04	0.72
1:D:362:ASN:HB3	2:D:1002:NAG:HN2	1.54	0.72
1:A:690:ASP:HA	1:A:693:GLN:HG2	1.71	0.72
1:B:690:ASP:HA	1:B:693:GLN:HG2	1.72	0.72
1:C:690:ASP:HA	1:C:693:GLN:HG2	1.72	0.72
1:A:362:ASN:HB3	2:A:1002:NAG:HN2	1.55	0.72
1:C:656:LEU:O	1:C:659:ILE:N	2.23	0.72
1:A:667:PHE:O	1:A:671:ILE:N	2.22	0.72
1:C:690:ASP:OD1	1:C:693:GLN:NE2	2.22	0.72
1:D:656:LEU:O	1:D:659:ILE:N	2.23	0.72
1:A:634:PHE:CZ	1:B:658:PRO:HB3	2.24	0.72
1:D:323:GLN:OE1	1:D:414:TRP:NE1	2.22	0.72
1:D:690:ASP:HA	1:D:693:GLN:HG2	1.72	0.72
1:C:362:ASN:HB3	2:C:1002:NAG:HN2	1.55	0.71
1:B:323:GLN:OE1	1:B:414:TRP:NE1	2.22	0.71
1:B:580:ASN:OD1	1:B:581:ARG:N	2.20	0.71
1:D:525:ASN:O	1:D:529:THR:OG1	2.08	0.71
1:B:375:ASN:ND2	2:B:1003:NAG:C2	2.54	0.71
1:B:362:ASN:HB3	2:B:1002:NAG:HN2	1.55	0.71
1:C:580:ASN:OD1	1:C:581:ARG:N	2.20	0.71
2:C:1002:NAG:C3	2:C:1002:NAG:O7	2.38	0.71
1:C:323:GLN:OE1	1:C:414:TRP:NE1	2.22	0.71
2:A:1002:NAG:C3	2:A:1002:NAG:O7	2.38	0.71
1:A:656:LEU:O	1:A:659:ILE:N	2.23	0.71
1:B:656:LEU:O	1:B:659:ILE:N	2.23	0.71
2:D:1002:NAG:O7	2:D:1002:NAG:C3	2.38	0.71
1:C:667:PHE:O	1:C:671:ILE:N	2.22	0.70
2:B:1002:NAG:C3	2:B:1002:NAG:O7	2.38	0.70
1:B:574:PHE:O	1:B:578:ASN:ND2	2.22	0.70
1:C:375:ASN:ND2	2:C:1003:NAG:C2	2.54	0.70
1:A:525:ASN:O	1:A:529:THR:OG1	2.08	0.70
1:D:286:SER:O	1:D:290:GLY:N	2.25	0.70
1:D:667:PHE:O	1:D:671:ILE:N	2.22	0.70
1:D:429:TYR:HD1	1:D:436:PHE:HD1	1.39	0.70
1:C:419:THR:O	1:C:420:ARG:NH1	2.25	0.69
1:B:322:ARG:HH21	1:B:423:PHE:HE2	1.40	0.69
1:A:419:THR:O	1:A:420:ARG:NH1	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:429:TYR:HD1	1:C:436:PHE:HD1	1.39	0.69
1:C:322:ARG:HH21	1:C:423:PHE:HE2	1.40	0.69
1:A:429:TYR:HD1	1:A:436:PHE:HD1	1.40	0.69
1:B:286:SER:O	1:B:290:GLY:N	2.25	0.69
1:A:286:SER:O	1:A:290:GLY:N	2.25	0.69
1:A:455:TRP:NE1	1:B:651:GLU:OE2	2.25	0.69
1:B:525:ASN:O	1:B:529:THR:OG1	2.08	0.68
1:C:525:ASN:O	1:C:529:THR:OG1	2.08	0.68
1:A:554:TRP:O	1:A:558:PHE:N	2.27	0.68
1:C:286:SER:O	1:C:290:GLY:N	2.25	0.68
1:B:429:TYR:HD1	1:B:436:PHE:HD1	1.40	0.68
1:D:419:THR:O	1:D:420:ARG:NH1	2.25	0.68
1:D:554:TRP:O	1:D:558:PHE:N	2.27	0.68
1:A:290:GLY:O	1:A:293:TRP:NE1	2.27	0.68
1:B:624:ASP:OD1	1:B:625:ASP:N	2.27	0.68
1:D:322:ARG:HH21	1:D:423:PHE:HE2	1.40	0.68
1:C:290:GLY:O	1:C:293:TRP:NE1	2.27	0.68
1:D:624:ASP:OD1	1:D:625:ASP:N	2.27	0.67
1:C:574:PHE:O	1:C:578:ASN:ND2	2.22	0.67
1:D:409:LEU:HB3	1:D:414:TRP:CZ3	2.30	0.67
1:A:223:GLU:O	1:A:226:THR:OG1	2.13	0.67
1:A:322:ARG:HH21	1:A:423:PHE:HE2	1.40	0.67
1:C:409:LEU:HB3	1:C:414:TRP:CZ3	2.30	0.67
1:C:554:TRP:O	1:C:558:PHE:N	2.27	0.67
1:D:290:GLY:O	1:D:293:TRP:NE1	2.27	0.67
1:A:409:LEU:HB3	1:A:414:TRP:CZ3	2.30	0.67
1:C:624:ASP:OD1	1:C:625:ASP:N	2.27	0.67
1:D:223:GLU:O	1:D:226:THR:OG1	2.13	0.67
1:B:409:LEU:HB3	1:B:414:TRP:CZ3	2.29	0.67
1:B:223:GLU:O	1:B:226:THR:OG1	2.13	0.67
1:B:290:GLY:O	1:B:293:TRP:NE1	2.27	0.67
1:B:554:TRP:O	1:B:558:PHE:N	2.27	0.67
1:A:624:ASP:OD1	1:A:625:ASP:N	2.27	0.67
1:A:677:LEU:HD21	1:B:673:LEU:HD22	1.76	0.67
1:B:493:LEU:HD22	1:B:496:ARG:HH11	1.61	0.66
1:D:493:LEU:HD22	1:D:496:ARG:HH11	1.61	0.66
1:A:405:GLN:O	1:A:409:LEU:N	2.29	0.66
1:A:493:LEU:HD22	1:A:496:ARG:HH11	1.61	0.66
1:D:574:PHE:O	1:D:578:ASN:ND2	2.22	0.66
1:C:405:GLN:O	1:C:409:LEU:N	2.29	0.66
1:B:419:THR:O	1:B:420:ARG:NH1	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:PRO:HB2	2:C:1002:NAG:H82	1.72	0.65
1:A:360:PRO:HB2	2:A:1002:NAG:H82	1.72	0.65
1:B:360:PRO:HB2	2:B:1002:NAG:H82	1.72	0.65
1:C:493:LEU:HD22	1:C:496:ARG:HH11	1.61	0.65
1:D:405:GLN:O	1:D:409:LEU:N	2.29	0.65
1:B:405:GLN:O	1:B:409:LEU:N	2.29	0.65
1:A:221:LEU:O	1:A:225:VAL:N	2.21	0.64
1:B:668:MET:HA	1:B:671:ILE:HG22	1.80	0.64
1:C:223:GLU:O	1:C:226:THR:OG1	2.13	0.64
1:C:634:PHE:CZ	1:D:658:PRO:HB3	2.32	0.64
1:A:668:MET:HA	1:A:671:ILE:HG22	1.80	0.64
1:A:580:ASN:OD1	1:A:583:MET:SD	2.55	0.64
1:C:644:ILE:HG23	1:C:646:PHE:H	1.63	0.64
1:C:355:ARG:HG2	1:C:368:TYR:CZ	2.33	0.64
1:D:355:ARG:HG2	1:D:368:TYR:CZ	2.33	0.64
1:D:668:MET:HA	1:D:671:ILE:HG22	1.79	0.64
1:A:355:ARG:HG2	1:A:368:TYR:CZ	2.33	0.63
1:D:644:ILE:HG23	1:D:646:PHE:H	1.63	0.63
1:B:355:ARG:HG2	1:B:368:TYR:CZ	2.33	0.63
1:A:279:PHE:HE1	1:A:443:VAL:HG21	1.64	0.63
1:C:279:PHE:HE1	1:C:443:VAL:HG21	1.64	0.63
1:D:279:PHE:HE1	1:D:443:VAL:HG21	1.64	0.63
1:D:637:PHE:O	1:D:640:ILE:N	2.32	0.63
1:A:574:PHE:O	1:A:578:ASN:ND2	2.22	0.63
1:C:586:LEU:O	1:C:589:THR:OG1	2.16	0.63
1:B:296:GLN:HE22	1:C:417:ARG:HB2	1.63	0.63
1:A:637:PHE:O	1:A:640:ILE:N	2.32	0.62
1:A:644:ILE:HG23	1:A:646:PHE:H	1.63	0.62
1:C:221:LEU:O	1:C:225:VAL:N	2.21	0.62
1:B:279:PHE:HE1	1:B:443:VAL:HG21	1.64	0.62
1:B:634:PHE:CZ	1:C:658:PRO:HB3	2.35	0.62
1:B:637:PHE:O	1:B:640:ILE:N	2.32	0.62
1:B:644:ILE:HG23	1:B:646:PHE:H	1.63	0.62
1:C:227:TYR:HA	1:C:230:PHE:HB3	1.81	0.62
1:C:668:MET:HA	1:C:671:ILE:HG22	1.79	0.62
1:B:227:TYR:HA	1:B:230:PHE:HB3	1.81	0.62
1:A:227:TYR:HA	1:A:230:PHE:HB3	1.81	0.62
1:C:637:PHE:O	1:C:640:ILE:N	2.32	0.62
1:D:594:ALA:O	1:D:598:PHE:N	2.32	0.62
1:A:594:ALA:O	1:A:598:PHE:N	2.32	0.62
1:B:586:LEU:O	1:B:589:THR:OG1	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:GLU:HA	2:D:1001:NAG:C6	2.30	0.61
1:A:658:PRO:HB3	1:D:634:PHE:CZ	2.33	0.61
1:B:519:VAL:HA	1:B:522:ILE:HD12	1.82	0.61
1:D:586:LEU:O	1:D:589:THR:OG1	2.16	0.61
1:D:227:TYR:HA	1:D:230:PHE:HB3	1.81	0.61
1:C:535:LEU:HD12	1:C:536:LEU:HD12	1.83	0.61
1:D:519:VAL:HA	1:D:522:ILE:HD12	1.81	0.61
1:A:519:VAL:HA	1:A:522:ILE:HD12	1.81	0.61
1:C:361:ARG:HA	1:C:366:TRP:HB3	1.83	0.61
1:B:400:GLU:O	1:B:404:ALA:N	2.34	0.60
1:C:594:ALA:O	1:C:598:PHE:N	2.32	0.60
1:D:361:ARG:HA	1:D:366:TRP:HB3	1.83	0.60
1:C:519:VAL:HA	1:C:522:ILE:HD12	1.81	0.60
1:D:535:LEU:HD12	1:D:536:LEU:HD12	1.83	0.60
1:A:586:LEU:O	1:A:589:THR:OG1	2.16	0.60
1:A:383:ILE:HG13	1:A:384:ALA:H	1.67	0.60
1:B:416:ASP:OD1	1:B:417:ARG:N	2.35	0.60
1:C:498:HIS:HB3	1:C:501:HIS:HB3	1.84	0.60
1:B:221:LEU:O	1:B:225:VAL:N	2.21	0.60
1:C:416:ASP:OD1	1:C:417:ARG:N	2.35	0.60
1:D:383:ILE:HG13	1:D:384:ALA:H	1.67	0.60
1:A:440:ARG:HD2	1:A:549:GLU:HG3	1.84	0.60
1:A:535:LEU:HD12	1:A:536:LEU:HD12	1.83	0.60
1:B:383:ILE:HG13	1:B:384:ALA:H	1.67	0.60
1:B:498:HIS:HB3	1:B:501:HIS:HB3	1.84	0.60
1:D:500:LEU:HA	1:D:503:PHE:HB2	1.84	0.60
1:B:294:LYS:HG2	1:B:295:MET:H	1.67	0.59
1:B:535:LEU:HD12	1:B:536:LEU:HD12	1.83	0.59
1:B:594:ALA:O	1:B:598:PHE:N	2.32	0.59
1:C:440:ARG:HD2	1:C:549:GLU:HG3	1.84	0.59
1:A:409:LEU:HB3	1:A:414:TRP:HZ3	1.67	0.59
1:A:500:LEU:HA	1:A:503:PHE:HB2	1.84	0.59
1:D:294:LYS:HG2	1:D:295:MET:H	1.67	0.59
1:D:440:ARG:HD2	1:D:549:GLU:HG3	1.84	0.59
1:B:409:LEU:HB3	1:B:414:TRP:HZ3	1.67	0.59
1:B:440:ARG:HD2	1:B:549:GLU:HG3	1.84	0.59
1:B:500:LEU:HA	1:B:503:PHE:HB2	1.84	0.59
1:C:400:GLU:O	1:C:404:ALA:N	2.34	0.59
1:D:498:HIS:HB3	1:D:501:HIS:HB3	1.84	0.59
1:A:349:SER:O	1:A:353:GLU:HG3	2.02	0.59
1:B:293:TRP:CZ2	1:B:310:PHE:HD1	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:656:LEU:HA	1:B:659:ILE:HG22	1.84	0.59
1:D:349:SER:O	1:D:353:GLU:HG3	2.02	0.59
1:A:293:TRP:CZ2	1:A:310:PHE:HD1	2.21	0.59
1:A:400:GLU:O	1:A:404:ALA:N	2.34	0.59
1:A:498:HIS:HB3	1:A:501:HIS:HB3	1.84	0.59
1:C:383:ILE:HG13	1:C:384:ALA:H	1.67	0.59
1:C:455:TRP:NE1	1:D:651:GLU:OE2	2.36	0.59
1:D:360:PRO:HB2	2:D:1002:NAG:H82	1.75	0.59
1:A:294:LYS:HG2	1:A:295:MET:H	1.67	0.59
1:C:409:LEU:HB3	1:C:414:TRP:HZ3	1.67	0.59
1:B:361:ARG:HA	1:B:366:TRP:HB3	1.83	0.59
1:D:221:LEU:O	1:D:225:VAL:N	2.21	0.59
1:A:361:ARG:HA	1:A:366:TRP:HB3	1.83	0.59
1:C:343:GLU:HA	2:C:1001:NAG:C6	2.33	0.59
5:A:1010:CHS:OH	5:A:1010:CHS:O	2.18	0.59
1:B:619:PHE:HB2	1:B:626:PHE:HD2	1.68	0.59
1:D:416:ASP:OD1	1:D:417:ARG:N	2.35	0.59
1:A:656:LEU:HA	1:A:659:ILE:HG22	1.84	0.58
1:C:500:LEU:HA	1:C:503:PHE:HB2	1.84	0.58
1:B:349:SER:O	1:B:353:GLU:HG3	2.02	0.58
1:D:619:PHE:HB2	1:D:626:PHE:HD2	1.68	0.58
1:A:416:ASP:OD1	1:A:417:ARG:N	2.35	0.58
1:A:619:PHE:HB2	1:A:626:PHE:HD2	1.68	0.58
1:C:656:LEU:HA	1:C:659:ILE:HG22	1.84	0.58
1:C:597:LEU:HA	1:C:600:PHE:HB3	1.84	0.58
1:D:409:LEU:HB3	1:D:414:TRP:HZ3	1.67	0.58
1:A:460:LEU:HD13	1:A:555:GLN:HG2	1.86	0.58
1:B:455:TRP:NE1	1:C:651:GLU:OE2	2.36	0.58
1:D:293:TRP:CZ2	1:D:310:PHE:HD1	2.20	0.58
1:C:460:LEU:HD13	1:C:555:GLN:HG2	1.86	0.58
1:A:651:GLU:OE2	1:D:455:TRP:NE1	2.37	0.58
1:C:293:TRP:CZ2	1:C:310:PHE:HD1	2.20	0.58
1:D:250:THR:O	1:D:254:SER:N	2.23	0.58
1:D:400:GLU:O	1:D:404:ALA:N	2.34	0.58
1:D:656:LEU:HA	1:D:659:ILE:HG22	1.84	0.58
1:C:335:GLN:OE1	1:C:335:GLN:N	2.34	0.58
1:D:460:LEU:HD13	1:D:555:GLN:HG2	1.86	0.58
1:A:597:LEU:HA	1:A:600:PHE:HB3	1.85	0.58
1:B:343:GLU:HA	2:B:1001:NAG:C6	2.33	0.58
1:C:294:LYS:HG2	1:C:295:MET:H	1.67	0.58
1:C:619:PHE:HB2	1:C:626:PHE:HD2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:597:LEU:HA	1:D:600:PHE:HB3	1.85	0.58
1:A:289:ASP:OD1	1:A:399:ARG:NH1	2.36	0.57
1:A:523:GLY:O	1:A:527:TYR:N	2.36	0.57
1:D:335:GLN:N	1:D:335:GLN:OE1	2.34	0.57
1:B:460:LEU:HD13	1:B:555:GLN:HG2	1.86	0.57
1:C:349:SER:O	1:C:353:GLU:HG3	2.02	0.57
1:D:507:TRP:HB3	1:D:575:LYS:NZ	2.20	0.57
1:A:583:MET:HA	1:A:586:LEU:HB2	1.87	0.57
1:D:523:GLY:O	1:D:527:TYR:N	2.36	0.57
5:B:1010:CHS:O	5:B:1010:CHS:OH	2.18	0.57
1:A:343:GLU:HA	2:A:1001:NAG:C6	2.33	0.57
1:A:296:GLN:HE22	1:B:417:ARG:HB2	1.69	0.57
1:D:289:ASP:OD1	1:D:399:ARG:NH1	2.36	0.57
1:B:597:LEU:HA	1:B:600:PHE:HB3	1.85	0.56
1:D:524:ILE:O	1:D:528:ARG:HB2	2.05	0.56
1:A:335:GLN:OE1	1:A:335:GLN:N	2.34	0.56
1:A:507:TRP:HB3	1:A:575:LYS:NZ	2.20	0.56
1:C:250:THR:O	1:C:254:SER:N	2.23	0.56
1:B:523:GLY:O	1:B:527:TYR:N	2.36	0.56
1:C:507:TRP:HB3	1:C:575:LYS:NZ	2.20	0.56
1:B:382:ILE:HG23	1:B:383:ILE:H	1.71	0.56
1:D:593:CYS:SG	1:D:594:ALA:N	2.79	0.56
1:C:524:ILE:O	1:C:528:ARG:HB2	2.05	0.56
1:D:382:ILE:HG23	1:D:383:ILE:H	1.71	0.56
1:C:382:ILE:HG23	1:C:383:ILE:H	1.71	0.56
1:A:593:CYS:SG	1:A:594:ALA:N	2.79	0.56
1:B:289:ASP:OD1	1:B:399:ARG:NH1	2.36	0.56
1:C:523:GLY:O	1:C:527:TYR:N	2.36	0.56
5:D:1010:CHS:OH	5:D:1010:CHS:O	2.19	0.56
1:D:365:ALA:HA	1:D:391:TYR:HB3	1.88	0.56
1:A:382:ILE:HG23	1:A:383:ILE:H	1.71	0.56
1:B:524:ILE:O	1:B:528:ARG:HB2	2.05	0.56
1:B:686:GLU:O	1:B:690:ASP:N	2.39	0.56
1:A:365:ALA:HA	1:A:391:TYR:HB3	1.88	0.55
1:C:289:ASP:OD1	1:C:399:ARG:NH1	2.36	0.55
1:C:593:CYS:SG	1:C:594:ALA:N	2.79	0.55
1:B:507:TRP:HB3	1:B:575:LYS:NZ	2.20	0.55
1:A:524:ILE:O	1:A:528:ARG:HB2	2.05	0.55
1:A:686:GLU:O	1:A:690:ASP:N	2.39	0.55
1:D:293:TRP:HZ2	1:D:310:PHE:HD1	1.54	0.55
1:A:250:THR:O	1:A:254:SER:N	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:GLN:OE1	1:B:335:GLN:N	2.34	0.55
1:B:593:CYS:SG	1:B:594:ALA:N	2.79	0.55
1:D:602:ILE:O	1:D:606:ILE:N	2.33	0.55
1:A:417:ARG:HB2	1:D:296:GLN:HE22	1.72	0.55
1:C:686:GLU:O	1:C:690:ASP:N	2.39	0.55
1:D:331:CYS:HB3	1:D:346:ASP:HB3	1.89	0.55
1:A:583:MET:O	1:A:587:SER:N	2.38	0.55
1:B:583:MET:O	1:B:587:SER:N	2.40	0.55
1:A:644:ILE:HG23	1:A:646:PHE:HB3	1.89	0.55
1:C:331:CYS:HB3	1:C:346:ASP:HB3	1.89	0.55
1:D:644:ILE:HG23	1:D:646:PHE:HB3	1.89	0.55
1:B:293:TRP:HZ2	1:B:310:PHE:HD1	1.54	0.55
1:C:644:ILE:HG23	1:C:646:PHE:HB3	1.89	0.55
1:A:602:ILE:O	1:A:606:ILE:N	2.33	0.54
1:B:337:LEU:O	1:B:340:GLU:N	2.40	0.54
1:C:293:TRP:HZ2	1:C:310:PHE:HD1	1.54	0.54
1:D:337:LEU:O	1:D:340:GLU:N	2.40	0.54
1:B:331:CYS:HB3	1:B:346:ASP:HB3	1.89	0.54
1:D:686:GLU:O	1:D:690:ASP:N	2.39	0.54
1:A:331:CYS:HB3	1:A:346:ASP:HB3	1.89	0.54
1:C:337:LEU:O	1:C:340:GLU:N	2.40	0.54
1:B:644:ILE:HG23	1:B:646:PHE:HB3	1.89	0.54
1:C:365:ALA:HA	1:C:391:TYR:HB3	1.88	0.54
1:A:337:LEU:O	1:A:340:GLU:N	2.40	0.54
1:B:365:ALA:HA	1:B:391:TYR:HB3	1.88	0.54
1:A:293:TRP:HZ2	1:A:310:PHE:HD1	1.54	0.54
1:D:323:GLN:NE2	1:D:414:TRP:HD1	2.03	0.54
1:A:323:GLN:NE2	1:A:414:TRP:HD1	2.03	0.54
1:D:583:MET:O	1:D:587:SER:N	2.40	0.54
1:C:467:THR:HA	1:C:471:PHE:HE2	1.74	0.53
1:D:467:THR:HA	1:D:471:PHE:HE2	1.74	0.53
1:A:430:ASN:HD22	1:A:433:ILE:HG12	1.74	0.53
1:A:467:THR:HA	1:A:471:PHE:HE2	1.74	0.53
5:C:1010:CHS:OH	5:C:1010:CHS:O	2.18	0.53
1:B:327:ARG:N	1:B:354:ASP:HB2	2.24	0.53
1:C:292:TYR:HB3	1:C:399:ARG:HB2	1.91	0.53
1:C:327:ARG:N	1:C:354:ASP:HB2	2.24	0.53
1:B:665:VAL:O	1:B:669:PHE:HB3	2.09	0.53
1:A:526:ILE:HA	1:A:530:SER:HB3	1.91	0.53
1:C:309:ILE:HG13	1:C:310:PHE:N	2.18	0.53
1:C:665:VAL:O	1:C:669:PHE:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:VAL:O	1:A:669:PHE:HB3	2.09	0.53
1:C:224:LEU:O	1:C:228:LEU:N	2.26	0.53
1:C:430:ASN:HD22	1:C:433:ILE:HG12	1.74	0.53
1:C:583:MET:O	1:C:587:SER:N	2.40	0.53
1:A:680:ILE:HD13	1:B:674:ASN:HA	1.90	0.53
1:B:322:ARG:HD2	1:B:389:ALA:HB2	1.91	0.53
1:C:254:SER:HA	1:C:457:PHE:HE2	1.74	0.53
1:D:292:TYR:HB3	1:D:399:ARG:HB2	1.91	0.53
1:D:322:ARG:HD2	1:D:389:ALA:HB2	1.91	0.53
1:D:319:PRO:HG3	1:D:426:PHE:HB3	1.90	0.53
1:B:319:PRO:HG3	1:B:426:PHE:HB3	1.90	0.53
1:A:309:ILE:HD11	1:A:313:ASN:HB2	1.91	0.52
1:C:322:ARG:HD2	1:C:389:ALA:HB2	1.91	0.52
1:C:541:ASP:OD1	1:C:542:GLN:N	2.42	0.52
1:D:309:ILE:HG13	1:D:310:PHE:N	2.19	0.52
1:D:526:ILE:HA	1:D:530:SER:HB3	1.91	0.52
1:D:604:PHE:O	1:D:607:ILE:HG22	2.10	0.52
1:D:665:VAL:O	1:D:669:PHE:HB3	2.09	0.52
1:A:555:GLN:O	1:A:559:ASN:N	2.35	0.52
1:B:541:ASP:OD1	1:B:542:GLN:N	2.42	0.52
1:C:296:GLN:HE22	1:D:417:ARG:HB2	1.74	0.52
1:C:319:PRO:HB2	1:C:395:LEU:HD13	1.92	0.52
1:D:319:PRO:HB2	1:D:395:LEU:HD13	1.92	0.52
1:A:319:PRO:HB2	1:A:395:LEU:HD13	1.92	0.52
1:A:604:PHE:O	1:A:607:ILE:HG22	2.09	0.52
1:B:292:TYR:HB3	1:B:399:ARG:HB2	1.91	0.52
1:B:430:ASN:HD22	1:B:433:ILE:HG12	1.73	0.52
1:D:254:SER:HA	1:D:457:PHE:HE2	1.74	0.52
1:D:430:ASN:HD22	1:D:433:ILE:HG12	1.74	0.52
1:A:319:PRO:HG3	1:A:426:PHE:HB3	1.90	0.52
1:B:250:THR:O	1:B:254:SER:N	2.23	0.52
1:B:526:ILE:HA	1:B:530:SER:HB3	1.91	0.52
1:A:247:TYR:OH	1:B:624:ASP:HB3	2.09	0.52
1:C:634:PHE:O	1:C:637:PHE:N	2.41	0.52
1:D:309:ILE:HD11	1:D:313:ASN:HB2	1.91	0.52
1:D:555:GLN:O	1:D:559:ASN:N	2.35	0.52
1:A:541:ASP:OD1	1:A:542:GLN:N	2.42	0.52
1:B:319:PRO:HB2	1:B:395:LEU:HD13	1.92	0.52
1:D:470:ASP:O	1:D:474:ALA:N	2.36	0.52
1:A:292:TYR:HB3	1:A:399:ARG:HB2	1.91	0.52
1:A:573:LEU:HA	1:A:576:PHE:HD2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:THR:HA	1:B:471:PHE:HE2	1.74	0.52
1:C:383:ILE:HG13	1:C:384:ALA:N	2.25	0.52
1:C:319:PRO:HG3	1:C:426:PHE:HB3	1.90	0.52
1:A:322:ARG:HD2	1:A:389:ALA:HB2	1.91	0.52
1:C:526:ILE:HA	1:C:530:SER:HB3	1.91	0.52
1:D:283:THR:OG1	1:D:284:GLU:N	2.43	0.52
1:A:327:ARG:N	1:A:354:ASP:HB2	2.24	0.52
1:A:473:LEU:O	1:A:477:GLU:N	2.43	0.52
1:B:323:GLN:NE2	1:B:414:TRP:HD1	2.03	0.52
1:B:573:LEU:HA	1:B:576:PHE:HD2	1.75	0.52
1:C:283:THR:OG1	1:C:284:GLU:N	2.43	0.52
1:D:541:ASP:OD1	1:D:542:GLN:N	2.42	0.52
1:D:573:LEU:HA	1:D:576:PHE:HD2	1.75	0.52
1:A:383:ILE:HG13	1:A:384:ALA:N	2.25	0.51
1:A:447:ALA:O	1:D:432:ASN:ND2	2.38	0.51
1:B:254:SER:HA	1:B:457:PHE:HE2	1.74	0.51
1:C:217:LEU:HA	1:C:220:VAL:HB	1.92	0.51
1:A:254:SER:HA	1:A:457:PHE:HE2	1.74	0.51
1:D:280:TRP:NE1	1:D:415:LEU:HD12	2.26	0.51
1:D:327:ARG:N	1:D:354:ASP:HB2	2.24	0.51
1:D:634:PHE:O	1:D:637:PHE:N	2.41	0.51
1:D:688:LYS:HD2	1:D:691:LEU:HD11	1.92	0.51
1:A:254:SER:HA	1:A:457:PHE:CE2	2.45	0.51
1:C:309:ILE:HD11	1:C:313:ASN:HB2	1.91	0.51
1:C:323:GLN:NE2	1:C:414:TRP:HD1	2.03	0.51
1:A:280:TRP:NE1	1:A:415:LEU:HD12	2.26	0.51
1:A:283:THR:OG1	1:A:284:GLU:N	2.43	0.51
1:B:309:ILE:HD11	1:B:313:ASN:HB2	1.91	0.51
1:B:350:VAL:HA	1:B:353:GLU:CD	2.31	0.51
1:B:349:SER:N	1:B:352:SER:OG	2.43	0.51
1:C:604:PHE:O	1:C:607:ILE:HG22	2.09	0.51
1:C:688:LYS:HD2	1:C:691:LEU:HD11	1.92	0.51
1:B:602:ILE:O	1:B:606:ILE:N	2.33	0.51
1:B:688:LYS:HD2	1:B:691:LEU:HD11	1.93	0.51
1:C:362:ASN:HB2	2:C:1002:NAG:HN2	1.75	0.51
1:C:526:ILE:O	1:C:530:SER:OG	2.25	0.51
1:D:296:GLN:HG2	1:D:311:TYR:CD1	2.46	0.51
1:A:217:LEU:HA	1:A:220:VAL:HB	1.92	0.51
1:A:350:VAL:HA	1:A:353:GLU:CD	2.31	0.51
1:B:594:ALA:HB1	1:B:598:PHE:HB2	1.93	0.51
1:B:604:PHE:O	1:B:607:ILE:HG22	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:PHE:CE1	1:C:443:VAL:HG21	2.46	0.51
1:C:280:TRP:NE1	1:C:415:LEU:HD12	2.26	0.51
1:C:573:LEU:HA	1:C:576:PHE:HD2	1.75	0.51
1:D:254:SER:HA	1:D:457:PHE:CE2	2.45	0.51
1:A:349:SER:N	1:A:352:SER:OG	2.43	0.51
1:A:594:ALA:HB1	1:A:598:PHE:HB2	1.93	0.51
1:B:280:TRP:NE1	1:B:415:LEU:HD12	2.26	0.51
1:C:349:SER:N	1:C:352:SER:OG	2.43	0.51
1:D:217:LEU:HA	1:D:220:VAL:HB	1.92	0.51
1:D:350:VAL:HA	1:D:353:GLU:CD	2.31	0.51
1:D:406:VAL:HA	1:D:409:LEU:HB2	1.93	0.51
1:C:406:VAL:HA	1:C:409:LEU:HB2	1.93	0.51
1:A:309:ILE:HG13	1:A:310:PHE:N	2.18	0.51
1:A:634:PHE:O	1:A:637:PHE:N	2.41	0.51
1:A:678:ALA:O	1:A:681:ASN:N	2.44	0.51
1:B:254:SER:HA	1:B:457:PHE:CE2	2.45	0.51
1:C:432:ASN:ND2	1:D:447:ALA:O	2.38	0.51
1:A:430:ASN:ND2	1:A:433:ILE:HG12	2.26	0.50
1:B:296:GLN:HG2	1:B:311:TYR:CD1	2.46	0.50
1:B:678:ALA:O	1:B:681:ASN:N	2.44	0.50
1:C:247:TYR:OH	1:D:624:ASP:HB3	2.11	0.50
1:C:254:SER:HA	1:C:457:PHE:CE2	2.45	0.50
1:A:624:ASP:HB3	1:D:247:TYR:OH	2.11	0.50
1:C:261:PRO:HG3	1:C:269:ASN:HA	1.93	0.50
1:D:427:SER:OG	1:D:437:CYS:O	2.25	0.50
1:D:473:LEU:O	1:D:477:GLU:N	2.43	0.50
1:A:261:PRO:HG3	1:A:269:ASN:HA	1.93	0.50
1:A:406:VAL:HA	1:A:409:LEU:HB2	1.93	0.50
1:B:406:VAL:HA	1:B:409:LEU:HB2	1.93	0.50
1:C:216:TYR:O	1:C:220:VAL:N	2.39	0.50
1:C:296:GLN:HG2	1:C:311:TYR:CD1	2.46	0.50
1:A:427:SER:OG	1:A:437:CYS:O	2.25	0.50
1:B:554:TRP:HA	1:B:557:GLN:HB2	1.94	0.50
1:C:470:ASP:O	1:C:474:ALA:N	2.36	0.50
1:A:296:GLN:HG2	1:A:311:TYR:CD1	2.46	0.50
1:B:234:LEU:HD21	1:B:480:PHE:CE1	2.47	0.50
1:B:261:PRO:HG3	1:B:269:ASN:HA	1.93	0.50
1:B:279:PHE:CE1	1:B:443:VAL:HG21	2.46	0.50
1:C:473:LEU:O	1:C:477:GLU:N	2.43	0.50
1:C:554:TRP:HA	1:C:557:GLN:HB2	1.94	0.50
1:D:261:PRO:HG3	1:D:269:ASN:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:349:SER:N	1:D:352:SER:OG	2.43	0.50
1:D:383:ILE:HG13	1:D:384:ALA:N	2.25	0.50
1:D:582:THR:O	1:D:586:LEU:N	2.34	0.50
1:D:678:ALA:O	1:D:681:ASN:N	2.44	0.50
1:A:476:CYS:HA	1:A:479:ILE:HD12	1.94	0.50
1:A:234:LEU:HD21	1:A:480:PHE:CE1	2.47	0.50
1:A:688:LYS:HD2	1:A:691:LEU:HD11	1.92	0.50
1:B:237:LEU:O	1:B:241:MET:N	2.35	0.50
1:C:430:ASN:ND2	1:C:433:ILE:HG12	2.26	0.50
1:B:217:LEU:HA	1:B:220:VAL:HB	1.92	0.50
1:B:283:THR:OG1	1:B:284:GLU:N	2.43	0.50
1:B:383:ILE:HG13	1:B:384:ALA:N	2.25	0.50
1:D:234:LEU:HD21	1:D:480:PHE:CE1	2.47	0.50
1:A:432:ASN:ND2	1:B:447:ALA:O	2.37	0.50
1:B:555:GLN:O	1:B:559:ASN:N	2.35	0.50
1:C:427:SER:OG	1:C:437:CYS:O	2.25	0.50
1:C:583:MET:HA	1:C:586:LEU:HB2	1.94	0.50
1:C:678:ALA:O	1:C:681:ASN:N	2.44	0.50
1:D:554:TRP:HA	1:D:557:GLN:HB2	1.94	0.50
1:D:570:TRP:O	1:D:573:LEU:HG	2.12	0.50
1:D:594:ALA:HB1	1:D:598:PHE:HB2	1.93	0.50
1:A:570:TRP:O	1:A:573:LEU:HG	2.12	0.49
1:B:430:ASN:ND2	1:B:433:ILE:HG12	2.26	0.49
1:B:583:MET:HA	1:B:586:LEU:HB2	1.94	0.49
1:C:234:LEU:HD21	1:C:480:PHE:CE1	2.47	0.49
1:C:350:VAL:HA	1:C:353:GLU:CD	2.31	0.49
1:C:570:TRP:O	1:C:573:LEU:HG	2.12	0.49
1:C:594:ALA:HB1	1:C:598:PHE:HB2	1.93	0.49
1:C:597:LEU:HD12	1:C:600:PHE:HB3	1.94	0.49
1:D:430:ASN:ND2	1:D:433:ILE:HG12	2.26	0.49
1:D:597:LEU:HD12	1:D:600:PHE:HB3	1.94	0.49
1:A:536:LEU:HA	1:A:539:LEU:HB3	1.94	0.49
1:A:554:TRP:HA	1:A:557:GLN:HB2	1.94	0.49
1:B:476:CYS:HA	1:B:479:ILE:HD12	1.94	0.49
1:B:473:LEU:O	1:B:477:GLU:N	2.43	0.49
1:B:536:LEU:HA	1:B:539:LEU:HB3	1.94	0.49
1:B:570:TRP:O	1:B:573:LEU:HG	2.12	0.49
1:B:611:TYR:O	1:B:615:ALA:N	2.45	0.49
1:C:684:TYR:HA	1:C:687:VAL:HG22	1.95	0.49
1:A:597:LEU:HD12	1:A:600:PHE:HB3	1.94	0.49
1:B:247:TYR:OH	1:C:624:ASP:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:597:LEU:HD12	1:B:600:PHE:HB3	1.94	0.49
1:D:357:PRO:HB2	1:D:361:ARG:HE	1.77	0.49
1:D:611:TYR:O	1:D:615:ALA:N	2.45	0.49
1:A:357:PRO:HB2	1:A:361:ARG:HE	1.77	0.49
1:D:378:SER:HA	1:D:387:SER:HA	1.94	0.49
1:A:682:ASP:OD1	1:A:683:THR:N	2.43	0.49
1:B:325:ARG:NH2	1:B:358:PHE:HB2	2.28	0.49
1:B:357:PRO:HB2	1:B:361:ARG:HE	1.78	0.49
1:B:460:LEU:HD23	1:B:548:PHE:HZ	1.78	0.49
1:B:684:TYR:HA	1:B:687:VAL:HG22	1.95	0.49
1:C:476:CYS:HA	1:C:479:ILE:HD12	1.94	0.49
1:C:460:LEU:HD23	1:C:548:PHE:HZ	1.78	0.49
1:D:476:CYS:HA	1:D:479:ILE:HD12	1.94	0.49
1:D:532:VAL:HG11	1:D:551:LEU:HB3	1.95	0.49
1:A:325:ARG:NH2	1:A:358:PHE:HB2	2.28	0.49
1:A:532:VAL:HG11	1:A:551:LEU:HB3	1.95	0.49
1:A:583:MET:O	1:A:586:LEU:N	2.45	0.49
1:B:378:SER:HA	1:B:387:SER:HA	1.94	0.49
1:D:460:LEU:HD23	1:D:548:PHE:HZ	1.78	0.49
1:D:583:MET:HA	1:D:586:LEU:HB2	1.94	0.49
1:A:328:ASN:HA	1:A:345:TYR:CE2	2.48	0.49
1:B:682:ASP:OD1	1:B:682:ASP:N	2.46	0.49
1:B:560:ASN:HB2	1:C:656:LEU:HD11	1.94	0.49
1:C:682:ASP:OD1	1:C:683:THR:N	2.43	0.49
1:D:484:ILE:O	1:D:488:VAL:HG23	2.13	0.49
1:D:566:VAL:HG12	1:D:570:TRP:CZ3	2.48	0.49
1:B:566:VAL:HG12	1:B:570:TRP:CZ3	2.48	0.49
1:C:328:ASN:HA	1:C:345:TYR:CE2	2.48	0.49
1:D:216:TYR:O	1:D:220:VAL:N	2.39	0.49
1:D:323:GLN:OE1	1:D:414:TRP:CD1	2.66	0.49
1:D:684:TYR:HA	1:D:687:VAL:HG22	1.95	0.49
1:A:367:ILE:O	1:A:367:ILE:CG2	2.61	0.49
1:A:224:LEU:HD22	1:A:577:ILE:HD11	1.95	0.49
1:B:328:ASN:HA	1:B:345:TYR:CE2	2.48	0.49
1:B:427:SER:OG	1:B:437:CYS:O	2.25	0.49
1:C:357:PRO:HB2	1:C:361:ARG:HE	1.77	0.49
1:D:362:ASN:H	1:D:366:TRP:HB2	1.78	0.49
1:B:224:LEU:O	1:B:228:LEU:N	2.26	0.48
1:B:362:ASN:H	1:B:366:TRP:HB2	1.78	0.48
1:C:237:LEU:O	1:C:241:MET:N	2.35	0.48
1:A:216:TYR:O	1:A:220:VAL:N	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:TYR:HA	1:A:390:GLY:O	2.14	0.48
1:A:484:ILE:O	1:A:488:VAL:HG23	2.13	0.48
1:C:325:ARG:NH2	1:C:358:PHE:HB2	2.28	0.48
1:C:378:SER:HA	1:C:387:SER:HA	1.94	0.48
1:C:582:THR:O	1:C:586:LEU:N	2.34	0.48
1:D:367:ILE:O	1:D:367:ILE:CG2	2.61	0.48
1:D:536:LEU:HA	1:D:539:LEU:HB3	1.94	0.48
1:A:378:SER:HA	1:A:387:SER:HA	1.94	0.48
1:B:367:ILE:O	1:B:367:ILE:CG2	2.61	0.48
1:C:269:ASN:OD1	1:C:271:LYS:N	2.47	0.48
1:C:323:GLN:OE1	1:C:414:TRP:CD1	2.66	0.48
1:A:566:VAL:HG12	1:A:570:TRP:CZ3	2.48	0.48
1:A:670:PHE:HA	1:A:673:LEU:HD12	1.96	0.48
1:B:368:TYR:HA	1:B:390:GLY:O	2.14	0.48
1:B:224:LEU:HD22	1:B:577:ILE:HD11	1.95	0.48
1:D:586:LEU:HA	1:D:589:THR:HG23	1.95	0.48
1:B:247:TYR:OH	1:B:251:ARG:HD2	2.14	0.48
1:B:280:TRP:O	1:B:284:GLU:HG2	2.14	0.48
1:B:484:ILE:O	1:B:488:VAL:HG23	2.13	0.48
1:C:367:ILE:CG2	1:C:367:ILE:O	2.61	0.48
1:C:484:ILE:O	1:C:488:VAL:HG23	2.13	0.48
1:C:532:VAL:HG11	1:C:551:LEU:HB3	1.95	0.48
1:C:555:GLN:O	1:C:559:ASN:N	2.35	0.48
1:C:566:VAL:HG12	1:C:570:TRP:CZ3	2.48	0.48
1:D:644:ILE:HG23	1:D:646:PHE:N	2.28	0.48
1:D:682:ASP:OD1	1:D:683:THR:N	2.43	0.48
1:A:280:TRP:O	1:A:284:GLU:HG2	2.14	0.48
1:A:319:PRO:HB2	1:A:395:LEU:HD22	1.95	0.48
1:B:362:ASN:HB2	2:B:1002:NAG:HN2	1.75	0.48
1:B:532:VAL:HG11	1:B:551:LEU:HB3	1.95	0.48
1:D:237:LEU:O	1:D:241:MET:N	2.35	0.48
1:D:269:ASN:OD1	1:D:271:LYS:N	2.47	0.48
1:A:684:TYR:HA	1:A:687:VAL:HG22	1.95	0.48
1:C:682:ASP:OD1	1:C:682:ASP:N	2.46	0.48
1:A:323:GLN:OE1	1:A:414:TRP:CD1	2.66	0.48
1:A:460:LEU:HD23	1:A:548:PHE:HZ	1.78	0.48
1:A:493:LEU:HD23	1:A:496:ARG:HE	1.79	0.48
1:C:536:LEU:HA	1:C:539:LEU:HB3	1.94	0.48
1:B:560:ASN:CB	1:C:656:LEU:HD11	2.44	0.48
1:D:328:ASN:HA	1:D:345:TYR:CE2	2.48	0.48
1:D:224:LEU:HD22	1:D:577:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:MET:O	1:A:279:PHE:HB3	2.14	0.48
1:A:362:ASN:H	1:A:366:TRP:HB2	1.77	0.48
1:A:611:TYR:O	1:A:615:ALA:N	2.45	0.48
1:A:644:ILE:HG23	1:A:646:PHE:N	2.28	0.48
1:B:309:ILE:HG13	1:B:310:PHE:N	2.19	0.48
1:C:362:ASN:H	1:C:366:TRP:HB2	1.78	0.48
1:C:602:ILE:O	1:C:606:ILE:N	2.33	0.48
1:C:644:ILE:HG23	1:C:646:PHE:N	2.28	0.48
1:D:280:TRP:O	1:D:284:GLU:HG2	2.14	0.48
1:A:682:ASP:OD1	1:A:682:ASP:N	2.46	0.48
1:B:323:GLN:OE1	1:B:414:TRP:CD1	2.66	0.48
1:B:493:LEU:HD23	1:B:496:ARG:HE	1.79	0.48
1:B:634:PHE:O	1:B:637:PHE:N	2.41	0.48
1:C:586:LEU:HA	1:C:589:THR:HG23	1.95	0.48
1:D:325:ARG:NH2	1:D:358:PHE:HB2	2.28	0.48
1:D:368:TYR:HA	1:D:390:GLY:O	2.13	0.48
1:A:256:LEU:HD22	1:A:257:PHE:CZ	2.49	0.47
1:A:269:ASN:OD1	1:A:271:LYS:N	2.47	0.47
1:A:317:GLY:O	1:A:318:VAL:HG13	2.14	0.47
1:B:586:LEU:HA	1:B:589:THR:HG23	1.95	0.47
1:A:247:TYR:OH	1:A:251:ARG:HD2	2.14	0.47
1:B:269:ASN:OD1	1:B:271:LYS:N	2.47	0.47
1:B:644:ILE:HG23	1:B:646:PHE:N	2.28	0.47
1:B:670:PHE:HA	1:B:673:LEU:HD12	1.96	0.47
1:C:256:LEU:HD22	1:C:257:PHE:CZ	2.49	0.47
1:C:280:TRP:O	1:C:284:GLU:HG2	2.14	0.47
1:C:317:GLY:O	1:C:318:VAL:HG13	2.14	0.47
1:C:670:PHE:HA	1:C:673:LEU:HD12	1.96	0.47
1:A:362:ASN:HB2	2:A:1002:NAG:HN2	1.75	0.47
1:A:310:PHE:HD2	1:A:311:TYR:CD2	2.33	0.47
1:A:586:LEU:HA	1:A:589:THR:HG23	1.95	0.47
1:C:276:MET:O	1:C:279:PHE:HB3	2.14	0.47
1:D:319:PRO:HB2	1:D:395:LEU:HD22	1.95	0.47
1:D:493:LEU:HD23	1:D:496:ARG:HE	1.79	0.47
1:D:690:ASP:O	1:D:693:GLN:HG2	2.15	0.47
1:B:276:MET:O	1:B:279:PHE:HB3	2.14	0.47
1:B:310:PHE:HD2	1:B:311:TYR:CD2	2.32	0.47
1:B:317:GLY:O	1:B:318:VAL:HG13	2.14	0.47
1:B:432:ASN:ND2	1:C:447:ALA:O	2.37	0.47
1:B:249:TYR:HD1	1:C:448:THR:HB	1.80	0.47
1:A:634:PHE:CE1	1:B:658:PRO:HB3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:ASN:HA	1:B:678:ALA:HB2	1.94	0.47
1:C:319:PRO:HB2	1:C:395:LEU:HD22	1.95	0.47
1:C:626:PHE:HE1	1:C:635:THR:HG21	1.80	0.47
1:D:325:ARG:HG2	1:D:326:VAL:N	2.30	0.47
1:D:626:PHE:HE1	1:D:635:THR:HG21	1.80	0.47
1:A:297:PRO:O	1:A:298:SER:OG	2.28	0.47
1:B:296:GLN:OE1	1:C:417:ARG:NH1	2.48	0.47
1:C:325:ARG:HG2	1:C:326:VAL:N	2.30	0.47
1:C:532:VAL:HG13	1:C:551:LEU:HD13	1.97	0.47
1:D:256:LEU:HD22	1:D:257:PHE:CZ	2.49	0.47
1:D:317:GLY:O	1:D:318:VAL:HG13	2.14	0.47
1:A:690:ASP:O	1:A:693:GLN:HG2	2.15	0.47
1:B:256:LEU:HD22	1:B:257:PHE:CZ	2.49	0.47
1:C:690:ASP:O	1:C:693:GLN:HG2	2.15	0.47
1:A:532:VAL:HG13	1:A:551:LEU:HD13	1.97	0.47
1:B:532:VAL:HG13	1:B:551:LEU:HD13	1.97	0.47
1:C:368:TYR:HA	1:C:390:GLY:O	2.14	0.47
1:C:322:ARG:HB3	1:C:423:PHE:HB2	1.97	0.47
1:C:493:LEU:HD23	1:C:496:ARG:HE	1.79	0.47
1:D:247:TYR:OH	1:D:251:ARG:HD2	2.14	0.47
1:A:605:PHE:HA	1:A:608:PHE:HB3	1.97	0.47
1:C:224:LEU:HD22	1:C:577:ILE:HD11	1.95	0.47
1:C:312:GLU:OE1	1:D:449:GLY:N	2.48	0.47
1:D:276:MET:O	1:D:279:PHE:HB3	2.14	0.47
1:D:279:PHE:CE1	1:D:443:VAL:HG21	2.46	0.47
1:D:532:VAL:HG13	1:D:551:LEU:HD13	1.97	0.47
1:C:560:ASN:HB2	1:D:656:LEU:HD11	1.96	0.47
3:A:1006:PX6:H61	3:A:1006:PX6:H54	1.70	0.47
1:B:547:ASN:O	1:B:549:GLU:N	2.48	0.47
1:D:518:SER:O	1:D:522:ILE:HG13	2.15	0.47
1:D:605:PHE:HA	1:D:608:PHE:HB3	1.97	0.47
1:A:325:ARG:HG2	1:A:326:VAL:N	2.30	0.47
1:A:449:GLY:N	1:D:312:GLU:OE1	2.48	0.47
1:C:611:TYR:O	1:C:615:ALA:N	2.45	0.47
1:D:536:LEU:HD12	1:D:539:LEU:HD23	1.97	0.47
1:A:518:SER:O	1:A:522:ILE:HG13	2.16	0.46
1:A:536:LEU:HD12	1:A:539:LEU:HD23	1.97	0.46
1:A:626:PHE:HE1	1:A:635:THR:HG21	1.80	0.46
1:B:297:PRO:O	1:B:298:SER:OG	2.28	0.46
1:B:319:PRO:HB2	1:B:395:LEU:HD22	1.95	0.46
1:B:536:LEU:HD12	1:B:539:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:TYR:OH	1:C:251:ARG:HD2	2.14	0.46
1:C:677:LEU:HD21	1:D:673:LEU:HB3	1.97	0.46
1:D:322:ARG:HB3	1:D:423:PHE:HB2	1.97	0.46
1:B:322:ARG:HB3	1:B:423:PHE:HB2	1.97	0.46
1:B:320:ARG:N	1:B:425:ASP:O	2.44	0.46
1:B:626:PHE:HE1	1:B:635:THR:HG21	1.80	0.46
3:C:1006:PX6:H49	3:C:1006:PX6:H42	1.53	0.46
1:C:310:PHE:HD2	1:C:311:TYR:CD2	2.32	0.46
1:C:605:PHE:HA	1:C:608:PHE:HB3	1.97	0.46
1:D:547:ASN:O	1:D:549:GLU:N	2.48	0.46
1:D:687:VAL:HA	1:D:690:ASP:HB3	1.97	0.46
1:A:656:LEU:HD11	1:D:560:ASN:HB2	1.95	0.46
1:A:687:VAL:HA	1:A:690:ASP:HB3	1.97	0.46
3:C:1006:PX6:H46	3:C:1006:PX6:H53	1.47	0.46
1:C:518:SER:O	1:C:522:ILE:HG13	2.16	0.46
1:A:279:PHE:CE1	1:A:443:VAL:HG21	2.46	0.46
1:B:325:ARG:HG2	1:B:326:VAL:N	2.30	0.46
1:C:349:SER:H	1:C:352:SER:HG	1.62	0.46
1:C:536:LEU:HD12	1:C:539:LEU:HD23	1.97	0.46
1:D:310:PHE:HD2	1:D:311:TYR:CD2	2.33	0.46
1:D:670:PHE:HA	1:D:673:LEU:HD12	1.96	0.46
1:B:216:TYR:O	1:B:220:VAL:N	2.39	0.46
1:A:296:GLN:OE1	1:B:417:ARG:NH1	2.49	0.46
1:C:634:PHE:CE1	1:D:658:PRO:HB3	2.51	0.46
1:A:470:ASP:O	1:A:474:ALA:N	2.36	0.46
1:B:410:LYS:O	1:B:413:VAL:N	2.49	0.46
1:A:547:ASN:O	1:A:549:GLU:N	2.48	0.46
1:B:605:PHE:HA	1:B:608:PHE:HB3	1.97	0.46
1:A:590:MET:HB2	1:B:675:MET:HE1	1.98	0.46
1:C:547:ASN:O	1:C:549:GLU:N	2.48	0.46
1:A:619:PHE:HB2	1:A:626:PHE:CD2	2.51	0.46
4:B:1007:PLM:HC2	4:B:1007:PLM:HF1	1.75	0.46
1:B:470:ASP:O	1:B:474:ALA:N	2.36	0.46
1:D:349:SER:O	1:D:353:GLU:N	2.49	0.46
1:B:568:PHE:HD1	1:B:571:ILE:HD11	1.80	0.46
1:B:690:ASP:O	1:B:693:GLN:HG2	2.15	0.46
1:D:619:PHE:HB2	1:D:626:PHE:CD2	2.51	0.46
1:A:448:THR:HB	1:D:249:TYR:HD1	1.81	0.45
1:B:349:SER:H	1:B:352:SER:HG	1.64	0.45
1:A:677:LEU:HD21	1:B:673:LEU:HB3	1.98	0.45
1:A:322:ARG:HB3	1:A:423:PHE:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:ASN:CB	1:A:648:GLU:OE2	2.56	0.45
1:A:658:PRO:HB3	1:D:634:PHE:CE1	2.51	0.45
3:B:1006:PX6:H49	3:B:1006:PX6:H42	1.53	0.45
1:B:349:SER:O	1:B:353:GLU:N	2.49	0.45
1:C:323:GLN:NE2	1:C:414:TRP:CD1	2.82	0.45
1:C:597:LEU:O	1:C:600:PHE:N	2.50	0.45
1:A:224:LEU:O	1:A:228:LEU:N	2.26	0.45
1:A:349:SER:H	1:A:352:SER:HG	1.64	0.45
4:B:1007:PLM:HA2	4:B:1007:PLM:HD1	1.67	0.45
4:C:1008:PLM:H21	4:C:1008:PLM:H52	1.83	0.45
1:C:687:VAL:HA	1:C:690:ASP:HB3	1.97	0.45
1:A:656:LEU:HD11	1:D:560:ASN:CB	2.46	0.45
1:D:597:LEU:O	1:D:600:PHE:N	2.50	0.45
1:D:560:ASN:O	1:D:563:ALA:N	2.50	0.45
1:A:410:LYS:O	1:A:413:VAL:N	2.49	0.45
1:A:568:PHE:HD1	1:A:571:ILE:HD11	1.80	0.45
1:B:687:VAL:HA	1:B:690:ASP:HB3	1.97	0.45
1:C:568:PHE:HD1	1:C:571:ILE:HD11	1.80	0.45
1:D:682:ASP:OD1	1:D:682:ASP:N	2.46	0.45
1:A:278:ASP:O	1:A:282:PHE:N	2.49	0.45
3:C:1006:PX6:H67	3:C:1006:PX6:H60	1.73	0.45
1:C:410:LYS:O	1:C:413:VAL:N	2.49	0.45
1:B:611:TYR:HA	1:B:614:LEU:HB3	1.99	0.45
1:C:507:TRP:HB3	1:C:575:LYS:HZ3	1.81	0.45
1:C:249:TYR:HD1	1:D:448:THR:HB	1.82	0.45
1:A:673:LEU:HB3	1:D:677:LEU:HD21	1.98	0.45
1:A:406:VAL:HA	1:A:409:LEU:HD12	1.99	0.45
1:D:410:LYS:O	1:D:413:VAL:N	2.49	0.45
1:B:518:SER:O	1:B:522:ILE:HG13	2.16	0.45
4:A:1007:PLM:H91	1:B:667:PHE:CE2	2.52	0.45
1:C:349:SER:O	1:C:353:GLU:N	2.49	0.45
1:C:681:ASN:HA	1:D:678:ALA:HB2	1.98	0.45
1:D:362:ASN:HB2	2:D:1002:NAG:HN2	1.78	0.45
3:D:1006:PX6:H60	3:D:1006:PX6:H67	1.71	0.45
1:A:349:SER:O	1:A:353:GLU:N	2.49	0.45
1:C:560:ASN:O	1:C:563:ALA:N	2.50	0.45
1:D:406:VAL:HA	1:D:409:LEU:HD12	1.99	0.45
1:D:568:PHE:HD1	1:D:571:ILE:HD11	1.81	0.45
1:C:296:GLN:HG2	1:C:311:TYR:HD1	1.82	0.44
4:A:1007:PLM:HA2	4:A:1007:PLM:HD1	1.71	0.44
1:A:237:LEU:O	1:A:241:MET:N	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:PHE:CD1	1:A:571:ILE:HD11	2.52	0.44
1:A:582:THR:O	1:A:586:LEU:N	2.34	0.44
1:C:321:ILE:HG13	1:C:395:LEU:HD11	1.99	0.44
1:D:224:LEU:O	1:D:228:LEU:N	2.26	0.44
1:D:484:ILE:O	1:D:488:VAL:N	2.48	0.44
1:B:308:PHE:HB3	1:B:315:LEU:H	1.83	0.44
1:B:321:ILE:HG13	1:B:395:LEU:HD11	1.99	0.44
1:B:570:TRP:O	1:B:573:LEU:N	2.51	0.44
1:C:382:ILE:HG23	1:C:383:ILE:N	2.32	0.44
1:C:570:TRP:O	1:C:573:LEU:N	2.51	0.44
1:D:349:SER:H	1:D:352:SER:HG	1.62	0.44
1:D:611:TYR:HA	1:D:614:LEU:HB3	1.99	0.44
1:A:667:PHE:CE2	4:D:1007:PLM:H91	2.53	0.44
1:A:677:LEU:O	1:A:681:ASN:N	2.46	0.44
1:B:296:GLN:HG2	1:B:311:TYR:HD1	1.83	0.44
1:C:320:ARG:N	1:C:425:ASP:O	2.44	0.44
1:C:226:THR:HB	1:C:483:PHE:HZ	1.83	0.44
1:C:568:PHE:CD1	1:C:571:ILE:HD11	2.52	0.44
1:D:235:CYS:O	1:D:238:THR:OG1	2.32	0.44
1:D:568:PHE:CD1	1:D:571:ILE:HD11	2.52	0.44
1:D:677:LEU:O	1:D:681:ASN:N	2.46	0.44
1:A:507:TRP:HB3	1:A:575:LYS:HZ1	1.82	0.44
1:A:574:PHE:HE1	1:B:603:MET:HG3	1.82	0.44
1:D:626:PHE:O	1:D:627:SER:C	2.56	0.44
1:C:560:ASN:CB	1:D:656:LEU:HD11	2.47	0.44
1:A:308:PHE:HB3	1:A:315:LEU:H	1.83	0.44
1:A:296:GLN:HG2	1:A:311:TYR:HD1	1.83	0.44
1:A:570:TRP:O	1:A:573:LEU:N	2.51	0.44
1:B:406:VAL:HA	1:B:409:LEU:HD12	1.99	0.44
1:B:451:VAL:O	1:B:452:ILE:HD13	2.18	0.44
1:C:308:PHE:HB3	1:C:315:LEU:H	1.83	0.44
1:C:645:ASN:CB	1:C:648:GLU:OE2	2.56	0.44
3:D:1006:PX6:H53	3:D:1006:PX6:H46	1.47	0.44
1:D:226:THR:HB	1:D:483:PHE:HZ	1.83	0.44
1:A:564:VAL:O	1:A:567:PHE:HB3	2.18	0.44
1:B:235:CYS:O	1:B:238:THR:OG1	2.32	0.44
1:B:597:LEU:O	1:B:600:PHE:N	2.50	0.44
4:C:1007:PLM:H91	1:D:667:PHE:CE2	2.53	0.44
1:C:238:THR:OG1	1:C:239:TYR:N	2.51	0.44
1:C:451:VAL:O	1:C:452:ILE:HD13	2.18	0.44
1:D:228:LEU:HA	1:D:231:LEU:HD23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1006:PX6:H53	3:A:1006:PX6:H46	1.47	0.44
1:A:310:PHE:HD2	1:A:311:TYR:HD2	1.65	0.44
1:A:484:ILE:O	1:A:488:VAL:N	2.48	0.44
1:A:611:TYR:HA	1:A:614:LEU:HB3	1.99	0.44
1:B:226:THR:HB	1:B:483:PHE:HZ	1.83	0.44
1:B:560:ASN:O	1:B:563:ALA:N	2.50	0.44
1:C:235:CYS:O	1:C:238:THR:OG1	2.32	0.44
1:C:560:ASN:OD1	1:C:561:ILE:N	2.51	0.44
1:A:228:LEU:HA	1:A:231:LEU:HD23	2.00	0.44
1:A:560:ASN:O	1:A:563:ALA:N	2.50	0.44
1:A:686:GLU:O	1:A:689:SER:OG	2.26	0.44
4:B:1007:PLM:H91	1:C:667:PHE:CE2	2.53	0.44
1:B:568:PHE:CD1	1:B:571:ILE:HD11	2.52	0.44
1:C:247:TYR:CZ	1:C:251:ARG:HB2	2.53	0.44
1:C:611:TYR:HA	1:C:614:LEU:HB3	1.99	0.44
1:D:656:LEU:HD23	1:D:656:LEU:HA	1.72	0.44
1:A:312:GLU:OE1	1:B:449:GLY:N	2.50	0.43
1:B:634:PHE:CE1	1:C:658:PRO:HB3	2.53	0.43
1:D:570:TRP:O	1:D:573:LEU:N	2.51	0.43
1:C:680:ILE:HD13	1:D:674:ASN:HA	2.00	0.43
1:A:323:GLN:NE2	1:A:414:TRP:CD1	2.82	0.43
1:A:382:ILE:HG23	1:A:383:ILE:N	2.32	0.43
1:A:638:ARG:NE	1:A:643:ASP:OD2	2.48	0.43
1:B:319:PRO:HA	1:B:425:ASP:O	2.18	0.43
1:C:319:PRO:HA	1:C:425:ASP:O	2.18	0.43
1:D:247:TYR:CZ	1:D:251:ARG:HB2	2.53	0.43
4:A:1007:PLM:HF1	4:A:1007:PLM:HC2	1.76	0.43
1:A:321:ILE:HG13	1:A:395:LEU:HD11	1.99	0.43
1:B:564:VAL:O	1:B:567:PHE:HB3	2.18	0.43
1:C:564:VAL:O	1:C:567:PHE:HB3	2.18	0.43
1:D:308:PHE:HB3	1:D:315:LEU:H	1.83	0.43
1:A:326:VAL:HG13	1:A:352:SER:O	2.19	0.43
1:B:560:ASN:OD1	1:B:560:ASN:N	2.51	0.43
1:C:406:VAL:HA	1:C:409:LEU:HD12	1.99	0.43
1:C:626:PHE:O	1:C:627:SER:C	2.56	0.43
1:D:321:ILE:HG13	1:D:395:LEU:HD11	1.99	0.43
1:D:326:VAL:HG13	1:D:352:SER:O	2.19	0.43
1:A:451:VAL:O	1:A:452:ILE:HD13	2.18	0.43
1:A:678:ALA:HB2	1:D:681:ASN:HA	2.00	0.43
1:A:249:TYR:HD1	1:B:448:THR:HB	1.84	0.43
1:B:608:PHE:O	1:B:636:GLN:NE2	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1007:PLM:HF1	4:D:1007:PLM:HC2	1.76	0.43
1:D:560:ASN:OD1	1:D:560:ASN:N	2.51	0.43
1:A:226:THR:HB	1:A:483:PHE:HZ	1.83	0.43
1:A:247:TYR:CZ	1:A:251:ARG:HB2	2.53	0.43
1:A:597:LEU:O	1:A:600:PHE:N	2.50	0.43
1:B:238:THR:OG1	1:B:239:TYR:N	2.51	0.43
1:B:382:ILE:HG23	1:B:383:ILE:N	2.32	0.43
1:D:278:ASP:O	1:D:282:PHE:N	2.49	0.43
1:D:451:VAL:O	1:D:452:ILE:HD13	2.18	0.43
1:A:379:HIS:HB2	1:A:440:ARG:HH22	1.84	0.43
1:A:677:LEU:HD23	1:A:677:LEU:HA	1.74	0.43
1:B:310:PHE:HD2	1:B:311:TYR:HD2	1.65	0.43
1:B:508:ASN:HA	1:B:511:ASP:OD2	2.19	0.43
1:A:684:TYR:HE2	1:B:682:ASP:OD2	2.02	0.43
1:C:228:LEU:HA	1:C:231:LEU:HD23	2.00	0.43
1:C:293:TRP:CH2	1:C:310:PHE:HB3	2.54	0.43
1:C:405:GLN:O	1:C:409:LEU:HG	2.19	0.43
1:D:319:PRO:HA	1:D:425:ASP:O	2.18	0.43
1:B:293:TRP:CH2	1:B:310:PHE:HB3	2.54	0.43
1:B:379:HIS:HB2	1:B:440:ARG:HH22	1.84	0.43
1:B:582:THR:O	1:B:586:LEU:N	2.34	0.43
1:B:677:LEU:HA	1:B:677:LEU:HD23	1.74	0.43
1:C:508:ASN:HA	1:C:511:ASP:OD2	2.19	0.43
1:D:238:THR:OG1	1:D:239:TYR:N	2.51	0.43
1:D:564:VAL:O	1:D:567:PHE:HB3	2.18	0.43
1:A:656:LEU:HA	1:A:656:LEU:HD23	1.72	0.43
1:B:247:TYR:CZ	1:B:251:ARG:HB2	2.53	0.43
1:B:611:TYR:HB3	1:B:660:TYR:HE1	1.84	0.43
1:C:560:ASN:N	1:C:560:ASN:OD1	2.51	0.43
1:D:382:ILE:HG23	1:D:383:ILE:N	2.32	0.43
1:A:319:PRO:HA	1:A:425:ASP:O	2.18	0.43
1:A:690:ASP:CA	1:A:693:GLN:HG2	2.46	0.43
1:C:532:VAL:O	1:C:535:LEU:HG	2.19	0.43
1:C:677:LEU:CD2	1:D:673:LEU:HB3	2.49	0.43
1:D:310:PHE:HD2	1:D:311:TYR:HD2	1.65	0.43
1:A:293:TRP:CH2	1:A:310:PHE:HB3	2.54	0.42
1:A:508:ASN:HA	1:A:511:ASP:OD2	2.19	0.42
1:B:532:VAL:O	1:B:535:LEU:HG	2.19	0.42
1:B:656:LEU:HA	1:B:656:LEU:HD23	1.72	0.42
1:C:297:PRO:O	1:C:298:SER:OG	2.28	0.42
1:C:326:VAL:HG13	1:C:352:SER:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:405:GLN:O	1:D:409:LEU:HG	2.19	0.42
1:B:326:VAL:HG13	1:B:352:SER:O	2.19	0.42
1:C:611:TYR:HB3	1:C:660:TYR:HE1	1.84	0.42
1:D:611:TYR:HB3	1:D:660:TYR:HE1	1.84	0.42
1:A:536:LEU:HD23	1:A:540:GLU:HB3	2.02	0.42
1:A:611:TYR:HB3	1:A:660:TYR:HE1	1.84	0.42
1:A:626:PHE:O	1:A:627:SER:C	2.56	0.42
1:B:592:ARG:HA	1:B:592:ARG:HD2	1.85	0.42
1:D:226:THR:HB	1:D:483:PHE:CZ	2.55	0.42
1:D:293:TRP:CH2	1:D:310:PHE:HB3	2.54	0.42
1:D:324:LEU:HD13	1:D:348:TYR:CZ	2.55	0.42
1:D:690:ASP:CA	1:D:693:GLN:HG2	2.46	0.42
1:A:418:GLY:O	1:A:420:ARG:HG2	2.19	0.42
1:A:532:VAL:O	1:A:535:LEU:HG	2.19	0.42
4:B:1008:PLM:H21	4:B:1008:PLM:H52	1.83	0.42
1:B:228:LEU:HA	1:B:231:LEU:HD23	2.00	0.42
1:B:588:THR:HA	1:B:591:SER:HB3	2.01	0.42
1:C:324:LEU:HD13	1:C:348:TYR:CZ	2.55	0.42
1:C:379:HIS:HB2	1:C:440:ARG:HH22	1.84	0.42
4:B:1007:PLM:H91	1:C:667:PHE:HE2	1.84	0.42
3:D:1006:PX6:H42	3:D:1006:PX6:H49	1.53	0.42
1:D:379:HIS:HB2	1:D:440:ARG:HH22	1.84	0.42
1:D:487:TYR:HB3	1:D:491:GLU:CD	2.40	0.42
1:A:588:THR:HA	1:A:591:SER:HB3	2.01	0.42
1:B:470:ASP:O	1:B:473:LEU:N	2.53	0.42
1:B:626:PHE:O	1:B:627:SER:C	2.56	0.42
1:C:310:PHE:HD2	1:C:311:TYR:HD2	1.65	0.42
1:C:484:ILE:O	1:C:488:VAL:N	2.48	0.42
1:D:536:LEU:HD23	1:D:540:GLU:HB3	2.02	0.42
1:A:673:LEU:HB3	1:D:677:LEU:CD2	2.49	0.42
1:A:405:GLN:O	1:A:409:LEU:HG	2.19	0.42
1:A:653:ASN:ND2	1:A:656:LEU:HD12	2.35	0.42
1:B:418:GLY:O	1:B:420:ARG:HG2	2.19	0.42
1:B:226:THR:HB	1:B:483:PHE:CZ	2.55	0.42
1:B:538:PHE:HA	1:B:541:ASP:CG	2.40	0.42
1:C:487:TYR:HB3	1:C:491:GLU:CD	2.40	0.42
1:D:470:ASP:O	1:D:473:LEU:N	2.53	0.42
1:A:226:THR:HB	1:A:483:PHE:CZ	2.55	0.42
1:A:560:ASN:OD1	1:A:561:ILE:N	2.51	0.42
1:B:324:LEU:HD13	1:B:348:TYR:CZ	2.54	0.42
1:B:487:TYR:HB3	1:B:491:GLU:CD	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:653:ASN:ND2	1:B:656:LEU:HD12	2.35	0.42
1:C:226:THR:HB	1:C:483:PHE:CZ	2.55	0.42
1:B:312:GLU:OE1	1:C:449:GLY:N	2.53	0.42
1:D:508:ASN:HA	1:D:511:ASP:OD2	2.19	0.42
1:D:532:VAL:O	1:D:535:LEU:HG	2.19	0.42
1:A:238:THR:OG1	1:A:239:TYR:N	2.51	0.42
1:A:538:PHE:HA	1:A:541:ASP:CG	2.40	0.42
1:A:574:PHE:CE1	1:B:603:MET:HG3	2.55	0.42
1:B:405:GLN:O	1:B:409:LEU:HG	2.19	0.42
3:C:1006:PX6:H61	3:C:1006:PX6:H54	1.65	0.42
1:C:418:GLY:O	1:C:420:ARG:HG2	2.19	0.42
1:C:653:ASN:ND2	1:C:656:LEU:HD12	2.35	0.42
1:D:333:ILE:HG13	1:D:334:PRO:HD2	2.01	0.42
1:A:324:LEU:HD13	1:A:348:TYR:CZ	2.54	0.42
1:A:487:TYR:HB3	1:A:491:GLU:CD	2.40	0.42
1:B:310:PHE:HB2	1:B:311:TYR:CD2	2.55	0.42
1:B:323:GLN:NE2	1:B:414:TRP:CD1	2.82	0.42
1:B:619:PHE:HB2	1:B:626:PHE:CD2	2.51	0.42
1:D:418:GLY:O	1:D:420:ARG:HG2	2.19	0.42
1:D:653:ASN:ND2	1:D:656:LEU:HD12	2.35	0.42
1:C:536:LEU:HD23	1:C:540:GLU:HB3	2.02	0.42
1:B:681:ASN:HA	1:C:678:ALA:HB2	2.02	0.42
1:A:470:ASP:O	1:A:473:LEU:N	2.53	0.41
1:A:512:VAL:O	1:A:516:VAL:HG23	2.20	0.41
1:B:512:VAL:O	1:B:516:VAL:HG23	2.20	0.41
1:B:645:ASN:CB	1:B:648:GLU:OE2	2.56	0.41
1:B:682:ASP:OD1	1:B:683:THR:N	2.43	0.41
4:C:1007:PLM:H91	1:D:667:PHE:HE2	1.85	0.41
1:C:470:ASP:O	1:C:473:LEU:N	2.53	0.41
1:C:538:PHE:HA	1:C:541:ASP:CG	2.40	0.41
1:D:588:THR:HA	1:D:591:SER:HB3	2.01	0.41
1:A:310:PHE:HB2	1:A:311:TYR:CD2	2.55	0.41
1:A:644:ILE:HG23	1:A:646:PHE:CB	2.50	0.41
3:B:1006:PX6:H60	3:B:1006:PX6:H67	1.71	0.41
1:B:560:ASN:ND2	3:B:1006:PX6:H43	2.35	0.41
1:D:323:GLN:NE2	1:D:414:TRP:CD1	2.82	0.41
1:B:278:ASP:O	1:B:282:PHE:N	2.49	0.41
1:B:333:ILE:HG13	1:B:334:PRO:HD2	2.01	0.41
1:B:420:ARG:HD3	1:B:420:ARG:HA	1.88	0.41
1:B:590:MET:HB2	1:C:675:MET:HE1	2.02	0.41
1:B:638:ARG:NE	1:B:643:ASP:OD2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:588:THR:HA	1:C:591:SER:HB3	2.01	0.41
1:C:677:LEU:O	1:C:681:ASN:N	2.46	0.41
1:A:235:CYS:O	1:A:238:THR:OG1	2.32	0.41
1:B:417:ARG:HG2	1:B:418:GLY:N	2.36	0.41
1:B:536:LEU:HD23	1:B:540:GLU:HB3	2.02	0.41
4:A:1007:PLM:H91	1:B:667:PHE:HE2	1.86	0.41
1:C:333:ILE:HG13	1:C:334:PRO:HD2	2.01	0.41
1:C:342:LYS:HB3	1:C:343:GLU:CD	2.41	0.41
1:D:560:ASN:ND2	3:D:1006:PX6:H43	2.35	0.41
1:A:560:ASN:OD1	1:A:560:ASN:N	2.51	0.41
1:C:644:ILE:HG23	1:C:646:PHE:CB	2.50	0.41
1:D:320:ARG:N	1:D:425:ASP:O	2.44	0.41
1:D:644:ILE:HG23	1:D:646:PHE:CB	2.50	0.41
1:A:683:THR:O	1:A:687:VAL:HG22	2.21	0.41
1:C:310:PHE:HB2	1:C:311:TYR:CD2	2.55	0.41
1:D:274:SER:OG	1:D:275:SER:N	2.54	0.41
1:D:310:PHE:HB2	1:D:311:TYR:CD2	2.55	0.41
1:D:342:LYS:HB3	1:D:343:GLU:CD	2.41	0.41
1:D:538:PHE:HA	1:D:541:ASP:CG	2.40	0.41
1:A:274:SER:OG	1:A:275:SER:N	2.54	0.41
1:A:409:LEU:HB3	1:A:414:TRP:CH2	2.56	0.41
1:A:320:ARG:N	1:A:425:ASP:O	2.43	0.41
1:B:644:ILE:HG23	1:B:646:PHE:CB	2.50	0.41
1:D:284:GLU:HA	1:D:288:LEU:HD13	2.03	0.41
1:D:296:GLN:HG2	1:D:311:TYR:HD1	1.83	0.41
1:D:568:PHE:HA	1:D:571:ILE:HG12	2.03	0.41
1:B:310:PHE:CD2	1:B:311:TYR:CD2	3.09	0.41
1:C:568:PHE:HA	1:C:571:ILE:HG12	2.03	0.41
1:C:619:PHE:HB2	1:C:626:PHE:CD2	2.51	0.41
5:D:1011:CHS:O	5:D:1011:CHS:OH	2.37	0.41
4:A:1008:PLM:H52	4:A:1008:PLM:H21	1.87	0.41
1:A:284:GLU:HA	1:A:288:LEU:HD13	2.03	0.41
1:A:310:PHE:CD2	1:A:311:TYR:CD2	3.09	0.41
1:A:333:ILE:HG13	1:A:334:PRO:HD2	2.01	0.41
1:A:483:PHE:O	1:A:486:TYR:HB3	2.21	0.41
1:A:677:LEU:CD2	1:B:673:LEU:HB3	2.51	0.41
1:C:444:GLU:HB2	1:C:452:ILE:HB	2.03	0.41
1:C:512:VAL:O	1:C:516:VAL:HG23	2.20	0.41
1:C:560:ASN:ND2	3:C:1006:PX6:H43	2.36	0.41
1:D:483:PHE:O	1:D:486:TYR:HB3	2.21	0.41
1:C:681:ASN:HD22	1:D:678:ALA:CB	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:SER:OG	1:A:378:SER:N	2.54	0.41
1:B:683:THR:O	1:B:687:VAL:HG22	2.21	0.41
1:C:417:ARG:HG2	1:C:418:GLY:N	2.36	0.41
1:C:656:LEU:HA	1:C:656:LEU:HD23	1.72	0.41
1:D:512:VAL:O	1:D:516:VAL:HG23	2.20	0.41
1:D:560:ASN:OD1	1:D:561:ILE:N	2.51	0.41
1:A:342:LYS:HB3	1:A:343:GLU:CD	2.41	0.41
1:B:444:GLU:HB2	1:B:452:ILE:HB	2.03	0.41
1:C:483:PHE:O	1:C:486:TYR:HB3	2.21	0.41
1:D:377:SER:OG	1:D:378:SER:N	2.54	0.41
1:D:417:ARG:HG2	1:D:418:GLY:N	2.36	0.41
1:A:264:LYS:HZ1	1:A:281:LYS:HD2	1.86	0.40
1:A:396:SER:HG	1:A:402:THR:HG1	1.66	0.40
1:A:462:LEU:CD1	1:A:533:GLU:HG2	2.51	0.40
1:B:280:TRP:HE1	1:B:415:LEU:HD12	1.86	0.40
1:B:483:PHE:O	1:B:486:TYR:HB3	2.21	0.40
1:B:526:ILE:O	1:B:530:SER:OG	2.25	0.40
1:B:568:PHE:HA	1:B:571:ILE:HG12	2.03	0.40
1:C:462:LEU:CD1	1:C:533:GLU:HG2	2.51	0.40
1:C:683:THR:O	1:C:687:VAL:HG22	2.21	0.40
4:D:1009:PLM:H72	4:D:1009:PLM:H42	1.95	0.40
1:D:592:ARG:HD2	1:D:592:ARG:HA	1.85	0.40
1:A:674:ASN:HA	1:D:680:ILE:HD13	2.02	0.40
1:B:409:LEU:HB3	1:B:414:TRP:CH2	2.56	0.40
1:C:278:ASP:O	1:C:282:PHE:N	2.49	0.40
1:C:284:GLU:HA	1:C:288:LEU:HD13	2.03	0.40
1:C:661:PHE:O	1:C:665:VAL:HG12	2.21	0.40
1:D:396:SER:OG	1:D:402:THR:OG1	2.38	0.40
1:D:444:GLU:HB2	1:D:452:ILE:HB	2.03	0.40
1:D:638:ARG:NE	1:D:643:ASP:OD2	2.48	0.40
1:D:661:PHE:O	1:D:665:VAL:HG12	2.21	0.40
5:A:1011:CHS:HD13	5:A:1011:CHS:HA	1.92	0.40
1:A:661:PHE:O	1:A:665:VAL:HG12	2.21	0.40
1:A:667:PHE:HE2	4:D:1007:PLM:H91	1.85	0.40
3:B:1006:PX6:H54	3:B:1006:PX6:H61	1.68	0.40
1:B:377:SER:OG	1:B:378:SER:N	2.54	0.40
1:B:507:TRP:HB3	1:B:575:LYS:HZ3	1.84	0.40
4:C:1007:PLM:HD1	4:C:1007:PLM:HA2	1.69	0.40
1:C:677:LEU:HA	1:C:677:LEU:HD23	1.74	0.40
1:A:452:ILE:HD11	1:D:248:TYR:CD1	2.56	0.40
1:D:302:GLU:O	1:D:306:ARG:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:310:PHE:CD2	1:D:311:TYR:CD2	3.09	0.40
1:D:374:LEU:HA	2:D:1003:NAG:H82	2.03	0.40
1:D:462:LEU:CD1	1:D:533:GLU:HG2	2.51	0.40
1:A:644:ILE:HA	1:A:644:ILE:HD13	1.86	0.40
5:B:1011:CHS:HD13	5:B:1011:CHS:HA	1.84	0.40
1:C:377:SER:OG	1:C:378:SER:N	2.54	0.40
1:D:683:THR:O	1:D:687:VAL:HG22	2.21	0.40
1:A:417:ARG:HG2	1:A:418:GLY:N	2.36	0.40
1:A:568:PHE:HA	1:A:571:ILE:HG12	2.03	0.40
1:A:682:ASP:CG	1:A:683:THR:H	2.24	0.40
1:B:484:ILE:O	1:B:488:VAL:N	2.48	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	479/968 (50%)	419 (88%)	56 (12%)	4 (1%)	24	69
1	B	479/968 (50%)	419 (88%)	56 (12%)	4 (1%)	24	69
1	C	479/968 (50%)	419 (88%)	56 (12%)	4 (1%)	24	69
1	D	479/968 (50%)	419 (88%)	56 (12%)	4 (1%)	24	69
All	All	1916/3872 (50%)	1676 (88%)	224 (12%)	16 (1%)	29	69

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	628	THR
1	B	628	THR
1	C	628	THR
1	D	628	THR

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Mol	Chain	Res	Type
1	A	674	ASN
1	B	674	ASN
1	C	674	ASN
1	D	674	ASN
1	A	309	ILE
1	B	309	ILE
1	C	309	ILE
1	D	309	ILE
1	A	413	VAL
1	B	413	VAL
1	C	413	VAL
1	D	413	VAL

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	432/837 (52%)	429 (99%)	3 (1%)	88	94
1	B	431/837 (52%)	429 (100%)	2 (0%)	92	96
1	C	431/837 (52%)	429 (100%)	2 (0%)	92	96
1	D	431/837 (52%)	429 (100%)	2 (0%)	92	96
All	All	1725/3348 (52%)	1716 (100%)	9 (0%)	92	96

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

Mol	Chain	Res	Type
1	A	503	PHE
1	A	583	MET
1	A	623	VAL
1	B	503	PHE
1	B	623	VAL
1	C	503	PHE
1	C	623	VAL
1	D	503	PHE
1	D	623	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	299	ASN
1	A	379	HIS
1	A	430	ASN
1	A	630	GLN
1	B	299	ASN
1	B	379	HIS
1	B	430	ASN
1	B	630	GLN
1	C	299	ASN
1	C	379	HIS
1	C	430	ASN
1	C	630	GLN
1	D	299	ASN
1	D	379	HIS
1	D	430	ASN
1	D	630	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 49 ligands modelled in this entry, 5 are monoatomic - leaving 44 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	NAG	A	1001	1	14,14,15	0.31	0	15,19,21	0.42	0
2	NAG	A	1002	1	14,14,15	0.35	0	15,19,21	0.19	0
2	NAG	A	1003	2	14,14,15	0.33	0	15,19,21	0.55	0
2	NAG	A	1004	2	14,14,15	0.95	1 (7%)	15,19,21	0.50	0
2	NAG	A	1005	-	14,14,15	0.32	0	15,19,21	0.28	0
3	PX6	A	1006	-	39,39,43	1.41	5 (12%)	43,44,48	1.53	5 (11%)
4	PLM	A	1007	-	14,17,17	0.22	0	14,17,17	0.43	0
4	PLM	A	1008	-	14,17,17	0.17	0	14,17,17	0.67	0
4	PLM	A	1009	-	14,17,17	0.23	0	14,17,17	0.47	0
5	CHS	A	1010	-	12,15,15	0.52	0	12,19,19	0.63	0
5	CHS	A	1011	-	12,15,15	0.34	0	12,19,19	0.76	0
2	NAG	B	1001	1	14,14,15	0.32	0	15,19,21	0.42	0
2	NAG	B	1002	1	14,14,15	0.35	0	15,19,21	0.19	0
2	NAG	B	1003	2	14,14,15	0.34	0	15,19,21	0.54	0
2	NAG	B	1004	2	14,14,15	0.96	1 (7%)	15,19,21	0.51	0
2	NAG	B	1005	-	14,14,15	0.30	0	15,19,21	0.28	0
3	PX6	B	1006	-	39,39,43	1.41	5 (12%)	43,44,48	1.52	5 (11%)
4	PLM	B	1007	-	14,17,17	0.23	0	14,17,17	0.43	0
4	PLM	B	1008	-	14,17,17	0.17	0	14,17,17	0.67	0
4	PLM	B	1009	-	14,17,17	0.23	0	14,17,17	0.45	0
5	CHS	B	1010	-	12,15,15	0.50	0	12,19,19	0.63	0
5	CHS	B	1011	-	12,15,15	0.34	0	12,19,19	0.72	0
2	NAG	C	1001	1	14,14,15	0.32	0	15,19,21	0.43	0
2	NAG	C	1002	1	14,14,15	0.34	0	15,19,21	0.19	0
2	NAG	C	1003	2	14,14,15	0.34	0	15,19,21	0.54	0
2	NAG	C	1004	2	14,14,15	0.95	1 (7%)	15,19,21	0.50	0
2	NAG	C	1005	-	14,14,15	0.30	0	15,19,21	0.28	0
3	PX6	C	1006	-	39,39,43	1.42	5 (12%)	43,44,48	1.52	5 (11%)
4	PLM	C	1007	-	14,17,17	0.23	0	14,17,17	0.43	0
4	PLM	C	1008	-	14,17,17	0.17	0	14,17,17	0.67	0
4	PLM	C	1009	-	14,17,17	0.23	0	14,17,17	0.45	0
5	CHS	C	1010	-	12,15,15	0.50	0	12,19,19	0.62	0
5	CHS	C	1011	-	12,15,15	0.36	0	12,19,19	0.76	0
2	NAG	D	1001	1	14,14,15	0.32	0	15,19,21	0.42	0
2	NAG	D	1002	1	14,14,15	0.35	0	15,19,21	0.19	0
2	NAG	D	1003	2	14,14,15	0.34	0	15,19,21	0.54	0
2	NAG	D	1004	2	14,14,15	0.96	1 (7%)	15,19,21	0.50	0
2	NAG	D	1005	-	14,14,15	0.30	0	15,19,21	0.28	0
3	PX6	D	1006	-	39,39,43	1.42	5 (12%)	43,44,48	1.52	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PLM	D	1007	-	14,17,17	0.23	0	14,17,17	0.43	0
4	PLM	D	1008	-	14,17,17	0.17	0	14,17,17	0.68	0
4	PLM	D	1009	-	14,17,17	0.23	0	14,17,17	0.45	0
5	CHS	D	1010	-	12,15,15	0.50	0	12,19,19	0.61	0
5	CHS	D	1011	-	12,15,15	0.36	0	12,19,19	0.74	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	NAG	A	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1002	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1003	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1004	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1005	-	-	0/6/23/26	0/1/1/1
3	PX6	A	1006	-	-	0/41/41/45	0/0/0/0
4	PLM	A	1007	-	-	0/13/15/15	0/0/0/0
4	PLM	A	1008	-	-	0/13/15/15	0/0/0/0
4	PLM	A	1009	-	-	0/13/15/15	0/0/0/0
5	CHS	A	1010	-	-	0/10/20/20	0/1/1/1
5	CHS	A	1011	-	-	0/10/20/20	0/1/1/1
2	NAG	B	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1002	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1003	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1004	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1005	-	-	0/6/23/26	0/1/1/1
3	PX6	B	1006	-	-	0/41/41/45	0/0/0/0
4	PLM	B	1007	-	-	0/13/15/15	0/0/0/0
4	PLM	B	1008	-	-	0/13/15/15	0/0/0/0
4	PLM	B	1009	-	-	0/13/15/15	0/0/0/0
5	CHS	B	1010	-	-	0/10/20/20	0/1/1/1
5	CHS	B	1011	-	-	0/10/20/20	0/1/1/1
2	NAG	C	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1002	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1003	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1004	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1005	-	-	0/6/23/26	0/1/1/1
3	PX6	C	1006	-	-	0/41/41/45	0/0/0/0
4	PLM	C	1007	-	-	0/13/15/15	0/0/0/0
4	PLM	C	1008	-	-	0/13/15/15	0/0/0/0
4	PLM	C	1009	-	-	0/13/15/15	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CHS	C	1010	-	-	0/10/20/20	0/1/1/1
5	CHS	C	1011	-	-	0/10/20/20	0/1/1/1
2	NAG	D	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1002	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1003	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1004	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1005	-	-	0/6/23/26	0/1/1/1
3	PX6	D	1006	-	-	0/41/41/45	0/0/0/0
4	PLM	D	1007	-	-	0/13/15/15	0/0/0/0
4	PLM	D	1008	-	-	0/13/15/15	0/0/0/0
4	PLM	D	1009	-	-	0/13/15/15	0/0/0/0
5	CHS	D	1010	-	-	0/10/20/20	0/1/1/1
5	CHS	D	1011	-	-	0/10/20/20	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1006	PX6	O7-C2	-2.86	1.38	1.46
3	B	1006	PX6	O7-C2	-2.86	1.38	1.46
3	D	1006	PX6	O7-C2	-2.83	1.39	1.46
3	A	1006	PX6	O7-C2	-2.82	1.39	1.46
3	D	1006	PX6	P1-O3	-2.28	1.46	1.55
3	C	1006	PX6	P1-O3	-2.28	1.46	1.55
3	B	1006	PX6	P1-O3	-2.27	1.46	1.55
3	A	1006	PX6	P1-O3	-2.27	1.46	1.55
3	D	1006	PX6	O7-C20	2.35	1.41	1.34
3	A	1006	PX6	O7-C20	2.36	1.41	1.34
3	B	1006	PX6	O7-C20	2.36	1.41	1.34
3	C	1006	PX6	O7-C20	2.37	1.41	1.34
3	A	1006	PX6	O5-C4	2.84	1.41	1.33
3	D	1006	PX6	O5-C4	2.85	1.41	1.33
3	B	1006	PX6	O5-C4	2.86	1.41	1.33
3	C	1006	PX6	O5-C4	2.86	1.41	1.33
2	C	1004	NAG	C1-C2	3.07	1.56	1.52
2	A	1004	NAG	C1-C2	3.10	1.56	1.52
2	D	1004	NAG	C1-C2	3.10	1.56	1.52
2	B	1004	NAG	C1-C2	3.14	1.56	1.52
3	A	1006	PX6	P1-O2	4.86	1.65	1.50
3	B	1006	PX6	P1-O2	4.87	1.65	1.50
3	D	1006	PX6	P1-O2	4.88	1.65	1.50
3	C	1006	PX6	P1-O2	4.88	1.65	1.50

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1006	PX6	O3-P1-O1	-2.42	100.95	110.60
3	B	1006	PX6	O3-P1-O1	-2.41	100.99	110.60
3	C	1006	PX6	O3-P1-O1	-2.41	100.99	110.60
3	D	1006	PX6	O3-P1-O1	-2.40	101.01	110.60
3	D	1006	PX6	O3-P1-O4	2.17	110.60	105.33
3	B	1006	PX6	O3-P1-O4	2.18	110.64	105.33
3	C	1006	PX6	O3-P1-O4	2.20	110.70	105.33
3	A	1006	PX6	O3-P1-O4	2.21	110.72	105.33
3	D	1006	PX6	O5-C4-C5	2.50	119.54	111.85
3	C	1006	PX6	O5-C4-C5	2.50	119.56	111.85
3	B	1006	PX6	O5-C4-C5	2.51	119.58	111.85
3	A	1006	PX6	O5-C4-C5	2.54	119.66	111.85
3	D	1006	PX6	O7-C20-C21	3.39	118.67	111.53
3	B	1006	PX6	O7-C20-C21	3.42	118.74	111.53
3	C	1006	PX6	O7-C20-C21	3.42	118.74	111.53
3	A	1006	PX6	O7-C20-C21	3.43	118.76	111.53
3	C	1006	PX6	O5-C3-C2	7.41	128.70	108.70
3	B	1006	PX6	O5-C3-C2	7.42	128.73	108.70
3	D	1006	PX6	O5-C3-C2	7.44	128.78	108.70
3	A	1006	PX6	O5-C3-C2	7.45	128.82	108.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

34 monomers are involved in 107 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	NAG	3	0
2	A	1002	NAG	10	0
2	A	1005	NAG	2	0
3	A	1006	PX6	2	0
4	A	1007	PLM	4	0
4	A	1008	PLM	1	0
5	A	1010	CHS	1	0
5	A	1011	CHS	1	0
2	B	1001	NAG	3	0
2	B	1002	NAG	10	0
2	B	1003	NAG	3	0
2	B	1005	NAG	2	0
3	B	1006	PX6	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1007	PLM	4	0
4	B	1008	PLM	1	0
5	B	1010	CHS	1	0
5	B	1011	CHS	1	0
2	C	1001	NAG	3	0
2	C	1002	NAG	10	0
2	C	1003	NAG	3	0
2	C	1005	NAG	2	0
3	C	1006	PX6	5	0
4	C	1007	PLM	3	0
4	C	1008	PLM	1	0
5	C	1010	CHS	1	0
2	D	1001	NAG	3	0
2	D	1002	NAG	10	0
2	D	1003	NAG	1	0
2	D	1005	NAG	2	0
3	D	1006	PX6	4	0
4	D	1007	PLM	3	0
4	D	1009	PLM	1	0
5	D	1010	CHS	1	0
5	D	1011	CHS	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.