



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:39 AM UTC

PDB ID : 1DDX / pdb_00001ddx
Title : CRYSTAL STRUCTURE OF A MIXTURE OF ARACHIDONIC ACID AND PROSTAGLANDIN BOUND TO THE CYCLOOXYGENASE ACTIVE SITE OF COX-2: PROSTAGLANDIN STRUCTURE
Authors : Kiefer, J.R.; Pawlitz, J.L.; Moreland, K.T.; Stegeman, R.A.; Gierse, J.K.; Stevens, A.M.; Goodwin, D.C.; Rowlinson, S.W.; Marnett, L.J.; Stallings, W.C.; Kurumbail, R.G.
Deposited on : 1999-11-11
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

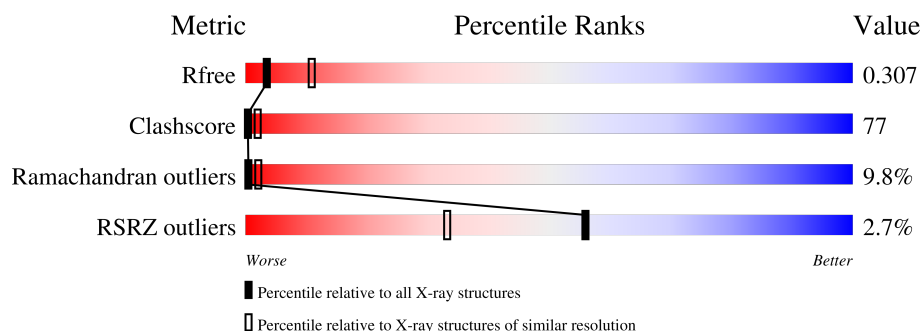
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

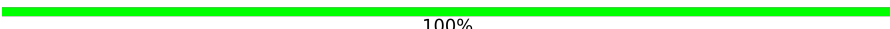
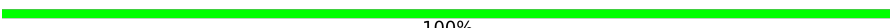
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	552	2% 18% 71% 11%
1	B	552	2% 18% 72% 10%
1	C	552	4% 18% 70% 12%
1	D	552	3% 18% 72% 11%
2	E	2	100%

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
2	F	2	 50%50%
2	G	2	 100%
2	H	2	 100%

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
5	PGX	A	701	-	-	X	-
5	PGX	B	1701	-	-	X	-
5	PGX	C	2701	-	-	X	-
5	PGX	D	3701	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18477 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 PROTEIN (PROSTAGLANDIN H2 SYNTHASE-2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4475	2885	750	815	25			
1	B	552	Total	C	N	O	S	0	0	0
			4475	2885	750	815	25			
1	C	552	Total	C	N	O	S	0	0	0
			4475	2885	750	815	25			
1	D	552	Total	C	N	O	S	0	0	0
			4475	2885	750	815	25			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



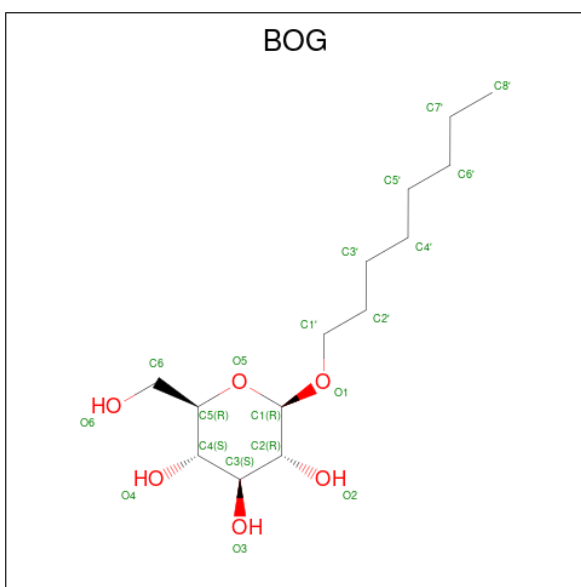
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



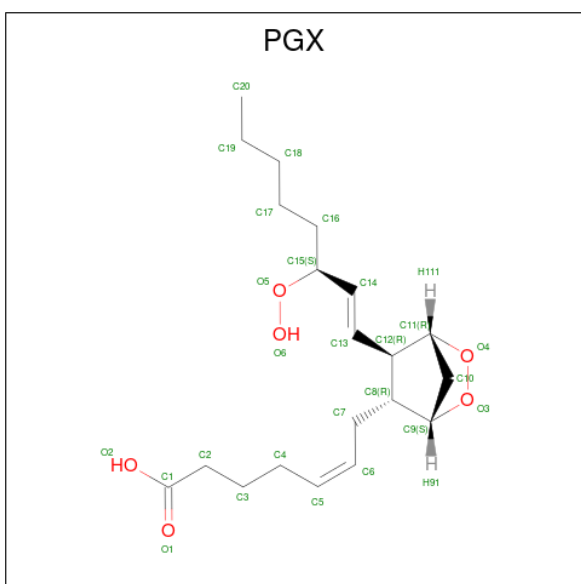
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	14	6		
4	B	1	Total	C	O	0	0
			20	14	6		
4	C	1	Total	C	O	0	0
			20	14	6		
4	D	1	Total	C	O	0	0
			20	14	6		

- Molecule 5 is 7-[6-(3-HYDROPEROXY-OCT-1-ENYL)-2,3-DIOXA-BICYCLO[2.2.1]HEPT-5-YL]-HEPT-5-ENOIC ACID (CCD ID: PGX) (formula: $C_{20}H_{32}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			25	20	5		
5	B	1	Total	C	O	0	0
			25	20	5		
5	C	1	Total	C	O	0	0
			25	20	5		
5	D	1	Total	C	O	0	0
			25	20	5		

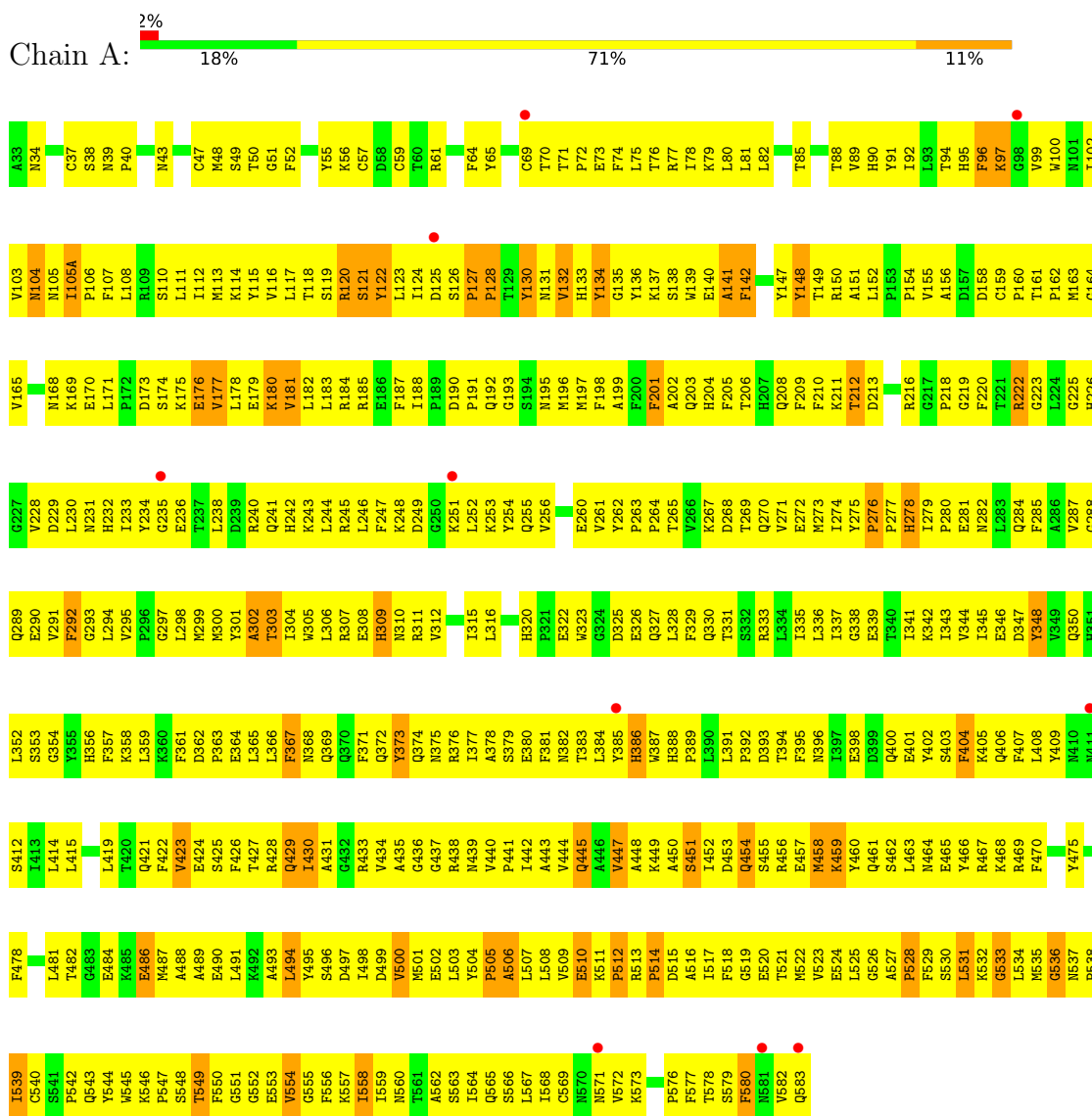
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	45	Total	O	0	0
			45	45		
6	B	39	Total	O	0	0
			39	39		
6	C	46	Total	O	0	0
			46	46		
6	D	43	Total	O	0	0
			43	43		

3 Residue-property plots

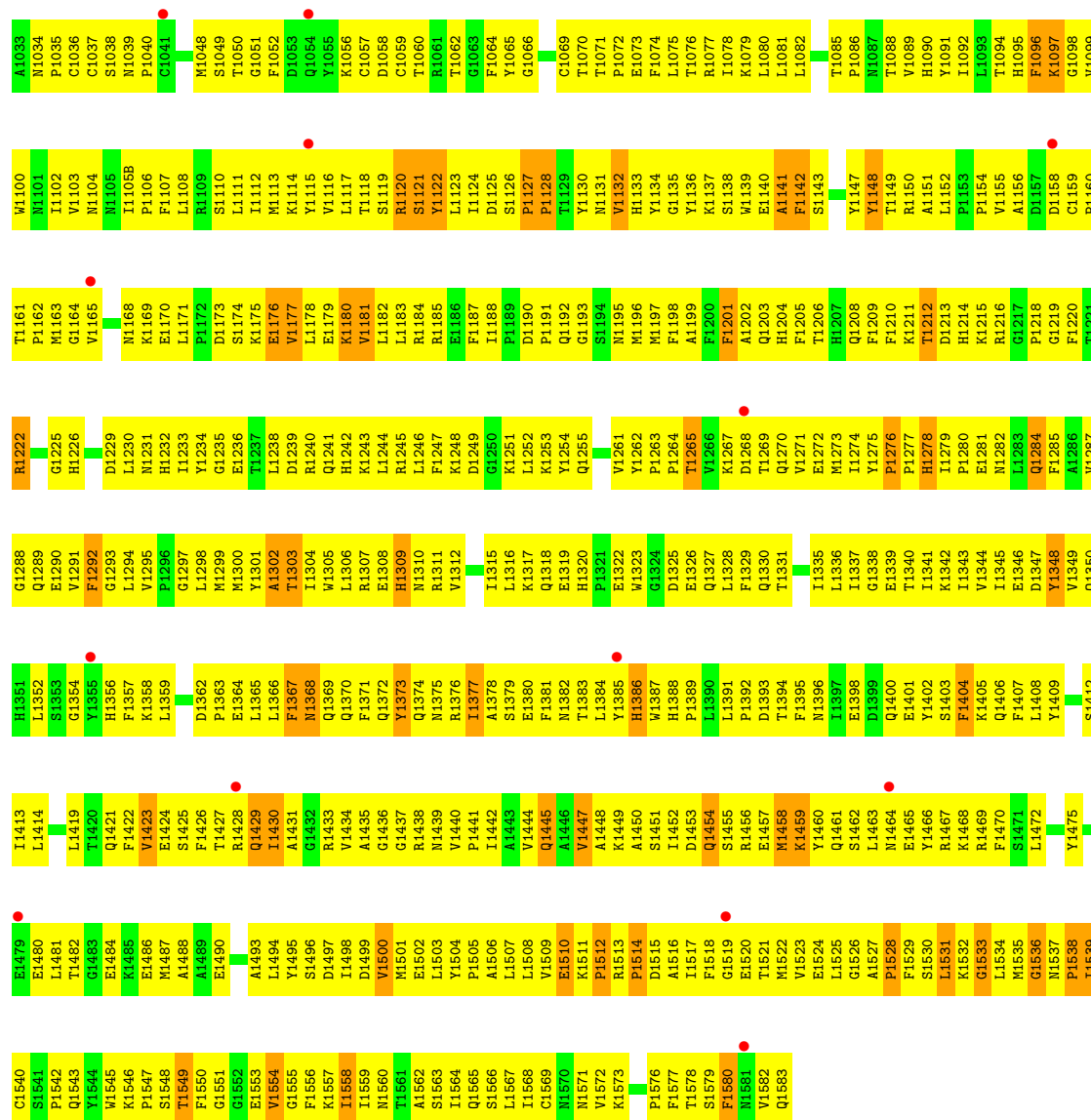
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: PROTEIN (PROSTAGLANDIN H2 SYNTHASE-2)

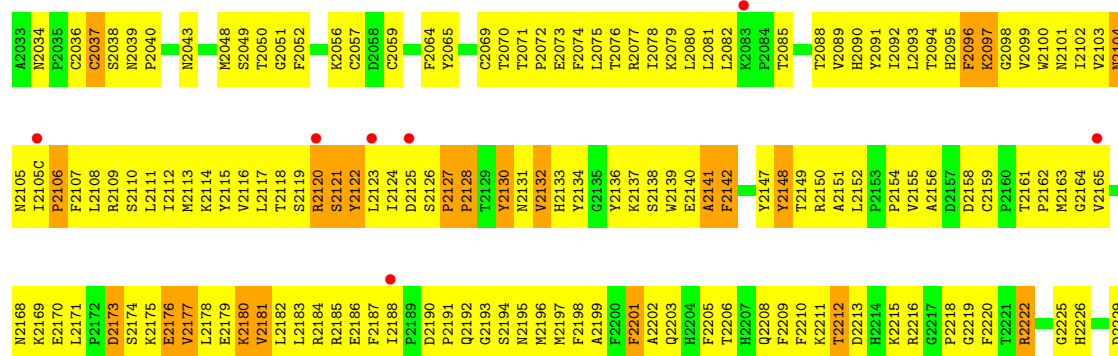


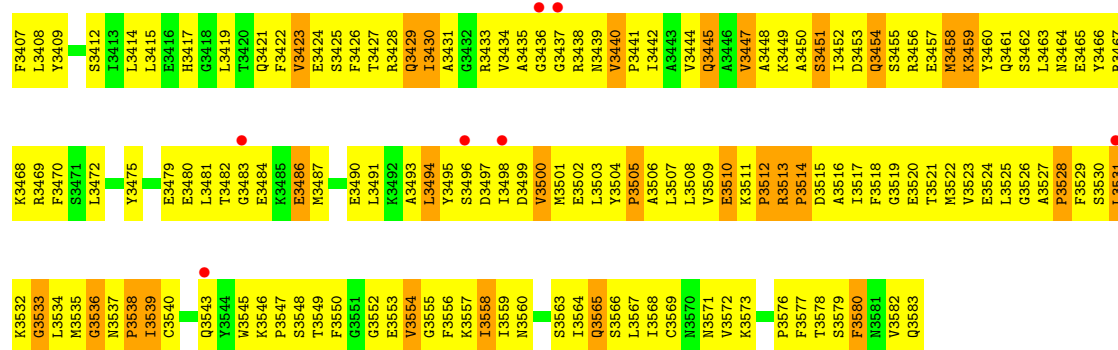
• Molecule 1: PROTEIN (PROSTAGLANDIN H2 SYNTHASE-2)



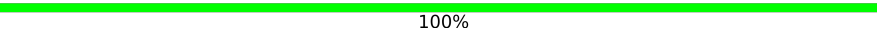


• Molecule 1: PROTEIN (PROSTAGLANDIN H2 SYNTHASE-2)





- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%

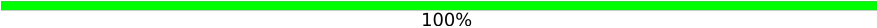


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  50%

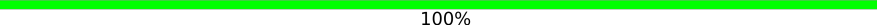


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	180.24Å 134.80Å 122.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	76.1 (20.00-3.00) 75.7 (20.00-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.00Å)	Xtrriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.267 , 0.324 0.252 , 0.307	Depositor DCC
R_{free} test set	4329 reflections (9.43%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtrriage
Anisotropy	0.915	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	18477	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.3521e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BOG, PGX

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	0.52	0/4602	1.00	21/6239 (0.3%)
1	B	0.51	0/4602	0.99	18/6239 (0.3%)
1	C	0.51	0/4602	1.01	20/6239 (0.3%)
1	D	0.52	0/4602	0.99	18/6239 (0.3%)
All	All	0.52	0/18408	1.00	77/24956 (0.3%)

There are no bond length outliers.

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2580	PHE	N-CA-C	-8.39	102.60	112.92
1	B	1580	PHE	N-CA-C	-7.99	103.43	113.02
1	D	3580	PHE	N-CA-C	-7.96	103.47	113.02
1	A	580	PHE	N-CA-C	-7.95	103.48	113.02
1	A	494	LEU	N-CA-C	7.68	119.73	111.36
1	C	2494	LEU	N-CA-C	7.41	119.43	111.36
1	D	3494	LEU	N-CA-C	7.12	118.83	111.14
1	C	2440	VAL	N-CA-C	7.11	114.59	107.55
1	B	1494	LEU	N-CA-C	7.08	119.07	111.36
1	C	2127	PRO	CA-C-N	6.84	128.38	119.84
1	C	2127	PRO	C-N-CA	6.84	128.38	119.84
1	A	440	VAL	N-CA-C	6.70	114.19	107.55
1	B	1440	VAL	N-CA-C	6.61	114.09	107.55
1	C	2368	ASN	N-CA-C	-6.58	104.00	113.21
1	D	3440	VAL	N-CA-C	6.58	114.06	107.55
1	D	3127	PRO	CA-C-N	6.53	128.00	119.84
1	D	3127	PRO	C-N-CA	6.53	128.00	119.84
1	A	276	PRO	CA-C-N	6.52	127.99	119.84
1	A	276	PRO	C-N-CA	6.52	127.99	119.84
1	C	2148	TYR	N-CA-C	-6.46	98.37	108.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1148	TYR	N-CA-C	-6.39	98.48	108.90
1	D	3368	ASN	N-CA-C	-6.38	104.28	113.21
1	B	1368	ASN	N-CA-C	-6.24	104.47	113.21
1	C	2276	PRO	CA-C-N	6.22	127.61	119.84
1	C	2276	PRO	C-N-CA	6.22	127.61	119.84
1	A	127	PRO	CA-C-N	6.17	127.55	119.84
1	A	127	PRO	C-N-CA	6.17	127.55	119.84
1	A	148	TYR	N-CA-C	-6.16	98.86	108.90
1	B	1276	PRO	CA-C-N	6.15	127.52	119.84
1	B	1276	PRO	C-N-CA	6.15	127.52	119.84
1	D	3276	PRO	CA-C-N	6.10	127.47	119.84
1	D	3276	PRO	C-N-CA	6.10	127.47	119.84
1	B	1404	PHE	N-CA-C	-6.09	104.56	111.07
1	A	398	GLU	CB-CA-C	-6.07	109.59	116.63
1	B	1398	GLU	CB-CA-C	-6.04	109.62	116.63
1	B	1412	SER	N-CA-C	-6.02	104.78	111.71
1	A	375	ASN	N-CA-C	6.02	118.30	108.55
1	D	3412	SER	N-CA-C	-5.90	104.93	111.71
1	B	1127	PRO	CA-C-N	5.83	127.12	119.84
1	B	1127	PRO	C-N-CA	5.83	127.12	119.84
1	B	1265	THR	N-CA-C	5.82	118.41	110.55
1	D	3398	GLU	CB-CA-C	-5.81	109.89	116.63
1	A	105(A)	ILE	CA-C-N	5.79	127.07	119.84
1	A	105(A)	ILE	C-N-CA	5.79	127.07	119.84
1	B	1346	GLU	N-CA-C	5.79	118.53	111.82
1	C	2398	GLU	CB-CA-C	-5.75	109.95	116.63
1	C	2375	ASN	N-CA-C	5.68	117.75	108.55
1	C	2412	SER	N-CA-C	-5.58	104.57	111.33
1	B	1375	ASN	N-CA-C	5.58	117.59	108.55
1	C	2222	ARG	N-CA-C	-5.56	106.49	113.72
1	A	404	PHE	N-CA-C	-5.55	104.44	111.11
1	C	2278	HIS	N-CA-C	5.55	117.33	111.28
1	B	1222	ARG	N-CA-C	-5.48	106.59	113.72
1	A	130	TYR	N-CA-C	5.43	117.54	110.53
1	C	2265	THR	N-CA-C	5.43	117.70	110.53
1	B	1278	HIS	N-CA-C	5.38	117.22	111.36
1	A	443	ALA	N-CA-C	-5.34	105.46	111.28
1	D	3130	TYR	N-CA-C	5.34	117.42	110.53
1	D	3375	ASN	N-CA-C	5.32	117.17	108.55
1	A	222	ARG	N-CA-C	-5.29	106.85	113.72
1	D	3278	HIS	N-CA-C	5.28	117.12	111.36
1	A	134	TYR	N-CA-C	5.26	117.22	108.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2551	GLY	N-CA-C	-5.26	106.98	115.08
1	C	2513	ARG	N-CA-C	-5.25	103.33	110.36
1	A	493	ALA	N-CA-C	-5.23	105.49	111.14
1	A	412	SER	N-CA-C	-5.22	105.07	111.75
1	C	2130	TYR	N-CA-C	5.22	117.26	110.53
1	D	3222	ARG	N-CA-C	-5.20	106.96	113.72
1	A	346	GLU	N-CA-C	5.19	118.77	112.23
1	D	3265	THR	N-CA-C	5.16	117.52	110.55
1	D	3148	TYR	N-CA-C	-5.11	100.57	108.90
1	A	278	HIS	N-CA-C	5.10	116.92	111.36
1	C	2173	ASP	N-CA-C	-5.09	103.42	110.35
1	D	3134	TYR	N-CA-C	5.08	116.91	108.02
1	D	3513	ARG	N-CA-C	-5.06	103.58	110.36
1	C	2328	LEU	N-CA-C	-5.06	105.46	110.97
1	B	1377	ILE	N-CA-C	5.04	116.00	108.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4475	0	4373	706	0
1	B	4475	0	4373	708	0
1	C	4475	0	4373	720	0
1	D	4475	0	4373	722	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
3	C	28	0	26	0	0
3	D	28	0	26	0	0
4	A	20	0	28	0	0
4	B	20	0	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	20	0	28	0	0
4	D	20	0	28	1	0
5	A	25	0	30	9	0
5	B	25	0	30	14	0
5	C	25	0	30	15	0
5	D	25	0	30	11	0
6	A	45	0	0	14	0
6	B	39	0	0	12	0
6	C	46	0	0	20	0
6	D	43	0	0	15	0
All	All	18477	0	17928	2799	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 77.

All (2799) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:LEU:HD22	1:A:522:MET:HE3	1.22	1.21
1:D:3312:VAL:HA	1:D:3315:ILE:HD12	1.33	1.09
1:A:312:VAL:HA	1:A:315:ILE:HD12	1.33	1.08
1:D:3507:LEU:HD22	1:D:3522:MET:HE3	1.30	1.08
1:B:1312:VAL:HA	1:B:1315:ILE:HD12	1.36	1.07
1:B:1301:TYR:HA	1:B:1304:ILE:HD12	1.37	1.07
1:A:99:VAL:HA	1:A:102:ILE:HD12	1.37	1.06
1:C:2301:TYR:HA	1:C:2304:ILE:HD12	1.35	1.05
1:B:1507:LEU:HD22	1:B:1522:MET:HE3	1.34	1.05
1:C:2507:LEU:HD22	1:C:2522:MET:HE3	1.33	1.05
1:B:1099:VAL:HA	1:B:1102:ILE:HD12	1.38	1.05
1:D:3230:LEU:HB3	1:D:3233:ILE:HD12	1.39	1.04
1:D:3099:VAL:HA	1:D:3102:ILE:HD12	1.38	1.04
1:D:3301:TYR:HA	1:D:3304:ILE:HD12	1.35	1.03
1:C:2312:VAL:HA	1:C:2315:ILE:HD12	1.34	1.03
1:A:301:TYR:HA	1:A:304:ILE:HD12	1.37	1.02
1:B:1230:LEU:HB3	1:B:1233:ILE:HD12	1.39	1.01
1:C:2099:VAL:HA	1:C:2102:ILE:HD12	1.39	1.01
1:A:389:PRO:HG2	1:A:434:VAL:HG13	1.42	1.01
1:A:230:LEU:HB3	1:A:233:ILE:HD12	1.43	1.00
1:C:2208:GLN:HB3	1:C:2232:HIS:HD2	1.28	0.99
1:B:1208:GLN:HB3	1:B:1232:HIS:HD2	1.26	0.98
1:D:3389:PRO:HG2	1:D:3434:VAL:HG13	1.44	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:GLN:HB3	1:A:232:HIS:HD2	1.29	0.96
1:C:2273:MET:HE1	1:C:2287:VAL:HG22	1.46	0.96
1:B:1389:PRO:HG2	1:B:1434:VAL:HG13	1.48	0.96
1:C:2526:GLY:HA3	5:C:2701:PGX:H61	1.46	0.94
1:C:2385:TYR:HA	5:C:2701:PGX:O3	1.68	0.94
1:C:2308:GLU:HB2	1:C:2571:ASN:HD21	1.31	0.94
1:D:3191:PRO:HD2	1:D:3433:ARG:HG3	1.50	0.94
1:D:3208:GLN:HB3	1:D:3232:HIS:HD2	1.32	0.94
1:A:308:GLU:HG3	1:A:336:LEU:HD11	1.49	0.93
1:B:1203:GLN:HG2	1:B:1298:LEU:HD11	1.49	0.93
1:A:191:PRO:HD2	1:A:433:ARG:HG3	1.50	0.93
1:B:1385:TYR:HA	5:B:1701:PGX:O3	1.68	0.93
1:A:308:GLU:HB2	1:A:571:ASN:HD21	1.31	0.93
1:B:1463:LEU:HD13	1:B:1506:ALA:HB3	1.48	0.92
1:B:1191:PRO:HD2	1:B:1433:ARG:HG3	1.51	0.92
1:C:2389:PRO:HG2	1:C:2434:VAL:HG13	1.50	0.92
1:A:463:LEU:HD13	1:A:506:ALA:HB3	1.50	0.92
1:B:1184:ARG:HD3	1:B:1187:PHE:HA	1.51	0.92
1:C:2463:LEU:HD13	1:C:2506:ALA:HB3	1.49	0.92
1:B:1245:ARG:HH22	1:B:1326:GLU:HG2	1.33	0.92
1:C:2191:PRO:HD2	1:C:2433:ARG:HG3	1.50	0.92
1:D:3463:LEU:HD13	1:D:3506:ALA:HB3	1.51	0.92
1:C:2230:LEU:HB3	1:C:2233:ILE:HD12	1.51	0.92
1:A:414:LEU:HA	1:A:422:PHE:CE1	2.05	0.91
1:B:1308:GLU:HB2	1:B:1571:ASN:HD21	1.35	0.91
1:D:3308:GLU:HB2	1:D:3571:ASN:HD21	1.35	0.90
1:A:203:GLN:HG2	1:A:298:LEU:HD11	1.54	0.90
1:C:2308:GLU:HG3	1:C:2336:LEU:HD11	1.52	0.90
1:A:275:TYR:HE1	1:A:293:GLY:HA3	1.37	0.89
1:B:1308:GLU:HG3	1:B:1336:LEU:HD11	1.52	0.89
1:D:3308:GLU:HG3	1:D:3336:LEU:HD11	1.54	0.89
1:C:2184:ARG:HD3	1:C:2187:PHE:HA	1.55	0.89
1:C:2414:LEU:HA	1:C:2422:PHE:CE1	2.08	0.88
1:D:3203:GLN:HG2	1:D:3298:LEU:HD11	1.56	0.88
1:C:2203:GLN:HG2	1:C:2298:LEU:HD11	1.56	0.88
1:B:1273:MET:HE1	1:B:1287:VAL:HG22	1.56	0.87
1:C:2051:GLY:C	1:D:3322:GLU:HG2	1.98	0.87
1:C:2507:LEU:HD22	1:C:2522:MET:CE	2.04	0.87
1:D:3396:ASN:ND2	1:D:3401:GLU:HG2	1.89	0.87
1:D:3507:LEU:HD22	1:D:3522:MET:CE	2.03	0.87
1:B:1526:GLY:HA3	5:B:1701:PGX:H61	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2391:LEU:HD23	1:C:2392:PRO:HD2	1.57	0.87
1:C:2502:GLU:HB2	1:C:2505:PRO:HG2	1.57	0.87
1:D:3414:LEU:HA	1:D:3422:PHE:CE1	2.10	0.87
1:A:245:ARG:HH22	1:A:326:GLU:HG2	1.39	0.86
1:A:502:GLU:HB2	1:A:505:PRO:HG2	1.57	0.86
1:B:1502:GLU:HB2	1:B:1505:PRO:HG2	1.56	0.86
1:A:526:GLY:HA3	5:A:701:PGX:H61	1.57	0.86
1:C:2275:TYR:HE1	1:C:2293:GLY:HA3	1.39	0.86
1:A:88:THR:HG22	1:A:92:ILE:HD11	1.58	0.86
1:A:350:GLN:HE22	1:A:358:LYS:HA	1.41	0.86
1:C:2245:ARG:HH22	1:C:2326:GLU:HG2	1.36	0.86
1:C:2350:GLN:HE22	1:C:2358:LYS:HA	1.39	0.86
1:D:3245:ARG:HH22	1:D:3326:GLU:HG2	1.40	0.86
1:D:3275:TYR:HE1	1:D:3293:GLY:HA3	1.41	0.86
1:D:3391:LEU:HD23	1:D:3392:PRO:HD2	1.58	0.86
1:B:1507:LEU:HD22	1:B:1522:MET:CE	2.05	0.85
1:D:3184:ARG:HD3	1:D:3187:PHE:HA	1.58	0.85
1:B:1275:TYR:HE1	1:B:1293:GLY:HA3	1.39	0.85
1:D:3088:THR:HG22	1:D:3092:ILE:HD11	1.58	0.85
1:C:2088:THR:HG22	1:C:2092:ILE:HD11	1.56	0.85
1:B:1088:THR:HG22	1:B:1092:ILE:HD11	1.59	0.84
1:A:507:LEU:HD22	1:A:522:MET:CE	2.05	0.84
1:C:2103:VAL:HG22	1:C:2108:LEU:HB3	1.59	0.84
1:D:3273:MET:HE1	1:D:3287:VAL:HG22	1.58	0.84
1:A:103:VAL:HG22	1:A:108:LEU:HB3	1.60	0.84
1:C:2419:LEU:O	1:C:2423:VAL:HG23	1.78	0.84
1:B:1350:GLN:HE22	1:B:1358:LYS:HA	1.42	0.84
1:A:184:ARG:HD3	1:A:187:PHE:HA	1.58	0.83
1:A:273:MET:HE1	1:A:287:VAL:HG22	1.58	0.83
1:B:1414:LEU:HA	1:B:1422:PHE:CE1	2.13	0.83
1:A:51:GLY:C	1:B:1322:GLU:HG2	2.03	0.83
1:C:2322:GLU:HG2	1:D:3052:PHE:N	1.94	0.83
1:B:1396:ASN:ND2	1:B:1401:GLU:HG2	1.92	0.83
1:D:3338:GLY:HA3	1:D:3559:ILE:HD13	1.60	0.83
1:D:3350:GLN:HE22	1:D:3358:LYS:HA	1.42	0.82
1:C:2396:ASN:ND2	1:C:2401:GLU:HG2	1.94	0.82
1:D:3502:GLU:HB2	1:D:3505:PRO:HG2	1.59	0.82
1:A:391:LEU:HD23	1:A:392:PRO:HD2	1.60	0.82
1:C:2322:GLU:HG2	1:D:3051:GLY:C	2.03	0.82
1:D:3103:VAL:HG22	1:D:3108:LEU:HB3	1.62	0.82
1:B:1391:LEU:HD23	1:B:1392:PRO:HD2	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3230:LEU:HG	1:D:3337:ILE:HG13	1.63	0.81
1:B:1208:GLN:HB3	1:B:1232:HIS:CD2	2.14	0.81
1:C:2387:TRP:CZ2	5:C:2701:PGX:H71	2.16	0.81
1:D:3526:GLY:HA3	5:D:3701:PGX:H61	1.62	0.81
1:A:396:ASN:ND2	1:A:401:GLU:HG2	1.95	0.81
1:A:216:ARG:HB3	1:A:220:PHE:CD1	2.17	0.80
1:D:3273:MET:SD	1:D:3290:GLU:HA	2.20	0.80
1:A:537:ASN:OD1	1:A:539:ILE:HG23	1.81	0.80
1:C:2534:LEU:HD22	5:C:2701:PGX:H182	1.62	0.80
1:A:275:TYR:CE1	1:A:293:GLY:HA3	2.16	0.80
1:A:322:GLU:HG2	1:B:1051:GLY:C	2.06	0.80
1:B:1103:VAL:HG22	1:B:1108:LEU:HB3	1.64	0.80
1:A:338:GLY:HA3	1:A:559:ILE:HD13	1.62	0.80
1:C:2208:GLN:HB3	1:C:2232:HIS:CD2	2.14	0.80
1:C:2218:PRO:HB2	1:C:2458:MET:HE3	1.64	0.80
1:C:2456:ARG:HA	6:C:4117:HOH:O	1.80	0.80
1:B:1338:GLY:HA3	1:B:1559:ILE:HD13	1.63	0.80
1:A:218:PRO:HB2	1:A:458:MET:HE3	1.64	0.79
1:A:384:LEU:HB3	1:A:522:MET:HE2	1.62	0.79
1:A:322:GLU:HG2	1:B:1052:PHE:N	1.96	0.79
1:B:1178:LEU:HA	1:B:1182:LEU:HD12	1.65	0.79
1:C:2578:THR:HG22	1:C:2579:SER:N	1.98	0.79
1:D:3208:GLN:HB3	1:D:3232:HIS:CD2	2.18	0.79
1:D:3578:THR:HG22	1:D:3579:SER:N	1.96	0.79
1:D:3182:LEU:O	1:D:3438:ARG:HA	1.82	0.79
1:A:419:LEU:O	1:A:423:VAL:HG23	1.82	0.79
1:A:88:THR:O	1:A:91:TYR:HB3	1.83	0.79
1:C:2275:TYR:CE1	1:C:2293:GLY:HA3	2.18	0.78
1:A:161:THR:HG21	1:A:165:VAL:O	1.83	0.78
1:D:3275:TYR:CE1	1:D:3293:GLY:HA3	2.18	0.78
1:A:208:GLN:HB3	1:A:232:HIS:CD2	2.15	0.78
1:A:578:THR:HG22	1:A:579:SER:N	1.98	0.78
1:B:1218:PRO:HB2	1:B:1458:MET:HE3	1.66	0.78
1:C:2273:MET:SD	1:C:2290:GLU:HA	2.24	0.78
1:D:3312:VAL:HA	1:D:3315:ILE:CD1	2.14	0.78
1:A:276:PRO:HD2	1:A:279:ILE:HG13	1.66	0.78
1:B:1275:TYR:CE1	1:B:1293:GLY:HA3	2.17	0.78
1:C:2387:TRP:HZ2	5:C:2701:PGX:H71	1.48	0.78
1:B:1088:THR:O	1:B:1091:TYR:HB3	1.84	0.78
1:A:414:LEU:HD11	1:A:419:LEU:HD22	1.66	0.77
1:B:1216:ARG:HB3	1:B:1220:PHE:CD1	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1182:LEU:O	1:B:1438:ARG:HA	1.84	0.77
1:D:3161:THR:HG21	1:D:3165:VAL:O	1.83	0.77
1:D:3449:LYS:HA	1:D:3452:ILE:HD12	1.66	0.77
1:B:1273:MET:HE2	1:B:1287:VAL:H	1.49	0.77
1:C:2449:LYS:HA	1:C:2452:ILE:HD12	1.65	0.77
1:D:3149:THR:O	1:D:3378:ALA:HA	1.84	0.77
1:A:185:ARG:HH21	1:A:438:ARG:NE	1.83	0.77
1:B:1553:GLU:OE1	1:B:1553:GLU:HA	1.83	0.77
1:D:3188:ILE:HD12	1:D:3439:ASN:HB2	1.66	0.77
1:D:3216:ARG:HB3	1:D:3220:PHE:CD1	2.20	0.77
1:D:3414:LEU:HD11	1:D:3419:LEU:HD22	1.67	0.77
1:C:2230:LEU:HG	1:C:2337:ILE:HG13	1.67	0.77
1:A:525:LEU:O	1:A:528:PRO:HD2	1.85	0.77
1:D:3273:MET:HG3	1:D:3285:PHE:O	1.85	0.77
1:D:3419:LEU:O	1:D:3423:VAL:HG23	1.85	0.77
1:B:1273:MET:SD	1:B:1290:GLU:HA	2.25	0.77
1:B:1504:TYR:HB3	1:B:1505:PRO:HD3	1.67	0.77
1:C:2052:PHE:N	1:D:3322:GLU:HG2	1.99	0.77
1:C:2273:MET:HG3	1:C:2285:PHE:O	1.85	0.77
1:C:2276:PRO:HD2	1:C:2279:ILE:HG13	1.65	0.77
1:B:1414:LEU:HD11	1:B:1419:LEU:HD22	1.66	0.76
1:C:2184:ARG:HB2	1:C:2439:ASN:C	2.10	0.76
1:C:2216:ARG:HB3	1:C:2220:PHE:CD1	2.19	0.76
1:D:3525:LEU:O	1:D:3528:PRO:HD2	1.84	0.76
1:C:2088:THR:O	1:C:2091:TYR:HB3	1.84	0.76
1:A:273:MET:HG3	1:A:285:PHE:O	1.84	0.76
1:B:1463:LEU:HD12	1:B:1503:LEU:HD12	1.67	0.76
1:B:1578:THR:HG22	1:B:1579:SER:N	2.01	0.76
1:C:2174:SER:OG	1:C:2449:LYS:HE2	1.85	0.76
1:D:3276:PRO:HD2	1:D:3279:ILE:HG13	1.67	0.76
1:D:3573:LYS:O	1:D:3576:PRO:HD3	1.85	0.76
1:D:3389:PRO:HB2	1:D:3434:VAL:HG22	1.68	0.76
1:A:403:SER:OG	1:A:406:GLN:HG3	1.86	0.76
1:B:1276:PRO:HD2	1:B:1279:ILE:HG13	1.68	0.76
1:C:2308:GLU:CB	1:C:2571:ASN:HD21	1.98	0.76
1:A:308:GLU:CB	1:A:571:ASN:HD21	1.99	0.76
1:C:2389:PRO:HB2	1:C:2434:VAL:HG22	1.68	0.76
1:B:1105(B):ILE:HG21	1:B:1108:LEU:HD12	1.68	0.76
1:B:1573:LYS:O	1:B:1576:PRO:HD3	1.86	0.76
1:D:3088:THR:O	1:D:3091:TYR:HB3	1.87	0.75
1:A:430:ILE:HG13	1:A:431:ALA:N	2.00	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:ASP:HB3	1:A:500:VAL:HG23	1.68	0.75
1:D:3537:ASN:OD1	1:D:3539:ILE:HG23	1.87	0.75
1:B:1449:LYS:HA	1:B:1452:ILE:HD12	1.67	0.75
1:C:2178:LEU:HA	1:C:2182:LEU:HD12	1.66	0.75
1:C:2244:LEU:O	1:C:2252:LEU:HD23	1.87	0.75
1:C:2497:ASP:HB3	1:C:2500:VAL:HG23	1.69	0.75
1:A:534:LEU:HD22	5:A:701:PGX:H182	1.68	0.75
1:B:1510:GLU:O	1:B:1512:PRO:HD3	1.85	0.75
1:C:2504:TYR:HB3	1:C:2505:PRO:HD3	1.67	0.75
1:C:2553:GLU:OE1	1:C:2553:GLU:HA	1.87	0.75
1:C:2281:GLU:HA	1:C:2284:GLN:HG3	1.69	0.75
1:C:2338:GLY:HA3	1:C:2559:ILE:HD13	1.67	0.75
1:C:2573:LYS:O	1:C:2576:PRO:HD3	1.86	0.75
1:B:1230:LEU:HG	1:B:1337:ILE:HG13	1.68	0.74
1:B:1430:ILE:HG13	1:B:1431:ALA:N	2.02	0.74
1:A:184:ARG:HB2	1:A:439:ASN:C	2.12	0.74
1:C:2182:LEU:O	1:C:2438:ARG:HA	1.87	0.74
1:C:2312:VAL:HA	1:C:2315:ILE:CD1	2.16	0.74
1:D:3430:ILE:HG13	1:D:3431:ALA:N	2.02	0.74
1:D:3185:ARG:HH21	1:D:3438:ARG:NE	1.86	0.74
1:B:1184:ARG:HB2	1:B:1439:ASN:C	2.12	0.74
1:A:553:GLU:OE1	1:A:553:GLU:HA	1.86	0.74
1:C:2161:THR:HG21	1:C:2165:VAL:O	1.87	0.74
1:D:3463:LEU:HD12	1:D:3503:LEU:HD12	1.69	0.74
1:D:3497:ASP:HB3	1:D:3500:VAL:HG23	1.68	0.74
1:A:273:MET:SD	1:A:290:GLU:HA	2.27	0.74
1:B:1273:MET:HE2	1:B:1287:VAL:N	2.02	0.74
1:C:2442:ILE:O	1:C:2445:GLN:HB2	1.87	0.74
1:C:2463:LEU:HD12	1:C:2503:LEU:HD12	1.70	0.74
1:D:3402:TYR:HA	1:D:3406:GLN:OE1	1.87	0.74
1:C:2210:PHE:CE1	1:C:2382:ASN:HA	2.23	0.74
1:A:573:LYS:O	1:A:576:PRO:HD3	1.88	0.74
1:B:1161:THR:HG21	1:B:1165:VAL:O	1.88	0.74
1:A:402:TYR:HA	1:A:406:GLN:OE1	1.87	0.73
1:B:1402:TYR:HA	1:B:1406:GLN:OE1	1.88	0.73
1:A:510:GLU:O	1:A:512:PRO:HD3	1.87	0.73
1:C:2537:ASN:OD1	1:C:2539:ILE:HG23	1.87	0.73
1:C:2185:ARG:HH21	1:C:2438:ARG:NE	1.85	0.73
1:D:3162:PRO:O	1:D:3163:MET:HE2	1.88	0.73
1:A:178:LEU:HA	1:A:182:LEU:HD12	1.70	0.73
1:B:1185:ARG:HH21	1:B:1438:ARG:NE	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1273:MET:HG3	1:B:1285:PHE:O	1.89	0.73
1:C:2510:GLU:O	1:C:2512:PRO:HD3	1.86	0.73
1:D:3190:ASP:OD1	1:D:3517:ILE:HB	1.88	0.73
1:D:3273:MET:HE2	1:D:3287:VAL:H	1.54	0.73
1:A:188:ILE:HD12	1:A:439:ASN:HB2	1.70	0.73
1:B:1442:ILE:O	1:B:1445:GLN:HB2	1.89	0.73
1:A:52:PHE:N	1:B:1322:GLU:HG2	2.03	0.72
1:A:174:SER:OG	1:A:449:LYS:HE2	1.88	0.72
1:A:182:LEU:O	1:A:438:ARG:HA	1.89	0.72
1:B:1196:MET:HE2	1:B:1196:MET:HA	1.71	0.72
1:D:3504:TYR:HB3	1:D:3505:PRO:HD3	1.70	0.72
1:B:1389:PRO:HB2	1:B:1434:VAL:HG22	1.71	0.72
1:B:1525:LEU:O	1:B:1528:PRO:HD2	1.89	0.72
1:B:1537:ASN:OD1	1:B:1539:ILE:HG23	1.89	0.72
1:D:3178:LEU:HA	1:D:3182:LEU:HD12	1.71	0.72
1:A:244:LEU:O	1:A:252:LEU:HD23	1.88	0.72
1:B:1387:TRP:CZ2	5:B:1701:PGX:H71	2.25	0.72
1:D:3218:PRO:HB2	1:D:3458:MET:HE3	1.70	0.72
1:D:3510:GLU:O	1:D:3512:PRO:HD3	1.88	0.72
1:A:389:PRO:HB2	1:A:434:VAL:HG22	1.70	0.72
1:B:1312:VAL:HA	1:B:1315:ILE:CD1	2.16	0.72
1:D:3442:ILE:O	1:D:3445:GLN:HB2	1.88	0.72
1:C:2178:LEU:O	1:C:2182:LEU:HB2	1.90	0.72
1:C:2402:TYR:HA	1:C:2406:GLN:OE1	1.89	0.72
1:A:312:VAL:HA	1:A:315:ILE:CD1	2.15	0.72
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.72	0.72
1:B:1210:PHE:CE1	1:B:1382:ASN:HA	2.25	0.72
1:C:2188:ILE:HD12	1:C:2439:ASN:HB2	1.72	0.72
1:C:2525:LEU:O	1:C:2528:PRO:HD2	1.89	0.72
1:B:1178:LEU:O	1:B:1182:LEU:HB2	1.90	0.72
1:C:2414:LEU:HD11	1:C:2419:LEU:HD22	1.69	0.72
1:C:2430:ILE:HG13	1:C:2431:ALA:N	2.04	0.72
1:B:1149:THR:O	1:B:1378:ALA:HA	1.90	0.72
1:B:1534:LEU:HD22	5:B:1701:PGX:H182	1.71	0.72
1:C:2273:MET:HE2	1:C:2287:VAL:H	1.55	0.72
1:D:3385:TYR:HA	5:D:3701:PGX:O4	1.89	0.72
1:A:449:LYS:HA	1:A:452:ILE:HD12	1.69	0.71
1:D:3311:ARG:HB2	6:D:4149:HOH:O	1.90	0.71
1:B:1308:GLU:CB	1:B:1571:ASN:HD21	2.02	0.71
1:D:3184:ARG:HB2	1:D:3439:ASN:C	2.15	0.71
1:A:442:ILE:O	1:A:445:GLN:HB2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1382:ASN:O	1:B:1385:TYR:HB3	1.91	0.71
1:B:1497:ASP:HB3	1:B:1500:VAL:HG23	1.72	0.71
1:C:2218:PRO:HD2	6:C:4099:HOH:O	1.91	0.71
1:C:2273:MET:HE2	1:C:2287:VAL:N	2.05	0.71
1:C:2196:MET:HA	1:C:2196:MET:HE2	1.73	0.71
1:D:3553:GLU:OE1	1:D:3553:GLU:HA	1.89	0.71
1:C:2527:ALA:HB3	1:C:2528:PRO:HD3	1.72	0.71
1:B:1244:LEU:HD23	1:B:1271:VAL:HG21	1.71	0.70
1:A:232:HIS:O	1:A:288:GLY:HA3	1.90	0.70
1:A:454:GLN:HA	1:A:457:GLU:OE2	1.91	0.70
1:C:2335:ILE:HA	1:C:2559:ILE:HD11	1.72	0.70
1:D:3527:ALA:HB3	1:D:3528:PRO:HD3	1.73	0.70
1:A:190:ASP:OD1	1:A:517:ILE:HB	1.91	0.70
1:B:1403:SER:OG	1:B:1406:GLN:HG3	1.91	0.70
1:D:3387:TRP:CZ2	5:D:3701:PGX:H121	2.27	0.70
1:A:404:PHE:HB2	1:A:405:LYS:HE3	1.74	0.70
1:B:1188:ILE:HD12	1:B:1439:ASN:HB2	1.72	0.70
1:B:1293:GLY:HA2	1:B:1299:MET:CE	2.22	0.70
1:D:3308:GLU:CB	1:D:3571:ASN:HD21	2.03	0.70
1:D:3563:SER:OG	1:D:3565:GLN:HB3	1.90	0.70
1:A:230:LEU:HG	1:A:337:ILE:HG13	1.73	0.70
1:B:1385:TYR:HB2	5:B:1701:PGX:H101	1.73	0.70
1:D:3138:SER:O	1:D:3141:ALA:HB3	1.92	0.70
1:C:2377:ILE:HA	6:C:4133:HOH:O	1.92	0.70
1:D:3273:MET:HE2	1:D:3287:VAL:N	2.07	0.70
1:D:3454:GLN:HA	1:D:3457:GLU:OE2	1.92	0.70
1:A:385:TYR:O	1:A:387:TRP:N	2.25	0.69
1:B:1162:PRO:O	1:B:1163:MET:HE2	1.91	0.69
1:C:2274:ILE:HG13	1:C:2290:GLU:O	1.92	0.69
1:C:2190:ASP:OD1	1:C:2517:ILE:HB	1.92	0.69
1:D:3178:LEU:O	1:D:3182:LEU:HB2	1.90	0.69
1:B:1281:GLU:HA	1:B:1284:GLN:HG3	1.74	0.69
1:B:1513:ARG:CZ	1:B:1520:GLU:HA	2.22	0.69
1:D:3306:LEU:HD23	1:D:3306:LEU:C	2.17	0.69
1:D:3513:ARG:CZ	1:D:3520:GLU:HA	2.22	0.69
1:B:1404:PHE:HB2	1:B:1405:LYS:HE3	1.72	0.69
1:C:2404:PHE:HB2	1:C:2405:LYS:HE3	1.74	0.69
1:A:335:ILE:HA	1:A:559:ILE:HD11	1.74	0.69
1:D:3350:GLN:NE2	1:D:3358:LYS:HA	2.08	0.69
1:A:281:GLU:HA	1:A:284:GLN:HG3	1.74	0.69
1:A:350:GLN:NE2	1:A:358:LYS:HA	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:GLU:OE2	1:A:524:GLU:HA	1.92	0.69
1:B:1275:TYR:CE2	1:B:1284:GLN:HA	2.28	0.69
1:C:2149:THR:O	1:C:2378:ALA:HA	1.92	0.69
1:C:2350:GLN:NE2	1:C:2358:LYS:HA	2.06	0.69
1:A:132:VAL:HG12	1:A:133:HIS:N	2.06	0.69
1:A:196:MET:HE2	1:A:196:MET:HA	1.74	0.69
1:A:210:PHE:CE1	1:A:382:ASN:HA	2.27	0.69
1:B:1206:THR:HG21	5:B:1701:PGX:H111	1.74	0.69
1:A:513:ARG:CZ	1:A:520:GLU:HA	2.23	0.69
1:B:1244:LEU:O	1:B:1252:LEU:HD23	1.93	0.69
1:B:1414:LEU:HD11	1:B:1419:LEU:CD2	2.22	0.69
1:C:2226:HIS:ND1	1:C:2376:ARG:HD2	2.07	0.69
1:C:2148:TYR:HD1	1:C:2377:ILE:HG22	1.58	0.69
1:C:2322:GLU:OE1	1:D:3049:SER:HB2	1.93	0.69
1:D:3210:PHE:CE1	1:D:3382:ASN:HA	2.28	0.69
1:A:306:LEU:C	1:A:306:LEU:HD23	2.18	0.68
1:D:3281:GLU:HA	1:D:3284:GLN:HG3	1.75	0.68
1:D:3382:ASN:O	1:D:3385:TYR:HB3	1.93	0.68
1:B:1132:VAL:HG12	1:B:1133:HIS:N	2.07	0.68
1:D:3404:PHE:HB2	1:D:3405:LYS:HE3	1.73	0.68
1:A:184:ARG:HB2	1:A:439:ASN:HA	1.76	0.68
1:B:1274:ILE:HG13	1:B:1290:GLU:O	1.94	0.68
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.74	0.68
1:B:1138:SER:O	1:B:1141:ALA:HB3	1.93	0.68
1:B:1203:GLN:CG	1:B:1298:LEU:HD11	2.22	0.68
1:C:2180:LYS:O	1:C:2181:VAL:HG13	1.93	0.68
1:D:3384:LEU:HB3	1:D:3522:MET:HE2	1.75	0.68
1:A:293:GLY:HA2	1:A:299:MET:CE	2.24	0.68
1:A:463:LEU:HD12	1:A:503:LEU:HD12	1.75	0.68
1:C:2308:GLU:HB2	1:C:2571:ASN:ND2	2.07	0.68
1:C:2385:TYR:O	1:C:2387:TRP:N	2.27	0.68
1:A:149:THR:O	1:A:378:ALA:HA	1.94	0.68
1:A:178:LEU:O	1:A:182:LEU:HB2	1.94	0.68
1:C:2384:LEU:HB3	1:C:2522:MET:HE2	1.75	0.68
1:A:273:MET:HE2	1:A:287:VAL:N	2.09	0.68
1:C:2537:ASN:HB2	6:C:4123:HOH:O	1.93	0.68
1:D:3385:TYR:O	1:D:3387:TRP:N	2.26	0.68
1:B:1385:TYR:O	1:B:1387:TRP:N	2.26	0.68
1:D:3534:LEU:HD22	5:D:3701:PGX:H182	1.76	0.68
1:B:1179:GLU:HA	1:B:1183:LEU:HD12	1.75	0.67
1:C:2403:SER:OG	1:C:2406:GLN:HG3	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2513:ARG:CZ	1:C:2520:GLU:HA	2.24	0.67
1:D:3219:GLY:HA2	1:D:3458:MET:HE2	1.76	0.67
1:C:2293:GLY:HA2	1:C:2299:MET:CE	2.24	0.67
1:A:219:GLY:HA2	1:A:458:MET:HE2	1.75	0.67
1:D:3134:TYR:HD2	1:D:3136:TYR:CE1	2.12	0.67
1:C:2275:TYR:CE2	1:C:2284:GLN:HA	2.30	0.67
1:C:2563:SER:OG	1:C:2565:GLN:HB3	1.94	0.67
1:C:2463:LEU:HD13	1:C:2506:ALA:CB	2.23	0.67
1:A:148:TYR:HD1	1:A:377:ILE:HG22	1.59	0.67
1:B:1190:ASP:OD1	1:B:1517:ILE:HB	1.95	0.67
1:B:1563:SER:OG	1:B:1565:GLN:HB3	1.94	0.67
1:C:2219:GLY:HA2	1:C:2458:MET:HE2	1.77	0.67
1:A:89:VAL:HA	1:A:92:ILE:HG13	1.75	0.67
1:B:1419:LEU:O	1:B:1423:VAL:HG23	1.94	0.67
1:C:2244:LEU:HD23	1:C:2271:VAL:HG21	1.77	0.67
1:A:226:HIS:ND1	1:A:376:ARG:HD2	2.09	0.67
1:A:148:TYR:CD1	1:A:377:ILE:HG22	2.30	0.67
1:C:2382:ASN:O	1:C:2385:TYR:HB3	1.94	0.67
1:D:3179:GLU:HA	1:D:3183:LEU:HD12	1.75	0.67
1:A:381:PHE:CD1	1:A:529:PHE:HB3	2.30	0.66
1:B:1384:LEU:HB3	1:B:1522:MET:HE2	1.76	0.66
1:A:308:GLU:HB2	1:A:571:ASN:ND2	2.08	0.66
1:B:1425:SER:O	1:B:1428:ARG:HG2	1.95	0.66
1:C:2148:TYR:CD1	1:C:2377:ILE:HG22	2.30	0.66
1:C:2150:ARG:HD3	6:C:4134:HOH:O	1.95	0.66
1:D:3567:LEU:HD12	1:D:3567:LEU:O	1.96	0.66
1:A:132:VAL:O	1:A:154:PRO:HG3	1.93	0.66
1:B:1381:PHE:CD1	1:B:1529:PHE:HB3	2.31	0.66
1:B:1463:LEU:HD13	1:B:1506:ALA:CB	2.23	0.66
1:D:3293:GLY:HA2	1:D:3299:MET:CE	2.24	0.66
1:B:1350:GLN:NE2	1:B:1358:LYS:HA	2.09	0.66
1:D:3148:TYR:HD1	1:D:3377:ILE:HG22	1.60	0.66
1:A:563:SER:OG	1:A:565:GLN:HB3	1.96	0.66
1:B:1454:GLN:HA	1:B:1457:GLU:OE2	1.95	0.66
1:D:3453:ASP:O	1:D:3456:ARG:HB2	1.96	0.66
1:B:1148:TYR:HD1	1:B:1377:ILE:HG22	1.60	0.66
1:D:3113:MET:HE3	1:D:3116:VAL:HG22	1.78	0.66
1:A:263:PRO:HD3	1:A:303:THR:HG23	1.77	0.66
1:A:482:THR:HG22	6:A:4032:HOH:O	1.96	0.66
1:D:3428:ARG:HA	1:D:3582:VAL:HG23	1.78	0.66
1:D:3501:MET:CE	1:D:3505:PRO:HB2	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1174:SER:OG	1:B:1449:LYS:HE2	1.94	0.66
1:C:2132:VAL:HG12	1:C:2133:HIS:N	2.10	0.66
1:C:2184:ARG:HB2	1:C:2439:ASN:HA	1.76	0.66
1:C:2425:SER:O	1:C:2428:ARG:HG2	1.94	0.66
1:D:3176:GLU:OE1	1:D:3180:LYS:HE2	1.96	0.66
1:D:3403:SER:OG	1:D:3406:GLN:HG3	1.95	0.66
1:B:1132:VAL:O	1:B:1154:PRO:HG3	1.95	0.66
1:C:2076:THR:O	1:C:2080:LEU:HG	1.96	0.66
1:D:3132:VAL:O	1:D:3154:PRO:HG3	1.95	0.66
1:A:179:GLU:HA	1:A:183:LEU:HD12	1.78	0.66
1:A:453:ASP:O	1:A:456:ARG:HB2	1.96	0.66
1:B:1148:TYR:CD1	1:B:1377:ILE:HG22	2.31	0.66
1:B:1205:PHE:O	1:B:1208:GLN:HG2	1.96	0.66
1:C:2280:PRO:HB2	1:C:2282:ASN:OD1	1.95	0.66
1:D:3180:LYS:O	1:D:3181:VAL:HG13	1.96	0.66
1:D:3274:ILE:HG13	1:D:3290:GLU:O	1.94	0.66
1:C:2089:VAL:HA	1:C:2092:ILE:HG13	1.76	0.65
1:D:3174:SER:OG	1:D:3449:LYS:HE2	1.95	0.65
1:B:1527:ALA:HB3	1:B:1528:PRO:HD3	1.77	0.65
1:C:2381:PHE:CD1	1:C:2529:PHE:HB3	2.31	0.65
1:B:1335:ILE:HA	1:B:1559:ILE:HD11	1.78	0.65
1:B:1524:GLU:HA	1:B:1524:GLU:OE2	1.97	0.65
1:C:2179:GLU:HA	1:C:2183:LEU:HD12	1.78	0.65
1:C:2453:ASP:O	1:C:2456:ARG:HB2	1.96	0.65
1:C:2524:GLU:OE2	1:C:2524:GLU:HA	1.95	0.65
1:D:3148:TYR:CD1	1:D:3377:ILE:HG22	2.30	0.65
1:D:3335:ILE:HA	1:D:3559:ILE:HD11	1.78	0.65
1:A:456:ARG:HA	6:A:4021:HOH:O	1.96	0.65
1:C:2203:GLN:CG	1:C:2298:LEU:HD11	2.26	0.65
1:C:2454:GLN:HA	1:C:2457:GLU:OE2	1.96	0.65
1:D:3089:VAL:HA	1:D:3092:ILE:HG13	1.78	0.65
1:D:3226:HIS:ND1	1:D:3376:ARG:HD2	2.12	0.65
1:C:2238:LEU:HD22	1:C:2242:HIS:NE2	2.11	0.65
1:B:1219:GLY:HA2	1:B:1458:MET:HE2	1.78	0.65
1:C:2138:SER:O	1:C:2141:ALA:HB3	1.97	0.65
1:C:2176:GLU:OE1	1:C:2180:LYS:HE2	1.96	0.65
1:B:1206:THR:HA	1:B:1209:PHE:CZ	2.32	0.65
1:B:1532:LYS:O	1:B:1534:LEU:N	2.30	0.65
1:D:3347:ASP:O	1:D:3348:TYR:C	2.40	0.65
1:D:3381:PHE:CD1	1:D:3529:PHE:HB3	2.32	0.65
1:A:134:TYR:HD2	1:A:136:TYR:CE1	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:PHE:O	1:A:208:GLN:HG2	1.96	0.65
1:B:1232:HIS:O	1:B:1288:GLY:HA3	1.97	0.65
1:D:3208:GLN:HG3	1:D:3209:PHE:CD1	2.32	0.65
1:D:3414:LEU:HD11	1:D:3419:LEU:CD2	2.26	0.65
1:D:3578:THR:CG2	1:D:3579:SER:N	2.60	0.65
1:A:428:ARG:HA	1:A:582:VAL:HG23	1.79	0.65
1:C:2232:HIS:O	1:C:2288:GLY:HA3	1.97	0.65
1:C:2388:HIS:HB3	1:C:2444:VAL:HG11	1.79	0.65
1:C:2428:ARG:HA	1:C:2582:VAL:HG23	1.77	0.65
1:C:2567:LEU:O	1:C:2567:LEU:HD12	1.97	0.65
1:D:3085:THR:O	1:D:3089:VAL:HG23	1.97	0.65
1:D:3563:SER:HB2	6:D:4157:HOH:O	1.96	0.65
1:A:218:PRO:HD2	6:A:4003:HOH:O	1.97	0.64
1:B:1391:LEU:HD22	1:B:1404:PHE:CZ	2.32	0.64
1:A:388:HIS:HB3	1:A:444:VAL:HG11	1.79	0.64
1:D:3238:LEU:HD22	1:D:3242:HIS:NE2	2.12	0.64
1:A:238:LEU:HD22	1:A:242:HIS:NE2	2.12	0.64
1:D:3388:HIS:HB3	1:D:3444:VAL:HG11	1.80	0.64
1:A:97:LYS:HB2	1:A:356:HIS:CE1	2.32	0.64
1:A:203:GLN:CG	1:A:298:LEU:HD11	2.27	0.64
1:D:3206:THR:HA	1:D:3209:PHE:CZ	2.32	0.64
1:D:3293:GLY:HA2	1:D:3299:MET:HE3	1.79	0.64
1:A:85:THR:O	1:A:89:VAL:HG23	1.98	0.64
1:A:389:PRO:CG	1:A:434:VAL:HG13	2.21	0.64
1:B:1176:GLU:OE1	1:B:1180:LYS:HE2	1.97	0.64
1:B:1295:VAL:HB	1:B:1298:LEU:HD22	1.79	0.64
1:C:2113:MET:HE3	1:C:2116:VAL:HG22	1.80	0.64
1:C:2385:TYR:HA	5:C:2701:PGX:O4	1.97	0.64
1:A:414:LEU:HD11	1:A:419:LEU:CD2	2.27	0.64
1:B:1229:ASP:OD2	1:B:1231:ASN:HB3	1.98	0.64
1:C:2134:TYR:HD2	1:C:2136:TYR:CE1	2.15	0.64
1:C:2306:LEU:C	1:C:2306:LEU:HD23	2.23	0.64
1:D:3280:PRO:HB2	1:D:3282:ASN:OD1	1.98	0.64
1:A:425:SER:O	1:A:428:ARG:HG2	1.97	0.64
1:A:273:MET:HE2	1:A:287:VAL:H	1.62	0.64
1:A:275:TYR:CE2	1:A:284:GLN:HA	2.33	0.64
1:C:2532:LYS:O	1:C:2534:LEU:N	2.31	0.64
1:D:3205:PHE:O	1:D:3208:GLN:HG2	1.98	0.64
1:D:3244:LEU:O	1:D:3252:LEU:HD23	1.97	0.64
1:D:3463:LEU:HD13	1:D:3506:ALA:CB	2.24	0.64
1:D:3524:GLU:HA	1:D:3524:GLU:OE2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:MET:HE3	1:A:116:VAL:HG22	1.80	0.63
1:A:138:SER:O	1:A:141:ALA:HB3	1.97	0.63
1:D:3130:TYR:HB3	1:D:3134:TYR:O	1.97	0.63
1:D:3191:PRO:CD	1:D:3433:ARG:HG3	2.27	0.63
1:B:1238:LEU:HD22	1:B:1242:HIS:NE2	2.13	0.63
1:C:2130:TYR:HB3	1:C:2134:TYR:O	1.98	0.63
1:C:2396:ASN:ND2	1:C:2396:ASN:N	2.45	0.63
1:A:347:ASP:O	1:A:348:TYR:C	2.40	0.63
1:B:1089:VAL:HA	1:B:1092:ILE:HG13	1.79	0.63
1:D:3057:CYS:HB3	1:D:3069:CYS:SG	2.38	0.63
1:D:3244:LEU:HD23	1:D:3271:VAL:HG21	1.79	0.63
1:A:245:ARG:NH2	1:A:326:GLU:HG2	2.12	0.63
1:A:274:ILE:HG13	1:A:290:GLU:O	1.97	0.63
1:A:501:MET:HE1	1:A:505:PRO:HB2	1.79	0.63
1:B:1057:CYS:HB3	1:B:1069:CYS:SG	2.38	0.63
1:D:3132:VAL:HG12	1:D:3133:HIS:N	2.13	0.63
1:D:3578:THR:HG22	1:D:3579:SER:H	1.61	0.63
1:B:1184:ARG:HB2	1:B:1439:ASN:HA	1.80	0.63
1:C:2272:GLU:HA	6:C:4108:HOH:O	1.97	0.63
1:C:2347:ASP:O	1:C:2348:TYR:C	2.41	0.63
1:A:280:PRO:HB2	1:A:282:ASN:OD1	1.99	0.63
1:B:1203:GLN:HG2	1:B:1298:LEU:CD1	2.27	0.63
1:B:1567:LEU:HD12	1:B:1567:LEU:O	1.99	0.63
1:D:3403:SER:HB2	1:D:3405:LYS:HZ2	1.64	0.63
1:A:226:HIS:CE1	1:A:376:ARG:HD2	2.33	0.63
1:A:463:LEU:HD13	1:A:506:ALA:CB	2.25	0.63
1:C:2226:HIS:CE1	1:C:2376:ARG:HD2	2.34	0.63
1:A:532:LYS:O	1:A:534:LEU:N	2.31	0.63
1:B:1306:LEU:HD23	1:B:1306:LEU:C	2.24	0.63
1:B:1465:GLU:OE2	1:B:1465:GLU:HA	1.98	0.63
1:C:2132:VAL:O	1:C:2154:PRO:HG3	1.97	0.63
1:C:2502:GLU:HB3	6:C:4124:HOH:O	1.99	0.63
1:D:3203:GLN:CG	1:D:3298:LEU:HD11	2.27	0.63
1:A:208:GLN:HG3	1:A:209:PHE:CD1	2.34	0.63
1:A:391:LEU:HD22	1:A:404:PHE:CZ	2.34	0.63
1:A:465:GLU:HA	1:A:465:GLU:OE2	1.98	0.62
1:D:3196:MET:HE2	1:D:3196:MET:HA	1.80	0.62
1:D:3308:GLU:O	1:D:3311:ARG:HB3	1.99	0.62
1:D:3482:THR:C	1:D:3511:LYS:HB2	2.24	0.62
1:A:180:LYS:O	1:A:181:VAL:HG13	1.99	0.62
1:A:382:ASN:O	1:A:385:TYR:HB3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:THR:CG2	1:A:579:SER:N	2.61	0.62
1:B:1245:ARG:NH2	1:B:1326:GLU:HG2	2.09	0.62
1:C:2578:THR:CG2	1:C:2579:SER:N	2.61	0.62
1:A:118:THR:HA	1:A:121:SER:OG	2.00	0.62
1:A:293:GLY:HA2	1:A:299:MET:HE3	1.78	0.62
1:B:1308:GLU:HB2	1:B:1571:ASN:ND2	2.11	0.62
1:B:1447:VAL:HG12	1:B:1448:ALA:N	2.13	0.62
1:D:3229:ASP:OD2	1:D:3231:ASN:HB3	1.99	0.62
1:D:3275:TYR:CE2	1:D:3284:GLN:HA	2.34	0.62
1:A:385:TYR:HA	5:A:701:PGX:O4	1.98	0.62
1:B:1510:GLU:OE1	1:B:1519:GLY:HA3	1.98	0.62
1:C:2391:LEU:HD22	1:C:2404:PHE:CZ	2.34	0.62
1:A:353:SER:HA	6:A:4023:HOH:O	2.00	0.62
1:B:1428:ARG:HA	1:B:1582:VAL:HG23	1.80	0.62
1:B:1442:ILE:N	1:B:1442:ILE:HD12	2.15	0.62
1:C:2085:THR:O	1:C:2089:VAL:HG23	2.00	0.62
1:D:3578:THR:CG2	1:D:3579:SER:H	2.13	0.62
1:C:2205:PHE:O	1:C:2208:GLN:HG2	1.99	0.62
1:D:3184:ARG:NH1	1:D:3441:PRO:HG3	2.13	0.62
1:B:1208:GLN:HG3	1:B:1209:PHE:CD1	2.35	0.62
1:D:3532:LYS:O	1:D:3534:LEU:N	2.33	0.62
1:A:327:GLN:NE2	1:B:1136:TYR:CD2	2.68	0.62
1:C:2208:GLN:HG3	1:C:2209:PHE:CD1	2.34	0.62
1:C:2201:PHE:O	1:C:2202:ALA:C	2.43	0.62
1:C:2229:ASP:OD2	1:C:2231:ASN:HB3	2.00	0.62
1:C:2245:ARG:NH2	1:C:2326:GLU:HG2	2.11	0.62
1:D:3078:ILE:O	1:D:3082:LEU:HD12	2.00	0.62
1:D:3197:MET:CE	1:D:3423:VAL:HG13	2.29	0.62
1:D:3425:SER:O	1:D:3428:ARG:HG2	1.99	0.62
1:A:76:THR:O	1:A:80:LEU:HG	1.99	0.62
1:B:1134:TYR:HD2	1:B:1136:TYR:CE1	2.17	0.62
1:C:2131:ASN:ND2	1:C:2147:TYR:CD2	2.68	0.62
1:C:2193:GLY:O	1:C:2582:VAL:HG12	2.00	0.62
1:D:3184:ARG:HB2	1:D:3439:ASN:HA	1.82	0.62
1:A:136:TYR:HD2	1:B:1327:GLN:NE2	1.98	0.61
1:B:1293:GLY:HA2	1:B:1299:MET:HE3	1.82	0.61
1:C:2465:GLU:HA	1:C:2465:GLU:OE2	2.00	0.61
1:D:3308:GLU:HB2	1:D:3571:ASN:ND2	2.12	0.61
1:A:386:HIS:HB3	1:A:388:HIS:CE1	2.36	0.61
1:B:1072:PRO:HG2	1:B:1077:ARG:HE	1.64	0.61
1:A:206:THR:HA	1:A:209:PHE:CZ	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ASP:OD2	1:A:231:ASN:HB3	2.00	0.61
1:C:2198:PHE:CE1	1:C:2352:LEU:HD13	2.35	0.61
1:D:3232:HIS:O	1:D:3288:GLY:HA3	2.01	0.61
1:D:3245:ARG:NH2	1:D:3326:GLU:HG2	2.14	0.61
1:D:3454:GLN:O	1:D:3457:GLU:HG3	2.00	0.61
1:B:1347:ASP:O	1:B:1348:TYR:C	2.43	0.61
1:B:1226:HIS:ND1	1:B:1376:ARG:HD2	2.15	0.61
1:C:2210:PHE:O	1:C:2211:LYS:HG3	2.01	0.61
1:D:3263:PRO:HD3	1:D:3303:THR:HG23	1.82	0.61
1:B:1387:TRP:HZ2	5:B:1701:PGX:H71	1.65	0.61
1:C:2203:GLN:HG2	1:C:2298:LEU:CD1	2.30	0.61
1:C:2241:GLN:HG3	1:C:2242:HIS:N	2.14	0.61
1:A:295:VAL:HB	1:A:298:LEU:HD22	1.83	0.61
1:B:1191:PRO:CD	1:B:1433:ARG:HG3	2.29	0.61
1:D:3197:MET:HE2	1:D:3423:VAL:HG13	1.80	0.61
1:A:130:TYR:HB3	1:A:134:TYR:O	2.00	0.61
1:A:136:TYR:CD2	1:B:1327:GLN:NE2	2.69	0.61
1:C:2306:LEU:HD23	1:C:2307:ARG:N	2.15	0.61
1:A:100:TRP:CD1	1:A:356:HIS:HB2	2.35	0.61
1:A:176:GLU:OE1	1:A:180:LYS:HE2	2.00	0.61
1:C:2074:PHE:HA	1:C:2077:ARG:HG3	1.83	0.61
1:D:3118:THR:HA	1:D:3121:SER:OG	2.01	0.61
1:D:3465:GLU:HA	1:D:3465:GLU:OE2	2.00	0.61
1:A:396:ASN:ND2	1:A:396:ASN:N	2.45	0.60
1:A:403:SER:HB2	1:A:405:LYS:HZ2	1.64	0.60
1:C:2118:THR:HA	1:C:2121:SER:OG	2.00	0.60
1:C:2327:GLN:NE2	1:D:3136:TYR:HD2	1.98	0.60
1:C:2339:GLU:O	1:C:2342:LYS:HB3	2.00	0.60
1:C:2385:TYR:HB2	5:C:2701:PGX:H101	1.82	0.60
1:D:3095:HIS:HA	6:D:4153:HOH:O	2.01	0.60
1:D:3389:PRO:CG	1:D:3434:VAL:HG13	2.26	0.60
1:A:120:ARG:NH1	1:A:527:ALA:HB1	2.16	0.60
1:B:1076:THR:O	1:B:1080:LEU:HG	2.01	0.60
1:B:1120:ARG:NH1	1:B:1527:ALA:HB1	2.16	0.60
1:B:1171:LEU:HD12	1:B:1502:GLU:OE2	2.01	0.60
1:B:1454:GLN:O	1:B:1457:GLU:HG3	2.02	0.60
1:D:3113:MET:C	1:D:3116:VAL:HG13	2.25	0.60
1:B:1197:MET:CE	1:B:1423:VAL:HG13	2.31	0.60
1:B:1210:PHE:O	1:B:1211:LYS:HG3	2.01	0.60
1:C:2113:MET:CA	1:C:2116:VAL:HG13	2.32	0.60
1:C:2184:ARG:HB2	1:C:2439:ASN:CA	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2327:GLN:NE2	1:D:3136:TYR:CD2	2.70	0.60
1:C:2409:TYR:N	1:C:2409:TYR:CD2	2.69	0.60
1:C:2295:VAL:HB	1:C:2298:LEU:HD22	1.82	0.60
1:B:1118:THR:HA	1:B:1121:SER:OG	2.01	0.60
1:B:1501:MET:CE	1:B:1505:PRO:HB2	2.31	0.60
1:B:1562:ALA:HA	6:B:4092:HOH:O	2.01	0.60
1:B:1578:THR:CG2	1:B:1579:SER:N	2.64	0.60
1:D:3171:LEU:HD12	1:D:3502:GLU:OE2	2.01	0.60
1:D:3203:GLN:HG2	1:D:3298:LEU:CD1	2.29	0.60
1:D:3409:TYR:N	1:D:3409:TYR:CD2	2.68	0.60
1:C:2184:ARG:NH2	1:C:2441:PRO:HD3	2.17	0.60
1:C:2414:LEU:HD11	1:C:2419:LEU:CD2	2.31	0.60
1:D:3181:VAL:HG12	1:D:3487:MET:HG2	1.84	0.60
1:A:526:GLY:CA	5:A:701:PGX:H61	2.30	0.60
1:D:3295:VAL:HB	1:D:3298:LEU:HD22	1.83	0.60
1:D:3457:GLU:C	1:D:3459:LYS:H	2.10	0.60
1:A:184:ARG:HB2	1:A:439:ASN:CA	2.31	0.60
1:A:197:MET:HE2	1:A:423:VAL:HG13	1.83	0.60
1:A:327:GLN:NE2	1:B:1136:TYR:HD2	2.00	0.60
1:B:1241:GLN:HG3	1:B:1242:HIS:N	2.15	0.60
1:C:2184:ARG:HA	1:C:2438:ARG:O	2.02	0.60
1:C:2197:MET:HE1	1:C:2300:MET:HE1	1.83	0.60
1:D:3072:PRO:HG2	1:D:3077:ARG:HE	1.65	0.60
1:D:3241:GLN:HG3	1:D:3242:HIS:N	2.11	0.60
1:A:203:GLN:HG2	1:A:298:LEU:CD1	2.30	0.60
1:B:1124:ILE:HD11	1:B:1528:PRO:HB2	1.84	0.60
1:A:409:TYR:N	1:A:409:TYR:CD2	2.69	0.60
1:B:1113:MET:HE3	1:B:1116:VAL:HG22	1.82	0.60
1:B:1113:MET:C	1:B:1116:VAL:HG13	2.26	0.60
1:B:1453:ASP:O	1:B:1456:ARG:HB2	2.01	0.60
1:B:1482:THR:C	1:B:1511:LYS:HB2	2.26	0.60
1:D:3274:ILE:HG13	1:D:3290:GLU:C	2.27	0.60
1:A:180:LYS:HD2	1:A:490:GLU:OE1	2.02	0.59
1:B:1074:PHE:HA	1:B:1077:ARG:HG3	1.84	0.59
1:B:1180:LYS:O	1:B:1181:VAL:HG13	2.02	0.59
1:C:2105(C):ILE:HG21	1:C:2108:LEU:HD12	1.84	0.59
1:A:197:MET:CE	1:A:423:VAL:HG13	2.32	0.59
1:A:244:LEU:HD23	1:A:271:VAL:HG21	1.82	0.59
1:A:343:ILE:O	1:A:347:ASP:HB2	2.02	0.59
1:A:389:PRO:HG3	1:A:508:LEU:HD22	1.84	0.59
1:A:501:MET:CE	1:A:505:PRO:HB2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1089:VAL:HA	1:B:1092:ILE:CG1	2.32	0.59
1:B:1495:TYR:HE2	1:B:1502:GLU:HG3	1.67	0.59
1:B:1193:GLY:O	1:B:1582:VAL:HG12	2.02	0.59
1:C:2184:ARG:NH1	1:C:2441:PRO:HG3	2.18	0.59
1:A:78:ILE:O	1:A:82:LEU:HD12	2.01	0.59
1:B:1184:ARG:HD3	1:B:1187:PHE:CA	2.29	0.59
1:B:1267:LYS:HG2	1:B:1267:LYS:O	2.03	0.59
1:D:3136:TYR:O	1:D:3136:TYR:HD1	1.85	0.59
1:D:3504:TYR:HA	1:D:3507:LEU:HD12	1.84	0.59
1:A:276:PRO:O	1:A:279:ILE:HG12	2.02	0.59
1:B:1343:ILE:O	1:B:1347:ASP:HB2	2.01	0.59
1:C:2276:PRO:HD2	1:C:2279:ILE:CG1	2.32	0.59
1:D:3193:GLY:O	1:D:3582:VAL:HG12	2.02	0.59
1:B:1213:ASP:HB2	1:B:1222:ARG:HG3	1.85	0.59
1:C:2274:ILE:HG13	1:C:2290:GLU:C	2.27	0.59
1:C:2293:GLY:HA2	1:C:2299:MET:HE3	1.84	0.59
1:D:3341:ILE:HG23	1:D:3534:LEU:HD12	1.85	0.59
1:B:1403:SER:HB2	1:B:1405:LYS:HZ2	1.66	0.59
1:D:3192:GLN:OE1	1:D:3517:ILE:HG22	2.02	0.59
1:D:3442:ILE:HD12	1:D:3442:ILE:N	2.18	0.59
1:A:57:CYS:HB3	1:A:69:CYS:SG	2.43	0.59
1:B:1130:TYR:HB3	1:B:1134:TYR:O	2.02	0.59
1:D:3076:THR:O	1:D:3080:LEU:HG	2.03	0.59
1:D:3447:VAL:HG12	1:D:3448:ALA:N	2.17	0.59
1:A:306:LEU:HD23	1:A:307:ARG:N	2.18	0.59
1:A:562:ALA:HA	6:A:4043:HOH:O	2.02	0.59
1:B:1388:HIS:HB3	1:B:1444:VAL:HG11	1.84	0.59
1:B:1554:VAL:HG12	1:B:1555:GLY:N	2.18	0.59
1:C:2273:MET:CE	1:C:2287:VAL:HG22	2.26	0.59
1:C:2276:PRO:O	1:C:2279:ILE:HG12	2.03	0.59
1:C:2578:THR:HG22	1:C:2579:SER:H	1.66	0.59
1:D:3184:ARG:NH2	1:D:3441:PRO:HD3	2.18	0.59
1:D:3391:LEU:HD22	1:D:3404:PHE:CZ	2.38	0.59
1:A:72:PRO:HG2	1:A:77:ARG:HE	1.67	0.58
1:C:2113:MET:C	1:C:2116:VAL:HG13	2.28	0.58
1:C:2362:ASP:O	1:C:2365:LEU:HG	2.01	0.58
1:C:2495:TYR:HE2	1:C:2502:GLU:HG3	1.67	0.58
1:D:3128:PRO:HG3	1:D:3376:ARG:HB2	1.85	0.58
1:D:3495:TYR:HE2	1:D:3502:GLU:HG3	1.68	0.58
1:D:3501:MET:HE1	1:D:3505:PRO:HB2	1.83	0.58
1:A:74:PHE:HA	1:A:77:ARG:HG3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:PHE:O	1:A:202:ALA:C	2.46	0.58
1:A:362:ASP:O	1:A:365:LEU:HG	2.03	0.58
1:B:1197:MET:HE2	1:B:1423:VAL:HG13	1.85	0.58
1:D:3427:THR:HG21	1:D:3578:THR:HA	1.85	0.58
1:A:269:THR:OG1	1:A:271:VAL:HG23	2.02	0.58
1:A:457:GLU:C	1:A:459:LYS:H	2.11	0.58
1:C:2457:GLU:C	1:C:2459:LYS:H	2.11	0.58
1:A:276:PRO:HD2	1:A:279:ILE:CG1	2.34	0.58
1:A:387:TRP:CH2	5:A:701:PGX:H121	2.38	0.58
1:B:1201:PHE:O	1:B:1202:ALA:C	2.45	0.58
1:C:2097:LYS:HB2	1:C:2356:HIS:CE1	2.37	0.58
1:C:2403:SER:HB2	1:C:2405:LYS:HZ2	1.68	0.58
1:D:3097:LYS:HB2	1:D:3356:HIS:CE1	2.38	0.58
1:D:3205:PHE:HE2	5:D:3701:PGX:H171	1.68	0.58
1:D:3218:PRO:C	1:D:3458:MET:HE3	2.29	0.58
1:A:113:MET:C	1:A:116:VAL:HG13	2.28	0.58
1:A:191:PRO:HG3	1:A:433:ARG:NH1	2.18	0.58
1:A:554:VAL:HG12	1:A:555:GLY:N	2.18	0.58
1:B:1085:THR:O	1:B:1089:VAL:HG23	2.03	0.58
1:C:2120:ARG:NH1	1:C:2527:ALA:HB1	2.19	0.58
1:C:2171:LEU:HD12	1:C:2502:GLU:OE2	2.04	0.58
1:C:2507:LEU:HD21	1:C:2521:THR:HG22	1.85	0.58
1:A:184:ARG:NH1	1:A:441:PRO:HG3	2.19	0.58
1:A:341:ILE:HG23	1:A:534:LEU:HD12	1.86	0.58
1:A:389:PRO:HG2	1:A:434:VAL:CG1	2.26	0.58
1:B:1184:ARG:HB2	1:B:1439:ASN:CA	2.34	0.58
1:B:1255:GLN:HG2	1:B:1263:PRO:O	2.04	0.58
1:B:1274:ILE:HG13	1:B:1290:GLU:C	2.27	0.58
1:C:2414:LEU:HA	1:C:2422:PHE:HE1	1.67	0.58
1:D:3201:PHE:O	1:D:3202:ALA:C	2.46	0.58
1:D:3269:THR:OG1	1:D:3271:VAL:HG23	2.04	0.58
1:A:128:PRO:CG	1:A:376:ARG:NH1	2.67	0.58
1:A:193:GLY:O	1:A:582:VAL:HG12	2.03	0.58
1:B:1131:ASN:ND2	1:B:1147:TYR:CD2	2.72	0.58
1:B:1180:LYS:HD2	1:B:1490:GLU:OE1	2.04	0.58
1:C:2108:LEU:HD23	1:C:2111:LEU:CD2	2.34	0.58
1:C:2136:TYR:CD2	1:D:3327:GLN:NE2	2.72	0.58
1:C:2263:PRO:HD3	1:C:2303:THR:HG23	1.83	0.58
1:D:3113:MET:CA	1:D:3116:VAL:HG13	2.34	0.58
1:D:3226:HIS:CE1	1:D:3376:ARG:HD2	2.39	0.58
1:D:3554:VAL:HG12	1:D:3555:GLY:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1192:GLN:OE1	1:B:1517:ILE:HG22	2.04	0.58
1:B:1254:TYR:C	1:B:1254:TYR:HD1	2.12	0.58
1:B:1322:GLU:HA	6:B:4068:HOH:O	2.03	0.58
1:C:2173:ASP:O	1:C:2177:VAL:HG23	2.03	0.58
1:A:171:LEU:HD12	1:A:502:GLU:OE2	2.04	0.58
1:A:495:TYR:HE2	1:A:502:GLU:HG3	1.68	0.58
1:B:1254:TYR:C	1:B:1254:TYR:CD1	2.82	0.58
1:B:1457:GLU:C	1:B:1459:LYS:H	2.11	0.58
1:C:2150:ARG:HH22	1:C:2154:PRO:HA	1.69	0.58
1:D:3074:PHE:HA	1:D:3077:ARG:HG3	1.86	0.58
1:D:3329:PHE:C	1:D:3329:PHE:CD2	2.82	0.58
1:D:3507:LEU:CD2	1:D:3521:THR:HG22	2.33	0.58
1:B:1507:LEU:HD21	1:B:1521:THR:HG22	1.86	0.57
1:A:210:PHE:O	1:A:211:LYS:HG3	2.03	0.57
1:A:388:HIS:N	1:A:389:PRO:HD2	2.19	0.57
1:B:1244:LEU:CD2	1:B:1271:VAL:HG21	2.35	0.57
1:B:1276:PRO:HD2	1:B:1279:ILE:CG1	2.35	0.57
1:B:1396:ASN:ND2	1:B:1396:ASN:N	2.51	0.57
1:C:2162:PRO:O	1:C:2163:MET:HE2	2.04	0.57
1:D:3173:ASP:O	1:D:3177:VAL:HG23	2.03	0.57
1:A:414:LEU:HA	1:A:422:PHE:HE1	1.64	0.57
1:B:1386:HIS:HB3	1:B:1388:HIS:CE1	2.39	0.57
1:B:1501:MET:HE1	1:B:1505:PRO:HB2	1.85	0.57
1:C:2100:TRP:CD1	1:C:2356:HIS:HB2	2.39	0.57
1:A:113:MET:CA	1:A:116:VAL:HG13	2.34	0.57
1:A:241:GLN:HG3	1:A:242:HIS:N	2.14	0.57
1:B:1078:ILE:O	1:B:1082:LEU:HD12	2.04	0.57
1:B:1280:PRO:HB2	1:B:1282:ASN:OD1	2.04	0.57
1:D:3338:GLY:HA3	1:D:3559:ILE:CD1	2.31	0.57
1:D:3343:ILE:O	1:D:3347:ASP:HB2	2.05	0.57
1:A:267:LYS:O	1:A:267:LYS:HG2	2.03	0.57
1:C:2124:ILE:HD11	1:C:2528:PRO:HB2	1.85	0.57
1:C:2183:LEU:HD21	1:C:2445:GLN:HG3	1.86	0.57
1:A:94:THR:HG22	1:A:354:GLY:O	2.04	0.57
1:B:1097:LYS:HB2	1:B:1356:HIS:CE1	2.39	0.57
1:B:1427:THR:HG21	1:B:1578:THR:HA	1.85	0.57
1:C:2089:VAL:HA	1:C:2092:ILE:CG1	2.33	0.57
1:C:2206:THR:HA	1:C:2209:PHE:CZ	2.40	0.57
1:C:2386:HIS:HB3	1:C:2388:HIS:CE1	2.40	0.57
1:D:3205:PHE:CE2	1:D:3209:PHE:HZ	2.23	0.57
1:A:183:LEU:HD21	1:A:445:GLN:HG3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:HIS:C	1:A:288:GLY:HA3	2.30	0.57
1:B:1182:LEU:C	1:B:1438:ARG:HA	2.29	0.57
1:C:2072:PRO:HG2	1:C:2077:ARG:HE	1.70	0.57
1:C:2501:MET:HE1	1:C:2505:PRO:HB2	1.87	0.57
1:C:2507:LEU:CD2	1:C:2521:THR:HG22	2.35	0.57
1:C:2578:THR:CG2	1:C:2579:SER:H	2.17	0.57
1:D:3191:PRO:HG3	1:D:3433:ARG:NH1	2.19	0.57
1:A:49:SER:HB2	1:B:1322:GLU:OE1	2.04	0.57
1:C:2530:SER:OG	5:C:2701:PGX:H162	2.05	0.57
1:D:3131:ASN:ND2	1:D:3147:TYR:CD2	2.72	0.57
1:D:3507:LEU:HD21	1:D:3521:THR:HG22	1.87	0.57
1:A:578:THR:HG22	1:A:579:SER:H	1.68	0.57
1:B:1263:PRO:HD3	1:B:1303:THR:HG23	1.87	0.57
1:B:1308:GLU:O	1:B:1311:ARG:HB3	2.05	0.57
1:B:1464:ASN:OD1	1:B:1499:ASP:HA	2.05	0.57
1:C:2180:LYS:HD2	1:C:2490:GLU:OE1	2.04	0.57
1:C:2388:HIS:N	1:C:2389:PRO:HD2	2.19	0.57
1:D:3108:LEU:HD23	1:D:3111:LEU:CD2	2.35	0.57
1:D:3124:ILE:HD11	1:D:3528:PRO:HB2	1.87	0.57
1:D:3254:TYR:C	1:D:3254:TYR:CD1	2.82	0.57
1:D:3386:HIS:HB3	1:D:3388:HIS:CE1	2.39	0.57
1:A:504:TYR:HA	1:A:507:LEU:HD12	1.87	0.57
1:B:1329:PHE:C	1:B:1329:PHE:CD2	2.82	0.57
1:D:3188:ILE:HD12	1:D:3439:ASN:CB	2.34	0.57
1:D:3210:PHE:O	1:D:3211:LYS:HG3	2.05	0.57
1:D:3396:ASN:ND2	1:D:3396:ASN:N	2.51	0.57
1:D:3454:GLN:HA	1:D:3457:GLU:HG3	1.87	0.57
1:A:108:LEU:HD23	1:A:111:LEU:CD2	2.35	0.56
1:A:197:MET:HE1	1:A:300:MET:HE1	1.86	0.56
1:B:1173:ASP:O	1:B:1177:VAL:HG23	2.05	0.56
1:B:1557:LYS:O	1:B:1558:ILE:C	2.47	0.56
1:C:2234:TYR:CE1	1:C:2252:LEU:HD11	2.40	0.56
1:C:2554:VAL:HG12	1:C:2555:GLY:N	2.20	0.56
1:D:3184:ARG:HD3	1:D:3187:PHE:CA	2.34	0.56
1:D:3254:TYR:C	1:D:3254:TYR:HD1	2.12	0.56
1:D:3362:ASP:O	1:D:3365:LEU:HG	2.05	0.56
1:D:3363:PRO:C	1:D:3365:LEU:H	2.13	0.56
1:A:567:LEU:O	1:A:567:LEU:HD12	2.04	0.56
1:B:1108:LEU:HD23	1:B:1111:LEU:CD2	2.35	0.56
1:B:1537:ASN:HB2	6:B:4076:HOH:O	2.04	0.56
1:C:2078:ILE:O	1:C:2082:LEU:HD12	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2094:THR:HG22	1:C:2354:GLY:O	2.05	0.56
1:C:2113:MET:HA	1:C:2116:VAL:HG13	1.87	0.56
1:C:2389:PRO:CB	1:C:2434:VAL:HG22	2.35	0.56
1:D:3120:ARG:NH1	1:D:3527:ALA:HB1	2.19	0.56
1:D:3235:GLY:HA3	1:D:3240:ARG:HG2	1.86	0.56
1:A:184:ARG:NH2	1:A:441:PRO:HD3	2.19	0.56
1:A:211:LYS:NZ	1:A:236:GLU:HG3	2.21	0.56
1:A:582:VAL:HG13	1:A:582:VAL:O	2.06	0.56
1:B:1211:LYS:NZ	1:B:1236:GLU:HG3	2.20	0.56
1:B:1265:THR:HG23	1:B:1268:ASP:OD2	2.05	0.56
1:B:1578:THR:HG22	1:B:1579:SER:H	1.69	0.56
1:C:2057:CYS:HB3	1:C:2069:CYS:SG	2.45	0.56
1:C:2211:LYS:NZ	1:C:2236:GLU:HG3	2.20	0.56
1:C:2389:PRO:CG	1:C:2434:VAL:HG13	2.29	0.56
1:C:2408:LEU:HD13	1:C:2409:TYR:CE2	2.41	0.56
1:D:3089:VAL:HA	1:D:3092:ILE:CG1	2.34	0.56
1:D:3176:GLU:O	1:D:3177:VAL:C	2.48	0.56
1:D:3276:PRO:O	1:D:3279:ILE:HG12	2.05	0.56
1:A:89:VAL:HA	1:A:92:ILE:CG1	2.35	0.56
1:B:1034:ASN:HB3	1:B:1037:CYS:SG	2.46	0.56
1:B:1232:HIS:C	1:B:1288:GLY:HA3	2.31	0.56
1:C:2305:TRP:O	1:C:2308:GLU:HB3	2.05	0.56
1:D:3281:GLU:HB3	6:D:4185:HOH:O	2.05	0.56
1:A:161:THR:HG23	1:A:165:VAL:HA	1.87	0.56
1:A:213:ASP:HB2	1:A:222:ARG:HG3	1.88	0.56
1:A:218:PRO:C	1:A:458:MET:HE3	2.31	0.56
1:B:1577:PHE:C	1:B:1577:PHE:CD2	2.83	0.56
1:C:2192:GLN:OE1	1:C:2517:ILE:HG22	2.05	0.56
1:C:2198:PHE:C	1:C:2198:PHE:CD2	2.83	0.56
1:A:131:ASN:ND2	1:A:147:TYR:CD2	2.73	0.56
1:A:447:VAL:HG12	1:A:448:ALA:N	2.20	0.56
1:B:1409:TYR:CD2	1:B:1409:TYR:N	2.70	0.56
1:B:1454:GLN:HA	1:B:1457:GLU:HG3	1.86	0.56
1:C:2389:PRO:HG3	1:C:2508:LEU:HD22	1.87	0.56
1:C:2577:PHE:C	1:C:2577:PHE:CD2	2.83	0.56
1:D:3273:MET:CE	1:D:3287:VAL:HG22	2.34	0.56
1:A:329:PHE:C	1:A:329:PHE:CD2	2.83	0.56
1:B:1184:ARG:NH2	1:B:1441:PRO:HD3	2.20	0.56
1:B:1305:TRP:O	1:B:1308:GLU:HB3	2.06	0.56
1:D:3116:VAL:HA	1:D:3119:SER:OG	2.06	0.56
1:D:3238:LEU:HD23	1:D:3241:GLN:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3331:THR:O	1:D:3335:ILE:HD12	2.05	0.56
1:D:3357:PHE:CE2	1:D:3359:LEU:HD23	2.41	0.56
1:A:184:ARG:HA	1:A:438:ARG:O	2.05	0.56
1:B:1226:HIS:CE1	1:B:1376:ARG:HD2	2.40	0.56
1:C:2363:PRO:C	1:C:2365:LEU:H	2.12	0.56
1:D:3451:SER:HB2	1:D:3504:TYR:CE2	2.40	0.56
1:A:463:LEU:HG	1:A:463:LEU:O	2.04	0.56
1:B:1408:LEU:HD13	1:B:1409:TYR:CE2	2.40	0.56
1:D:3105(D):ILE:HG21	1:D:3108:LEU:HD12	1.86	0.56
1:D:3389:PRO:HG3	1:D:3508:LEU:HD22	1.87	0.56
1:A:128:PRO:HG3	1:A:376:ARG:HB2	1.87	0.56
1:A:128:PRO:HG2	1:A:376:ARG:NH1	2.20	0.56
1:A:362:ASP:OD1	1:A:364:GLU:HB2	2.06	0.56
1:B:1184:ARG:HA	1:B:1438:ARG:O	2.06	0.56
1:B:1362:ASP:O	1:B:1365:LEU:HG	2.05	0.56
1:B:1388:HIS:N	1:B:1389:PRO:HD2	2.21	0.56
1:B:1405:LYS:CD	1:B:1405:LYS:H	2.18	0.56
1:C:2128:PRO:CG	1:C:2376:ARG:NH1	2.68	0.56
1:C:2182:LEU:C	1:C:2438:ARG:HA	2.31	0.56
1:C:2184:ARG:HD3	1:C:2187:PHE:CA	2.33	0.56
1:C:2265:THR:HG23	1:C:2268:ASP:OD2	2.06	0.56
1:C:2329:PHE:HD2	1:C:2330:GLN:HG2	1.71	0.56
1:C:2454:GLN:HA	1:C:2457:GLU:HG3	1.88	0.56
1:C:2499:ASP:O	1:C:2501:MET:N	2.38	0.56
1:D:3161:THR:HG23	1:D:3165:VAL:HA	1.87	0.56
1:D:3364:GLU:HA	1:D:3367:PHE:CD1	2.41	0.56
1:A:363:PRO:C	1:A:365:LEU:H	2.14	0.55
1:A:454:GLN:HA	1:A:457:GLU:HG3	1.86	0.55
1:C:2267:LYS:O	1:C:2267:LYS:HG2	2.05	0.55
1:D:3428:ARG:O	1:D:3430:ILE:N	2.39	0.55
1:A:308:GLU:O	1:A:311:ARG:HB3	2.07	0.55
1:B:1428:ARG:O	1:B:1430:ILE:N	2.38	0.55
1:C:2219:GLY:CA	1:C:2458:MET:HE2	2.37	0.55
1:C:2232:HIS:C	1:C:2288:GLY:HA3	2.31	0.55
1:D:3121:SER:C	1:D:3123:LEU:H	2.15	0.55
1:D:3463:LEU:HB2	1:D:3503:LEU:HA	1.88	0.55
1:A:578:THR:CG2	1:A:579:SER:H	2.18	0.55
1:D:3185:ARG:HH21	1:D:3438:ARG:CD	2.20	0.55
1:A:162:PRO:O	1:A:163:MET:HE2	2.06	0.55
1:A:372:GLN:HE22	1:B:1373:TYR:H	1.52	0.55
1:B:1116:VAL:HA	1:B:1119:SER:OG	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2113:MET:HB2	1:C:2357:PHE:HZ	1.71	0.55
1:C:2343:ILE:O	1:C:2347:ASP:HB2	2.05	0.55
1:C:2501:MET:CE	1:C:2505:PRO:HB2	2.36	0.55
1:D:3389:PRO:CB	1:D:3434:VAL:HG22	2.36	0.55
1:A:104:ASN:ND2	1:A:358:LYS:HB2	2.20	0.55
1:A:577:PHE:CD2	1:A:577:PHE:C	2.84	0.55
1:B:1238:LEU:HD23	1:B:1241:GLN:HG2	1.89	0.55
1:C:2191:PRO:HG3	1:C:2433:ARG:NH1	2.21	0.55
1:C:2442:ILE:HD12	1:C:2442:ILE:N	2.22	0.55
1:C:2447:VAL:HG12	1:C:2448:ALA:N	2.20	0.55
1:A:185:ARG:HH21	1:A:438:ARG:CZ	2.20	0.55
1:B:1184:ARG:CD	1:B:1187:PHE:HA	2.32	0.55
1:B:1197:MET:HE1	1:B:1300:MET:HE1	1.87	0.55
1:B:1363:PRO:C	1:B:1365:LEU:H	2.14	0.55
1:B:1578:THR:CG2	1:B:1579:SER:H	2.20	0.55
1:C:2121:SER:C	1:C:2123:LEU:H	2.15	0.55
1:C:2489:ALA:HB2	6:C:4140:HOH:O	2.05	0.55
1:D:3134:TYR:HD2	1:D:3136:TYR:HE1	1.54	0.55
1:D:3211:LYS:NZ	1:D:3236:GLU:HG3	2.21	0.55
1:D:3513:ARG:NH2	1:D:3520:GLU:HB2	2.22	0.55
1:B:1039:ASN:N	1:B:1040:PRO:CD	2.69	0.55
1:B:1113:MET:HB2	1:B:1357:PHE:HZ	1.72	0.55
1:C:2198:PHE:CZ	1:C:2352:LEU:HD13	2.42	0.55
1:C:2218:PRO:C	1:C:2458:MET:HE3	2.32	0.55
1:C:2308:GLU:O	1:C:2311:ARG:HB3	2.07	0.55
1:D:3582:VAL:HG13	1:D:3582:VAL:O	2.06	0.55
1:A:454:GLN:O	1:A:457:GLU:HG3	2.07	0.55
1:C:2121:SER:O	1:C:2123:LEU:N	2.40	0.55
1:C:2128:PRO:HG3	1:C:2376:ARG:HB2	1.89	0.55
1:D:3339:GLU:O	1:D:3342:LYS:HB3	2.07	0.55
1:A:191:PRO:CD	1:A:433:ARG:HG3	2.30	0.55
1:A:482:THR:C	1:A:511:LYS:HB2	2.31	0.55
1:D:3184:ARG:HB2	1:D:3439:ASN:CA	2.37	0.55
1:D:3208:GLN:NE2	1:D:3232:HIS:NE2	2.55	0.55
1:D:3213:ASP:HB2	1:D:3222:ARG:HG3	1.88	0.55
1:D:3232:HIS:C	1:D:3288:GLY:HA3	2.32	0.55
1:D:3464:ASN:OD1	1:D:3499:ASP:HA	2.07	0.55
1:D:3566:SER:HA	1:D:3569:CYS:HB2	1.89	0.55
1:A:364:GLU:HA	1:A:367:PHE:CD1	2.42	0.54
1:A:387:TRP:CZ2	1:A:518:PHE:CZ	2.95	0.54
1:A:405:LYS:CD	1:A:405:LYS:H	2.18	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:ALA:HB3	1:A:512:PRO:HG3	1.88	0.54
1:B:1357:PHE:CE2	1:B:1359:LEU:HD23	2.42	0.54
1:C:2387:TRP:CH2	5:C:2701:PGX:H121	2.42	0.54
1:A:182:LEU:C	1:A:438:ARG:HA	2.32	0.54
1:A:308:GLU:HG3	1:A:336:LEU:CD1	2.32	0.54
1:A:387:TRP:CZ2	5:A:701:PGX:H121	2.41	0.54
1:A:451:SER:HB2	1:A:504:TYR:CE2	2.42	0.54
1:B:1582:VAL:O	1:B:1582:VAL:HG13	2.06	0.54
1:C:2226:HIS:C	1:C:2377:ILE:HD12	2.31	0.54
1:C:2254:TYR:C	1:C:2254:TYR:HD1	2.15	0.54
1:D:3305:TRP:O	1:D:3308:GLU:HB3	2.08	0.54
1:A:81:LEU:O	1:A:82:LEU:HG	2.07	0.54
1:A:184:ARG:HD3	1:A:187:PHE:CA	2.35	0.54
1:B:1380:GLU:HG3	1:B:1460:TYR:HE2	1.72	0.54
1:C:2208:GLN:NE2	1:C:2232:HIS:NE2	2.56	0.54
1:C:2514:PRO:O	1:C:2515:ASP:HB2	2.07	0.54
1:D:3100:TRP:CD1	1:D:3356:HIS:HB2	2.42	0.54
1:D:3255:GLN:HG2	1:D:3263:PRO:O	2.07	0.54
1:D:3265:THR:HG23	1:D:3268:ASP:OD2	2.07	0.54
1:D:3577:PHE:C	1:D:3577:PHE:CD2	2.84	0.54
1:A:150:ARG:HH22	1:A:154:PRO:HA	1.73	0.54
1:A:274:ILE:HG13	1:A:290:GLU:C	2.31	0.54
1:B:1341:ILE:HG23	1:B:1534:LEU:HD12	1.89	0.54
1:B:1364:GLU:HA	1:B:1367:PHE:CD1	2.42	0.54
1:B:1463:LEU:HG	1:B:1463:LEU:O	2.08	0.54
1:B:1507:LEU:CD2	1:B:1521:THR:HG22	2.38	0.54
1:C:2185:ARG:HH21	1:C:2438:ARG:CZ	2.19	0.54
1:C:2499:ASP:C	1:C:2501:MET:H	2.15	0.54
1:D:3121:SER:O	1:D:3123:LEU:N	2.41	0.54
1:A:121:SER:C	1:A:123:LEU:H	2.16	0.54
1:A:173:ASP:O	1:A:177:VAL:HG23	2.07	0.54
1:B:1379:SER:O	1:B:1382:ASN:HB3	2.07	0.54
1:B:1504:TYR:HA	1:B:1507:LEU:HD12	1.88	0.54
1:C:2253:LYS:O	1:C:2264:PRO:HG3	2.07	0.54
1:C:2482:THR:C	1:C:2511:LYS:HB2	2.33	0.54
1:C:2547:PRO:HB3	1:C:2553:GLU:N	2.23	0.54
1:D:3389:PRO:HG2	1:D:3434:VAL:CG1	2.28	0.54
1:A:39:ASN:HD22	1:A:39:ASN:N	2.05	0.54
1:A:124:ILE:HD11	1:A:528:PRO:HB2	1.89	0.54
1:A:162:PRO:HG2	1:A:171:LEU:HD23	1.90	0.54
1:A:219:GLY:CA	1:A:458:MET:HE2	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:GLU:OE1	1:B:1049:SER:HB2	2.07	0.54
1:B:1121:SER:C	1:B:1123:LEU:H	2.15	0.54
1:D:3219:GLY:CA	1:D:3458:MET:HE2	2.38	0.54
1:D:3352:LEU:HD21	1:D:3387:TRP:CH2	2.42	0.54
1:D:3408:LEU:HD13	1:D:3409:TYR:CE2	2.43	0.54
1:A:116:VAL:HA	1:A:119:SER:OG	2.08	0.54
1:B:1389:PRO:HG3	1:B:1508:LEU:HD22	1.90	0.54
1:C:2352:LEU:HD21	1:C:2387:TRP:CH2	2.42	0.54
1:D:3267:LYS:O	1:D:3267:LYS:HG2	2.06	0.54
1:A:302:ALA:O	1:A:303:THR:C	2.51	0.54
1:A:403:SER:N	1:A:406:GLN:OE1	2.41	0.54
1:A:407:PHE:HZ	1:A:426:PHE:HZ	1.54	0.54
1:B:1191:PRO:HG3	1:B:1433:ARG:NH1	2.23	0.54
1:B:1463:LEU:HB2	1:B:1503:LEU:HA	1.89	0.54
1:B:1482:THR:HG22	6:B:4081:HOH:O	2.07	0.54
1:C:2096:PHE:N	1:C:2096:PHE:CD1	2.75	0.54
1:C:2197:MET:HE2	1:C:2423:VAL:HG13	1.89	0.54
1:C:2341:ILE:HG23	1:C:2534:LEU:HD12	1.89	0.54
1:D:3131:ASN:C	1:D:3131:ASN:OD1	2.50	0.54
1:D:3182:LEU:C	1:D:3438:ARG:HA	2.32	0.54
1:D:3208:GLN:O	1:D:3211:LYS:HD3	2.08	0.54
1:A:357:PHE:CE2	1:A:359:LEU:HD23	2.43	0.54
1:C:2128:PRO:HG2	1:C:2376:ARG:NH1	2.23	0.54
1:C:2136:TYR:HD2	1:D:3327:GLN:NE2	2.05	0.54
1:C:2352:LEU:HD21	1:C:2387:TRP:HH2	1.72	0.54
1:D:3184:ARG:HH12	1:D:3441:PRO:HG3	1.72	0.54
1:D:3557:LYS:O	1:D:3558:ILE:C	2.51	0.54
1:A:568:ILE:HG23	1:A:572:VAL:HG21	1.90	0.54
1:B:1072:PRO:HG2	1:B:1077:ARG:NE	2.23	0.54
1:B:1113:MET:CA	1:B:1116:VAL:HG13	2.37	0.54
1:B:1306:LEU:HD23	1:B:1307:ARG:N	2.23	0.54
1:B:1482:THR:HB	1:B:1484:GLU:HG3	1.90	0.54
1:C:2104:ASN:ND2	1:C:2358:LYS:HB2	2.23	0.54
1:C:2152:LEU:HB2	1:C:2466:TYR:CE1	2.43	0.54
1:C:2191:PRO:CD	1:C:2433:ARG:HG3	2.29	0.54
1:C:2254:TYR:C	1:C:2254:TYR:CD1	2.85	0.54
1:C:2526:GLY:O	1:C:2530:SER:HB3	2.07	0.54
1:C:2582:VAL:HG13	1:C:2582:VAL:O	2.08	0.54
1:D:3396:ASN:HD22	1:D:3401:GLU:HG2	1.72	0.54
1:D:3563:SER:O	1:D:3564:ILE:C	2.51	0.54
1:A:113:MET:HA	1:A:116:VAL:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:LEU:HB2	1:A:503:LEU:HA	1.88	0.53
1:B:1161:THR:HG23	1:B:1165:VAL:HA	1.90	0.53
1:B:1573:LYS:HB2	6:B:4063:HOH:O	2.07	0.53
1:C:2048:MET:HA	6:C:4104:HOH:O	2.07	0.53
1:C:2238:LEU:HD23	1:C:2241:GLN:HG2	1.90	0.53
1:C:2357:PHE:CE2	1:C:2359:LEU:HD23	2.42	0.53
1:C:2435:ALA:HB3	1:C:2512:PRO:HG3	1.90	0.53
1:C:2450:ALA:O	1:C:2451:SER:C	2.51	0.53
1:D:3405:LYS:H	1:D:3405:LYS:CD	2.22	0.53
1:D:3467:ARG:NH1	1:D:3520:GLU:OE1	2.37	0.53
1:A:339:GLU:O	1:A:342:LYS:HB3	2.08	0.53
1:A:389:PRO:CB	1:A:434:VAL:HG22	2.37	0.53
1:A:454:GLN:O	1:A:457:GLU:N	2.41	0.53
1:B:1121:SER:O	1:B:1123:LEU:N	2.40	0.53
1:B:1184:ARG:NH1	1:B:1441:PRO:HG3	2.23	0.53
1:B:1208:GLN:NE2	1:B:1232:HIS:NE2	2.57	0.53
1:B:1535:MET:C	1:B:1537:ASN:H	2.16	0.53
1:C:2099:VAL:HG12	1:C:2100:TRP:N	2.23	0.53
1:C:2142:PHE:CE2	1:D:3538:PRO:HG3	2.43	0.53
1:D:3482:THR:HB	1:D:3484:GLU:HG3	1.89	0.53
1:A:105(A):ILE:O	1:A:108:LEU:HB2	2.09	0.53
1:A:208:GLN:NE2	1:A:232:HIS:NE2	2.56	0.53
1:A:330:GLN:HE22	1:B:1140:GLU:HB2	1.73	0.53
1:A:498:ILE:O	1:A:501:MET:HB2	2.08	0.53
1:C:2088:THR:O	1:C:2092:ILE:HG12	2.08	0.53
1:C:2301:TYR:O	1:C:2302:ALA:C	2.49	0.53
1:C:2308:GLU:CA	1:C:2571:ASN:HD21	2.20	0.53
1:D:3276:PRO:HD2	1:D:3279:ILE:CG1	2.36	0.53
1:A:88:THR:O	1:A:92:ILE:HG12	2.08	0.53
1:A:232:HIS:O	1:A:288:GLY:CA	2.55	0.53
1:A:380:GLU:HG3	1:A:460:TYR:HE2	1.73	0.53
1:A:530:SER:HB2	5:A:701:PGX:H161	1.89	0.53
1:B:1128:PRO:HG3	1:B:1376:ARG:HB2	1.90	0.53
1:B:1188:ILE:HD12	1:B:1439:ASN:CB	2.38	0.53
1:B:1218:PRO:C	1:B:1458:MET:HE3	2.34	0.53
1:B:1362:ASP:OD1	1:B:1364:GLU:HB2	2.08	0.53
1:B:1403:SER:N	1:B:1406:GLN:OE1	2.41	0.53
1:C:2405:LYS:CD	1:C:2405:LYS:H	2.20	0.53
1:C:2463:LEU:HB2	1:C:2503:LEU:HA	1.90	0.53
1:D:3039:ASN:HD22	1:D:3039:ASN:N	2.06	0.53
1:D:3108:LEU:O	1:D:3112:ILE:HG12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3180:LYS:HD2	1:D:3490:GLU:OE1	2.08	0.53
1:D:3481:LEU:CD1	1:D:3510:GLU:HA	2.39	0.53
1:A:105(A):ILE:O	1:A:105(A):ILE:HG22	2.08	0.53
1:B:1105(B):ILE:CG2	1:B:1108:LEU:HD12	2.38	0.53
1:B:1329:PHE:HD2	1:B:1330:GLN:HG2	1.74	0.53
1:C:2039:ASN:N	1:C:2039:ASN:HD22	2.05	0.53
1:C:2116:VAL:HA	1:C:2119:SER:OG	2.09	0.53
1:D:3184:ARG:HA	1:D:3438:ARG:O	2.09	0.53
1:D:3388:HIS:N	1:D:3389:PRO:HD2	2.24	0.53
1:A:176:GLU:O	1:A:177:VAL:C	2.51	0.53
1:B:1176:GLU:O	1:B:1177:VAL:C	2.51	0.53
1:B:1388:HIS:O	1:B:1391:LEU:HB2	2.09	0.53
1:C:2188:ILE:HD12	1:C:2439:ASN:CB	2.39	0.53
1:C:2206:THR:HG21	5:C:2701:PGX:H111	1.90	0.53
1:C:2244:LEU:CD2	1:C:2271:VAL:HG21	2.38	0.53
1:D:3198:PHE:C	1:D:3198:PHE:CD2	2.87	0.53
1:D:3377:ILE:HG13	6:D:4180:HOH:O	2.08	0.53
1:A:64:PHE:HD2	1:A:70:THR:O	1.91	0.53
1:A:103:VAL:C	1:A:105:ASN:H	2.16	0.53
1:A:261:VAL:O	1:A:307:ARG:NH1	2.42	0.53
1:A:304:ILE:O	1:A:307:ARG:HB2	2.09	0.53
1:A:566:SER:HA	1:A:569:CYS:HB2	1.90	0.53
1:B:1385:TYR:HA	5:B:1701:PGX:O4	2.07	0.53
1:B:1389:PRO:HG2	1:B:1434:VAL:CG1	2.31	0.53
1:C:2255:GLN:HG2	1:C:2263:PRO:O	2.09	0.53
1:C:2380:GLU:HG3	1:C:2460:TYR:HE2	1.74	0.53
1:C:2464:ASN:OD1	1:C:2499:ASP:HA	2.08	0.53
1:C:2482:THR:HB	1:C:2484:GLU:HG3	1.90	0.53
1:D:3124:ILE:HD11	1:D:3529:PHE:N	2.24	0.53
1:D:3526:GLY:CA	5:D:3701:PGX:H61	2.35	0.53
1:A:120:ARG:HD2	1:A:527:ALA:HB1	1.91	0.53
1:A:152:LEU:HB2	1:A:466:TYR:CE1	2.44	0.53
1:A:188:ILE:HD12	1:A:439:ASN:CB	2.37	0.53
1:A:245:ARG:HH22	1:A:326:GLU:HA	1.74	0.53
1:A:254:TYR:HD1	1:A:254:TYR:C	2.17	0.53
1:A:507:LEU:HD21	1:A:521:THR:HG22	1.89	0.53
1:B:1198:PHE:CE1	1:B:1352:LEU:HD13	2.44	0.53
1:C:2108:LEU:O	1:C:2112:ILE:HG12	2.09	0.53
1:C:2131:ASN:C	1:C:2131:ASN:OD1	2.52	0.53
1:C:2205:PHE:CE2	1:C:2209:PHE:HZ	2.27	0.53
1:C:2568:ILE:HG23	1:C:2572:VAL:HG21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3403:SER:N	1:D:3406:GLN:OE1	2.42	0.53
1:D:3450:ALA:O	1:D:3451:SER:C	2.52	0.53
1:A:197:MET:HE1	1:A:300:MET:CE	2.39	0.53
1:B:1131:ASN:C	1:B:1131:ASN:OD1	2.52	0.53
1:D:3407:PHE:HZ	1:D:3426:PHE:HZ	1.57	0.53
1:A:121:SER:O	1:A:123:LEU:N	2.41	0.53
1:A:205:PHE:CE2	1:A:209:PHE:HZ	2.26	0.53
1:A:225:GLY:HA3	1:A:229:ASP:OD1	2.07	0.53
1:A:229:ASP:OD2	1:A:229:ASP:C	2.51	0.53
1:C:2081:LEU:O	1:C:2082:LEU:HG	2.08	0.53
1:C:2155:VAL:HG23	1:C:2459:LYS:O	2.09	0.53
1:D:3387:TRP:CZ2	1:D:3518:PHE:CZ	2.97	0.53
1:D:3387:TRP:CH2	5:D:3701:PGX:H121	2.44	0.53
1:D:3414:LEU:HA	1:D:3422:PHE:HE1	1.71	0.53
1:A:113:MET:HE3	1:A:116:VAL:CG2	2.38	0.52
1:A:113:MET:HB2	1:A:357:PHE:HZ	1.74	0.52
1:A:379:SER:O	1:A:382:ASN:HB3	2.08	0.52
1:A:507:LEU:CD2	1:A:521:THR:HG22	2.39	0.52
1:B:1105(B):ILE:HG22	1:B:1105(B):ILE:O	2.10	0.52
1:B:1162:PRO:HG2	1:B:1171:LEU:HD23	1.90	0.52
1:C:2161:THR:HG23	1:C:2165:VAL:HA	1.91	0.52
1:D:3104:ASN:ND2	1:D:3358:LYS:HB2	2.24	0.52
1:D:3128:PRO:CG	1:D:3376:ARG:NH1	2.72	0.52
1:D:3243:LYS:HA	6:D:4189:HOH:O	2.10	0.52
1:A:96:PHE:N	1:A:96:PHE:CD1	2.77	0.52
1:A:124:ILE:HD11	1:A:529:PHE:N	2.24	0.52
1:A:234:TYR:CE1	1:A:252:LEU:HD11	2.44	0.52
1:A:265:THR:HG23	1:A:268:ASP:OD2	2.08	0.52
1:A:292:PHE:O	1:A:299:MET:HE2	2.09	0.52
1:B:1124:ILE:HD11	1:B:1529:PHE:N	2.25	0.52
1:B:1338:GLY:HA3	1:B:1559:ILE:CD1	2.35	0.52
1:B:1467:ARG:NH1	1:B:1520:GLU:OE1	2.41	0.52
1:C:2341:ILE:HD13	1:C:2534:LEU:HD12	1.91	0.52
1:D:3081:LEU:O	1:D:3082:LEU:HG	2.08	0.52
1:D:3352:LEU:HD21	1:D:3387:TRP:HH2	1.74	0.52
1:D:3454:GLN:O	1:D:3457:GLU:N	2.42	0.52
1:A:347:ASP:O	1:A:350:GLN:HB3	2.09	0.52
1:B:1096:PHE:N	1:B:1096:PHE:CD1	2.77	0.52
1:B:1197:MET:O	1:B:1198:PHE:C	2.52	0.52
1:B:1276:PRO:O	1:B:1279:ILE:HG12	2.08	0.52
1:B:1301:TYR:O	1:B:1302:ALA:C	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1389:PRO:CG	1:B:1434:VAL:HG13	2.29	0.52
1:C:2329:PHE:C	1:C:2329:PHE:CD2	2.87	0.52
1:C:2454:GLN:O	1:C:2457:GLU:HG3	2.09	0.52
1:D:3080:LEU:C	1:D:3082:LEU:H	2.18	0.52
1:D:3088:THR:O	1:D:3092:ILE:HG12	2.10	0.52
1:D:3244:LEU:CD2	1:D:3271:VAL:HG21	2.38	0.52
1:D:3435:ALA:HB3	1:D:3512:PRO:HG3	1.91	0.52
1:B:1435:ALA:HB3	1:B:1512:PRO:HG3	1.90	0.52
1:B:1500:VAL:O	1:B:1500:VAL:HG12	2.09	0.52
1:B:1538:PRO:O	1:B:1540:CYS:N	2.42	0.52
1:C:2120:ARG:HD2	1:C:2527:ALA:HB1	1.91	0.52
1:C:2197:MET:CE	1:C:2423:VAL:HG13	2.39	0.52
1:C:2308:GLU:HG3	1:C:2336:LEU:CD1	2.33	0.52
1:C:2362:ASP:OD1	1:C:2364:GLU:HB2	2.09	0.52
1:C:2403:SER:N	1:C:2406:GLN:OE1	2.43	0.52
1:C:2498:ILE:HG23	1:C:2499:ASP:N	2.24	0.52
1:D:3039:ASN:N	1:D:3040:PRO:CD	2.72	0.52
1:D:3495:TYR:CD2	1:D:3501:MET:HA	2.44	0.52
1:A:198:PHE:CD2	1:A:198:PHE:C	2.87	0.52
1:A:254:TYR:C	1:A:254:TYR:CD1	2.87	0.52
1:A:433:ARG:HD3	1:A:436:GLY:H	1.75	0.52
1:B:1389:PRO:CB	1:B:1434:VAL:HG22	2.38	0.52
1:B:1566:SER:HA	1:B:1569:CYS:HB2	1.91	0.52
1:C:2039:ASN:N	1:C:2040:PRO:CD	2.72	0.52
1:D:3128:PRO:HG2	1:D:3376:ARG:NH1	2.24	0.52
1:D:3162:PRO:HG2	1:D:3171:LEU:HD23	1.92	0.52
1:D:3206:THR:HA	1:D:3209:PHE:CE2	2.44	0.52
1:D:3463:LEU:O	1:D:3463:LEU:HG	2.10	0.52
1:A:39:ASN:N	1:A:40:PRO:CD	2.72	0.52
1:A:235:GLY:HA3	1:A:240:ARG:HG2	1.90	0.52
1:B:1038:SER:C	1:B:1040:PRO:HD3	2.34	0.52
1:B:1185:ARG:HH21	1:B:1438:ARG:CZ	2.22	0.52
1:C:2407:PHE:HZ	1:C:2426:PHE:HZ	1.58	0.52
1:C:2463:LEU:HG	1:C:2463:LEU:O	2.08	0.52
1:D:3096:PHE:CD1	1:D:3096:PHE:N	2.78	0.52
1:D:3112:ILE:O	1:D:3115:TYR:N	2.43	0.52
1:D:3113:MET:CE	1:D:3117:LEU:HD22	2.40	0.52
1:D:3380:GLU:HG3	1:D:3460:TYR:HE2	1.74	0.52
1:D:3543:GLN:CD	1:D:3543:GLN:H	2.18	0.52
1:A:246:LEU:HD23	1:A:251:LYS:HB2	1.91	0.52
1:A:499:ASP:C	1:A:501:MET:H	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1050:THR:HG21	1:B:1056:LYS:HB2	1.90	0.52
1:B:1202:ALA:CA	1:B:1348:TYR:HE1	2.23	0.52
1:C:2080:LEU:C	1:C:2082:LEU:H	2.17	0.52
1:D:3050:THR:HG21	1:D:3056:LYS:HB2	1.92	0.52
1:A:464:ASN:OD1	1:A:499:ASP:HA	2.09	0.52
1:A:482:THR:HG23	1:A:509:VAL:HG12	1.92	0.52
1:A:510:GLU:OE1	1:A:519:GLY:HA3	2.10	0.52
1:B:1234:TYR:CE1	1:B:1252:LEU:HD11	2.45	0.52
1:B:1304:ILE:O	1:B:1307:ARG:HB2	2.09	0.52
1:B:1352:LEU:HD21	1:B:1387:TRP:CH2	2.45	0.52
1:B:1467:ARG:NH1	1:B:1521:THR:OG1	2.42	0.52
1:B:1532:LYS:C	1:B:1534:LEU:N	2.68	0.52
1:C:2427:THR:HG21	1:C:2578:THR:HA	1.92	0.52
1:D:3241:GLN:OE1	1:D:3245:ARG:HD2	2.10	0.52
1:D:3379:SER:O	1:D:3382:ASN:HB3	2.10	0.52
1:A:140:GLU:HB2	1:B:1330:GLN:HE22	1.75	0.52
1:A:185:ARG:HH21	1:A:438:ARG:CD	2.22	0.52
1:A:255:GLN:HG2	1:A:263:PRO:O	2.09	0.52
1:A:377:ILE:HA	6:A:4037:HOH:O	2.10	0.52
1:A:458:MET:O	1:A:459:LYS:C	2.53	0.52
1:B:1273:MET:CE	1:B:1287:VAL:HG22	2.34	0.52
1:B:1302:ALA:O	1:B:1303:THR:C	2.51	0.52
1:C:2196:MET:CE	1:C:2431:ALA:HB2	2.40	0.52
1:C:2197:MET:HE1	1:C:2300:MET:CE	2.39	0.52
1:C:2349:VAL:HG22	5:C:2701:PGX:O5	2.09	0.52
1:C:2364:GLU:HA	1:C:2367:PHE:CD1	2.44	0.52
1:A:305:TRP:O	1:A:308:GLU:HB3	2.10	0.52
1:A:308:GLU:CA	1:A:571:ASN:HD21	2.23	0.52
1:A:498:ILE:HG23	1:A:499:ASP:N	2.25	0.52
1:B:1206:THR:HA	1:B:1209:PHE:CE2	2.45	0.52
1:B:1253:LYS:O	1:B:1264:PRO:HG3	2.10	0.52
1:B:1433:ARG:HD3	1:B:1436:GLY:H	1.74	0.52
1:C:2184:ARG:CD	1:C:2187:PHE:HA	2.35	0.52
1:C:2202:ALA:CA	1:C:2348:TYR:HE1	2.23	0.52
1:C:2347:ASP:O	1:C:2350:GLN:HB3	2.09	0.52
1:C:2543:GLN:H	1:C:2543:GLN:CD	2.18	0.52
1:C:2557:LYS:O	1:C:2558:ILE:C	2.51	0.52
1:D:3150:ARG:HH22	1:D:3154:PRO:HA	1.75	0.52
1:D:3306:LEU:HD23	1:D:3307:ARG:N	2.25	0.52
1:D:3567:LEU:HD12	1:D:3567:LEU:C	2.35	0.52
1:A:491:LEU:O	1:A:494:LEU:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2330:GLN:HE22	1:D:3140:GLU:HB2	1.75	0.51
1:D:3072:PRO:HG2	1:D:3077:ARG:NE	2.24	0.51
1:D:3347:ASP:O	1:D:3350:GLN:N	2.43	0.51
1:A:427:THR:HG21	1:A:578:THR:HA	1.91	0.51
1:A:442:ILE:HD12	1:A:442:ILE:N	2.24	0.51
1:A:514:PRO:O	1:A:515:ASP:HB2	2.10	0.51
1:B:1099:VAL:HG12	1:B:1100:TRP:N	2.24	0.51
1:B:1463:LEU:HD12	1:B:1503:LEU:CD1	2.39	0.51
1:C:2179:GLU:O	1:C:2181:VAL:N	2.43	0.51
1:D:3225:GLY:HA3	1:D:3229:ASP:OD1	2.10	0.51
1:A:64:PHE:HA	1:A:71:THR:O	2.11	0.51
1:A:72:PRO:HG2	1:A:77:ARG:NE	2.25	0.51
1:A:261:VAL:H	1:A:307:ARG:NH2	2.07	0.51
1:A:467:ARG:NH1	1:A:521:THR:OG1	2.43	0.51
1:B:1128:PRO:CG	1:B:1376:ARG:NH1	2.74	0.51
1:C:2241:GLN:OE1	1:C:2245:ARG:HD2	2.10	0.51
1:C:2294:LEU:HB3	1:C:2409:TYR:CD2	2.45	0.51
1:C:2379:SER:O	1:C:2382:ASN:HB3	2.11	0.51
1:D:3185:ARG:NH2	6:D:4167:HOH:O	2.43	0.51
1:D:3229:ASP:OD2	1:D:3229:ASP:C	2.53	0.51
1:B:1152:LEU:HB2	1:B:1466:TYR:CE1	2.46	0.51
1:B:1209:PHE:HB3	1:B:1377:ILE:CD1	2.40	0.51
1:B:1270:GLN:N	1:B:1270:GLN:OE1	2.43	0.51
1:C:2509:VAL:O	1:C:2510:GLU:O	2.28	0.51
1:A:50:THR:CG2	1:A:56:LYS:HB3	2.40	0.51
1:A:112:ILE:O	1:A:115:TYR:N	2.43	0.51
1:A:134:TYR:HD2	1:A:136:TYR:HE1	1.57	0.51
1:A:526:GLY:O	1:A:530:SER:HB3	2.10	0.51
1:B:1156:ALA:O	1:B:1159:CYS:HB2	2.11	0.51
1:C:2185:ARG:NH2	6:C:4120:HOH:O	2.44	0.51
1:C:2302:ALA:O	1:C:2303:THR:C	2.53	0.51
1:D:3183:LEU:HD21	1:D:3445:GLN:HG3	1.92	0.51
1:D:3535:MET:C	1:D:3537:ASN:H	2.19	0.51
1:D:3568:ILE:HG23	1:D:3572:VAL:HG21	1.92	0.51
1:A:48:MET:HE1	1:B:1551:GLY:O	2.10	0.51
1:A:156:ALA:O	1:A:159:CYS:HB2	2.11	0.51
1:A:209:PHE:CD1	1:A:209:PHE:N	2.78	0.51
1:A:394:THR:HA	1:A:402:TYR:O	2.10	0.51
1:B:1120:ARG:HD2	1:B:1527:ALA:HB1	1.92	0.51
1:B:1339:GLU:O	1:B:1342:LYS:HB3	2.10	0.51
1:B:1396:ASN:HD22	1:B:1401:GLU:HG2	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1568:ILE:HG23	1:B:1572:VAL:HG21	1.92	0.51
1:C:2103:VAL:C	1:C:2105:ASN:H	2.19	0.51
1:C:2394:THR:O	1:C:2429:GLN:NE2	2.40	0.51
1:D:3137:LYS:HD2	6:D:4174:HOH:O	2.10	0.51
1:D:3450:ALA:O	1:D:3452:ILE:N	2.43	0.51
1:A:80:LEU:C	1:A:82:LEU:H	2.18	0.51
1:A:513:ARG:NH2	1:A:520:GLU:HB2	2.26	0.51
1:B:1294:LEU:HB3	1:B:1409:TYR:CD2	2.45	0.51
1:B:1444:VAL:O	1:B:1444:VAL:CG1	2.59	0.51
1:C:2113:MET:HE3	1:C:2116:VAL:CG2	2.40	0.51
1:C:2187:PHE:C	1:C:2187:PHE:CD1	2.89	0.51
1:C:2433:ARG:HD3	1:C:2436:GLY:H	1.76	0.51
1:C:2482:THR:HG23	1:C:2509:VAL:HG12	1.91	0.51
1:C:2532:LYS:C	1:C:2534:LEU:N	2.68	0.51
1:C:2547:PRO:O	1:C:2552:GLY:N	2.41	0.51
1:D:3050:THR:CG2	1:D:3056:LYS:HB3	2.41	0.51
1:D:3095:HIS:O	1:D:3097:LYS:N	2.43	0.51
1:D:3463:LEU:HD12	1:D:3503:LEU:CD1	2.38	0.51
1:D:3547:PRO:HB3	1:D:3553:GLU:N	2.25	0.51
1:A:253:LYS:O	1:A:264:PRO:HG3	2.10	0.51
1:A:547:PRO:HB3	1:A:553:GLU:N	2.26	0.51
1:B:1181:VAL:HG12	1:B:1487:MET:HG2	1.93	0.51
1:C:2113:MET:HA	1:C:2116:VAL:CG1	2.41	0.51
1:C:2547:PRO:C	1:C:2552:GLY:HA2	2.36	0.51
1:C:2583:GLN:CD	1:C:2583:GLN:N	2.69	0.51
1:D:3156:ALA:O	1:D:3159:CYS:HB2	2.10	0.51
1:D:3347:ASP:O	1:D:3350:GLN:HB3	2.11	0.51
1:A:428:ARG:O	1:A:430:ILE:N	2.44	0.51
1:A:463:LEU:HD12	1:A:503:LEU:CD1	2.41	0.51
1:A:482:THR:HB	1:A:484:GLU:HG3	1.93	0.51
1:B:1198:PHE:C	1:B:1198:PHE:CD2	2.89	0.51
1:B:1208:GLN:O	1:B:1211:LYS:HD3	2.11	0.51
1:C:2185:ARG:HH21	1:C:2438:ARG:CD	2.23	0.51
1:C:2197:MET:O	1:C:2198:PHE:C	2.54	0.51
1:C:2211:LYS:HZ1	1:C:2236:GLU:HG3	1.76	0.51
1:D:3113:MET:HA	1:D:3116:VAL:HG13	1.93	0.51
1:D:3202:ALA:CA	1:D:3348:TYR:HE1	2.23	0.51
1:D:3301:TYR:O	1:D:3302:ALA:C	2.54	0.51
1:D:3509:VAL:O	1:D:3510:GLU:O	2.29	0.51
1:A:124:ILE:HD11	1:A:528:PRO:C	2.36	0.51
1:B:1183:LEU:HD21	1:B:1445:GLN:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1407:PHE:HZ	1:B:1426:PHE:HZ	1.58	0.51
1:B:1499:ASP:C	1:B:1501:MET:H	2.18	0.51
1:C:2124:ILE:HD11	1:C:2529:PHE:N	2.26	0.51
1:C:2176:GLU:O	1:C:2177:VAL:C	2.54	0.51
1:C:2566:SER:HA	1:C:2569:CYS:HB2	1.93	0.51
1:D:3206:THR:HB	1:D:3210:PHE:CD2	2.46	0.51
1:D:3465:GLU:OE2	1:D:3468:LYS:CE	2.59	0.51
1:A:238:LEU:HD23	1:A:241:GLN:HG2	1.92	0.50
1:A:352:LEU:HD21	1:A:387:TRP:CH2	2.46	0.50
1:A:433:ARG:HH21	1:A:512:PRO:HB3	1.76	0.50
1:A:450:ALA:O	1:A:452:ILE:N	2.44	0.50
1:A:557:LYS:HA	1:A:560:ASN:HD22	1.76	0.50
1:B:1482:THR:HG23	1:B:1509:VAL:HG12	1.93	0.50
1:C:2064:PHE:HA	1:C:2071:THR:O	2.11	0.50
1:C:2387:TRP:CZ2	1:C:2518:PHE:CZ	2.99	0.50
1:C:2454:GLN:O	1:C:2457:GLU:N	2.43	0.50
1:C:2463:LEU:HD12	1:C:2503:LEU:CD1	2.40	0.50
1:D:3188:ILE:HB	1:D:3439:ASN:ND2	2.26	0.50
1:D:3433:ARG:HD3	1:D:3436:GLY:H	1.75	0.50
1:D:3526:GLY:O	1:D:3530:SER:HB3	2.11	0.50
1:A:50:THR:HG21	1:A:56:LYS:HB2	1.92	0.50
1:A:247:PHE:HA	1:A:325:ASP:OD2	2.12	0.50
1:B:1243:LYS:HA	6:B:4095:HOH:O	2.12	0.50
1:C:2213:ASP:HB2	1:C:2222:ARG:HG3	1.94	0.50
1:A:179:GLU:O	1:A:181:VAL:N	2.44	0.50
1:B:1120:ARG:O	1:B:1122:TYR:N	2.44	0.50
1:B:1155:VAL:HG23	1:B:1459:LYS:O	2.11	0.50
1:B:1464:ASN:HD21	1:B:1475:TYR:H	1.59	0.50
1:B:1498:ILE:HG23	1:B:1499:ASP:N	2.26	0.50
1:B:1567:LEU:HD12	1:B:1567:LEU:C	2.37	0.50
1:C:2235:GLY:HA3	1:C:2240:ARG:HG2	1.92	0.50
1:C:2444:VAL:O	1:C:2444:VAL:CG1	2.60	0.50
1:D:3113:MET:HB2	1:D:3357:PHE:HZ	1.75	0.50
1:D:3421:GLN:O	1:D:3422:PHE:C	2.54	0.50
1:D:3482:THR:HG23	1:D:3509:VAL:HG12	1.93	0.50
1:A:131:ASN:C	1:A:131:ASN:OD1	2.53	0.50
1:A:329:PHE:HD2	1:A:330:GLN:HG2	1.76	0.50
1:D:3174:SER:O	1:D:3178:LEU:HB2	2.11	0.50
1:D:3187:PHE:CD1	1:D:3187:PHE:C	2.90	0.50
1:D:3514:PRO:O	1:D:3515:ASP:HB2	2.12	0.50
1:A:89:VAL:O	1:A:90:HIS:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:VAL:HG12	1:A:487:MET:HG2	1.93	0.50
1:A:326:GLU:HB2	6:A:4005:HOH:O	2.10	0.50
1:B:1050:THR:CG2	1:B:1056:LYS:HB3	2.41	0.50
1:B:1150:ARG:HH22	1:B:1154:PRO:HA	1.76	0.50
1:C:2089:VAL:O	1:C:2090:HIS:C	2.53	0.50
1:C:2101:ASN:O	1:C:2105:ASN:ND2	2.44	0.50
1:C:2105(C):ILE:HB	1:C:2108:LEU:HB2	1.93	0.50
1:C:2206:THR:HB	1:C:2210:PHE:CE2	2.46	0.50
1:C:2270:GLN:OE1	1:C:2270:GLN:N	2.45	0.50
1:C:2389:PRO:HG2	1:C:2434:VAL:CG1	2.32	0.50
1:D:3532:LYS:C	1:D:3534:LEU:N	2.69	0.50
1:B:1100:TRP:CD1	1:B:1356:HIS:HB2	2.47	0.50
1:B:1347:ASP:O	1:B:1350:GLN:HB3	2.11	0.50
1:B:1495:TYR:CD2	1:B:1501:MET:HA	2.46	0.50
1:D:3300:MET:O	1:D:3304:ILE:HG13	2.12	0.50
1:D:3394:THR:HA	1:D:3402:TYR:O	2.10	0.50
1:A:228:VAL:HG23	6:A:4027:HOH:O	2.11	0.50
1:A:532:LYS:C	1:A:534:LEU:N	2.68	0.50
1:A:546:LYS:HE3	1:B:1137:LYS:NZ	2.26	0.50
1:B:1245:ARG:HD2	1:B:1329:PHE:CE1	2.47	0.50
1:B:1394:THR:HA	1:B:1402:TYR:O	2.12	0.50
1:C:2202:ALA:HB2	1:C:2348:TYR:CE1	2.47	0.50
1:C:2396:ASN:N	1:C:2396:ASN:HD22	2.08	0.50
1:D:3132:VAL:HG23	6:D:4179:HOH:O	2.12	0.50
1:B:1088:THR:O	1:B:1092:ILE:HG12	2.12	0.50
1:B:1209:PHE:HB3	1:B:1377:ILE:HD11	1.93	0.50
1:B:1246:LEU:HD23	1:B:1251:LYS:HB2	1.94	0.50
1:B:1543:GLN:CD	1:B:1543:GLN:H	2.19	0.50
1:C:2095:HIS:O	1:C:2097:LYS:N	2.45	0.50
1:C:2456:ARG:NE	1:C:2502:GLU:OE2	2.44	0.50
1:D:3134:TYR:CD2	1:D:3136:TYR:HE1	2.29	0.50
1:D:3308:GLU:CA	1:D:3571:ASN:HD21	2.24	0.50
1:D:3491:LEU:O	1:D:3494:LEU:N	2.45	0.50
1:A:99:VAL:HG12	1:A:100:TRP:N	2.27	0.50
1:A:148:TYR:HB2	1:A:219:GLY:O	2.12	0.50
1:A:198:PHE:CE1	1:A:352:LEU:HD13	2.47	0.50
1:A:218:PRO:C	1:A:458:MET:CE	2.85	0.50
1:A:331:THR:O	1:A:335:ILE:HD12	2.11	0.50
1:B:1080:LEU:C	1:B:1082:LEU:H	2.19	0.50
1:B:1169:LYS:O	1:B:1170:GLU:HG3	2.12	0.50
1:B:1269:THR:OG1	1:B:1271:VAL:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2428:ARG:O	1:C:2430:ILE:N	2.45	0.50
1:C:2449:LYS:CA	1:C:2452:ILE:HD12	2.36	0.50
1:C:2451:SER:HB2	1:C:2504:TYR:CE2	2.46	0.50
1:C:2464:ASN:ND2	1:C:2475:TYR:H	2.10	0.50
1:D:3302:ALA:O	1:D:3303:THR:C	2.53	0.50
1:A:169:LYS:O	1:A:170:GLU:HG3	2.12	0.49
1:A:209:PHE:HB3	1:A:377:ILE:CD1	2.41	0.49
1:A:408:LEU:HD13	1:A:409:TYR:CE2	2.46	0.49
1:B:1113:MET:O	1:B:1116:VAL:HG13	2.12	0.49
1:B:1198:PHE:HA	1:B:1580:PHE:CD2	2.46	0.49
1:C:2388:HIS:O	1:C:2391:LEU:HB2	2.11	0.49
1:D:3077:ARG:O	1:D:3081:LEU:HG	2.11	0.49
1:D:3465:GLU:OE2	1:D:3468:LYS:HE2	2.12	0.49
1:A:43:ASN:ND2	1:A:69:CYS:O	2.45	0.49
1:A:168:ASN:C	1:A:170:GLU:N	2.69	0.49
1:B:1064:PHE:HA	1:B:1071:THR:O	2.12	0.49
1:B:1108:LEU:O	1:B:1112:ILE:HG12	2.12	0.49
1:B:1151:ALA:HB2	1:B:1529:PHE:HZ	1.77	0.49
1:B:1173:ASP:C	1:B:1173:ASP:OD2	2.55	0.49
1:B:1174:SER:O	1:B:1178:LEU:HB2	2.11	0.49
1:C:2132:VAL:HG23	6:C:4132:HOH:O	2.11	0.49
1:C:2225:GLY:HA3	1:C:2229:ASP:OD1	2.12	0.49
1:C:2246:LEU:HD23	1:C:2251:LYS:HB2	1.94	0.49
1:C:2464:ASN:HD21	1:C:2475:TYR:H	1.58	0.49
1:D:3196:MET:CE	1:D:3431:ALA:HB2	2.42	0.49
1:D:3563:SER:C	1:D:3565:GLN:N	2.69	0.49
1:A:196:MET:CE	1:A:431:ALA:HB2	2.42	0.49
1:B:1081:LEU:O	1:B:1082:LEU:HG	2.12	0.49
1:B:1196:MET:CE	1:B:1431:ALA:HB2	2.42	0.49
1:B:1229:ASP:HA	1:B:1337:ILE:HD11	1.94	0.49
1:B:1308:GLU:CA	1:B:1571:ASN:HD21	2.24	0.49
1:B:1347:ASP:O	1:B:1350:GLN:N	2.45	0.49
1:C:2049:SER:HB2	1:D:3322:GLU:OE1	2.13	0.49
1:C:2287:VAL:HG23	1:C:2289:GLN:H	1.77	0.49
1:C:2394:THR:HA	1:C:2402:TYR:O	2.12	0.49
1:D:3087:ASN:HB3	4:D:3702:BOG:H3	1.93	0.49
1:D:3197:MET:O	1:D:3198:PHE:C	2.55	0.49
1:D:3557:LYS:HA	1:D:3560:ASN:HD22	1.77	0.49
1:A:190:ASP:HB2	1:A:517:ILE:HD12	1.94	0.49
1:A:535:MET:C	1:A:537:ASN:H	2.20	0.49
1:A:545:TRP:CE3	1:A:545:TRP:HA	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1039:ASN:N	1:B:1039:ASN:HD22	2.10	0.49
1:C:2363:PRO:C	1:C:2365:LEU:N	2.70	0.49
1:D:3064:PHE:HD2	1:D:3070:THR:O	1.96	0.49
1:D:3103:VAL:C	1:D:3105:ASN:H	2.21	0.49
1:D:3209:PHE:CD1	1:D:3209:PHE:N	2.79	0.49
1:D:3245:ARG:HH22	1:D:3326:GLU:HA	1.78	0.49
1:D:3464:ASN:HD21	1:D:3475:TYR:H	1.59	0.49
1:D:3523:VAL:HG12	1:D:3524:GLU:OE2	2.12	0.49
1:D:3545:TRP:HA	1:D:3545:TRP:CE3	2.47	0.49
1:A:34:ASN:HB3	1:A:37:CYS:SG	2.52	0.49
1:A:241:GLN:OE1	1:A:245:ARG:HD2	2.11	0.49
1:A:352:LEU:HD21	1:A:387:TRP:HH2	1.78	0.49
1:B:1107:PHE:O	1:B:1111:LEU:HB3	2.12	0.49
1:B:1229:ASP:OD2	1:B:1229:ASP:C	2.55	0.49
1:C:2050:THR:HG21	1:C:2056:LYS:HB2	1.94	0.49
1:C:2435:ALA:O	1:C:2510:GLU:O	2.30	0.49
1:C:2504:TYR:HA	1:C:2507:LEU:HD12	1.93	0.49
1:D:3276:PRO:HG3	1:D:3409:TYR:CD1	2.48	0.49
1:D:3532:LYS:C	1:D:3534:LEU:H	2.21	0.49
1:A:90:HIS:CD2	1:A:513:ARG:HG2	2.46	0.49
1:A:155:VAL:HG23	1:A:459:LYS:O	2.12	0.49
1:A:454:GLN:O	1:A:455:SER:C	2.55	0.49
1:A:495:TYR:CD2	1:A:501:MET:HA	2.47	0.49
1:B:1226:HIS:C	1:B:1377:ILE:HD12	2.38	0.49
1:B:1458:MET:O	1:B:1459:LYS:C	2.56	0.49
1:C:2128:PRO:HG3	1:C:2376:ARG:NH1	2.27	0.49
1:C:2150:ARG:NH2	1:C:2154:PRO:HA	2.27	0.49
1:C:2184:ARG:HH12	1:C:2441:PRO:HG3	1.77	0.49
1:C:2566:SER:O	1:C:2567:LEU:C	2.56	0.49
1:D:3064:PHE:HA	1:D:3071:THR:O	2.12	0.49
1:D:3099:VAL:HG12	1:D:3100:TRP:N	2.27	0.49
1:D:3246:LEU:HD23	1:D:3251:LYS:HB2	1.93	0.49
1:D:3500:VAL:O	1:D:3500:VAL:HG12	2.11	0.49
1:D:3510:GLU:OE1	1:D:3519:GLY:HA3	2.13	0.49
1:A:244:LEU:CD2	1:A:271:VAL:HG21	2.42	0.49
1:B:1465:GLU:OE2	1:B:1468:LYS:CE	2.61	0.49
1:C:2156:ALA:O	1:C:2159:CYS:HB2	2.12	0.49
1:C:2162:PRO:HG2	1:C:2171:LEU:HD23	1.94	0.49
1:C:2209:PHE:HB3	1:C:2377:ILE:HD11	1.94	0.49
1:D:3197:MET:HE1	1:D:3300:MET:HE1	1.94	0.49
1:A:206:THR:HB	1:A:210:PHE:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:PRO:C	1:A:365:LEU:N	2.71	0.49
1:A:500:VAL:O	1:A:500:VAL:HG12	2.12	0.49
1:A:523:VAL:HG12	1:A:524:GLU:OE2	2.13	0.49
1:B:1187:PHE:CD1	1:B:1187:PHE:C	2.90	0.49
1:B:1206:THR:HB	1:B:1210:PHE:CD2	2.48	0.49
1:B:1241:GLN:OE1	1:B:1245:ARG:HD2	2.13	0.49
1:B:1456:ARG:NE	1:B:1502:GLU:OE2	2.45	0.49
1:B:1535:MET:O	1:B:1537:ASN:N	2.45	0.49
1:C:2120:ARG:O	1:C:2122:TYR:N	2.46	0.49
1:C:2195:ASN:OD1	1:C:2197:MET:HB2	2.13	0.49
1:C:2395:PHE:O	1:C:2402:TYR:HD2	1.95	0.49
1:C:2433:ARG:HH21	1:C:2512:PRO:HB3	1.78	0.49
1:D:3096:PHE:O	1:D:3099:VAL:N	2.46	0.49
1:D:3113:MET:HE3	1:D:3116:VAL:CG2	2.41	0.49
1:D:3113:MET:O	1:D:3116:VAL:HG13	2.12	0.49
1:A:128:PRO:HG3	1:A:376:ARG:NH1	2.28	0.49
1:A:270:GLN:OE1	1:A:270:GLN:N	2.45	0.49
1:A:347:ASP:O	1:A:350:GLN:N	2.46	0.49
1:B:1202:ALA:HB2	1:B:1348:TYR:CE1	2.48	0.49
1:B:1205:PHE:CE2	5:B:1701:PGX:H171	2.48	0.49
1:B:1545:TRP:HA	1:B:1545:TRP:CE3	2.48	0.49
1:C:2072:PRO:HG2	1:C:2077:ARG:NE	2.27	0.49
1:C:2206:THR:HB	1:C:2210:PHE:CD2	2.48	0.49
1:C:2322:GLU:HB3	1:D:3052:PHE:CD2	2.48	0.49
1:C:2347:ASP:O	1:C:2350:GLN:N	2.46	0.49
1:D:3136:TYR:O	1:D:3136:TYR:CD1	2.66	0.49
1:A:95:HIS:O	1:A:97:LYS:N	2.46	0.49
1:A:450:ALA:O	1:A:451:SER:C	2.55	0.49
1:B:1195:ASN:OD1	1:B:1197:MET:HB2	2.13	0.49
1:B:1339:GLU:OE2	1:B:1558:ILE:CG2	2.61	0.49
1:B:1513:ARG:NH2	1:B:1520:GLU:HB2	2.28	0.49
1:B:1523:VAL:HG12	1:B:1524:GLU:OE2	2.13	0.49
1:C:2107:PHE:O	1:C:2111:LEU:HB3	2.13	0.49
1:C:2209:PHE:HB3	1:C:2377:ILE:CD1	2.43	0.49
1:C:2467:ARG:NH1	1:C:2521:THR:OG1	2.44	0.49
1:D:3253:LYS:O	1:D:3264:PRO:HG3	2.12	0.49
1:A:464:ASN:HD21	1:A:475:TYR:H	1.60	0.48
1:A:513:ARG:HB2	1:A:516:ALA:HB3	1.95	0.48
1:A:583:GLN:CD	1:A:583:GLN:N	2.70	0.48
1:B:1449:LYS:CA	1:B:1452:ILE:HD12	2.40	0.48
1:B:1507:LEU:HD22	1:B:1522:MET:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1530:SER:OG	5:B:1701:PGX:H162	2.13	0.48
1:B:1547:PRO:HB3	1:B:1553:GLU:N	2.28	0.48
1:C:2112:ILE:O	1:C:2115:TYR:N	2.46	0.48
1:C:2151:ALA:HB2	1:C:2529:PHE:HZ	1.78	0.48
1:C:2450:ALA:O	1:C:2452:ILE:N	2.46	0.48
1:D:3151:ALA:HB2	1:D:3529:PHE:HZ	1.78	0.48
1:D:3173:ASP:OD2	1:D:3173:ASP:C	2.55	0.48
1:D:3198:PHE:CE1	1:D:3352:LEU:HD13	2.48	0.48
1:D:3537:ASN:HB2	6:D:4170:HOH:O	2.13	0.48
1:A:371:PHE:HZ	1:A:536:GLY:N	2.11	0.48
1:B:1064:PHE:HD2	1:B:1070:THR:O	1.96	0.48
1:B:1352:LEU:HD21	1:B:1387:TRP:HH2	1.76	0.48
1:C:2495:TYR:CD2	1:C:2501:MET:HA	2.48	0.48
1:C:2567:LEU:HD12	1:C:2567:LEU:C	2.37	0.48
1:D:3198:PHE:HA	1:D:3580:PHE:CD2	2.48	0.48
1:D:3294:LEU:HB3	1:D:3409:TYR:CD2	2.47	0.48
1:D:3362:ASP:OD1	1:D:3364:GLU:HB2	2.13	0.48
1:D:3444:VAL:O	1:D:3445:GLN:C	2.56	0.48
1:C:2187:PHE:HB2	1:C:2393:ASP:OD1	2.12	0.48
1:C:2467:ARG:NH1	1:C:2520:GLU:OE1	2.42	0.48
1:C:2532:LYS:C	1:C:2534:LEU:H	2.20	0.48
1:C:2545:TRP:CE3	1:C:2545:TRP:HA	2.47	0.48
1:D:3403:SER:OG	1:D:3405:LYS:HD2	2.13	0.48
1:A:187:PHE:CD1	1:A:187:PHE:C	2.91	0.48
1:A:564:ILE:O	1:A:568:ILE:HD12	2.14	0.48
1:B:1235:GLY:HA3	1:B:1240:ARG:HG2	1.94	0.48
1:B:1331:THR:O	1:B:1335:ILE:HD12	2.13	0.48
1:B:1344:VAL:HG12	1:B:1345:ILE:N	2.27	0.48
1:C:2140:GLU:HB2	1:D:3330:GLN:HE22	1.78	0.48
1:C:2316:LEU:O	1:C:2319:GLU:N	2.47	0.48
1:C:2495:TYR:CE2	1:C:2502:GLU:HG3	2.48	0.48
1:C:2503:LEU:O	1:C:2504:TYR:C	2.55	0.48
1:D:3124:ILE:HD11	1:D:3528:PRO:C	2.39	0.48
1:D:3130:TYR:CE2	1:D:3135:GLY:O	2.66	0.48
1:D:3169:LYS:O	1:D:3170:GLU:HG3	2.13	0.48
1:D:3583:GLN:N	1:D:3583:GLN:CD	2.72	0.48
1:B:1394:THR:O	1:B:1429:GLN:NE2	2.44	0.48
1:B:1454:GLN:O	1:B:1457:GLU:N	2.46	0.48
1:C:2320:HIS:C	1:C:2322:GLU:H	2.21	0.48
1:D:3152:LEU:HB2	1:D:3466:TYR:CE1	2.47	0.48
1:D:3363:PRO:C	1:D:3365:LEU:N	2.70	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:VAL:HG22	1:A:117:LEU:N	2.27	0.48
1:A:120:ARG:O	1:A:122:TYR:N	2.47	0.48
1:A:464:ASN:ND2	1:A:475:TYR:H	2.12	0.48
1:A:532:LYS:C	1:A:534:LEU:H	2.21	0.48
1:A:538:PRO:HG2	1:B:1139:TRP:HZ3	1.78	0.48
1:A:557:LYS:O	1:A:558:ILE:C	2.56	0.48
1:B:1113:MET:CE	1:B:1117:LEU:HD22	2.43	0.48
1:B:1190:ASP:HB2	1:B:1517:ILE:HD12	1.95	0.48
1:B:1387:TRP:CZ2	1:B:1518:PHE:CZ	3.01	0.48
1:B:1523:VAL:HG11	6:B:4064:HOH:O	2.12	0.48
1:B:1563:SER:C	1:B:1565:GLN:N	2.70	0.48
1:C:2077:ARG:O	1:C:2081:LEU:HG	2.14	0.48
1:C:2315:ILE:HD13	1:C:2558:ILE:HD11	1.95	0.48
1:C:2316:LEU:CD1	1:C:2331:THR:HB	2.44	0.48
1:C:2389:PRO:HB2	1:C:2433:ARG:O	2.13	0.48
1:D:3034:ASN:HB3	1:D:3037:CYS:SG	2.53	0.48
1:D:3090:HIS:CD2	1:D:3513:ARG:HG2	2.49	0.48
1:D:3113:MET:HA	1:D:3116:VAL:CG1	2.44	0.48
1:D:3187:PHE:HB2	1:D:3393:ASP:OD1	2.13	0.48
1:D:3371:PHE:CE1	1:D:3532:LYS:HE2	2.49	0.48
1:D:3509:VAL:O	1:D:3510:GLU:C	2.56	0.48
1:D:3525:LEU:C	1:D:3528:PRO:HD2	2.38	0.48
1:D:3528:PRO:O	1:D:3529:PHE:C	2.56	0.48
1:D:3538:PRO:O	1:D:3540:CYS:N	2.46	0.48
1:A:173:ASP:OD2	1:A:173:ASP:C	2.57	0.48
1:A:206:THR:HB	1:A:210:PHE:CE2	2.48	0.48
1:A:396:ASN:N	1:A:396:ASN:HD22	2.10	0.48
1:B:1090:HIS:CD2	1:B:1513:ARG:HG2	2.49	0.48
1:B:1092:ILE:HG12	1:B:1092:ILE:H	1.36	0.48
1:B:1206:THR:HB	1:B:1210:PHE:CE2	2.49	0.48
1:B:1232:HIS:O	1:B:1288:GLY:CA	2.61	0.48
1:B:1303:THR:O	1:B:1307:ARG:HG3	2.14	0.48
1:B:1363:PRO:C	1:B:1365:LEU:N	2.72	0.48
1:B:1467:ARG:O	1:B:1472:LEU:HB2	2.13	0.48
1:C:2137:LYS:NZ	1:D:3546:LYS:HE3	2.28	0.48
1:C:2463:LEU:CD1	1:C:2503:LEU:HA	2.44	0.48
1:D:3120:ARG:O	1:D:3122:TYR:N	2.46	0.48
1:D:3120:ARG:HD2	1:D:3527:ALA:HB1	1.95	0.48
1:D:3185:ARG:HH21	1:D:3438:ARG:CZ	2.27	0.48
1:D:3513:ARG:HB2	1:D:3516:ALA:HB3	1.96	0.48
1:A:185:ARG:NH2	6:A:4024:HOH:O	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:HIS:O	1:A:391:LEU:HB2	2.14	0.48
1:A:524:GLU:OE2	1:A:524:GLU:CA	2.60	0.48
1:B:1532:LYS:C	1:B:1534:LEU:H	2.22	0.48
1:C:2050:THR:CG2	1:C:2056:LYS:HB3	2.44	0.48
1:D:3148:TYR:HB2	1:D:3219:GLY:O	2.12	0.48
1:D:3206:THR:HB	1:D:3210:PHE:CE2	2.48	0.48
1:D:3234:TYR:CE1	1:D:3252:LEU:HD11	2.48	0.48
1:D:3247:PHE:HA	1:D:3325:ASP:OD2	2.13	0.48
1:D:3344:VAL:HG12	1:D:3345:ILE:N	2.28	0.48
1:D:3388:HIS:O	1:D:3391:LEU:HB2	2.13	0.48
1:D:3521:THR:HG22	1:D:3522:MET:N	2.29	0.48
1:B:1187:PHE:HB2	1:B:1393:ASP:OD1	2.14	0.48
1:B:1451:SER:HB2	1:B:1504:TYR:CE2	2.49	0.48
1:C:2428:ARG:HB3	6:C:4126:HOH:O	2.13	0.48
1:D:3209:PHE:HB3	1:D:3377:ILE:CD1	2.43	0.48
1:D:3566:SER:O	1:D:3567:LEU:C	2.56	0.48
1:A:191:PRO:HG2	1:A:515:ASP:O	2.13	0.48
1:A:192:GLN:OE1	1:A:517:ILE:HG22	2.14	0.48
1:A:209:PHE:HB3	1:A:377:ILE:HD11	1.96	0.48
1:A:301:TYR:O	1:A:302:ALA:C	2.56	0.48
1:A:373:TYR:H	1:B:1372:GLN:HE22	1.62	0.48
1:A:551:GLY:O	1:B:1048:MET:HE1	2.14	0.48
1:B:1272:GLU:HA	6:B:4061:HOH:O	2.13	0.48
1:B:1308:GLU:HG3	1:B:1336:LEU:CD1	2.35	0.48
1:C:2134:TYR:HD2	1:C:2136:TYR:HE1	1.59	0.48
1:D:3089:VAL:O	1:D:3090:HIS:C	2.56	0.48
1:A:462:SER:CB	1:A:465:GLU:HG2	2.43	0.47
1:A:462:SER:HB3	1:A:465:GLU:HG2	1.96	0.47
1:B:1499:ASP:O	1:B:1501:MET:N	2.47	0.47
1:C:2231:ASN:C	1:C:2231:ASN:OD1	2.56	0.47
1:C:2381:PHE:HB2	1:C:2529:PHE:CD1	2.49	0.47
1:C:2383:THR:C	1:C:2385:TYR:N	2.70	0.47
1:C:2551:GLY:O	1:D:3048:MET:HE1	2.14	0.47
1:C:2563:SER:O	1:C:2564:ILE:C	2.57	0.47
1:D:3387:TRP:HZ2	5:D:3701:PGX:H71	1.79	0.47
1:A:38:SER:C	1:A:40:PRO:HD3	2.39	0.47
1:A:208:GLN:O	1:A:211:LYS:HD3	2.14	0.47
1:A:287:VAL:HG23	1:A:289:GLN:H	1.78	0.47
1:B:1056:LYS:HG3	1:B:1057:CYS:N	2.29	0.47
1:B:1108:LEU:HA	1:B:1111:LEU:HD23	1.95	0.47
1:B:1116:VAL:HG22	1:B:1117:LEU:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1185:ARG:HH21	1:B:1438:ARG:CD	2.26	0.47
1:C:2155:VAL:HG12	1:C:2159:CYS:SG	2.54	0.47
1:C:2304:ILE:O	1:C:2307:ARG:HB2	2.14	0.47
1:C:2320:HIS:C	1:C:2322:GLU:N	2.72	0.47
1:D:3463:LEU:CD1	1:D:3503:LEU:HA	2.44	0.47
1:A:202:ALA:CA	1:A:348:TYR:HE1	2.27	0.47
1:C:2208:GLN:O	1:C:2211:LYS:HD3	2.14	0.47
1:D:3179:GLU:O	1:D:3181:VAL:N	2.47	0.47
1:A:108:LEU:O	1:A:112:ILE:HG12	2.15	0.47
1:A:113:MET:HA	1:A:116:VAL:CG1	2.43	0.47
1:A:198:PHE:HA	1:A:580:PHE:CD2	2.50	0.47
1:A:303:THR:O	1:A:307:ARG:HG3	2.15	0.47
1:A:338:GLY:HA3	1:A:559:ILE:CD1	2.39	0.47
1:B:1128:PRO:HG2	1:B:1376:ARG:NH1	2.30	0.47
1:B:1150:ARG:NH2	1:B:1154:PRO:HA	2.29	0.47
1:B:1295:VAL:CB	1:B:1298:LEU:HD22	2.43	0.47
1:B:1309:HIS:HD2	1:B:1310:ASN:OD1	1.97	0.47
1:B:1316:LEU:CD1	1:B:1331:THR:HB	2.45	0.47
1:C:2183:LEU:HD21	1:C:2445:GLN:CG	2.44	0.47
1:C:2463:LEU:HB3	6:C:4112:HOH:O	2.15	0.47
1:C:2535:MET:C	1:C:2537:ASN:H	2.21	0.47
1:D:3038:SER:C	1:D:3040:PRO:HD3	2.38	0.47
1:D:3226:HIS:C	1:D:3377:ILE:HD12	2.39	0.47
1:A:205:PHE:HE2	5:A:701:PGX:H171	1.78	0.47
1:A:481:LEU:CD1	1:A:510:GLU:HA	2.44	0.47
1:B:1168:ASN:C	1:B:1170:GLU:N	2.70	0.47
1:B:1287:VAL:HG23	1:B:1289:GLN:H	1.80	0.47
1:B:1463:LEU:CD1	1:B:1503:LEU:HA	2.44	0.47
1:C:2090:HIS:CD2	1:C:2513:ARG:HG2	2.49	0.47
1:C:2169:LYS:O	1:C:2170:GLU:HG3	2.13	0.47
1:C:2403:SER:OG	1:C:2405:LYS:HD2	2.13	0.47
1:C:2454:GLN:O	1:C:2455:SER:C	2.54	0.47
1:D:3245:ARG:O	1:D:3253:LYS:HG3	2.15	0.47
1:D:3435:ALA:O	1:D:3510:GLU:O	2.32	0.47
1:A:120:ARG:HH11	1:A:527:ALA:HB1	1.80	0.47
1:A:150:ARG:NH2	1:A:154:PRO:HA	2.29	0.47
1:A:175:LYS:O	1:A:179:GLU:HG3	2.14	0.47
1:A:197:MET:O	1:A:198:PHE:C	2.56	0.47
1:B:1126:SER:HA	1:B:1127:PRO:C	2.38	0.47
1:B:1190:ASP:OD2	1:B:1193:GLY:N	2.48	0.47
1:B:1450:ALA:O	1:B:1454:GLN:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1530:SER:C	1:B:1532:LYS:H	2.23	0.47
1:B:1563:SER:O	1:B:1564:ILE:C	2.57	0.47
1:B:1564:ILE:O	1:B:1568:ILE:HD12	2.15	0.47
1:C:2178:LEU:HD22	1:C:2183:LEU:CD1	2.45	0.47
1:C:2191:PRO:HG2	1:C:2515:ASP:O	2.15	0.47
1:C:2387:TRP:CZ2	5:C:2701:PGX:C7	2.95	0.47
1:D:3487:MET:O	1:D:3490:GLU:HB3	2.13	0.47
1:D:3501:MET:HE3	1:D:3505:PRO:HB2	1.96	0.47
1:A:50:THR:HG21	1:A:56:LYS:CB	2.45	0.47
1:A:546:LYS:HE3	1:B:1137:LYS:HZ1	1.80	0.47
1:B:1050:THR:HG21	1:B:1056:LYS:CB	2.44	0.47
1:B:1089:VAL:O	1:B:1090:HIS:C	2.57	0.47
1:B:1108:LEU:HD23	1:B:1111:LEU:HD23	1.97	0.47
1:B:1142:PHE:O	1:B:1376:ARG:NH2	2.36	0.47
1:B:1183:LEU:HD22	1:B:1442:ILE:HG13	1.96	0.47
1:B:1247:PHE:HA	1:B:1325:ASP:OD2	2.15	0.47
1:B:1276:PRO:HB2	1:B:1278:HIS:CE1	2.49	0.47
1:B:1287:VAL:O	1:B:1288:GLY:C	2.56	0.47
1:B:1421:GLN:O	1:B:1422:PHE:C	2.58	0.47
1:B:1444:VAL:O	1:B:1445:GLN:C	2.58	0.47
1:C:2113:MET:CE	1:C:2117:LEU:HD22	2.44	0.47
1:C:2168:ASN:C	1:C:2170:GLU:N	2.70	0.47
1:C:2181:VAL:HG12	1:C:2487:MET:HG2	1.97	0.47
1:C:2232:HIS:O	1:C:2288:GLY:CA	2.61	0.47
1:C:2396:ASN:HD22	1:C:2401:GLU:HG2	1.79	0.47
1:C:2458:MET:O	1:C:2459:LYS:C	2.56	0.47
1:C:2481:LEU:CD1	1:C:2510:GLU:HA	2.45	0.47
1:C:2491:LEU:O	1:C:2494:LEU:N	2.47	0.47
1:C:2546:LYS:HE3	1:D:3137:LYS:NZ	2.29	0.47
1:D:3096:PHE:O	1:D:3098:GLY:N	2.47	0.47
1:D:3126:SER:HA	1:D:3127:PRO:C	2.39	0.47
1:D:3183:LEU:HD21	1:D:3445:GLN:CG	2.45	0.47
1:D:3304:ILE:HG22	1:D:3571:ASN:HD22	1.79	0.47
1:D:3530:SER:C	1:D:3532:LYS:H	2.23	0.47
1:A:107:PHE:O	1:A:111:LEU:HB3	2.15	0.47
1:A:134:TYR:CD2	1:A:136:TYR:HE1	2.33	0.47
1:A:320:HIS:C	1:A:322:GLU:H	2.22	0.47
1:B:1086:PRO:HG2	6:B:4096:HOH:O	2.14	0.47
1:B:1124:ILE:HD11	1:B:1528:PRO:C	2.40	0.47
1:B:1240:ARG:HH12	1:B:1272:GLU:HB2	1.80	0.47
1:C:2056:LYS:HE2	6:C:4097:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2573:LYS:HB2	6:C:4110:HOH:O	2.14	0.47
1:D:3150:ARG:NH2	1:D:3154:PRO:HA	2.30	0.47
1:D:3209:PHE:HB3	1:D:3377:ILE:HD11	1.96	0.47
1:D:3211:LYS:O	1:D:3212:THR:C	2.58	0.47
1:D:3449:LYS:CA	1:D:3452:ILE:HD12	2.39	0.47
1:D:3458:MET:O	1:D:3459:LYS:C	2.58	0.47
1:D:3481:LEU:HD12	1:D:3481:LEU:O	2.14	0.47
1:A:206:THR:HA	1:A:209:PHE:CE2	2.50	0.47
1:A:316:LEU:CD1	1:A:331:THR:HB	2.45	0.47
1:A:433:ARG:HH21	1:A:512:PRO:CB	2.28	0.47
1:B:1076:THR:O	1:B:1079:LYS:HB2	2.14	0.47
1:B:1219:GLY:CA	1:B:1458:MET:HE2	2.42	0.47
1:B:1316:LEU:O	1:B:1319:GLU:N	2.48	0.47
1:B:1372:GLN:O	1:B:1374:GLN:N	2.47	0.47
1:B:1389:PRO:HG2	1:B:1434:VAL:HG22	1.97	0.47
1:B:1403:SER:OG	1:B:1405:LYS:HD2	2.15	0.47
1:B:1509:VAL:O	1:B:1510:GLU:O	2.31	0.47
1:B:1514:PRO:O	1:B:1515:ASP:HB2	2.14	0.47
1:C:2132:VAL:HG21	1:C:2219:GLY:HA3	1.97	0.47
1:D:3095:HIS:O	1:D:3100:TRP:CD1	2.68	0.47
1:D:3215:LYS:H	1:D:3215:LYS:HG2	1.51	0.47
1:D:3270:GLN:OE1	1:D:3270:GLN:N	2.47	0.47
1:D:3308:GLU:HG3	1:D:3336:LEU:CD1	2.35	0.47
1:D:3467:ARG:NH1	1:D:3521:THR:OG1	2.47	0.47
1:D:3503:LEU:O	1:D:3504:TYR:C	2.58	0.47
1:A:184:ARG:CD	1:A:187:PHE:HA	2.38	0.47
1:A:229:ASP:HA	1:A:337:ILE:HD11	1.97	0.47
1:A:429:GLN:O	1:A:429:GLN:HG2	2.14	0.47
1:A:509:VAL:O	1:A:510:GLU:O	2.32	0.47
1:A:547:PRO:O	1:A:552:GLY:N	2.43	0.47
1:C:2105(C):ILE:O	1:C:2108:LEU:HB2	2.15	0.47
1:C:2218:PRO:CB	1:C:2458:MET:HE3	2.42	0.47
1:C:2261:VAL:H	1:C:2307:ARG:NH2	2.13	0.47
1:C:2510:GLU:OE1	1:C:2519:GLY:HA3	2.15	0.47
1:C:2528:PRO:O	1:C:2529:PHE:C	2.58	0.47
1:D:3108:LEU:HD23	1:D:3111:LEU:HD23	1.97	0.47
1:D:3116:VAL:HG22	1:D:3117:LEU:N	2.30	0.47
1:A:386:HIS:HB2	1:A:504:TYR:CE1	2.50	0.46
1:A:465:GLU:OE2	1:A:468:LYS:CE	2.63	0.46
1:A:503:LEU:O	1:A:504:TYR:C	2.56	0.46
1:B:1225:GLY:HA3	1:B:1229:ASP:OD1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1444:VAL:O	1:B:1444:VAL:HG12	2.15	0.46
1:B:1450:ALA:O	1:B:1451:SER:C	2.57	0.46
1:C:2110:SER:O	1:C:2111:LEU:C	2.57	0.46
1:C:2176:GLU:O	1:C:2179:GLU:N	2.48	0.46
1:C:2209:PHE:CD1	1:C:2209:PHE:N	2.79	0.46
1:C:2211:LYS:O	1:C:2212:THR:C	2.59	0.46
1:C:2295:VAL:CB	1:C:2298:LEU:HD22	2.46	0.46
1:A:226:HIS:C	1:A:377:ILE:HD12	2.40	0.46
1:A:444:VAL:O	1:A:444:VAL:CG1	2.62	0.46
1:A:538:PRO:HG2	1:B:1139:TRP:CZ3	2.50	0.46
1:B:1134:TYR:HD2	1:B:1136:TYR:HE1	1.61	0.46
1:B:1205:PHE:CE2	1:B:1209:PHE:HZ	2.33	0.46
1:B:1386:HIS:HD2	1:B:1451:SER:HB3	1.79	0.46
1:B:1528:PRO:O	1:B:1529:PHE:C	2.58	0.46
1:C:2303:THR:O	1:C:2307:ARG:HG3	2.15	0.46
1:C:2450:ALA:O	1:C:2454:GLN:HG3	2.15	0.46
1:D:3107:PHE:O	1:D:3111:LEU:HB3	2.15	0.46
1:A:183:LEU:HD21	1:A:445:GLN:CG	2.45	0.46
1:B:1124:ILE:H	1:B:1124:ILE:HG12	1.59	0.46
1:B:1197:MET:HE1	1:B:1300:MET:CE	2.46	0.46
1:B:1526:GLY:O	1:B:1530:SER:HB3	2.15	0.46
1:C:2038:SER:C	1:C:2040:PRO:HD3	2.40	0.46
1:C:2173:ASP:OD2	1:C:2173:ASP:C	2.58	0.46
1:C:2344:VAL:HG12	1:C:2345:ILE:N	2.30	0.46
1:D:3196:MET:HE2	1:D:3431:ALA:HB2	1.97	0.46
1:D:3303:THR:O	1:D:3307:ARG:HG3	2.16	0.46
1:D:3553:GLU:OE1	1:D:3553:GLU:CA	2.63	0.46
1:A:456:ARG:NE	1:A:502:GLU:OE2	2.48	0.46
1:B:1300:MET:O	1:B:1304:ILE:HG13	2.14	0.46
1:B:1435:ALA:HB2	1:B:1518:PHE:HA	1.97	0.46
1:C:2433:ARG:HH21	1:C:2512:PRO:CB	2.29	0.46
1:C:2513:ARG:NH2	1:C:2520:GLU:HB2	2.31	0.46
1:D:3190:ASP:OD2	1:D:3193:GLY:N	2.49	0.46
1:D:3304:ILE:O	1:D:3307:ARG:HB2	2.16	0.46
1:A:274:ILE:HD12	1:A:291:VAL:HA	1.96	0.46
1:A:295:VAL:CB	1:A:298:LEU:HD22	2.44	0.46
1:A:341:ILE:HD13	1:A:534:LEU:HD12	1.97	0.46
1:A:381:PHE:CD1	1:A:529:PHE:CB	2.97	0.46
1:B:1077:ARG:O	1:B:1081:LEU:HG	2.15	0.46
1:B:1389:PRO:HB2	1:B:1433:ARG:O	2.15	0.46
1:B:1414:LEU:HA	1:B:1422:PHE:HE1	1.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1481:LEU:CD1	1:B:1510:GLU:HA	2.46	0.46
1:C:2056:LYS:HG3	1:C:2057:CYS:N	2.30	0.46
1:C:2429:GLN:O	1:C:2429:GLN:HG2	2.15	0.46
1:D:3174:SER:N	6:D:4188:HOH:O	2.48	0.46
1:D:3232:HIS:O	1:D:3288:GLY:CA	2.63	0.46
1:D:3245:ARG:HD2	1:D:3329:PHE:CE1	2.50	0.46
1:D:3435:ALA:HB2	1:D:3518:PHE:HA	1.96	0.46
1:D:3498:ILE:HG23	1:D:3499:ASP:N	2.29	0.46
1:A:74:PHE:O	1:A:75:LEU:C	2.59	0.46
1:A:103:VAL:C	1:A:105:ASN:N	2.73	0.46
1:A:176:GLU:O	1:A:179:GLU:N	2.49	0.46
1:A:383:THR:C	1:A:385:TYR:N	2.71	0.46
1:A:499:ASP:O	1:A:501:MET:N	2.49	0.46
1:A:509:VAL:O	1:A:510:GLU:C	2.59	0.46
1:B:1095:HIS:O	1:B:1097:LYS:N	2.49	0.46
1:C:2174:SER:O	1:C:2178:LEU:HB2	2.16	0.46
1:C:2514:PRO:O	1:C:2515:ASP:CB	2.63	0.46
1:D:3219:GLY:HA2	1:D:3458:MET:CE	2.43	0.46
1:D:3261:VAL:O	1:D:3307:ARG:NH1	2.49	0.46
1:D:3276:PRO:HB2	1:D:3278:HIS:CE1	2.50	0.46
1:D:3405:LYS:HE3	1:D:3405:LYS:H	1.81	0.46
1:D:3513:ARG:O	1:D:3515:ASP:N	2.49	0.46
1:A:456:ARG:NH1	6:A:4045:HOH:O	2.48	0.46
1:A:489:ALA:HB2	6:A:4044:HOH:O	2.14	0.46
1:A:513:ARG:O	1:A:515:ASP:N	2.48	0.46
1:B:1137:LYS:N	6:B:4080:HOH:O	2.49	0.46
1:B:1179:GLU:O	1:B:1181:VAL:N	2.48	0.46
1:B:1395:PHE:O	1:B:1402:TYR:HD2	1.99	0.46
1:B:1583:GLN:CD	1:B:1583:GLN:N	2.74	0.46
1:C:2105(C):ILE:CB	1:C:2108:LEU:HD12	2.46	0.46
1:C:2116:VAL:HG22	1:C:2117:LEU:N	2.31	0.46
1:C:2490:GLU:O	1:C:2493:ALA:HB3	2.16	0.46
1:C:2525:LEU:C	1:C:2528:PRO:HD2	2.41	0.46
1:D:3162:PRO:HB2	1:D:3171:LEU:CD2	2.46	0.46
1:A:61:ARG:NH2	1:B:1545:TRP:O	2.48	0.46
1:A:383:THR:O	1:A:385:TYR:N	2.49	0.46
1:B:1096:PHE:O	1:B:1097:LYS:C	2.58	0.46
1:B:1391:LEU:HD13	1:B:1404:PHE:HE2	1.80	0.46
1:C:2105(C):ILE:CG2	1:C:2108:LEU:HD12	2.46	0.46
1:C:2381:PHE:CD1	1:C:2529:PHE:CB	2.99	0.46
1:C:2513:ARG:HB2	1:C:2516:ALA:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3175:LYS:O	1:D:3178:LEU:HB3	2.16	0.46
1:D:3261:VAL:H	1:D:3307:ARG:NH2	2.14	0.46
1:A:366:LEU:C	1:A:368:ASN:H	2.24	0.46
1:B:1116:VAL:O	1:B:1119:SER:OG	2.34	0.46
1:B:1323:TRP:CE3	1:B:1327:GLN:HG2	2.51	0.46
1:B:1535:MET:C	1:B:1537:ASN:N	2.74	0.46
1:C:2065:TYR:CD2	1:C:2065:TYR:N	2.84	0.46
1:D:3076:THR:O	1:D:3079:LYS:HB2	2.16	0.46
1:D:3078:ILE:HD13	1:D:3078:ILE:N	2.30	0.46
1:D:3089:VAL:O	1:D:3092:ILE:HG12	2.16	0.46
1:D:3096:PHE:O	1:D:3097:LYS:C	2.59	0.46
1:D:3274:ILE:HD12	1:D:3291:VAL:HA	1.98	0.46
1:D:3499:ASP:C	1:D:3501:MET:H	2.23	0.46
1:A:405:LYS:HE3	1:A:405:LYS:H	1.81	0.46
1:A:463:LEU:CD1	1:A:503:LEU:HA	2.46	0.46
1:B:1113:MET:HA	1:B:1116:VAL:HG13	1.96	0.46
1:B:1120:ARG:HH11	1:B:1527:ALA:HB1	1.80	0.46
1:B:1245:ARG:HH22	1:B:1326:GLU:HA	1.81	0.46
1:B:1487:MET:O	1:B:1488:ALA:C	2.59	0.46
1:C:2064:PHE:HD2	1:C:2070:THR:O	1.99	0.46
1:C:2229:ASP:OD2	1:C:2229:ASP:C	2.58	0.46
1:C:2504:TYR:O	1:C:2507:LEU:HB2	2.16	0.46
1:C:2530:SER:C	1:C:2532:LYS:H	2.23	0.46
1:C:2546:LYS:HE3	1:D:3137:LYS:HZ1	1.80	0.46
1:D:3059:CYS:HB3	1:D:3064:PHE:O	2.16	0.46
1:D:3195:ASN:OD1	1:D:3197:MET:HB2	2.15	0.46
1:D:3218:PRO:C	1:D:3458:MET:CE	2.88	0.46
1:D:3287:VAL:HG23	1:D:3289:GLN:H	1.80	0.46
1:A:563:SER:C	1:A:565:GLN:N	2.72	0.45
1:B:1110:SER:O	1:B:1111:LEU:C	2.59	0.45
1:B:1308:GLU:OE2	1:B:1308:GLU:HA	2.16	0.45
1:C:2183:LEU:HD22	1:C:2442:ILE:HG13	1.98	0.45
1:C:2218:PRO:C	1:C:2458:MET:CE	2.89	0.45
1:C:2276:PRO:HG3	1:C:2409:TYR:CD1	2.51	0.45
1:C:2464:ASN:HD21	1:C:2475:TYR:N	2.14	0.45
1:C:2509:VAL:O	1:C:2510:GLU:C	2.59	0.45
1:C:2549:THR:HG23	1:D:3137:LYS:HD3	1.98	0.45
1:D:3136:TYR:CD1	1:D:3136:TYR:C	2.94	0.45
1:D:3190:ASP:HB2	1:D:3517:ILE:HD12	1.97	0.45
1:D:3309:HIS:HD2	1:D:3310:ASN:OD1	1.98	0.45
1:D:3315:ILE:HD13	1:D:3558:ILE:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:PHE:HB2	1:A:393:ASP:OD1	2.16	0.45
1:A:256:VAL:HA	1:A:260:GLU:O	2.17	0.45
1:A:371:PHE:CE1	1:A:532:LYS:HE2	2.51	0.45
1:A:563:SER:O	1:A:564:ILE:C	2.59	0.45
1:B:1151:ALA:HB2	1:B:1529:PHE:CZ	2.51	0.45
1:B:1380:GLU:HG3	1:B:1460:TYR:CE2	2.50	0.45
1:C:2247:PHE:HA	1:C:2325:ASP:OD2	2.15	0.45
1:D:3043:ASN:ND2	1:D:3069:CYS:O	2.49	0.45
1:D:3103:VAL:C	1:D:3105:ASN:N	2.75	0.45
1:D:3383:THR:C	1:D:3385:TYR:N	2.74	0.45
1:A:148:TYR:HD2	1:A:219:GLY:O	1.98	0.45
1:A:168:ASN:C	1:A:170:GLU:H	2.24	0.45
1:A:240:ARG:HH12	1:A:272:GLU:HB2	1.81	0.45
1:A:357:PHE:HE2	1:A:359:LEU:HD23	1.81	0.45
1:A:530:SER:C	1:A:532:LYS:H	2.24	0.45
1:B:1105(B):ILE:HG21	1:B:1108:LEU:CD1	2.42	0.45
1:B:1495:TYR:CE2	1:B:1502:GLU:HG3	2.48	0.45
1:B:1509:VAL:O	1:B:1510:GLU:C	2.59	0.45
1:C:2043:ASN:ND2	1:C:2069:CYS:O	2.49	0.45
1:C:2331:THR:O	1:C:2335:ILE:HD12	2.16	0.45
1:D:3173:ASP:OD2	1:D:3175:LYS:N	2.49	0.45
1:D:3191:PRO:HG2	1:D:3515:ASP:O	2.16	0.45
1:D:3230:LEU:CG	1:D:3337:ILE:HG13	2.41	0.45
1:D:3301:TYR:O	1:D:3304:ILE:HB	2.16	0.45
1:D:3381:PHE:O	5:D:3701:PGX:H101	2.17	0.45
1:A:65:TYR:N	1:A:65:TYR:CD2	2.84	0.45
1:A:110:SER:O	1:A:111:LEU:C	2.60	0.45
1:A:184:ARG:CB	1:A:439:ASN:HA	2.44	0.45
1:A:184:ARG:HH12	1:A:441:PRO:HG3	1.80	0.45
1:A:347:ASP:OD2	1:A:564:ILE:HG22	2.17	0.45
1:A:421:GLN:O	1:A:422:PHE:C	2.59	0.45
1:B:1065:TYR:CD2	1:B:1065:TYR:N	2.84	0.45
1:B:1148:TYR:HB2	1:B:1219:GLY:O	2.17	0.45
1:B:1455:SER:HA	1:B:1460:TYR:CD1	2.51	0.45
1:B:1464:ASN:ND2	1:B:1475:TYR:H	2.14	0.45
1:C:2108:LEU:HA	1:C:2111:LEU:HD23	1.98	0.45
1:C:2142:PHE:O	1:C:2376:ARG:NH2	2.37	0.45
1:C:2292:PHE:O	1:C:2299:MET:HE2	2.16	0.45
1:C:2387:TRP:HZ2	5:C:2701:PGX:C7	2.24	0.45
1:C:2395:PHE:CD1	1:C:2407:PHE:CD2	3.04	0.45
1:C:2534:LEU:HD13	1:C:2534:LEU:HA	1.87	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3380:GLU:HG3	1:D:3460:TYR:CE2	2.52	0.45
1:D:3386:HIS:HB2	1:D:3504:TYR:CE1	2.50	0.45
1:A:383:THR:O	1:A:384:LEU:C	2.59	0.45
1:A:538:PRO:HG3	1:B:1142:PHE:CE2	2.51	0.45
1:B:1191:PRO:HG2	1:B:1515:ASP:O	2.17	0.45
1:B:1209:PHE:CD1	1:B:1209:PHE:N	2.79	0.45
1:B:1216:ARG:HB3	1:B:1220:PHE:HD1	1.76	0.45
1:B:1405:LYS:HE3	1:B:1405:LYS:H	1.82	0.45
1:B:1503:LEU:O	1:B:1504:TYR:C	2.59	0.45
1:C:2148:TYR:HB2	1:C:2219:GLY:O	2.16	0.45
1:C:2215:LYS:H	1:C:2215:LYS:HG2	1.50	0.45
1:C:2245:ARG:HH22	1:C:2326:GLU:HA	1.82	0.45
1:C:2287:VAL:O	1:C:2288:GLY:C	2.58	0.45
1:C:2371:PHE:HZ	1:C:2536:GLY:N	2.14	0.45
1:C:2380:GLU:HG3	1:C:2460:TYR:CE2	2.51	0.45
1:C:2523:VAL:HG12	1:C:2524:GLU:OE2	2.16	0.45
1:D:3050:THR:HG21	1:D:3056:LYS:CB	2.46	0.45
1:D:3095:HIS:O	1:D:3100:TRP:HD1	1.99	0.45
1:D:3176:GLU:O	1:D:3179:GLU:N	2.50	0.45
1:D:3389:PRO:HB2	1:D:3433:ARG:O	2.16	0.45
1:D:3464:ASN:ND2	1:D:3475:TYR:H	2.14	0.45
1:A:190:ASP:OD1	1:A:192:GLN:HG3	2.16	0.45
1:A:246:LEU:HB3	1:A:251:LYS:O	2.16	0.45
1:A:389:PRO:HB2	1:A:433:ARG:O	2.17	0.45
1:A:435:ALA:O	1:A:510:GLU:O	2.34	0.45
1:A:465:GLU:OE2	1:A:468:LYS:HE2	2.17	0.45
1:A:530:SER:OG	5:A:701:PGX:H162	2.17	0.45
1:A:564:ILE:O	1:A:568:ILE:CD1	2.65	0.45
1:B:1095:HIS:O	1:B:1100:TRP:CD1	2.70	0.45
1:B:1128:PRO:HG3	1:B:1376:ARG:NH1	2.30	0.45
1:B:1292:PHE:O	1:B:1299:MET:HE2	2.16	0.45
1:C:2190:ASP:OD1	1:C:2192:GLN:HG3	2.17	0.45
1:C:2198:PHE:HA	1:C:2580:PHE:CD2	2.52	0.45
1:C:2336:LEU:O	1:C:2337:ILE:C	2.59	0.45
1:C:2498:ILE:O	1:C:2501:MET:HB2	2.16	0.45
1:D:3065:TYR:N	1:D:3065:TYR:CD2	2.85	0.45
1:D:3095:HIS:C	1:D:3097:LYS:N	2.74	0.45
1:D:3151:ALA:HB2	1:D:3529:PHE:CZ	2.51	0.45
1:D:3198:PHE:CZ	1:D:3352:LEU:HD13	2.51	0.45
1:D:3369:GLN:O	1:D:3371:PHE:N	2.49	0.45
1:D:3535:MET:O	1:D:3537:ASN:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:SER:O	1:A:178:LEU:HB2	2.17	0.45
1:A:276:PRO:HB2	1:A:278:HIS:CE1	2.51	0.45
1:B:1176:GLU:O	1:B:1179:GLU:N	2.50	0.45
1:B:1198:PHE:CZ	1:B:1352:LEU:HD13	2.51	0.45
1:B:1276:PRO:HG3	1:B:1409:TYR:CD1	2.52	0.45
1:B:1437:GLY:O	1:B:1438:ARG:C	2.59	0.45
1:C:2124:ILE:HD11	1:C:2528:PRO:C	2.41	0.45
1:C:2383:THR:O	1:C:2385:TYR:N	2.49	0.45
1:C:2523:VAL:HG12	1:C:2524:GLU:N	2.31	0.45
1:C:2535:MET:O	1:C:2537:ASN:N	2.50	0.45
1:C:2568:ILE:HG23	1:C:2572:VAL:CG2	2.46	0.45
1:D:3198:PHE:O	1:D:3199:ALA:C	2.60	0.45
1:A:454:GLN:C	1:A:456:ARG:N	2.75	0.45
1:A:525:LEU:C	1:A:528:PRO:HD2	2.41	0.45
1:B:1274:ILE:HD12	1:B:1291:VAL:HG23	1.98	0.45
1:B:1504:TYR:O	1:B:1507:LEU:HB2	2.17	0.45
1:C:2190:ASP:OD2	1:C:2193:GLY:N	2.50	0.45
1:C:2347:ASP:O	1:C:2348:TYR:O	2.35	0.45
1:C:2455:SER:HA	1:C:2460:TYR:CD1	2.51	0.45
1:C:2513:ARG:O	1:C:2515:ASP:N	2.50	0.45
1:C:2538:PRO:O	1:C:2540:CYS:N	2.49	0.45
1:D:3036:CYS:O	1:D:3037:CYS:C	2.60	0.45
1:D:3155:VAL:HG23	1:D:3459:LYS:O	2.17	0.45
1:D:3161:THR:O	1:D:3164:GLY:N	2.48	0.45
1:D:3229:ASP:HA	1:D:3337:ILE:HD11	1.98	0.45
1:D:3386:HIS:HD2	1:D:3451:SER:HB3	1.81	0.45
1:D:3404:PHE:N	1:D:3404:PHE:CD1	2.85	0.45
1:D:3433:ARG:HH21	1:D:3512:PRO:HB3	1.81	0.45
1:A:294:LEU:HB3	1:A:409:TYR:CD2	2.52	0.45
1:A:320:HIS:C	1:A:322:GLU:N	2.74	0.45
1:A:381:PHE:HB2	1:A:529:PHE:CD1	2.51	0.45
1:B:1175:LYS:O	1:B:1178:LEU:HB3	2.16	0.45
1:B:1566:SER:O	1:B:1567:LEU:C	2.58	0.45
5:B:1701:PGX:H202	6:B:4074:HOH:O	2.17	0.45
1:C:2059:CYS:HB3	1:C:2064:PHE:O	2.16	0.45
1:C:2190:ASP:HB2	1:C:2517:ILE:HD12	1.97	0.45
1:C:2357:PHE:HE2	1:C:2359:LEU:HD23	1.81	0.45
1:D:3034:ASN:HA	1:D:3035:PRO:HD2	1.86	0.45
1:D:3201:PHE:O	1:D:3204:HIS:N	2.50	0.45
1:D:3415:LEU:HD23	1:D:3415:LEU:HA	1.82	0.45
1:A:107:PHE:H	1:A:107:PHE:HD2	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:PHE:CD1	1:A:535:MET:HE1	2.52	0.45
1:B:1201:PHE:O	1:B:1204:HIS:N	2.50	0.45
1:B:1465:GLU:OE2	1:B:1468:LYS:HE2	2.17	0.45
1:C:2184:ARG:CB	1:C:2439:ASN:HA	2.44	0.45
1:C:2261:VAL:O	1:C:2307:ARG:NH1	2.50	0.45
1:C:2276:PRO:HB2	1:C:2278:HIS:CE1	2.52	0.45
1:C:2487:MET:O	1:C:2490:GLU:HB3	2.17	0.45
1:D:3162:PRO:HB2	1:D:3171:LEU:HD21	1.99	0.45
1:D:3295:VAL:CB	1:D:3298:LEU:HD22	2.47	0.45
1:D:3481:LEU:HD12	1:D:3510:GLU:HA	1.98	0.45
1:D:3507:LEU:HD22	1:D:3522:MET:HB2	1.98	0.45
1:A:195:ASN:OD1	1:A:197:MET:HB2	2.17	0.44
1:A:231:ASN:OD1	1:A:231:ASN:C	2.60	0.44
1:A:300:MET:O	1:A:304:ILE:HG13	2.16	0.44
1:A:404:PHE:N	1:A:404:PHE:CD1	2.85	0.44
1:A:449:LYS:CA	1:A:452:ILE:HD12	2.41	0.44
1:B:1118:THR:C	1:B:1121:SER:HG	2.25	0.44
1:B:1156:ALA:C	1:B:1158:ASP:N	2.75	0.44
1:C:2099:VAL:HA	1:C:2102:ILE:CD1	2.28	0.44
1:C:2103:VAL:C	1:C:2105:ASN:N	2.75	0.44
1:C:2105(C):ILE:O	1:C:2106:PRO:C	2.60	0.44
1:C:2156:ALA:C	1:C:2158:ASP:N	2.73	0.44
1:D:3530:SER:HB2	5:D:3701:PGX:H161	1.99	0.44
1:A:183:LEU:HD22	1:A:442:ILE:HG13	1.98	0.44
1:A:405:LYS:H	1:A:405:LYS:CE	2.30	0.44
1:B:1188:ILE:HB	1:B:1439:ASN:ND2	2.33	0.44
1:B:1211:LYS:O	1:B:1212:THR:C	2.59	0.44
1:B:1381:PHE:HB2	1:B:1529:PHE:CD1	2.52	0.44
1:B:1383:THR:C	1:B:1385:TYR:N	2.72	0.44
1:B:1467:ARG:HH22	1:B:1520:GLU:CD	2.25	0.44
1:D:3065:TYR:HB2	1:D:3066:GLY:H	1.64	0.44
1:D:3292:PHE:O	1:D:3299:MET:HE2	2.17	0.44
1:D:3381:PHE:CD1	1:D:3529:PHE:CB	2.99	0.44
1:A:108:LEU:HD23	1:A:111:LEU:HD23	1.99	0.44
1:A:113:MET:CE	1:A:117:LEU:HD22	2.47	0.44
1:A:126:SER:HA	1:A:127:PRO:C	2.41	0.44
1:A:196:MET:HA	1:A:196:MET:CE	2.47	0.44
1:A:462:SER:O	1:A:465:GLU:HB2	2.16	0.44
1:A:566:SER:O	1:A:567:LEU:C	2.59	0.44
1:B:1113:MET:HE3	1:B:1116:VAL:CG2	2.47	0.44
1:B:1162:PRO:HB2	1:B:1171:LEU:CD2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1369:GLN:O	1:B:1371:PHE:N	2.50	0.44
1:B:1405:LYS:H	1:B:1405:LYS:CE	2.30	0.44
1:B:1513:ARG:HB2	1:B:1516:ALA:HB3	1.99	0.44
1:C:2366:LEU:C	1:C:2368:ASN:H	2.25	0.44
1:C:2389:PRO:HG2	1:C:2434:VAL:HG22	1.98	0.44
1:C:2507:LEU:HD22	1:C:2522:MET:HB2	2.00	0.44
1:D:3246:LEU:HB3	1:D:3251:LYS:O	2.17	0.44
1:D:3329:PHE:HD2	1:D:3330:GLN:HG2	1.82	0.44
1:A:37:CYS:O	1:A:39:ASN:ND2	2.50	0.44
1:A:136:TYR:O	1:A:136:TYR:HD1	2.01	0.44
1:A:538:PRO:O	1:A:540:CYS:N	2.51	0.44
1:A:567:LEU:HD12	1:A:567:LEU:C	2.41	0.44
1:B:1095:HIS:O	1:B:1100:TRP:HD1	2.00	0.44
1:B:1205:PHE:HE2	5:B:1701:PGX:H171	1.82	0.44
1:B:1381:PHE:CD1	1:B:1529:PHE:CB	3.00	0.44
1:B:1389:PRO:HB2	1:B:1434:VAL:HA	2.00	0.44
1:B:1487:MET:O	1:B:1490:GLU:HB3	2.18	0.44
1:C:2050:THR:HG21	1:C:2056:LYS:CB	2.47	0.44
1:C:2112:ILE:O	1:C:2115:TYR:HB3	2.17	0.44
1:C:2114:LYS:O	1:C:2115:TYR:C	2.60	0.44
1:C:2196:MET:HE2	1:C:2431:ALA:HB2	1.98	0.44
1:C:2339:GLU:OE2	1:C:2558:ILE:CG2	2.66	0.44
1:D:3308:GLU:HA	1:D:3308:GLU:OE2	2.17	0.44
1:D:3352:LEU:HG	1:D:3518:PHE:HE2	1.83	0.44
1:D:3371:PHE:HZ	1:D:3536:GLY:N	2.15	0.44
1:A:156:ALA:C	1:A:158:ASP:N	2.73	0.44
1:A:196:MET:HE2	1:A:431:ALA:HB2	2.00	0.44
1:A:323:TRP:CE3	1:A:327:GLN:HG2	2.53	0.44
1:A:384:LEU:HB3	1:A:522:MET:CE	2.42	0.44
1:A:395:PHE:O	1:A:402:TYR:HD2	2.00	0.44
1:A:548:SER:O	1:A:550:PHE:N	2.50	0.44
1:B:1490:GLU:O	1:B:1493:ALA:HB3	2.17	0.44
1:C:2137:LYS:HZ1	1:D:3546:LYS:HE3	1.82	0.44
1:C:2298:LEU:O	1:C:2299:MET:C	2.60	0.44
1:C:2405:LYS:HE3	1:C:2405:LYS:H	1.83	0.44
1:C:2524:GLU:OE2	1:C:2524:GLU:CA	2.62	0.44
1:D:3196:MET:HG2	1:D:3429:GLN:HG2	2.00	0.44
1:D:3202:ALA:HB2	1:D:3348:TYR:CE1	2.52	0.44
1:D:3316:LEU:CD1	1:D:3331:THR:HB	2.47	0.44
1:D:3513:ARG:HH21	1:D:3520:GLU:HB2	1.83	0.44
1:A:295:VAL:HB	1:A:298:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:ILE:HD13	1:A:558:ILE:HD11	1.99	0.44
1:A:339:GLU:OE2	1:A:558:ILE:CG2	2.66	0.44
1:A:435:ALA:HB2	1:A:518:PHE:HA	1.99	0.44
1:A:543:GLN:H	1:A:543:GLN:CD	2.23	0.44
1:B:1107:PHE:H	1:B:1107:PHE:HD2	1.64	0.44
1:B:1173:ASP:OD2	1:B:1175:LYS:N	2.51	0.44
1:B:1371:PHE:HZ	1:B:1536:GLY:N	2.15	0.44
1:B:1436:GLY:HA2	1:B:1512:PRO:HG2	2.00	0.44
1:B:1462:SER:HB3	1:B:1465:GLU:HG2	1.99	0.44
1:B:1513:ARG:O	1:B:1515:ASP:N	2.50	0.44
1:B:1530:SER:C	1:B:1532:LYS:N	2.75	0.44
1:C:2096:PHE:O	1:C:2097:LYS:C	2.60	0.44
1:C:2103:VAL:O	1:C:2105:ASN:N	2.51	0.44
1:C:2134:TYR:CD2	1:C:2136:TYR:HE1	2.35	0.44
1:C:2206:THR:HA	1:C:2209:PHE:CE2	2.52	0.44
1:C:2369:GLN:O	1:C:2371:PHE:N	2.50	0.44
1:C:2530:SER:C	1:C:2532:LYS:N	2.76	0.44
1:D:3056:LYS:HA	6:D:4150:HOH:O	2.17	0.44
1:D:3198:PHE:HB2	1:D:3580:PHE:HB3	1.99	0.44
1:A:150:ARG:HD2	1:A:380:GLU:OE1	2.17	0.44
1:A:198:PHE:CZ	1:A:352:LEU:HD13	2.52	0.44
1:A:247:PHE:HA	1:A:325:ASP:CG	2.43	0.44
1:A:287:VAL:O	1:A:288:GLY:C	2.60	0.44
1:A:470:PHE:CD2	1:A:470:PHE:N	2.85	0.44
1:A:521:THR:HG22	1:A:522:MET:N	2.32	0.44
1:A:568:ILE:HG23	1:A:572:VAL:CG2	2.47	0.44
1:B:1136:TYR:HD1	1:B:1136:TYR:O	2.00	0.44
1:B:1175:LYS:O	1:B:1179:GLU:HG3	2.18	0.44
1:B:1261:VAL:O	1:B:1307:ARG:NH1	2.51	0.44
1:B:1386:HIS:HB2	1:B:1504:TYR:CE1	2.52	0.44
1:B:1454:GLN:O	1:B:1455:SER:C	2.61	0.44
1:B:1461:GLN:H	1:B:1466:TYR:HE2	1.65	0.44
1:B:1548:SER:O	1:B:1550:PHE:N	2.50	0.44
1:C:2124:ILE:H	1:C:2124:ILE:HG12	1.61	0.44
1:C:2373:TYR:H	1:D:3372:GLN:HE22	1.65	0.44
1:C:2437:GLY:O	1:C:2438:ARG:C	2.60	0.44
1:C:2522:MET:HE3	1:C:2522:MET:HB2	1.80	0.44
1:D:3108:LEU:HA	1:D:3111:LEU:HD23	1.99	0.44
1:D:3156:ALA:C	1:D:3158:ASP:N	2.75	0.44
1:D:3352:LEU:HD12	1:D:3352:LEU:HA	1.81	0.44
1:D:3396:ASN:N	1:D:3396:ASN:HD22	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3535:MET:C	1:D:3537:ASN:N	2.76	0.44
1:A:59:CYS:HB3	1:A:64:PHE:O	2.18	0.44
1:A:112:ILE:O	1:A:115:TYR:HB3	2.17	0.44
1:A:219:GLY:HA2	1:A:458:MET:CE	2.46	0.44
1:A:380:GLU:O	1:A:381:PHE:C	2.61	0.44
1:A:507:LEU:HD22	1:A:522:MET:HB2	1.99	0.44
1:B:1113:MET:HA	1:B:1116:VAL:CG1	2.47	0.44
1:B:1178:LEU:HD22	1:B:1183:LEU:CD1	2.48	0.44
1:B:1482:THR:CG2	1:B:1509:VAL:HG12	2.48	0.44
1:C:2161:THR:O	1:C:2164:GLY:N	2.46	0.44
1:C:2269:THR:OG1	1:C:2271:VAL:HG23	2.17	0.44
1:C:2352:LEU:HG	1:C:2518:PHE:HE2	1.83	0.44
1:D:3444:VAL:O	1:D:3444:VAL:CG1	2.65	0.44
1:A:77:ARG:O	1:A:81:LEU:HG	2.18	0.44
1:A:137:LYS:NZ	1:B:1546:LYS:HE3	2.32	0.44
1:A:444:VAL:O	1:A:445:GLN:C	2.61	0.44
1:A:535:MET:O	1:A:537:ASN:N	2.51	0.44
1:B:1168:ASN:C	1:B:1170:GLU:H	2.26	0.44
1:B:1435:ALA:O	1:B:1510:GLU:O	2.36	0.44
1:C:2274:ILE:HD11	1:C:2290:GLU:HG3	2.00	0.44
1:C:2323:TRP:CE3	1:C:2327:GLN:HG2	2.52	0.44
1:C:2482:THR:HG22	6:C:4128:HOH:O	2.17	0.44
1:D:3105(D):ILE:CG2	1:D:3108:LEU:HD12	2.48	0.44
1:D:3405:LYS:H	1:D:3405:LYS:CE	2.30	0.44
1:A:112:ILE:HB	1:A:357:PHE:CE1	2.53	0.43
1:A:322:GLU:HB3	1:B:1052:PHE:CD2	2.52	0.43
1:A:352:LEU:HD12	1:A:352:LEU:HA	1.81	0.43
1:A:415:LEU:HD23	1:A:415:LEU:HA	1.85	0.43
1:A:467:ARG:NH1	1:A:520:GLU:OE1	2.44	0.43
1:A:543:GLN:O	1:B:1137:LYS:HE2	2.18	0.43
1:B:1160:PRO:HD2	1:B:1164:GLY:O	2.18	0.43
1:B:1295:VAL:C	1:B:1297:GLY:N	2.75	0.43
1:C:2105(C):ILE:O	1:C:2108:LEU:N	2.50	0.43
1:C:2112:ILE:HB	1:C:2357:PHE:CE1	2.53	0.43
1:C:2219:GLY:HA2	1:C:2458:MET:CE	2.46	0.43
1:D:3178:LEU:HD22	1:D:3183:LEU:CD1	2.48	0.43
1:D:3182:LEU:O	1:D:3438:ARG:CA	2.61	0.43
1:D:3184:ARG:CB	1:D:3439:ASN:HA	2.48	0.43
1:D:3381:PHE:HB2	1:D:3529:PHE:CD1	2.53	0.43
1:D:3450:ALA:C	1:D:3452:ILE:N	2.76	0.43
1:D:3491:LEU:C	1:D:3493:ALA:N	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3499:ASP:O	1:D:3501:MET:N	2.51	0.43
1:D:3524:GLU:OE2	1:D:3524:GLU:CA	2.65	0.43
1:D:3530:SER:C	1:D:3532:LYS:N	2.75	0.43
1:A:185:ARG:HE	1:A:438:ARG:HD3	1.83	0.43
1:A:248:LYS:N	1:A:325:ASP:OD1	2.51	0.43
1:A:461:GLN:H	1:A:466:TYR:HE2	1.65	0.43
1:B:1112:ILE:O	1:B:1116:VAL:HG13	2.18	0.43
1:B:1113:MET:HE3	1:B:1117:LEU:HD22	2.00	0.43
1:B:1304:ILE:HG22	1:B:1571:ASN:HD22	1.82	0.43
1:B:1442:ILE:N	1:B:1442:ILE:CD1	2.81	0.43
1:B:1524:GLU:OE2	1:B:1524:GLU:CA	2.65	0.43
1:C:2052:PHE:CD2	1:D:3322:GLU:HB3	2.53	0.43
1:C:2252:LEU:HD12	1:C:2309:HIS:CG	2.53	0.43
1:C:2273:MET:CE	1:C:2287:VAL:H	2.28	0.43
1:C:2440:VAL:O	1:C:2441:PRO:C	2.61	0.43
1:C:2557:LYS:HA	1:C:2560:ASN:HD22	1.82	0.43
1:D:3168:ASN:C	1:D:3170:GLU:N	2.72	0.43
1:D:3461:GLN:H	1:D:3466:TYR:HE2	1.66	0.43
1:D:3495:TYR:CE2	1:D:3502:GLU:HG3	2.51	0.43
1:D:3532:LYS:HB3	1:D:3533:GLY:H	1.70	0.43
1:A:61:ARG:HH12	1:B:1542:PRO:C	2.26	0.43
1:A:495:TYR:CE2	1:A:502:GLU:HG3	2.50	0.43
1:A:548:SER:C	1:A:550:PHE:N	2.76	0.43
1:B:1112:ILE:O	1:B:1115:TYR:HB3	2.18	0.43
1:B:1190:ASP:OD1	1:B:1192:GLN:HG3	2.18	0.43
1:B:1229:ASP:OD2	1:B:1231:ASN:N	2.51	0.43
1:B:1352:LEU:HD12	1:B:1352:LEU:HA	1.79	0.43
1:B:1383:THR:O	1:B:1384:LEU:C	2.61	0.43
1:C:2124:ILE:HG22	1:C:2125:ASP:N	2.33	0.43
1:C:2175:LYS:O	1:C:2179:GLU:HG3	2.19	0.43
1:C:2371:PHE:CE1	1:C:2532:LYS:HE2	2.53	0.43
1:C:2421:GLN:O	1:C:2422:PHE:C	2.60	0.43
1:D:3148:TYR:HD2	1:D:3219:GLY:O	2.01	0.43
1:D:3339:GLU:OE2	1:D:3558:ILE:CG2	2.66	0.43
1:D:3482:THR:CA	1:D:3511:LYS:HB2	2.48	0.43
1:A:161:THR:O	1:A:164:GLY:N	2.50	0.43
1:A:188:ILE:HB	1:A:439:ASN:ND2	2.34	0.43
1:B:1104:ASN:ND2	1:B:1358:LYS:HB2	2.33	0.43
1:B:1142:PHE:CD2	1:B:1142:PHE:C	2.96	0.43
1:B:1507:LEU:CD2	1:B:1522:MET:HB2	2.47	0.43
1:C:2304:ILE:HG22	1:C:2567:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2316:LEU:C	1:C:2318:GLN:N	2.76	0.43
1:C:2327:GLN:HB2	1:D:3136:TYR:HE2	1.83	0.43
1:C:2463:LEU:HD12	1:C:2503:LEU:HA	2.00	0.43
1:D:3185:ARG:HH21	1:D:3438:ARG:HD3	1.81	0.43
1:D:3249:ASP:HA	1:D:3328:LEU:CD1	2.48	0.43
1:D:3298:LEU:HD12	1:D:3298:LEU:HA	1.76	0.43
1:D:3454:GLN:O	1:D:3455:SER:C	2.61	0.43
1:D:3547:PRO:O	1:D:3552:GLY:N	2.48	0.43
1:A:107:PHE:CD2	1:A:107:PHE:N	2.86	0.43
1:A:114:LYS:O	1:A:115:TYR:C	2.61	0.43
1:A:216:ARG:HB3	1:A:220:PHE:HD1	1.73	0.43
1:A:249:ASP:HA	1:A:328:LEU:CD1	2.48	0.43
1:A:276:PRO:HG3	1:A:409:TYR:CD1	2.53	0.43
1:A:308:GLU:HA	1:A:308:GLU:OE2	2.18	0.43
1:A:380:GLU:HG3	1:A:460:TYR:CE2	2.52	0.43
1:A:389:PRO:HG2	1:A:434:VAL:HG22	2.01	0.43
1:A:449:LYS:O	1:A:450:ALA:C	2.61	0.43
1:A:455:SER:HA	1:A:460:TYR:CD1	2.53	0.43
1:A:457:GLU:C	1:A:459:LYS:N	2.77	0.43
1:B:1183:LEU:HD21	1:B:1445:GLN:CG	2.48	0.43
1:B:1241:GLN:OE1	1:B:1329:PHE:CZ	2.72	0.43
1:B:1252:LEU:HD12	1:B:1309:HIS:CG	2.53	0.43
1:B:1463:LEU:HD12	1:B:1503:LEU:HA	2.00	0.43
1:B:1548:SER:C	1:B:1550:PHE:N	2.76	0.43
1:C:2034:ASN:HB3	1:C:2037:CYS:SG	2.58	0.43
1:C:2240:ARG:HH12	1:C:2272:GLU:HB2	1.83	0.43
1:C:2427:THR:HG23	1:C:2578:THR:HG23	2.00	0.43
1:C:2465:GLU:OE2	1:C:2468:LYS:CE	2.66	0.43
6:C:4113:HOH:O	1:D:3140:GLU:HB2	2.18	0.43
1:D:3130:TYR:CD2	1:D:3135:GLY:O	2.72	0.43
1:D:3142:PHE:C	1:D:3142:PHE:CD2	2.94	0.43
1:D:3315:ILE:H	1:D:3315:ILE:HG13	1.52	0.43
1:D:3455:SER:HA	1:D:3460:TYR:CD1	2.53	0.43
1:D:3467:ARG:HH22	1:D:3520:GLU:CD	2.26	0.43
1:D:3490:GLU:O	1:D:3493:ALA:HB3	2.18	0.43
1:A:396:ASN:HD22	1:A:401:GLU:HG2	1.78	0.43
1:A:530:SER:C	1:A:532:LYS:N	2.76	0.43
1:B:1134:TYR:CD2	1:B:1136:TYR:HE1	2.37	0.43
1:B:1150:ARG:HD2	1:B:1380:GLU:OE1	2.17	0.43
1:B:1482:THR:CA	1:B:1511:LYS:HB2	2.48	0.43
1:B:1564:ILE:O	1:B:1568:ILE:CD1	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2168:ASN:C	1:C:2170:GLU:H	2.26	0.43
1:C:2312:VAL:O	1:C:2313:CYS:C	2.61	0.43
1:C:2341:ILE:HD12	1:C:2534:LEU:O	2.18	0.43
1:C:2462:SER:CB	1:C:2465:GLU:HG2	2.48	0.43
1:D:3124:ILE:H	1:D:3124:ILE:HG12	1.57	0.43
1:D:3240:ARG:HH12	1:D:3272:GLU:HB2	1.83	0.43
1:D:3368:ASN:OD1	1:D:3368:ASN:N	2.51	0.43
1:D:3522:MET:HE3	1:D:3522:MET:HB2	1.75	0.43
1:A:273:MET:CE	1:A:287:VAL:HG22	2.38	0.43
1:B:1130:TYR:CE2	1:B:1135:GLY:O	2.72	0.43
1:B:1136:TYR:CD1	1:B:1136:TYR:C	2.96	0.43
1:B:1155:VAL:HG12	1:B:1159:CYS:SG	2.58	0.43
1:B:1230:LEU:CG	1:B:1337:ILE:HG13	2.46	0.43
1:B:1320:HIS:CD2	1:B:1323:TRP:CE2	3.06	0.43
1:C:2383:THR:O	1:C:2384:LEU:C	2.61	0.43
1:D:3112:ILE:HB	1:D:3357:PHE:CE1	2.54	0.43
1:D:3456:ARG:NE	1:D:3502:GLU:OE2	2.51	0.43
1:D:3469:ARG:HA	1:D:3469:ARG:HD2	1.77	0.43
1:D:3564:ILE:O	1:D:3568:ILE:HD12	2.18	0.43
1:A:306:LEU:C	1:A:306:LEU:CD2	2.88	0.43
1:B:1065:TYR:HB2	1:B:1066:GLY:H	1.61	0.43
1:B:1089:VAL:O	1:B:1092:ILE:HG12	2.19	0.43
1:B:1096:PHE:O	1:B:1098:GLY:N	2.52	0.43
1:B:1124:ILE:HG22	1:B:1125:ASP:N	2.33	0.43
1:B:1184:ARG:HH12	1:B:1441:PRO:HG3	1.82	0.43
1:B:1298:LEU:O	1:B:1299:MET:C	2.61	0.43
1:B:1481:LEU:HD12	1:B:1481:LEU:O	2.19	0.43
1:B:1498:ILE:O	1:B:1501:MET:HB2	2.18	0.43
1:B:1533:GLY:C	5:B:1701:PGX:H203	2.44	0.43
1:B:1566:SER:HA	1:B:1569:CYS:CB	2.48	0.43
1:B:1577:PHE:CG	1:B:1578:THR:N	2.87	0.43
1:C:2108:LEU:HD23	1:C:2111:LEU:HD23	1.99	0.43
1:C:2444:VAL:O	1:C:2445:GLN:C	2.61	0.43
1:C:2546:LYS:HA	6:C:4145:HOH:O	2.19	0.43
1:C:2564:ILE:O	1:C:2568:ILE:CD1	2.66	0.43
1:D:3274:ILE:HD11	1:D:3290:GLU:HG3	2.00	0.43
1:D:3320:HIS:C	1:D:3322:GLU:N	2.76	0.43
1:D:3434:VAL:HG13	1:D:3508:LEU:CD2	2.49	0.43
1:D:3462:SER:CB	1:D:3465:GLU:HG2	2.48	0.43
1:D:3531:LEU:HD12	1:D:3531:LEU:HA	1.82	0.43
1:A:151:ALA:HB2	1:A:529:PHE:HZ	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ILE:HD12	1:A:291:VAL:CA	2.49	0.43
1:A:301:TYR:O	1:A:304:ILE:HB	2.18	0.43
1:A:327:GLN:CG	1:B:1136:TYR:CE2	3.02	0.43
1:A:403:SER:H	1:A:406:GLN:HB2	1.84	0.43
1:A:450:ALA:C	1:A:452:ILE:N	2.77	0.43
1:A:544:TYR:O	1:A:549:THR:OG1	2.33	0.43
1:B:1341:ILE:HD13	1:B:1534:LEU:HD12	2.00	0.43
1:B:1525:LEU:C	1:B:1528:PRO:HD2	2.43	0.43
1:C:2078:ILE:HD13	1:C:2078:ILE:N	2.33	0.43
1:C:2126:SER:HA	1:C:2127:PRO:C	2.42	0.43
1:C:2139:TRP:CZ3	1:D:3538:PRO:HG2	2.53	0.43
1:C:2243:LYS:O	1:C:2253:LYS:HE3	2.18	0.43
1:C:2301:TYR:O	1:C:2302:ALA:O	2.36	0.43
1:C:2380:GLU:O	1:C:2381:PHE:C	2.61	0.43
1:C:2386:HIS:HB2	1:C:2504:TYR:CE1	2.54	0.43
1:D:3074:PHE:O	1:D:3075:LEU:C	2.60	0.43
1:D:3372:GLN:O	1:D:3374:GLN:N	2.50	0.43
1:A:95:HIS:C	1:A:97:LYS:N	2.77	0.43
1:A:130:TYR:CE2	1:A:135:GLY:O	2.72	0.43
1:A:142:PHE:C	1:A:142:PHE:CD2	2.94	0.43
1:B:1078:ILE:HD13	1:B:1078:ILE:N	2.34	0.43
1:B:1120:ARG:O	1:B:1121:SER:C	2.61	0.43
1:B:1315:ILE:HD13	1:B:1558:ILE:HD11	1.99	0.43
1:B:1423:VAL:O	1:B:1424:GLU:C	2.62	0.43
1:B:1457:GLU:C	1:B:1459:LYS:N	2.77	0.43
1:B:1556:PHE:O	1:B:1557:LYS:C	2.62	0.43
1:C:2099:VAL:CA	1:C:2102:ILE:HD12	2.28	0.43
1:C:2173:ASP:OD2	1:C:2175:LYS:N	2.51	0.43
1:C:2499:ASP:C	1:C:2501:MET:N	2.75	0.43
1:D:3124:ILE:HG22	1:D:3125:ASP:N	2.34	0.43
1:D:3442:ILE:N	1:D:3442:ILE:CD1	2.81	0.43
1:D:3566:SER:HA	1:D:3569:CYS:CB	2.48	0.43
1:A:76:THR:O	1:A:79:LYS:HB2	2.19	0.42
1:A:185:ARG:NH2	1:A:438:ARG:NE	2.61	0.42
1:A:245:ARG:NH2	1:A:326:GLU:HA	2.33	0.42
1:A:262:TYR:HA	1:A:303:THR:HG23	2.00	0.42
1:A:427:THR:HG22	1:A:427:THR:O	2.19	0.42
1:A:427:THR:HG23	1:A:578:THR:HG23	2.01	0.42
1:A:437:GLY:O	1:A:438:ARG:C	2.62	0.42
1:B:1059:CYS:HB3	1:B:1064:PHE:O	2.18	0.42
1:B:1301:TYR:O	1:B:1304:ILE:HB	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1467:ARG:NH2	1:B:1520:GLU:OE1	2.49	0.42
1:B:1475:TYR:CD2	1:B:1480:GLU:HG2	2.54	0.42
1:C:2405:LYS:H	1:C:2405:LYS:CE	2.31	0.42
1:C:2535:MET:C	1:C:2537:ASN:N	2.77	0.42
1:D:3110:SER:O	1:D:3111:LEU:C	2.61	0.42
1:D:3112:ILE:O	1:D:3115:TYR:HB3	2.19	0.42
1:D:3267:LYS:HB3	6:D:4185:HOH:O	2.17	0.42
1:D:3306:LEU:C	1:D:3306:LEU:CD2	2.88	0.42
1:D:3383:THR:O	1:D:3384:LEU:C	2.61	0.42
1:D:3437:GLY:O	1:D:3438:ARG:C	2.62	0.42
1:A:142:PHE:O	1:A:376:ARG:NH2	2.40	0.42
1:A:202:ALA:HB2	1:A:348:TYR:CE1	2.55	0.42
1:A:218:PRO:CB	1:A:458:MET:HE3	2.43	0.42
1:A:229:ASP:OD2	1:A:231:ASN:N	2.50	0.42
1:A:243:LYS:O	1:A:253:LYS:HE3	2.19	0.42
1:A:478:PHE:O	1:A:482:THR:OG1	2.37	0.42
1:A:507:LEU:CD2	1:A:522:MET:HB2	2.49	0.42
1:A:531:LEU:HD12	1:A:531:LEU:HA	1.80	0.42
1:B:1073:GLU:O	1:B:1077:ARG:HG2	2.19	0.42
1:B:1427:THR:CG2	1:B:1578:THR:HA	2.48	0.42
1:C:2074:PHE:O	1:C:2075:LEU:C	2.61	0.42
1:C:2139:TRP:O	1:C:2140:GLU:C	2.62	0.42
1:C:2246:LEU:HG	1:C:2248:LYS:HB2	2.01	0.42
1:C:2280:PRO:HG2	1:C:2283:LEU:HG	2.01	0.42
1:C:2322:GLU:HA	6:C:4115:HOH:O	2.19	0.42
1:C:2462:SER:O	1:C:2465:GLU:HB2	2.19	0.42
1:D:3094:THR:HG22	1:D:3354:GLY:O	2.18	0.42
1:D:3114:LYS:O	1:D:3115:TYR:C	2.62	0.42
1:D:3150:ARG:HD2	1:D:3380:GLU:OE1	2.19	0.42
1:D:3160:PRO:HD2	1:D:3164:GLY:O	2.19	0.42
1:A:201:PHE:N	1:A:301:TYR:HE2	2.17	0.42
1:A:225:GLY:O	1:A:226:HIS:C	2.61	0.42
1:A:302:ALA:O	1:A:304:ILE:N	2.52	0.42
1:A:309:HIS:HD2	1:A:310:ASN:OD1	2.02	0.42
1:A:380:GLU:N	1:A:460:TYR:OH	2.52	0.42
1:A:481:LEU:HD12	1:A:481:LEU:O	2.19	0.42
1:B:1184:ARG:CB	1:B:1439:ASN:HA	2.47	0.42
1:B:1275:TYR:CE2	1:B:1284:GLN:CA	3.00	0.42
1:C:2073:GLU:O	1:C:2077:ARG:HG2	2.19	0.42
1:C:2274:ILE:HD12	1:C:2291:VAL:HA	2.01	0.42
1:C:2308:GLU:HA	1:C:2308:GLU:OE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2404:PHE:H	1:C:2404:PHE:HD1	1.67	0.42
1:C:2435:ALA:HB2	1:C:2518:PHE:HA	2.00	0.42
1:C:2487:MET:O	1:C:2488:ALA:C	2.62	0.42
1:C:2547:PRO:CB	1:C:2552:GLY:HA2	2.48	0.42
1:D:3107:PHE:CD2	1:D:3107:PHE:N	2.87	0.42
1:D:3181:VAL:HG12	1:D:3487:MET:CG	2.50	0.42
1:D:3320:HIS:C	1:D:3322:GLU:H	2.26	0.42
1:A:113:MET:O	1:A:116:VAL:HG13	2.20	0.42
1:A:136:TYR:CD1	1:A:136:TYR:C	2.97	0.42
1:A:198:PHE:O	1:A:199:ALA:C	2.61	0.42
1:A:469:ARG:HA	1:A:469:ARG:HD2	1.77	0.42
1:A:528:PRO:O	1:A:529:PHE:C	2.62	0.42
1:A:534:LEU:HD13	1:A:534:LEU:HA	1.90	0.42
1:B:1196:MET:HG2	1:B:1429:GLN:O	2.19	0.42
1:B:1261:VAL:H	1:B:1307:ARG:NH2	2.17	0.42
1:B:1510:GLU:CD	1:B:1519:GLY:HA3	2.44	0.42
1:C:2245:ARG:HD2	1:C:2329:PHE:CE1	2.54	0.42
1:C:2348:TYR:O	1:C:2349:VAL:C	2.62	0.42
1:C:2548:SER:O	1:C:2550:PHE:N	2.53	0.42
1:D:3202:ALA:HA	1:D:3348:TYR:HE1	1.83	0.42
1:D:3298:LEU:O	1:D:3299:MET:C	2.63	0.42
1:D:3323:TRP:CE3	1:D:3327:GLN:HG2	2.54	0.42
1:D:3379:SER:C	1:D:3460:TYR:OH	2.62	0.42
1:D:3395:PHE:O	1:D:3402:TYR:HD2	2.02	0.42
1:A:56:LYS:HA	6:A:4007:HOH:O	2.18	0.42
1:A:124:ILE:HG22	1:A:125:ASP:N	2.34	0.42
1:A:173:ASP:OD2	1:A:175:LYS:N	2.53	0.42
1:B:1094:THR:HG22	1:B:1354:GLY:O	2.20	0.42
1:B:1099:VAL:O	1:B:1102:ILE:HB	2.19	0.42
1:B:1162:PRO:HB2	1:B:1171:LEU:HD21	2.01	0.42
1:B:1174:SER:O	1:B:1175:LYS:C	2.63	0.42
1:B:1190:ASP:OD2	1:B:1192:GLN:HB2	2.18	0.42
1:B:1269:THR:C	1:B:1271:VAL:H	2.26	0.42
1:B:1429:GLN:O	1:B:1429:GLN:HG2	2.18	0.42
1:C:2095:HIS:O	1:C:2100:TRP:HD1	2.02	0.42
1:C:2500:VAL:O	1:C:2500:VAL:HG12	2.19	0.42
1:C:2531:LEU:HD12	1:C:2531:LEU:HA	1.80	0.42
1:C:2556:PHE:O	1:C:2557:LYS:C	2.63	0.42
1:D:3128:PRO:HG3	1:D:3376:ARG:NH1	2.34	0.42
1:D:3155:VAL:HG12	1:D:3159:CYS:SG	2.59	0.42
1:D:3357:PHE:HE2	1:D:3359:LEU:HD23	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3469:ARG:HD2	1:D:3469:ARG:C	2.44	0.42
1:D:3568:ILE:HG23	1:D:3572:VAL:CG2	2.48	0.42
1:A:344:VAL:HG12	1:A:345:ILE:N	2.34	0.42
1:A:404:PHE:N	1:A:404:PHE:HD1	2.18	0.42
1:B:1105(B):ILE:O	1:B:1108:LEU:HB2	2.19	0.42
1:B:1182:LEU:O	1:B:1438:ARG:CA	2.62	0.42
1:B:1205:PHE:CZ	1:B:1344:VAL:HG21	2.54	0.42
1:B:1219:GLY:HA2	1:B:1458:MET:CE	2.49	0.42
1:B:1245:ARG:O	1:B:1253:LYS:HG3	2.19	0.42
1:B:1396:ASN:N	1:B:1396:ASN:HD22	2.17	0.42
1:C:2036:CYS:O	1:C:2037:CYS:C	2.63	0.42
1:C:2150:ARG:HD2	1:C:2380:GLU:OE1	2.19	0.42
1:C:2379:SER:C	1:C:2460:TYR:OH	2.62	0.42
1:C:2390:LEU:HD21	1:C:2517:ILE:HD11	2.01	0.42
1:C:2452:ILE:O	1:C:2453:ASP:C	2.62	0.42
1:C:2462:SER:HB3	1:C:2465:GLU:HG2	2.02	0.42
1:C:2481:LEU:HD12	1:C:2510:GLU:HA	2.02	0.42
1:C:2521:THR:HG22	1:C:2522:MET:N	2.33	0.42
1:D:3168:ASN:C	1:D:3170:GLU:H	2.27	0.42
1:D:3184:ARG:CD	1:D:3187:PHE:HA	2.37	0.42
1:D:3185:ARG:HE	1:D:3438:ARG:HD3	1.85	0.42
1:D:3454:GLN:C	1:D:3456:ARG:N	2.77	0.42
1:D:3467:ARG:NH2	1:D:3520:GLU:OE1	2.52	0.42
1:D:3470:PHE:CD2	1:D:3470:PHE:N	2.87	0.42
1:A:92:ILE:HG12	1:A:92:ILE:H	1.34	0.42
1:A:95:HIS:O	1:A:100:TRP:CD1	2.73	0.42
1:A:151:ALA:HB2	1:A:529:PHE:CZ	2.55	0.42
1:A:155:VAL:HG12	1:A:159:CYS:SG	2.59	0.42
1:A:404:PHE:HD1	1:A:404:PHE:H	1.67	0.42
1:A:482:THR:CG2	1:A:509:VAL:HG12	2.49	0.42
1:B:1121:SER:C	1:B:1123:LEU:N	2.78	0.42
1:B:1198:PHE:HB2	1:B:1580:PHE:HB3	2.00	0.42
1:B:1230:LEU:HD11	1:B:1337:ILE:HA	2.02	0.42
1:B:1269:THR:C	1:B:1271:VAL:N	2.76	0.42
1:B:1531:LEU:HD12	1:B:1531:LEU:HA	1.79	0.42
1:C:2391:LEU:HD13	1:C:2404:PHE:HE2	1.84	0.42
1:C:2444:VAL:O	1:C:2444:VAL:HG12	2.18	0.42
1:C:2467:ARG:O	1:C:2472:LEU:HB2	2.19	0.42
1:C:2564:ILE:O	1:C:2568:ILE:HD12	2.19	0.42
1:D:3113:MET:HE2	1:D:3117:LEU:HD22	2.00	0.42
1:D:3136:TYR:HD1	1:D:3136:TYR:C	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3287:VAL:O	1:D:3288:GLY:C	2.62	0.42
1:D:3467:ARG:O	1:D:3472:LEU:HB2	2.19	0.42
1:B:1099:VAL:CA	1:B:1102:ILE:HD12	2.29	0.42
1:B:1112:ILE:HB	1:B:1357:PHE:CE1	2.55	0.42
1:B:1273:MET:CE	1:B:1287:VAL:H	2.28	0.42
1:B:1274:ILE:HD12	1:B:1291:VAL:HA	2.01	0.42
1:B:1404:PHE:N	1:B:1404:PHE:CD1	2.88	0.42
1:C:2302:ALA:O	1:C:2304:ILE:N	2.52	0.42
1:C:2348:TYR:HD2	1:C:2349:VAL:N	2.18	0.42
1:C:2532:LYS:HB3	1:C:2533:GLY:H	1.68	0.42
1:C:2564:ILE:HG23	1:C:2565:GLN:N	2.35	0.42
1:D:3141:ALA:O	1:D:3143:SER:N	2.53	0.42
1:D:3530:SER:O	1:D:3532:LYS:N	2.52	0.42
1:A:211:LYS:O	1:A:212:THR:C	2.61	0.42
1:A:523:VAL:HG12	1:A:524:GLU:N	2.33	0.42
1:A:532:LYS:O	1:A:535:MET:N	2.53	0.42
1:B:1389:PRO:CB	1:B:1434:VAL:HA	2.49	0.42
1:B:1532:LYS:O	1:B:1533:GLY:C	2.63	0.42
1:B:1568:ILE:HG23	1:B:1572:VAL:CG2	2.50	0.42
1:C:2113:MET:O	1:C:2117:LEU:HD22	2.20	0.42
1:C:2197:MET:HG3	1:C:2578:THR:HG21	2.01	0.42
1:C:2230:LEU:CG	1:C:2337:ILE:HG13	2.44	0.42
1:C:2320:HIS:HE1	1:D:3048:MET:HE3	1.84	0.42
1:D:3074:PHE:O	1:D:3077:ARG:N	2.53	0.42
1:D:3120:ARG:O	1:D:3121:SER:C	2.63	0.42
1:D:3174:SER:O	1:D:3175:LYS:C	2.62	0.42
1:D:3197:MET:HE1	1:D:3300:MET:CE	2.49	0.42
1:D:3256:VAL:HA	1:D:3260:GLU:O	2.20	0.42
1:D:3295:VAL:HB	1:D:3298:LEU:HB2	2.02	0.42
1:D:3384:LEU:HB2	5:D:3701:PGX:O3	2.19	0.42
1:D:3404:PHE:N	1:D:3404:PHE:HD1	2.17	0.42
1:D:3433:ARG:HH21	1:D:3512:PRO:CB	2.33	0.42
1:D:3520:GLU:O	1:D:3521:THR:C	2.63	0.42
1:D:3564:ILE:HG22	6:D:4157:HOH:O	2.19	0.42
1:D:3577:PHE:CG	1:D:3578:THR:N	2.87	0.42
1:A:116:VAL:CG2	1:A:117:LEU:N	2.82	0.42
1:A:160:PRO:HD2	1:A:164:GLY:O	2.20	0.42
1:A:185:ARG:HH21	1:A:438:ARG:HD3	1.85	0.42
1:A:234:TYR:HB2	1:A:333:ARG:NH1	2.35	0.42
1:A:315:ILE:H	1:A:315:ILE:HG13	1.56	0.42
1:A:350:GLN:NE2	1:A:359:LEU:H	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:MET:O	1:A:488:ALA:C	2.61	0.42
1:A:487:MET:O	1:A:490:GLU:HB3	2.20	0.42
1:A:535:MET:C	1:A:537:ASN:N	2.78	0.42
1:C:2247:PHE:HA	1:C:2325:ASP:CG	2.44	0.42
1:C:2331:THR:O	1:C:2332:SER:C	2.63	0.42
1:C:2404:PHE:CD1	1:C:2404:PHE:N	2.85	0.42
1:C:2507:LEU:CD2	1:C:2522:MET:HB2	2.50	0.42
1:C:2538:PRO:HG2	1:D:3139:TRP:HZ3	1.85	0.42
1:C:2553:GLU:OE1	1:C:2553:GLU:CA	2.62	0.42
1:D:3105(D):ILE:CB	1:D:3108:LEU:HD12	2.49	0.42
1:D:3231:ASN:O	1:D:3235:GLY:N	2.52	0.42
1:D:3295:VAL:HG12	1:D:3298:LEU:H	1.85	0.42
1:D:3318:GLN:OE1	1:D:3318:GLN:HA	2.19	0.42
1:D:3357:PHE:CD2	1:D:3359:LEU:HD23	2.55	0.42
1:D:3427:THR:HG23	1:D:3578:THR:HG23	2.02	0.42
1:D:3481:LEU:O	1:D:3511:LYS:N	2.53	0.42
1:D:3556:PHE:O	1:D:3557:LYS:C	2.62	0.42
1:A:454:GLN:O	1:A:456:ARG:N	2.52	0.41
1:B:1141:ALA:O	1:B:1143:SER:N	2.52	0.41
1:B:1371:PHE:CE1	1:B:1532:LYS:HE2	2.55	0.41
1:B:1465:GLU:OE2	1:B:1465:GLU:CA	2.68	0.41
1:C:2249:ASP:HA	1:C:2328:LEU:CD1	2.50	0.41
1:C:2262:TYR:HA	1:C:2303:THR:HG23	2.02	0.41
1:C:2530:SER:O	1:C:2532:LYS:N	2.52	0.41
1:D:3073:GLU:O	1:D:3076:THR:HB	2.20	0.41
1:D:3092:ILE:HG12	1:D:3092:ILE:H	1.36	0.41
1:D:3099:VAL:O	1:D:3102:ILE:HB	2.20	0.41
1:D:3229:ASP:OD2	1:D:3231:ASN:N	2.53	0.41
1:D:3345:ILE:CG1	1:D:3534:LEU:HG	2.50	0.41
1:D:3548:SER:O	1:D:3550:PHE:N	2.53	0.41
1:A:403:SER:OG	1:A:405:LYS:HD2	2.20	0.41
1:A:444:VAL:O	1:A:444:VAL:HG12	2.20	0.41
1:B:1099:VAL:HA	1:B:1102:ILE:CD1	2.29	0.41
1:B:1366:LEU:C	1:B:1368:ASN:H	2.28	0.41
1:B:1368:ASN:OD1	1:B:1368:ASN:N	2.53	0.41
1:B:1535:MET:O	1:B:1540:CYS:HB2	2.20	0.41
1:B:1557:LYS:HA	1:B:1560:ASN:HD22	1.85	0.41
1:C:2064:PHE:CE2	1:C:2072:PRO:HB3	2.54	0.41
1:D:3274:ILE:HD12	1:D:3291:VAL:CA	2.49	0.41
1:A:372:GLN:O	1:A:374:GLN:N	2.51	0.41
1:A:510:GLU:CD	1:A:521:THR:HB	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:LEU:O	1:A:535:MET:HB2	2.21	0.41
1:B:1095:HIS:C	1:B:1097:LYS:N	2.77	0.41
1:B:1136:TYR:HB2	6:B:4080:HOH:O	2.20	0.41
1:B:1196:MET:HE2	1:B:1431:ALA:HB2	2.01	0.41
1:B:1202:ALA:HA	1:B:1348:TYR:HE1	1.85	0.41
1:B:1275:TYR:HE2	1:B:1284:GLN:CA	2.34	0.41
1:B:1301:TYR:O	1:B:1302:ALA:O	2.38	0.41
1:C:2184:ARG:NE	1:C:2439:ASN:OD1	2.48	0.41
1:C:2350:GLN:NE2	1:C:2359:LEU:H	2.17	0.41
1:C:2404:PHE:HD1	1:C:2404:PHE:N	2.18	0.41
1:C:2504:TYR:HB3	1:C:2505:PRO:CD	2.45	0.41
1:D:3058:ASP:OD2	1:D:3060:THR:OG1	2.34	0.41
1:D:3113:MET:HE3	1:D:3117:LEU:HD22	2.02	0.41
1:D:3295:VAL:C	1:D:3297:GLY:N	2.77	0.41
1:D:3316:LEU:O	1:D:3319:GLU:N	2.52	0.41
1:A:108:LEU:HA	1:A:111:LEU:HD23	2.02	0.41
1:A:274:ILE:HD11	1:A:290:GLU:HG3	2.03	0.41
1:A:295:VAL:HG12	1:A:297:GLY:H	1.85	0.41
1:A:305:TRP:O	1:A:306:LEU:C	2.64	0.41
1:A:352:LEU:HG	1:A:518:PHE:HE2	1.86	0.41
1:A:361:PHE:HD1	1:A:535:MET:HE1	1.85	0.41
1:A:386:HIS:HD2	1:A:451:SER:HB3	1.85	0.41
1:A:394:THR:O	1:A:429:GLN:NE2	2.47	0.41
1:A:467:ARG:HH22	1:A:520:GLU:CD	2.29	0.41
1:A:532:LYS:HB3	1:A:533:GLY:H	1.70	0.41
1:B:1114:LYS:O	1:B:1115:TYR:C	2.64	0.41
1:B:1347:ASP:OD2	1:B:1564:ILE:HG22	2.20	0.41
1:B:1427:THR:HG23	1:B:1578:THR:HG23	2.02	0.41
1:B:1517:ILE:O	1:B:1517:ILE:HG13	2.20	0.41
1:B:1523:VAL:HG12	1:B:1524:GLU:N	2.36	0.41
1:B:1532:LYS:O	1:B:1535:MET:N	2.53	0.41
1:C:2074:PHE:O	1:C:2077:ARG:N	2.53	0.41
1:C:2096:PHE:O	1:C:2098:GLY:N	2.53	0.41
1:C:2120:ARG:HH11	1:C:2527:ALA:HB1	1.83	0.41
1:C:2151:ALA:HB2	1:C:2529:PHE:CZ	2.53	0.41
1:C:2275:TYR:CE2	1:C:2284:GLN:CA	3.03	0.41
1:C:2275:TYR:HE2	1:C:2284:GLN:HA	1.84	0.41
1:C:2423:VAL:O	1:C:2424:GLU:C	2.63	0.41
1:C:2563:SER:C	1:C:2565:GLN:N	2.72	0.41
1:D:3059:CYS:HA	1:D:3062:THR:HG21	2.01	0.41
1:D:3214:HIS:O	1:D:3215:LYS:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3404:PHE:HD1	1:D:3404:PHE:H	1.68	0.41
1:A:50:THR:CG2	1:A:56:LYS:CB	2.98	0.41
1:A:73:GLU:O	1:A:77:ARG:HG2	2.20	0.41
1:A:91:TYR:CD2	1:A:91:TYR:C	2.99	0.41
1:A:96:PHE:O	1:A:97:LYS:C	2.63	0.41
1:A:103:VAL:O	1:A:105:ASN:N	2.53	0.41
1:B:1074:PHE:O	1:B:1075:LEU:C	2.61	0.41
1:B:1246:LEU:HG	1:B:1248:LYS:HB2	2.02	0.41
1:B:1295:VAL:HG12	1:B:1298:LEU:H	1.85	0.41
1:B:1308:GLU:OE2	1:B:1311:ARG:HD3	2.21	0.41
1:B:1320:HIS:C	1:B:1322:GLU:N	2.78	0.41
1:B:1383:THR:O	1:B:1385:TYR:N	2.54	0.41
1:B:1464:ASN:HD21	1:B:1475:TYR:N	2.19	0.41
1:B:1530:SER:O	1:B:1532:LYS:N	2.53	0.41
1:C:2139:TRP:HZ3	1:D:3538:PRO:HG2	1.86	0.41
1:C:2185:ARG:HH21	1:C:2438:ARG:HD3	1.85	0.41
1:C:2309:HIS:HD2	1:C:2310:ASN:OD1	2.03	0.41
1:C:2389:PRO:CB	1:C:2434:VAL:HA	2.51	0.41
1:D:3148:TYR:CZ	1:D:3221:THR:HB	2.55	0.41
1:D:3196:MET:O	1:D:3197:MET:C	2.63	0.41
1:D:3274:ILE:HD12	1:D:3291:VAL:HG23	2.01	0.41
1:D:3380:GLU:N	1:D:3460:TYR:OH	2.53	0.41
1:D:3394:THR:O	1:D:3429:GLN:NE2	2.46	0.41
1:A:39:ASN:N	1:A:39:ASN:ND2	2.68	0.41
1:A:327:GLN:HG3	1:B:1136:TYR:CE2	2.55	0.41
1:B:1218:PRO:C	1:B:1458:MET:CE	2.94	0.41
1:B:1380:GLU:O	1:B:1381:PHE:C	2.63	0.41
1:B:1434:VAL:HG13	1:B:1508:LEU:CD2	2.50	0.41
1:B:1469:ARG:C	1:B:1469:ARG:HD2	2.44	0.41
1:B:1499:ASP:C	1:B:1501:MET:N	2.78	0.41
1:C:2120:ARG:O	1:C:2121:SER:C	2.63	0.41
1:C:2186:GLU:N	6:C:4100:HOH:O	2.52	0.41
1:C:2295:VAL:HB	1:C:2298:LEU:HB2	2.03	0.41
1:C:2389:PRO:HB2	1:C:2434:VAL:HA	2.03	0.41
1:D:3112:ILE:O	1:D:3116:VAL:HG13	2.21	0.41
1:D:3123:LEU:O	1:D:3469:ARG:NH2	2.54	0.41
1:D:3377:ILE:HA	6:D:4180:HOH:O	2.20	0.41
1:D:3440:VAL:O	1:D:3441:PRO:C	2.62	0.41
1:D:3450:ALA:O	1:D:3454:GLN:HG3	2.21	0.41
1:D:3507:LEU:CD2	1:D:3522:MET:HB2	2.51	0.41
1:A:95:HIS:O	1:A:100:TRP:HD1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:LYS:HD3	1:B:1549:THR:HG23	2.02	0.41
1:A:178:LEU:HD22	1:A:183:LEU:CD1	2.50	0.41
1:A:197:MET:HG3	1:A:578:THR:HG21	2.03	0.41
1:A:379:SER:C	1:A:460:TYR:OH	2.63	0.41
1:A:499:ASP:C	1:A:501:MET:N	2.78	0.41
1:A:514:PRO:O	1:A:515:ASP:CB	2.66	0.41
1:A:542:PRO:C	1:A:544:TYR:H	2.28	0.41
1:B:1481:LEU:O	1:B:1511:LYS:N	2.53	0.41
1:C:2454:GLN:O	1:C:2456:ARG:N	2.53	0.41
1:C:2533:GLY:C	5:C:2701:PGX:H203	2.45	0.41
1:D:3105(D):ILE:CG2	1:D:3108:LEU:HB2	2.51	0.41
1:D:3190:ASP:OD1	1:D:3192:GLN:HG3	2.20	0.41
1:D:3423:VAL:O	1:D:3424:GLU:C	2.63	0.41
1:A:184:ARG:NH2	1:A:391:LEU:O	2.48	0.41
1:A:516:ALA:HB1	6:A:4048:HOH:O	2.21	0.41
1:B:1060:THR:C	1:B:1062:THR:N	2.79	0.41
1:B:1198:PHE:O	1:B:1199:ALA:C	2.62	0.41
1:B:1309:HIS:O	1:B:1312:VAL:N	2.53	0.41
1:B:1316:LEU:C	1:B:1318:GLN:N	2.78	0.41
1:C:2065:TYR:N	1:C:2071:THR:O	2.49	0.41
1:C:2106:PRO:O	1:C:2107:PHE:C	2.64	0.41
1:C:2185:ARG:HE	1:C:2438:ARG:HD3	1.86	0.41
1:C:2372:GLN:O	1:C:2374:GLN:N	2.50	0.41
1:C:2415:LEU:HD23	1:C:2415:LEU:HA	1.83	0.41
1:D:3243:LYS:O	1:D:3253:LYS:HE3	2.21	0.41
1:D:3462:SER:HB3	1:D:3465:GLU:HG2	2.03	0.41
1:D:3486:GLU:HB3	1:D:3487:MET:H	1.73	0.41
1:D:3514:PRO:O	1:D:3515:ASP:CB	2.69	0.41
1:D:3535:MET:O	1:D:3540:CYS:HB2	2.21	0.41
1:A:56:LYS:HG3	1:A:57:CYS:N	2.35	0.41
1:A:117:LEU:HD13	1:A:117:LEU:HA	1.81	0.41
1:A:132:VAL:HG23	6:A:4038:HOH:O	2.21	0.41
1:A:156:ALA:HB3	1:A:159:CYS:SG	2.61	0.41
1:A:180:LYS:HD2	1:A:490:GLU:CD	2.45	0.41
1:A:298:LEU:O	1:A:299:MET:C	2.63	0.41
1:A:368:ASN:OD1	1:A:368:ASN:N	2.54	0.41
1:A:423:VAL:O	1:A:424:GLU:C	2.64	0.41
1:A:464:ASN:HD21	1:A:475:TYR:N	2.18	0.41
1:A:547:PRO:C	1:A:552:GLY:HA2	2.46	0.41
1:A:553:GLU:OE1	1:A:553:GLU:CA	2.60	0.41
1:B:1058:ASP:OD2	1:B:1060:THR:OG1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1132:VAL:HG21	1:B:1219:GLY:HA3	2.03	0.41
1:B:1320:HIS:C	1:B:1322:GLU:H	2.28	0.41
1:C:2039:ASN:N	1:C:2039:ASN:ND2	2.69	0.41
1:C:2089:VAL:O	1:C:2092:ILE:HG12	2.21	0.41
1:C:2091:TYR:CD2	1:C:2091:TYR:C	2.99	0.41
1:C:2096:PHE:O	1:C:2099:VAL:N	2.54	0.41
1:C:2121:SER:C	1:C:2123:LEU:N	2.77	0.41
1:C:2162:PRO:HB2	1:C:2171:LEU:CD2	2.51	0.41
1:C:2185:ARG:NH2	1:C:2438:ARG:NE	2.63	0.41
1:C:2269:THR:C	1:C:2271:VAL:N	2.78	0.41
1:C:2341:ILE:HD13	1:C:2534:LEU:CD1	2.50	0.41
1:C:2347:ASP:OD2	1:C:2564:ILE:HG22	2.21	0.41
1:C:2366:LEU:HA	1:C:2369:GLN:CG	2.51	0.41
1:C:2449:LYS:HA	1:C:2452:ILE:CD1	2.44	0.41
1:C:2482:THR:CG2	1:C:2509:VAL:HG12	2.51	0.41
1:D:3091:TYR:C	1:D:3091:TYR:CD2	2.99	0.41
1:D:3112:ILE:O	1:D:3113:MET:C	2.64	0.41
1:D:3124:ILE:HG22	1:D:3125:ASP:H	1.85	0.41
1:D:3152:LEU:HD12	1:D:3466:TYR:CD1	2.56	0.41
1:D:3175:LYS:O	1:D:3179:GLU:HG3	2.21	0.41
1:D:3231:ASN:OD1	1:D:3231:ASN:C	2.63	0.41
1:D:3366:LEU:C	1:D:3368:ASN:H	2.29	0.41
1:D:3429:GLN:HG2	1:D:3429:GLN:O	2.20	0.41
1:D:3479:GLU:O	1:D:3483:GLY:N	2.49	0.41
1:D:3504:TYR:O	1:D:3507:LEU:HB2	2.20	0.41
1:A:388:HIS:O	1:A:389:PRO:C	2.64	0.41
1:A:428:ARG:O	1:A:582:VAL:HG21	2.21	0.41
1:A:486:GLU:HB3	1:A:487:MET:H	1.70	0.41
1:B:1247:PHE:HA	1:B:1325:ASP:CG	2.46	0.41
1:B:1249:ASP:HA	1:B:1328:LEU:CD1	2.50	0.41
1:B:1379:SER:C	1:B:1460:TYR:OH	2.63	0.41
1:B:1454:GLN:C	1:B:1456:ARG:N	2.79	0.41
1:B:1470:PHE:CD2	1:B:1470:PHE:N	2.88	0.41
1:B:1522:MET:HE3	1:B:1522:MET:HB2	1.85	0.41
1:C:2142:PHE:CD2	1:C:2142:PHE:C	2.98	0.41
1:C:2216:ARG:HB3	1:C:2220:PHE:HD1	1.76	0.41
1:C:2256:VAL:HA	1:C:2260:GLU:O	2.21	0.41
1:C:2295:VAL:HG12	1:C:2298:LEU:H	1.86	0.41
1:C:2465:GLU:OE2	1:C:2468:LYS:HE2	2.21	0.41
1:D:3073:GLU:O	1:D:3077:ARG:HG2	2.21	0.41
1:D:3105(D):ILE:HG22	1:D:3108:LEU:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3150:ARG:HD2	1:D:3380:GLU:CD	2.46	0.41
1:D:3252:LEU:HD12	1:D:3309:HIS:CG	2.56	0.41
1:D:3280:PRO:HG2	1:D:3283:LEU:HG	2.03	0.41
1:D:3444:VAL:O	1:D:3444:VAL:HG12	2.21	0.41
1:A:105(A):ILE:O	1:A:108:LEU:N	2.55	0.40
1:A:113:MET:O	1:A:116:VAL:HG22	2.21	0.40
1:A:162:PRO:HB2	1:A:171:LEU:CD2	2.51	0.40
1:A:268:ASP:OD1	1:A:268:ASP:N	2.54	0.40
1:A:295:VAL:HG12	1:A:298:LEU:H	1.86	0.40
1:A:530:SER:O	1:A:532:LYS:N	2.54	0.40
1:A:556:PHE:O	1:A:557:LYS:C	2.64	0.40
1:B:1268:ASP:OD1	1:B:1268:ASP:N	2.53	0.40
1:B:1306:LEU:C	1:B:1306:LEU:CD2	2.94	0.40
1:B:1339:GLU:O	1:B:1340:THR:C	2.65	0.40
1:C:2076:THR:O	1:C:2079:LYS:HB2	2.21	0.40
1:C:2108:LEU:O	1:C:2109:ARG:C	2.64	0.40
1:C:2128:PRO:HG3	1:C:2376:ARG:HH11	1.86	0.40
1:C:2300:MET:O	1:C:2304:ILE:HG13	2.21	0.40
1:C:2491:LEU:C	1:C:2493:ALA:N	2.76	0.40
1:C:2498:ILE:CG2	1:C:2499:ASP:N	2.83	0.40
1:C:2534:LEU:HD22	5:C:2701:PGX:C18	2.43	0.40
1:D:3205:PHE:CZ	1:D:3344:VAL:HG21	2.56	0.40
1:D:3247:PHE:HA	1:D:3325:ASP:CG	2.46	0.40
1:D:3436:GLY:HA2	1:D:3512:PRO:HG2	2.02	0.40
1:D:3475:TYR:CD1	1:D:3481:LEU:HB2	2.56	0.40
1:A:132:VAL:HG21	1:A:219:GLY:HA3	2.03	0.40
1:A:341:ILE:HD13	1:A:534:LEU:CD1	2.51	0.40
1:A:389:PRO:HB2	1:A:434:VAL:HA	2.02	0.40
1:A:454:GLN:CA	1:A:457:GLU:HG3	2.51	0.40
1:B:1036:CYS:O	1:B:1037:CYS:C	2.63	0.40
1:B:1209:PHE:CZ	5:B:1701:PGX:H192	2.56	0.40
1:B:1302:ALA:O	1:B:1304:ILE:N	2.54	0.40
1:B:1320:HIS:CD2	1:B:1323:TRP:CZ2	3.09	0.40
1:B:1388:HIS:NE2	1:B:1447:VAL:CG1	2.85	0.40
1:B:1407:PHE:HD1	1:B:1413:ILE:HD13	1.87	0.40
1:B:1452:ILE:O	1:B:1453:ASP:C	2.65	0.40
1:C:2148:TYR:HD2	1:C:2219:GLY:O	2.04	0.40
1:C:2280:PRO:HG2	1:C:2283:LEU:CG	2.52	0.40
1:C:2454:GLN:C	1:C:2456:ARG:N	2.74	0.40
1:C:2470:PHE:CD2	1:C:2470:PHE:N	2.88	0.40
1:C:2503:LEU:HG	1:C:2507:LEU:CD1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3103:VAL:HG12	1:D:3104:ASN:N	2.37	0.40
1:D:3402:TYR:OH	1:D:3417:HIS:CE1	2.74	0.40
1:A:65:TYR:N	1:A:71:THR:O	2.52	0.40
1:A:204:HIS:CD2	1:A:292:PHE:CE2	3.09	0.40
1:A:295:VAL:C	1:A:297:GLY:N	2.77	0.40
1:A:369:GLN:O	1:A:371:PHE:N	2.54	0.40
1:A:481:LEU:O	1:A:511:LYS:N	2.55	0.40
1:A:522:MET:HE3	1:A:522:MET:HB2	1.87	0.40
1:B:1196:MET:O	1:B:1197:MET:C	2.64	0.40
1:B:1245:ARG:NH2	1:B:1326:GLU:HA	2.37	0.40
1:B:1274:ILE:HD11	1:B:1290:GLU:HG3	2.04	0.40
1:B:1433:ARG:HH21	1:B:1512:PRO:CB	2.35	0.40
1:C:2085:THR:O	1:C:2088:THR:HB	2.21	0.40
1:C:2093:LEU:HB3	1:C:2355:TYR:CD1	2.56	0.40
1:C:2162:PRO:HB2	1:C:2171:LEU:HD21	2.04	0.40
1:C:2308:GLU:OE2	1:C:2311:ARG:HD3	2.21	0.40
1:C:2428:ARG:O	1:C:2582:VAL:HG21	2.22	0.40
1:C:2481:LEU:HD12	1:C:2481:LEU:O	2.21	0.40
1:D:3050:THR:CG2	1:D:3056:LYS:CB	2.99	0.40
1:D:3427:THR:CG2	1:D:3578:THR:HA	2.50	0.40
1:D:3498:ILE:O	1:D:3501:MET:HB2	2.21	0.40
1:D:3548:SER:C	1:D:3550:PHE:N	2.77	0.40
1:A:47:CYS:SG	1:A:55:TYR:HD1	2.44	0.40
1:A:75:LEU:HD12	1:A:75:LEU:O	2.21	0.40
1:A:223:GLY:HA2	1:A:236:GLU:OE1	2.21	0.40
1:A:274:ILE:HD12	1:A:291:VAL:HG23	2.04	0.40
1:A:304:ILE:HG22	1:A:571:ASN:HD22	1.86	0.40
1:B:1112:ILE:O	1:B:1115:TYR:N	2.54	0.40
1:B:1214:HIS:O	1:B:1215:LYS:C	2.65	0.40
1:B:1262:TYR:HA	1:B:1303:THR:HG23	2.02	0.40
1:B:1295:VAL:O	1:B:1297:GLY:N	2.55	0.40
1:B:1357:PHE:CD2	1:B:1359:LEU:HD23	2.56	0.40
1:B:1450:ALA:O	1:B:1452:ILE:N	2.54	0.40
1:B:1514:PRO:O	1:B:1515:ASP:CB	2.70	0.40
1:C:2156:ALA:C	1:C:2158:ASP:H	2.29	0.40
1:C:2301:TYR:O	1:C:2304:ILE:HB	2.21	0.40
1:C:2449:LYS:O	1:C:2450:ALA:C	2.64	0.40
1:C:2548:SER:C	1:C:2550:PHE:N	2.77	0.40
1:D:3060:THR:C	1:D:3062:THR:N	2.78	0.40
1:D:3132:VAL:HG21	1:D:3219:GLY:HA3	2.03	0.40
1:D:3201:PHE:N	1:D:3301:TYR:HE2	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3225:GLY:O	1:D:3226:HIS:C	2.63	0.40
1:D:3383:THR:O	1:D:3385:TYR:N	2.54	0.40
1:D:3464:ASN:HD21	1:D:3475:TYR:N	2.19	0.40
1:A:99:VAL:O	1:A:102:ILE:HB	2.21	0.40
1:A:139:TRP:O	1:A:140:GLU:C	2.64	0.40
1:A:142:PHE:CE2	1:B:1538:PRO:HG3	2.56	0.40
1:A:231:ASN:O	1:A:235:GLY:N	2.55	0.40
1:A:245:ARG:O	1:A:253:LYS:HG3	2.21	0.40
1:A:295:VAL:O	1:A:298:LEU:N	2.55	0.40
1:A:481:LEU:HD12	1:A:510:GLU:HA	2.03	0.40
1:A:498:ILE:CG2	1:A:499:ASP:N	2.84	0.40
1:B:1034:ASN:HA	1:B:1035:PRO:HD2	1.86	0.40
1:B:1150:ARG:HD2	1:B:1380:GLU:CD	2.47	0.40
1:B:1238:LEU:O	1:B:1239:ASP:C	2.64	0.40
1:B:1348:TYR:HD2	1:B:1349:VAL:N	2.20	0.40
1:B:1531:LEU:O	1:B:1535:MET:HB2	2.21	0.40
1:C:2112:ILE:O	1:C:2116:VAL:HG13	2.21	0.40
1:C:2113:MET:HE2	1:C:2117:LEU:HD22	2.03	0.40
1:C:2150:ARG:HD2	1:C:2380:GLU:CD	2.47	0.40
1:C:2198:PHE:O	1:C:2199:ALA:C	2.63	0.40
1:C:2320:HIS:CD2	1:C:2323:TRP:CE2	3.10	0.40
1:C:2461:GLN:H	1:C:2466:TYR:HE2	1.67	0.40
1:C:2535:MET:O	1:C:2540:CYS:HB2	2.22	0.40
1:C:2538:PRO:HG2	1:D:3139:TRP:CZ3	2.57	0.40
1:D:3216:ARG:HB3	1:D:3220:PHE:HD1	1.79	0.40
1:D:3269:THR:C	1:D:3271:VAL:H	2.29	0.40
1:D:3428:ARG:O	1:D:3582:VAL:HG21	2.22	0.40
1:D:3475:TYR:CD2	1:D:3480:GLU:HG2	2.56	0.40
1:D:3564:ILE:HG13	1:D:3568:ILE:HD13	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	550/552 (100%)	374 (68%)	124 (22%)	52 (10%)	0	2
1	B	550/552 (100%)	379 (69%)	119 (22%)	52 (10%)	0	2
1	C	550/552 (100%)	372 (68%)	120 (22%)	58 (10%)	0	2
1	D	550/552 (100%)	376 (68%)	121 (22%)	53 (10%)	0	2
All	All	2200/2208 (100%)	1501 (68%)	484 (22%)	215 (10%)	0	2

All (215) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	SER
1	A	122	TYR
1	A	176	GLU
1	A	180	LYS
1	A	348	TYR
1	A	386	HIS
1	A	400	GLN
1	A	429	GLN
1	A	486	GLU
1	A	510	GLU
1	A	514	PRO
1	B	1121	SER
1	B	1122	TYR
1	B	1176	GLU
1	B	1180	LYS
1	B	1348	TYR
1	B	1386	HIS
1	B	1400	GLN
1	B	1429	GLN
1	B	1486	GLU
1	B	1510	GLU
1	C	2121	SER
1	C	2122	TYR
1	C	2176	GLU
1	C	2180	LYS
1	C	2181	VAL
1	C	2348	TYR
1	C	2386	HIS
1	C	2400	GLN
1	C	2429	GLN
1	C	2486	GLU
1	C	2500	VAL
1	C	2510	GLU

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Mol	Chain	Res	Type
1	C	2514	PRO
1	D	3121	SER
1	D	3122	TYR
1	D	3176	GLU
1	D	3180	LYS
1	D	3348	TYR
1	D	3386	HIS
1	D	3400	GLN
1	D	3429	GLN
1	D	3486	GLU
1	D	3510	GLU
1	A	96	PHE
1	A	120	ARG
1	A	141	ALA
1	A	142	PHE
1	A	177	VAL
1	A	181	VAL
1	A	292	PHE
1	A	500	VAL
1	A	533	GLY
1	A	536	GLY
1	A	539	ILE
1	A	549	THR
1	B	1096	PHE
1	B	1120	ARG
1	B	1141	ALA
1	B	1142	PHE
1	B	1181	VAL
1	B	1292	PHE
1	B	1302	ALA
1	B	1423	VAL
1	B	1458	MET
1	B	1500	VAL
1	B	1514	PRO
1	B	1533	GLY
1	B	1536	GLY
1	B	1539	ILE
1	B	1549	THR
1	C	2096	PHE
1	C	2120	ARG
1	C	2141	ALA
1	C	2142	PHE

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Mol	Chain	Res	Type
1	C	2177	VAL
1	C	2292	PHE
1	C	2302	ALA
1	C	2459	LYS
1	C	2512	PRO
1	C	2533	GLY
1	C	2539	ILE
1	D	3096	PHE
1	D	3097	LYS
1	D	3141	ALA
1	D	3142	PHE
1	D	3177	VAL
1	D	3181	VAL
1	D	3292	PHE
1	D	3500	VAL
1	D	3514	PRO
1	D	3533	GLY
1	D	3539	ILE
1	A	97	LYS
1	A	106	PRO
1	A	302	ALA
1	A	367	PHE
1	A	451	SER
1	A	458	MET
1	A	459	LYS
1	A	512	PRO
1	B	1097	LYS
1	B	1106	PRO
1	B	1177	VAL
1	B	1373	TYR
1	B	1512	PRO
1	C	2097	LYS
1	C	2104	ASN
1	C	2106	PRO
1	C	2303	THR
1	C	2367	PHE
1	C	2423	VAL
1	C	2458	MET
1	C	2531	LEU
1	C	2536	GLY
1	C	2549	THR
1	D	3120	ARG

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Mol	Chain	Res	Type
1	D	3302	ALA
1	D	3423	VAL
1	D	3451	SER
1	D	3458	MET
1	D	3459	LYS
1	D	3512	PRO
1	D	3536	GLY
1	D	3549	THR
1	A	104	ASN
1	A	303	THR
1	A	373	TYR
1	A	423	VAL
1	A	447	VAL
1	A	506	ALA
1	B	1201	PHE
1	B	1303	THR
1	B	1309	HIS
1	B	1317	LYS
1	B	1367	PHE
1	B	1370	GLN
1	B	1445	GLN
1	B	1459	LYS
1	B	1531	LEU
1	B	1558	ILE
1	C	2370	GLN
1	C	2451	SER
1	C	2496	SER
1	D	3106	PRO
1	D	3201	PHE
1	D	3367	PHE
1	D	3445	GLN
1	D	3454	GLN
1	D	3528	PRO
1	D	3531	LEU
1	D	3558	ILE
1	A	201	PHE
1	A	309	HIS
1	A	445	GLN
1	A	454	GLN
1	A	496	SER
1	A	528	PRO
1	A	531	LEU

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Mol	Chain	Res	Type
1	B	1212	THR
1	B	1284	GLN
1	B	1447	VAL
1	B	1454	GLN
1	B	1496	SER
1	B	1528	PRO
1	C	2037	CYS
1	C	2194	SER
1	C	2201	PHE
1	C	2212	THR
1	C	2309	HIS
1	C	2373	TYR
1	C	2384	LEU
1	C	2445	GLN
1	C	2454	GLN
1	C	2528	PRO
1	D	3228	VAL
1	D	3303	THR
1	D	3309	HIS
1	D	3370	GLN
1	D	3373	TYR
1	D	3447	VAL
1	D	3496	SER
1	D	3554	VAL
1	A	212	THR
1	A	277	PRO
1	A	554	VAL
1	A	558	ILE
1	B	1132	VAL
1	B	1277	PRO
1	B	1554	VAL
1	C	2364	GLU
1	C	2447	VAL
1	C	2506	ALA
1	C	2558	ILE
1	C	2565	GLN
1	D	3277	PRO
1	D	3565	GLN
1	A	132	VAL
1	C	2128	PRO
1	C	2277	PRO
1	C	2554	VAL

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Mol	Chain	Res	Type
1	B	1128	PRO
1	B	1430	ILE
1	C	2132	VAL
1	D	3132	VAL
1	A	430	ILE
1	A	505	PRO
1	B	1538	PRO
1	C	2505	PRO
1	D	3128	PRO
1	D	3430	ILE
1	A	128	PRO
1	C	2538	PRO
1	D	3505	PRO
1	D	3538	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	E	1	2,1	14,14,15	0.67	0	17,19,21	0.68	0
2	NAG	E	2	2	14,14,15	0.80	0	17,19,21	0.51	0
2	NAG	F	1	2,1	14,14,15	0.88	0	17,19,21	0.75	1 (5%)
2	NAG	F	2	2	14,14,15	0.93	0	17,19,21	0.53	0
2	NAG	G	1	2,1	14,14,15	0.67	0	17,19,21	0.71	0
2	NAG	G	2	2	14,14,15	0.80	0	17,19,21	0.52	0
2	NAG	H	1	2,1	14,14,15	0.76	0	17,19,21	0.70	0
2	NAG	H	2	2	14,14,15	0.85	0	17,19,21	0.57	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	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	C2-N2-C7	-2.08	120.11	122.90

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C1-C2-N2-C7
2	F	2	NAG	C1-C2-N2-C7
2	G	2	NAG	C1-C2-N2-C7

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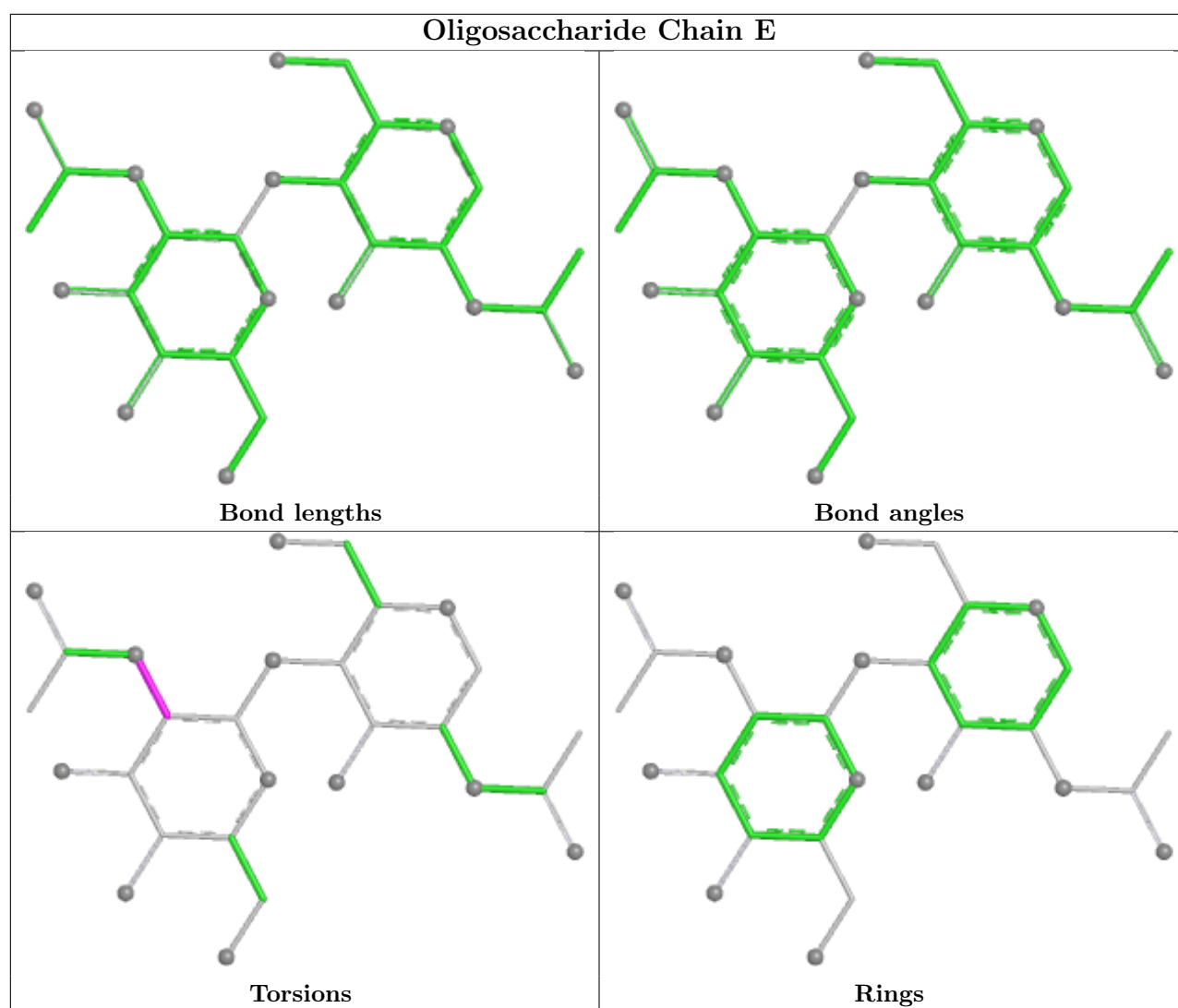
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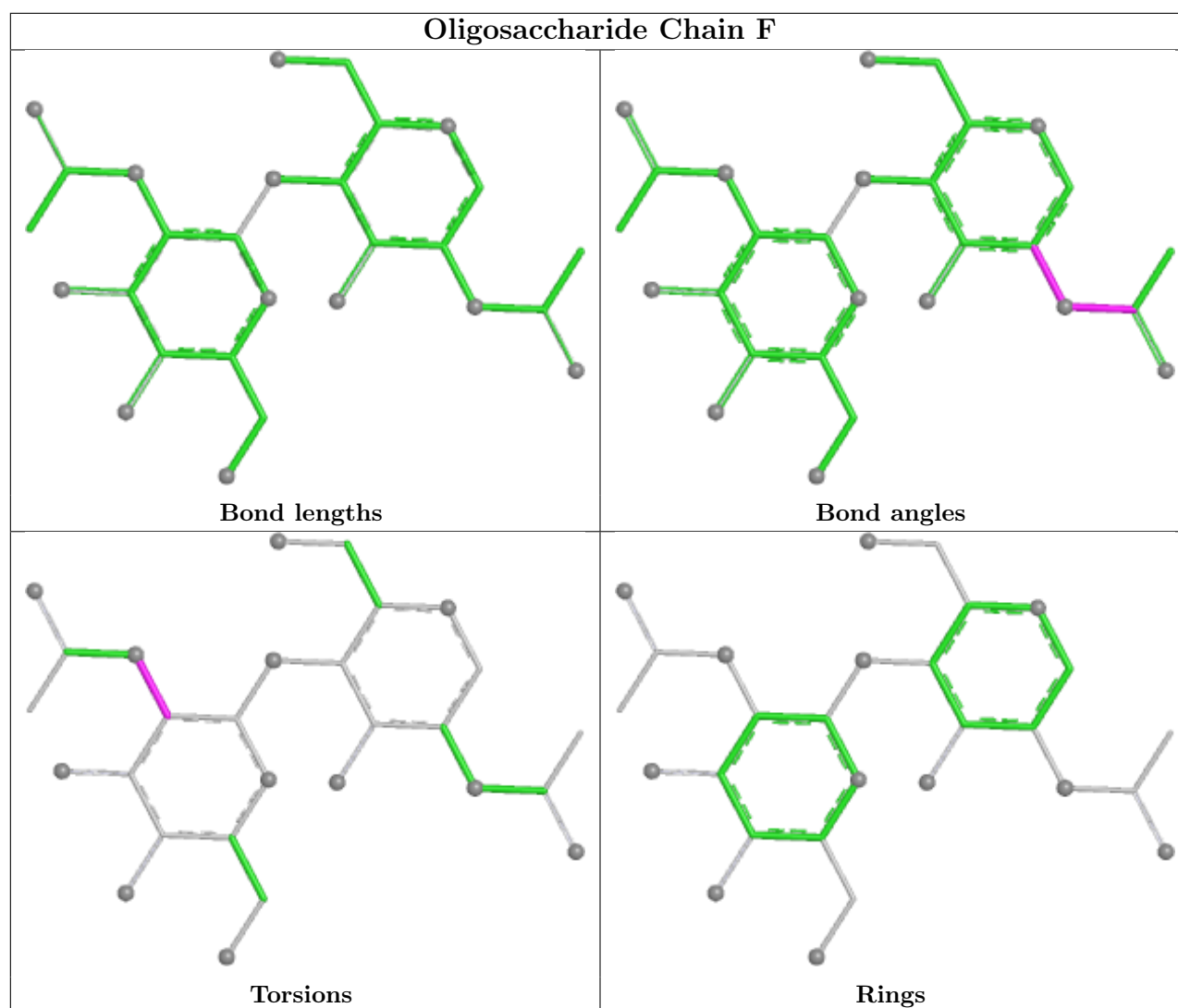
Mol	Chain	Res	Type	Atoms
2	H	2	NAG	C1-C2-N2-C7
2	F	2	NAG	C3-C2-N2-C7
2	E	2	NAG	C3-C2-N2-C7
2	G	2	NAG	C3-C2-N2-C7
2	H	2	NAG	C3-C2-N2-C7

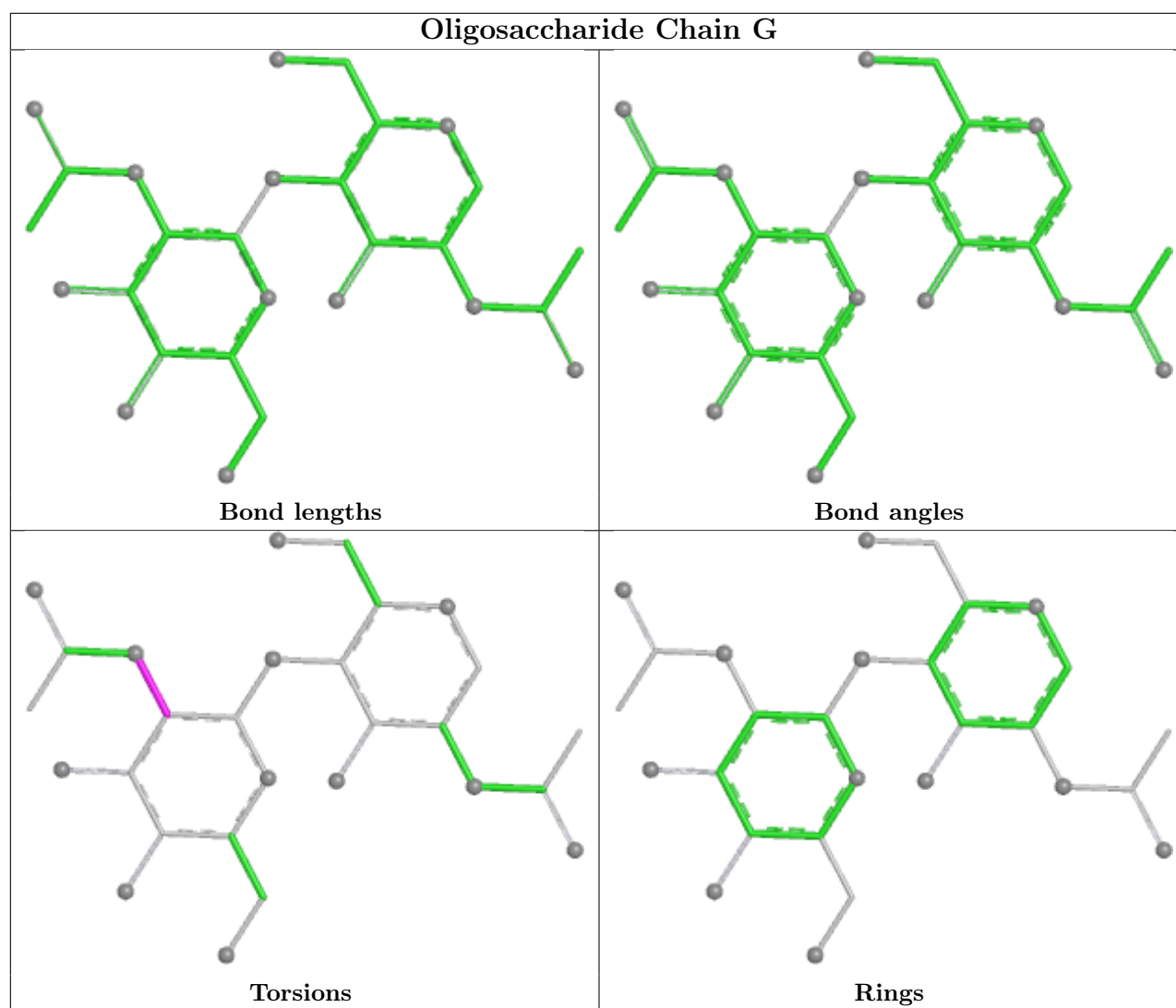
There are no ring outliers.

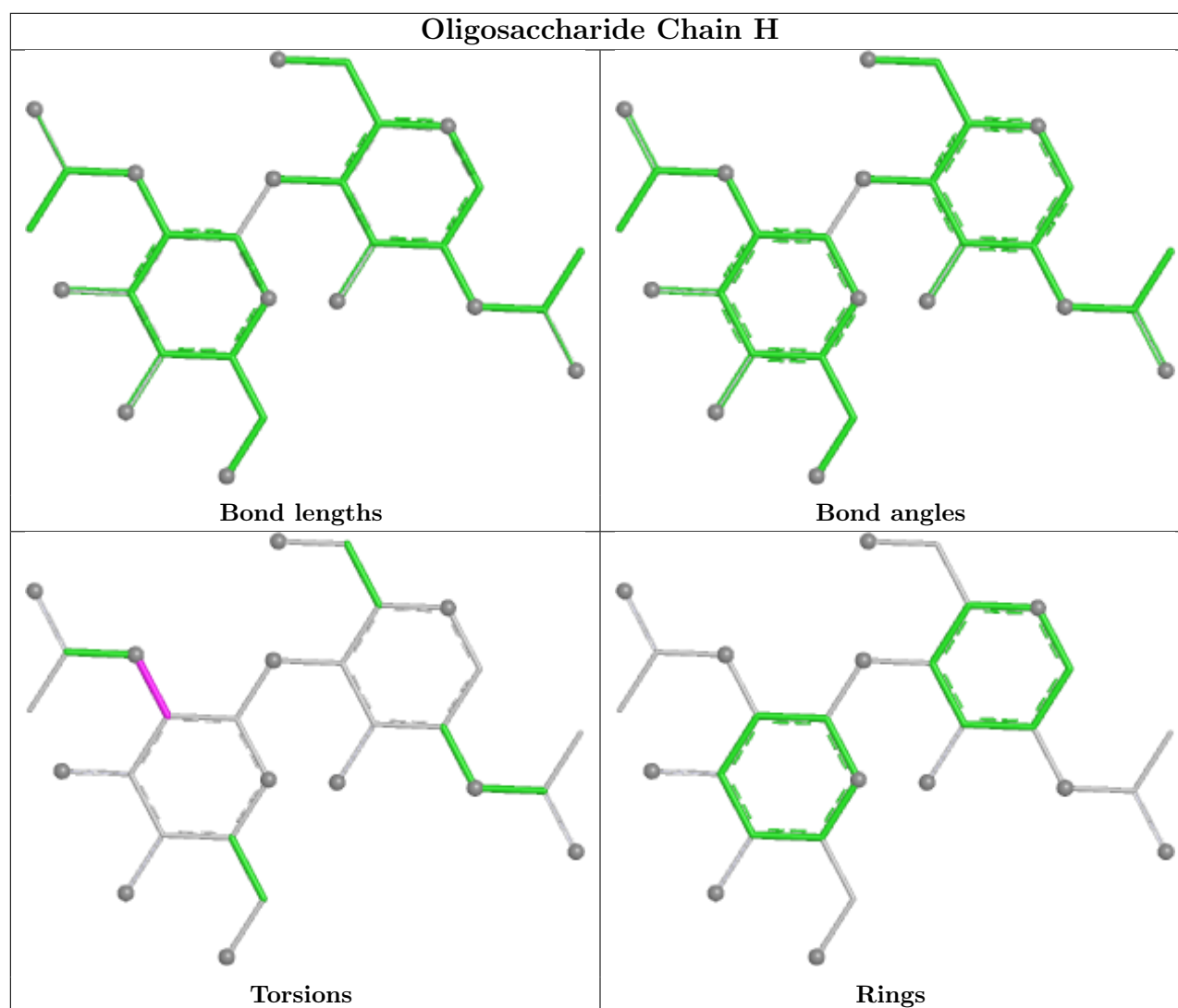
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	BOG	C	2702	-	20,20,20	0.97	2 (10%)	25,25,25	0.60	0
3	NAG	C	2671	1	14,14,15	0.72	0	17,19,21	1.07	1 (5%)
3	NAG	B	1671	1	14,14,15	0.57	0	17,19,21	0.89	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	D	3681	1	14,14,15	0.62	0	17,19,21	0.51	0
4	BOG	D	3702	-	20,20,20	0.89	2 (10%)	25,25,25	0.59	0
3	NAG	D	3671	1	14,14,15	0.61	0	17,19,21	1.00	2 (11%)
5	PGX	D	3701	-	24,26,27	1.50	1 (4%)	25,33,34	1.52	1 (4%)
3	NAG	C	2681	1	14,14,15	0.72	0	17,19,21	0.63	0
4	BOG	B	1702	-	20,20,20	0.87	2 (10%)	25,25,25	0.62	0
3	NAG	A	671	1	14,14,15	0.71	0	17,19,21	1.12	2 (11%)
4	BOG	A	702	-	20,20,20	0.90	2 (10%)	25,25,25	0.61	0
3	NAG	A	681	1	14,14,15	0.73	0	17,19,21	0.70	0
5	PGX	B	1701	-	24,26,27	1.52	2 (8%)	25,33,34	1.51	1 (4%)
3	NAG	B	1681	1	14,14,15	0.69	0	17,19,21	0.65	0
5	PGX	A	701	-	24,26,27	1.51	3 (12%)	25,33,34	1.52	1 (4%)
5	PGX	C	2701	-	24,26,27	1.47	1 (4%)	25,33,34	1.50	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BOG	C	2702	-	-	2/11/31/31	0/1/1/1
3	NAG	C	2671	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1671	1	-	2/6/23/26	0/1/1/1
3	NAG	D	3681	1	-	3/6/23/26	0/1/1/1
4	BOG	D	3702	-	-	2/11/31/31	0/1/1/1
3	NAG	D	3671	1	-	2/6/23/26	0/1/1/1
5	PGX	D	3701	-	-	11/19/40/42	0/2/2/2
3	NAG	C	2681	1	-	2/6/23/26	0/1/1/1
4	BOG	B	1702	-	-	2/11/31/31	0/1/1/1
3	NAG	A	671	1	-	2/6/23/26	0/1/1/1
4	BOG	A	702	-	-	2/11/31/31	0/1/1/1
3	NAG	A	681	1	-	2/6/23/26	0/1/1/1
5	PGX	B	1701	-	-	11/19/40/42	0/2/2/2
3	NAG	B	1681	1	-	3/6/23/26	0/1/1/1
5	PGX	A	701	-	-	11/19/40/42	0/2/2/2
5	PGX	C	2701	-	-	11/19/40/42	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1701	PGX	O4-O3	-5.68	1.24	1.46
5	D	3701	PGX	O4-O3	-5.64	1.24	1.46
5	C	2701	PGX	O4-O3	-5.63	1.24	1.46
5	A	701	PGX	O4-O3	-5.56	1.24	1.46
4	C	2702	BOG	O1-C1	2.91	1.45	1.40
4	A	702	BOG	O1-C1	2.33	1.44	1.40
4	D	3702	BOG	O1-C1	2.33	1.44	1.40
4	B	1702	BOG	O1-C1	2.25	1.43	1.40
4	B	1702	BOG	O5-C1	2.20	1.47	1.41
5	B	1701	PGX	C7-C8	2.13	1.57	1.54
4	A	702	BOG	O5-C1	2.13	1.47	1.41
5	A	701	PGX	C8-C9	2.10	1.57	1.53
5	A	701	PGX	C7-C8	2.08	1.57	1.54
4	C	2702	BOG	O5-C1	2.06	1.47	1.41
4	D	3702	BOG	O5-C1	2.00	1.47	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	3701	PGX	C11-C10-C9	-6.37	85.67	103.67
5	A	701	PGX	C11-C10-C9	-6.30	85.86	103.67
5	B	1701	PGX	C11-C10-C9	-6.27	85.95	103.67
5	C	2701	PGX	C11-C10-C9	-6.25	85.99	103.67
3	A	671	NAG	C2-N2-C7	-2.84	119.09	122.90
3	C	2671	NAG	C2-N2-C7	-2.53	119.51	122.90
3	D	3671	NAG	C1-O5-C5	2.38	115.38	112.19
3	A	671	NAG	C1-O5-C5	2.32	115.30	112.19
3	B	1671	NAG	C2-N2-C7	-2.13	120.04	122.90
3	D	3671	NAG	C2-N2-C7	-2.02	120.19	122.90

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	701	PGX	C6-C7-C8-C9
5	A	701	PGX	C6-C7-C8-C12
5	A	701	PGX	C8-C12-C13-C14
5	A	701	PGX	C11-C12-C13-C14
5	A	701	PGX	C14-C15-C16-C17
5	A	701	PGX	O5-C15-C16-C17
5	B	1701	PGX	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
5	B	1701	PGX	C6-C7-C8-C12
5	B	1701	PGX	C8-C12-C13-C14
5	B	1701	PGX	C11-C12-C13-C14
5	B	1701	PGX	C14-C15-C16-C17
5	B	1701	PGX	O5-C15-C16-C17
5	C	2701	PGX	C6-C7-C8-C9
5	C	2701	PGX	C6-C7-C8-C12
5	C	2701	PGX	C8-C12-C13-C14
5	C	2701	PGX	C11-C12-C13-C14
5	C	2701	PGX	C14-C15-C16-C17
5	C	2701	PGX	O5-C15-C16-C17
5	D	3701	PGX	C6-C7-C8-C9
5	D	3701	PGX	C6-C7-C8-C12
5	D	3701	PGX	C8-C12-C13-C14
5	D	3701	PGX	C11-C12-C13-C14
5	D	3701	PGX	C14-C15-C16-C17
5	D	3701	PGX	O5-C15-C16-C17
3	C	2671	NAG	O5-C5-C6-O6
3	A	671	NAG	O5-C5-C6-O6
3	B	1671	NAG	O5-C5-C6-O6
3	C	2671	NAG	C4-C5-C6-O6
3	A	671	NAG	C4-C5-C6-O6
3	B	1671	NAG	C4-C5-C6-O6
4	B	1702	BOG	C4-C5-C6-O6
4	D	3702	BOG	C4-C5-C6-O6
4	B	1702	BOG	O5-C5-C6-O6
4	A	702	BOG	C4-C5-C6-O6
3	D	3671	NAG	O5-C5-C6-O6
3	D	3671	NAG	C4-C5-C6-O6
5	A	701	PGX	C1-C2-C3-C4
5	B	1701	PGX	C1-C2-C3-C4
5	C	2701	PGX	C1-C2-C3-C4
4	D	3702	BOG	O5-C5-C6-O6
5	D	3701	PGX	C1-C2-C3-C4
4	A	702	BOG	O5-C5-C6-O6
4	C	2702	BOG	C4-C5-C6-O6
4	C	2702	BOG	O5-C5-C6-O6
3	C	2681	NAG	C4-C5-C6-O6
5	A	701	PGX	C13-C14-C15-O5
5	B	1701	PGX	C13-C14-C15-O5
5	C	2701	PGX	C13-C14-C15-O5
5	D	3701	PGX	C13-C14-C15-O5

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Mol	Chain	Res	Type	Atoms
3	C	2681	NAG	O5-C5-C6-O6
3	A	681	NAG	C4-C5-C6-O6
3	B	1681	NAG	C4-C5-C6-O6
3	A	681	NAG	O5-C5-C6-O6
3	D	3681	NAG	C4-C5-C6-O6
3	B	1681	NAG	C1-C2-N2-C7
3	D	3681	NAG	C1-C2-N2-C7
3	B	1681	NAG	O5-C5-C6-O6
5	A	701	PGX	C13-C14-C15-C16
5	C	2701	PGX	C13-C14-C15-C16
5	D	3701	PGX	C13-C14-C15-C16
3	D	3681	NAG	O5-C5-C6-O6
5	A	701	PGX	O2-C1-C2-C3
5	B	1701	PGX	O2-C1-C2-C3
5	D	3701	PGX	O1-C1-C2-C3
5	A	701	PGX	O1-C1-C2-C3
5	B	1701	PGX	O1-C1-C2-C3
5	C	2701	PGX	O1-C1-C2-C3
5	C	2701	PGX	O2-C1-C2-C3
5	D	3701	PGX	O2-C1-C2-C3
5	B	1701	PGX	C13-C14-C15-C16

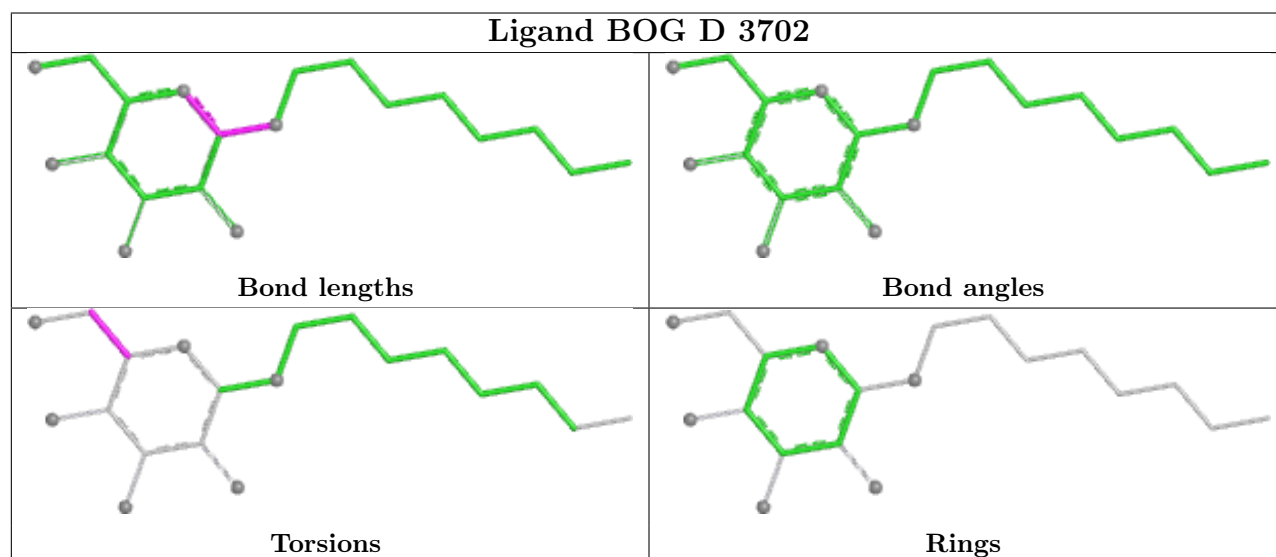
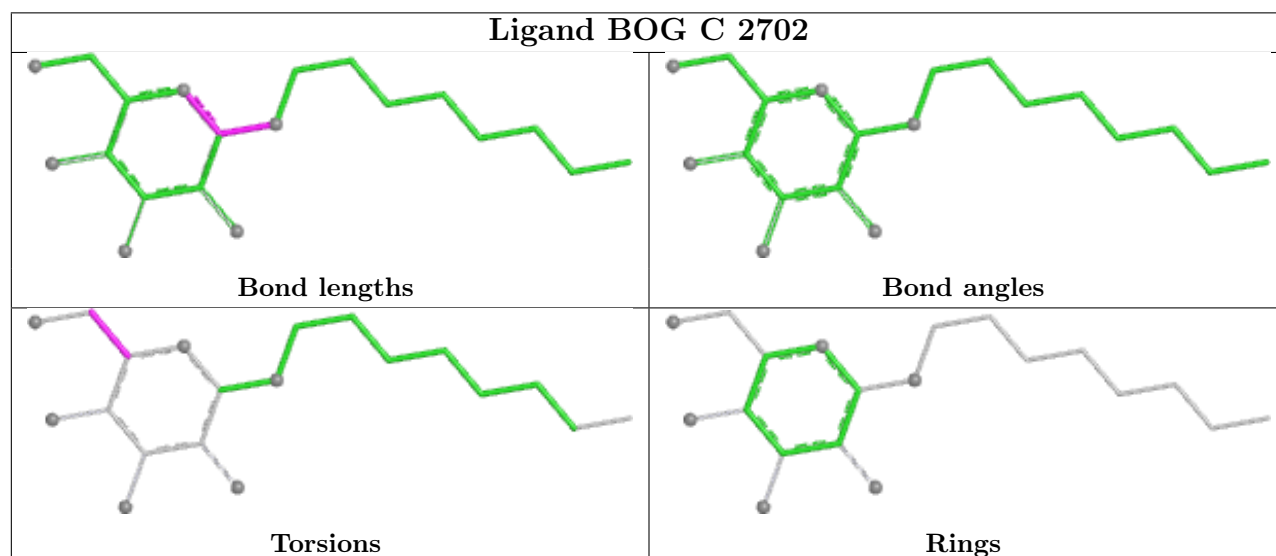
There are no ring outliers.

5 monomers are involved in 50 short contacts:

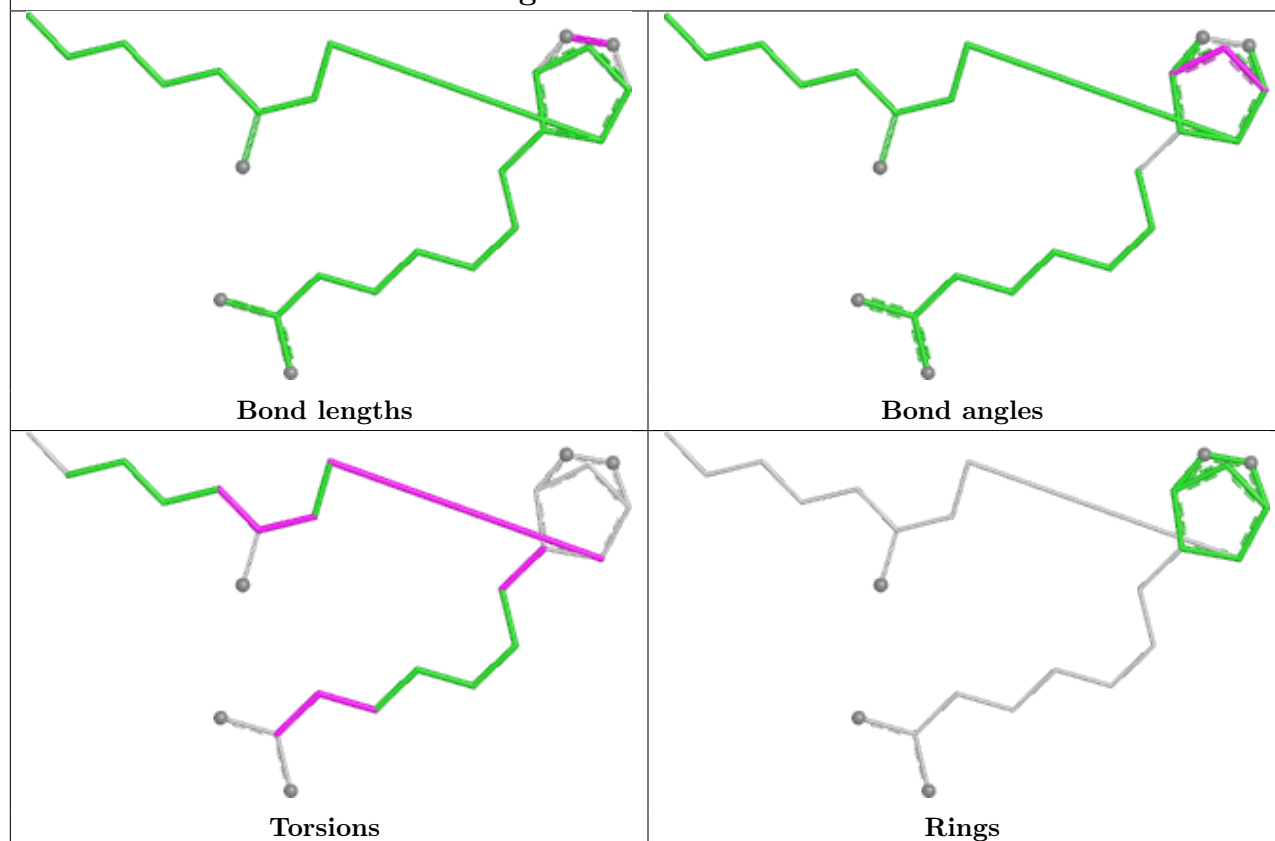
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	3702	BOG	1	0
5	D	3701	PGX	11	0
5	B	1701	PGX	14	0
5	A	701	PGX	9	0
5	C	2701	PGX	15	0

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.

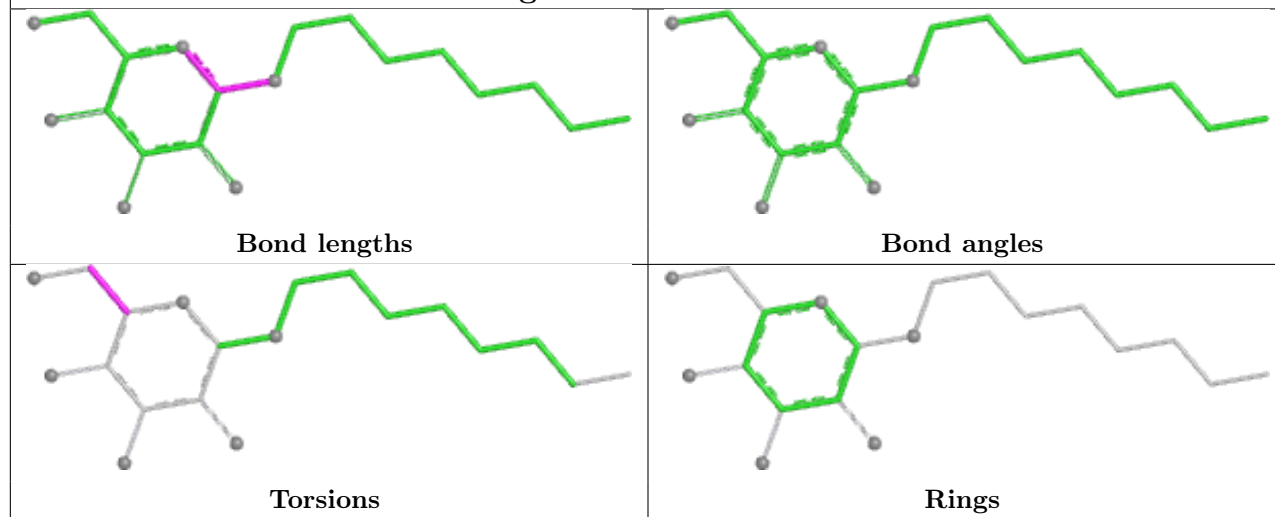
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

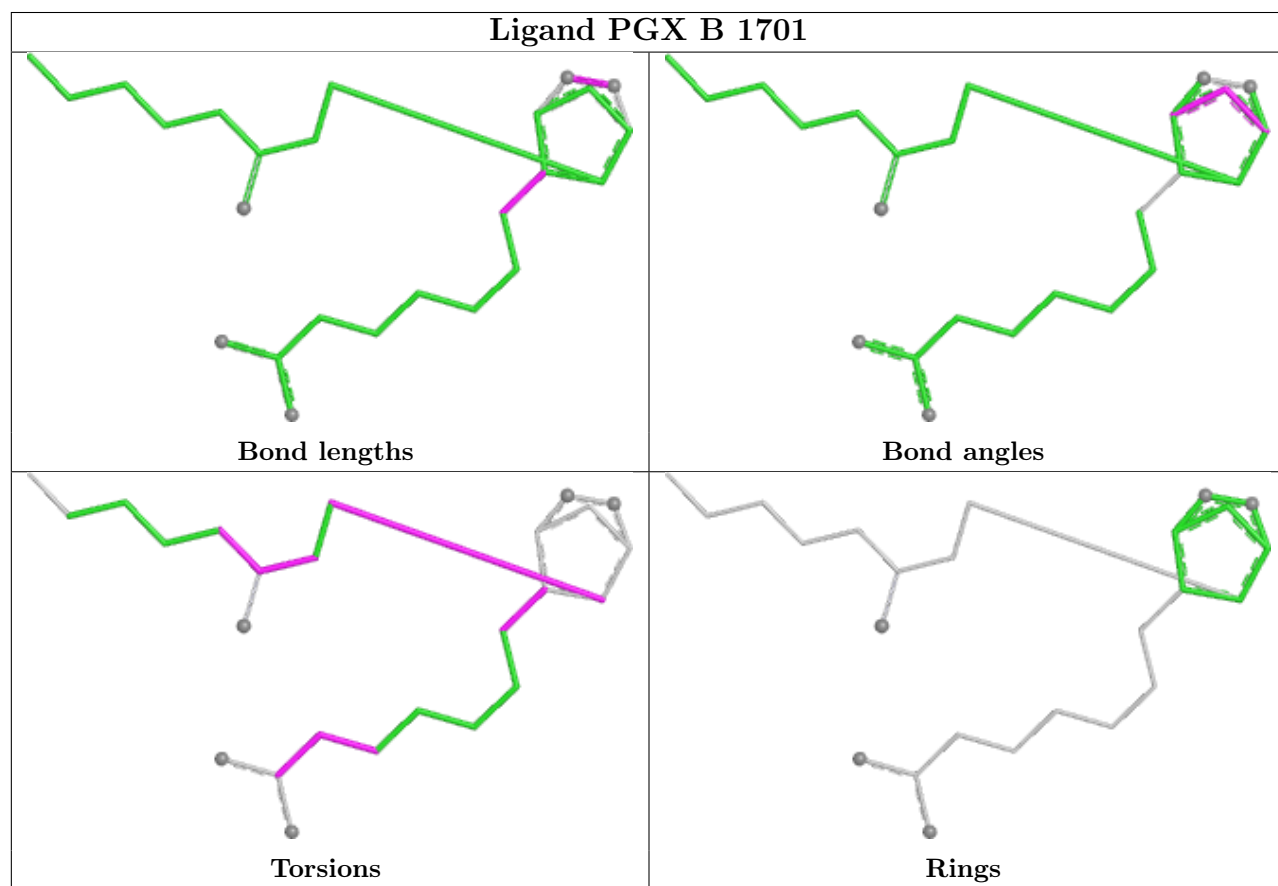
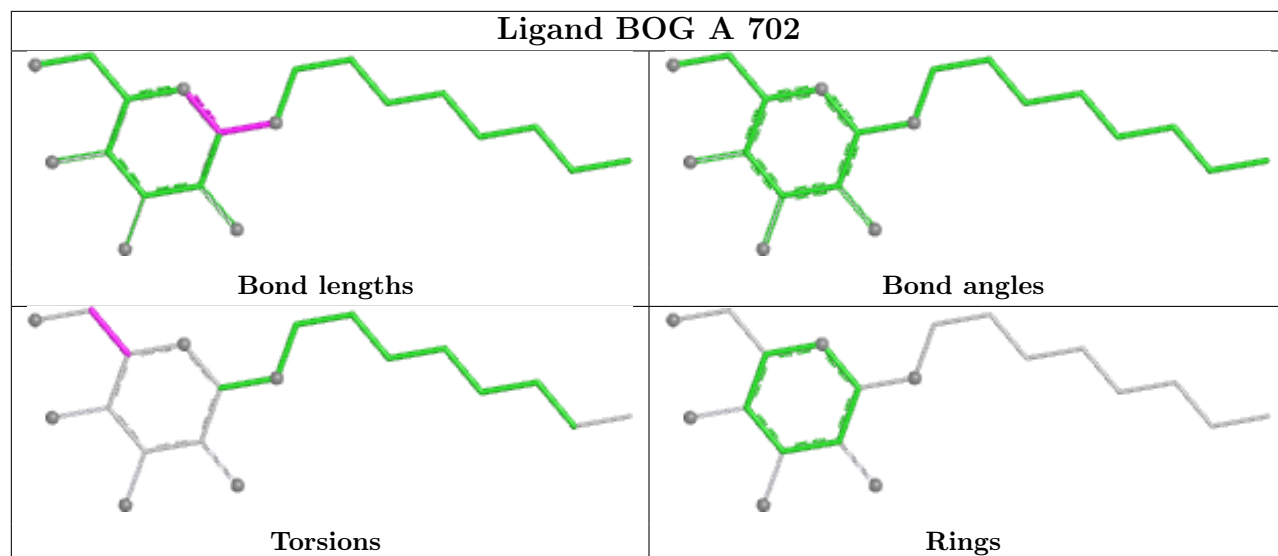


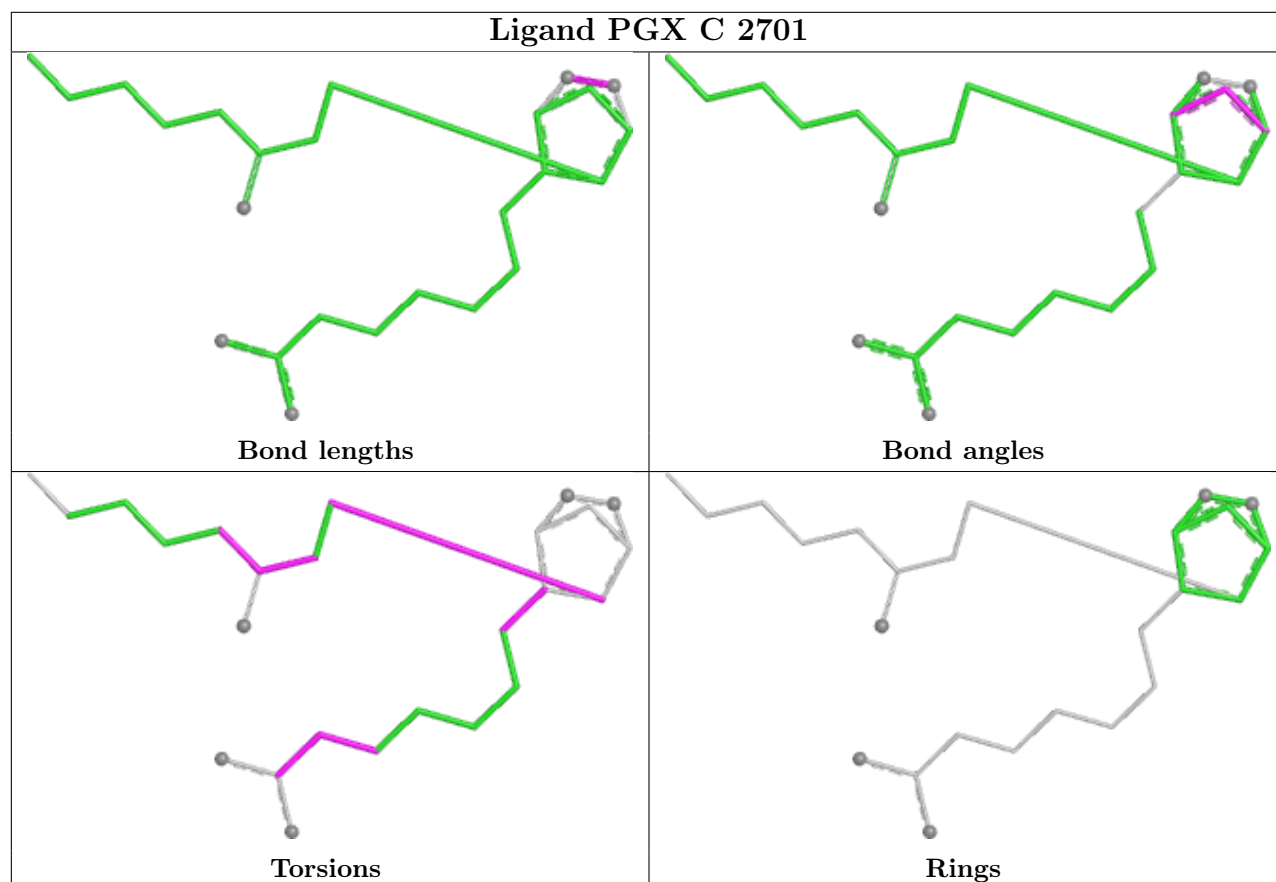
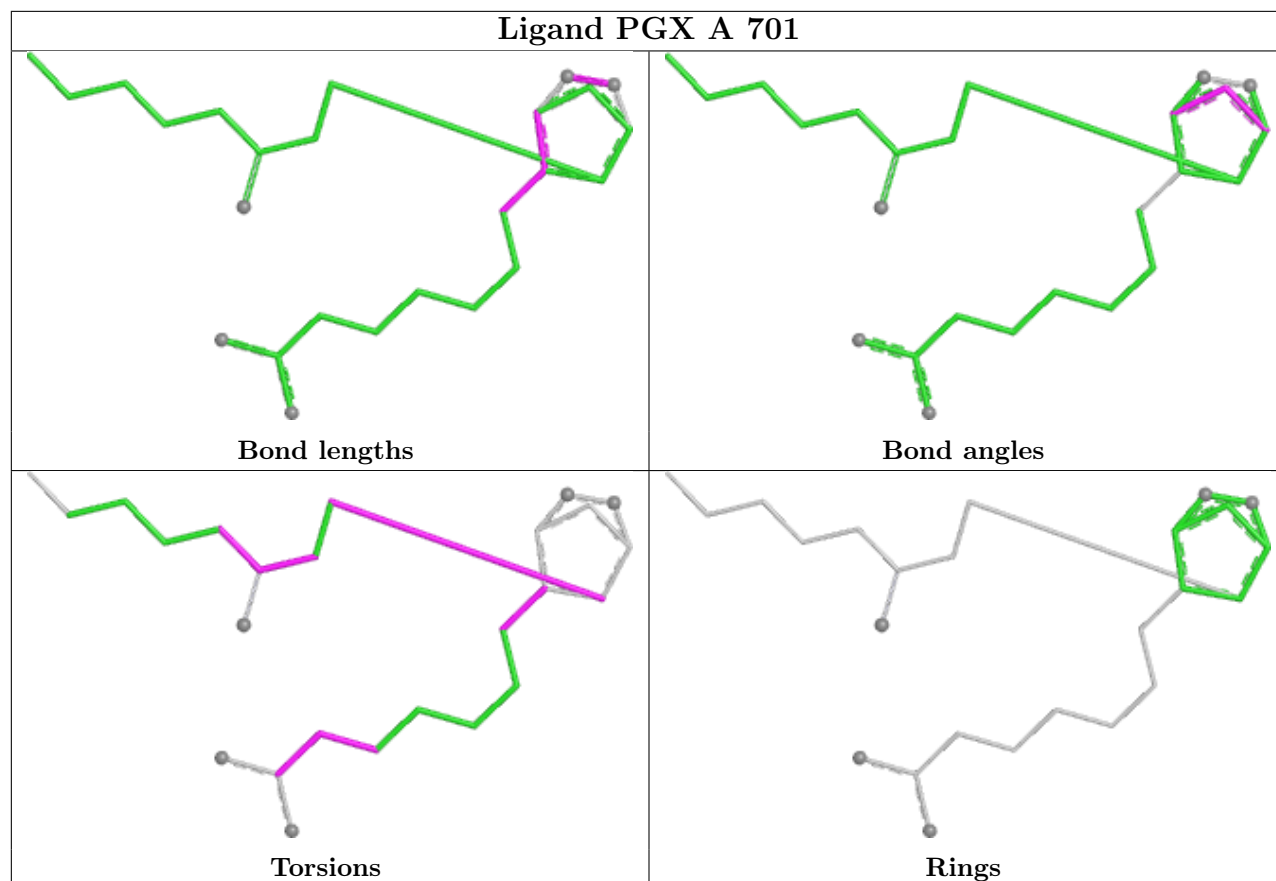
Ligand PGX D 3701



Ligand BOG B 1702







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	552/552 (100%)	0.41	10 (1%) 67 44	2, 25, 52, 71	0
1	B	552/552 (100%)	0.42	13 (2%) 59 36	3, 25, 51, 70	0
1	C	552/552 (100%)	0.44	21 (3%) 44 24	2, 25, 51, 70	0
1	D	552/552 (100%)	0.40	16 (2%) 53 31	3, 25, 51, 70	0
All	All	2208/2208 (100%)	0.42	60 (2%) 56 33	2, 25, 51, 71	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2486	GLU	3.9
1	D	3268	ASP	3.8
1	C	2357	PHE	3.1
1	B	1158	ASP	3.1
1	C	2531	LEU	3.0
1	A	411	ASN	2.9
1	C	2282	ASN	2.9
1	D	3054	GLN	2.8
1	D	3122	TYR	2.8
1	C	2123	LEU	2.8
1	D	3436	GLY	2.7
1	C	2388	HIS	2.7
1	C	2385	TYR	2.7
1	C	2188	ILE	2.6
1	B	1581	ASN	2.6
1	B	1054	GLN	2.5
1	C	2583	GLN	2.5
1	A	251	LYS	2.5
1	B	1268	ASP	2.5
1	C	2416	GLU	2.5
1	C	2409	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	2083	LYS	2.5
1	B	1464	ASN	2.5
1	A	581	ASN	2.4
1	D	3531	LEU	2.4
1	B	1041	CYS	2.4
1	A	385	TYR	2.4
1	B	1428	ARG	2.4
1	C	2581	ASN	2.4
1	B	1355	TYR	2.4
1	D	3051	GLY	2.4
1	B	1385	TYR	2.4
1	D	3437	GLY	2.3
1	A	583	GLN	2.3
1	A	98	GLY	2.3
1	C	2105(C)	ILE	2.3
1	A	571	ASN	2.3
1	C	2165	VAL	2.3
1	B	1165	VAL	2.3
1	D	3214	HIS	2.2
1	B	1519	GLY	2.2
1	D	3496	SER	2.2
1	B	1479	GLU	2.2
1	C	2120	ARG	2.2
1	D	3239	ASP	2.2
1	B	1115	TYR	2.1
1	C	2283	LEU	2.1
1	D	3543	GLN	2.1
1	D	3483	GLY	2.1
1	C	2464	ASN	2.1
1	D	3075	LEU	2.1
1	A	125	ASP	2.1
1	C	2125	ASP	2.1
1	D	3393	ASP	2.1
1	A	69	CYS	2.1
1	C	2571	ASN	2.0
1	C	2393	ASP	2.0
1	A	235	GLY	2.0
1	D	3041	CYS	2.0
1	D	3498	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

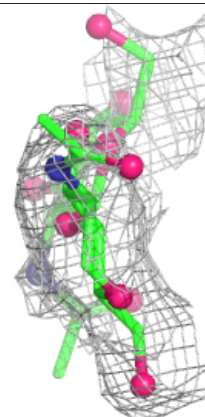
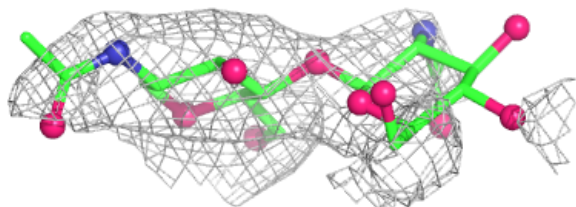
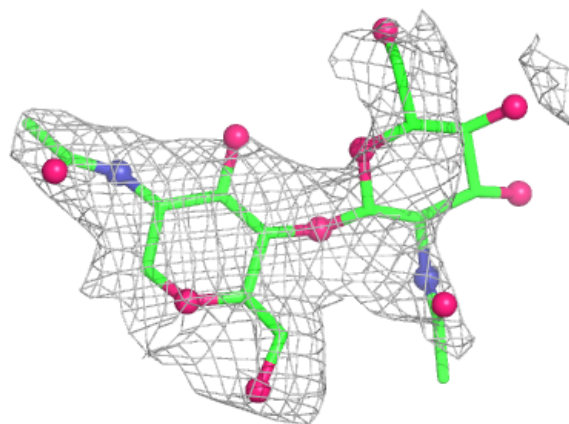
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	F	2	14/15	0.46	0.20	78,81,84,84	0
2	NAG	E	2	14/15	0.55	0.17	77,81,84,84	0
2	NAG	G	2	14/15	0.59	0.18	78,81,85,85	0
2	NAG	H	2	14/15	0.60	0.18	77,80,85,86	0
2	NAG	F	1	14/15	0.74	0.14	52,60,67,74	0
2	NAG	G	1	14/15	0.76	0.16	51,59,64,72	0
2	NAG	H	1	14/15	0.77	0.14	51,62,66,71	0
2	NAG	E	1	14/15	0.78	0.13	52,59,65,72	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

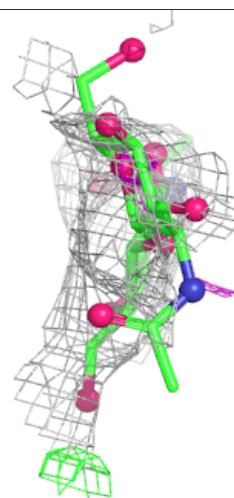
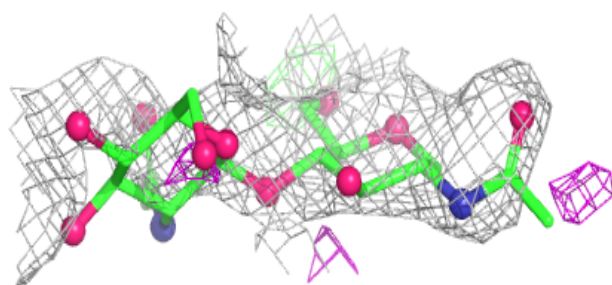
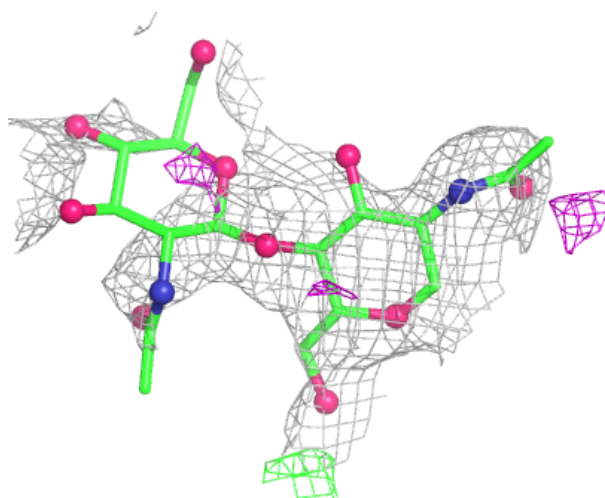
Electron density around Chain E:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



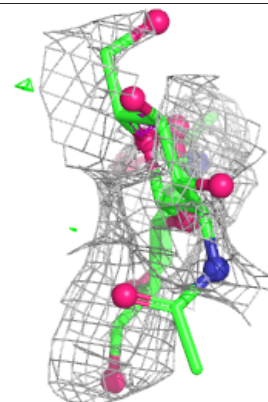
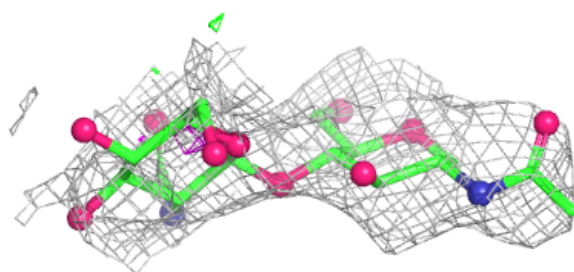
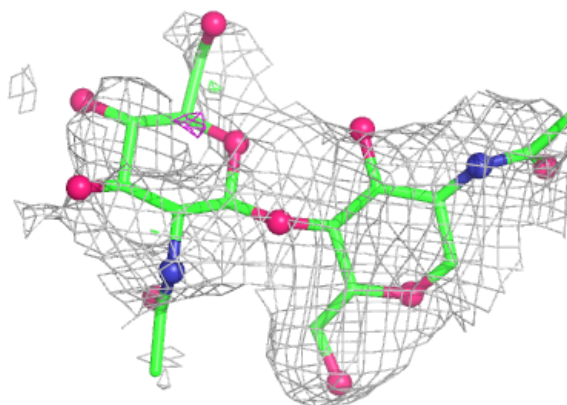
Electron density around Chain F:

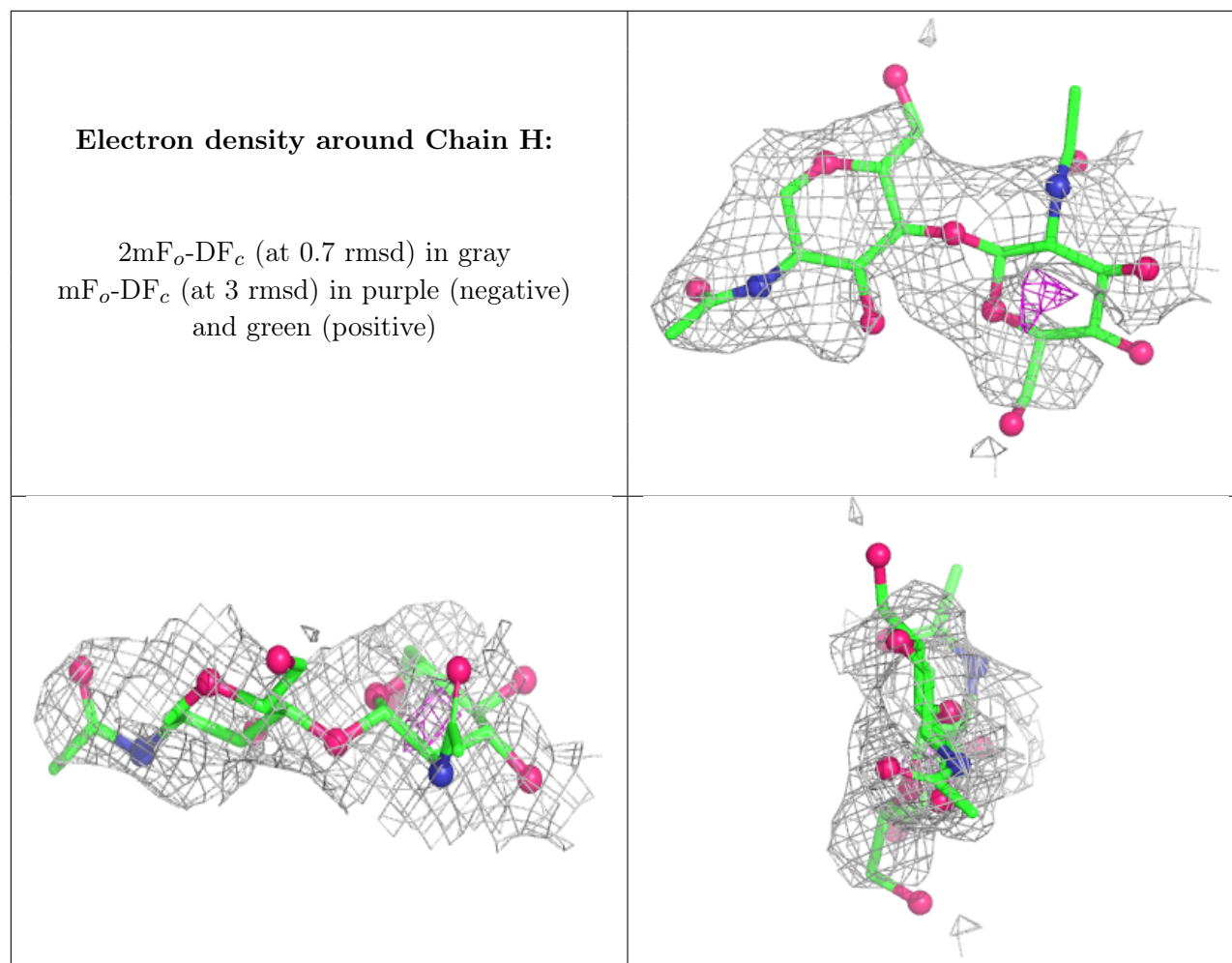
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain G:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	C	2681	14/15	0.46	0.22	66,69,73,73	0
3	NAG	A	681	14/15	0.56	0.19	67,70,73,74	0
4	BOG	B	1702	20/20	0.64	0.19	50,54,59,59	0
4	BOG	A	702	20/20	0.65	0.19	54,58,62,65	0
3	NAG	B	1681	14/15	0.67	0.17	66,71,73,75	0
3	NAG	D	3681	14/15	0.67	0.15	66,70,72,73	0
4	BOG	C	2702	20/20	0.67	0.22	56,60,64,66	0
5	PGX	C	2701	25/26	0.68	0.33	75,79,84,84	0
5	PGX	A	701	25/26	0.69	0.35	73,78,86,87	0
5	PGX	D	3701	25/26	0.69	0.34	74,78,86,87	0

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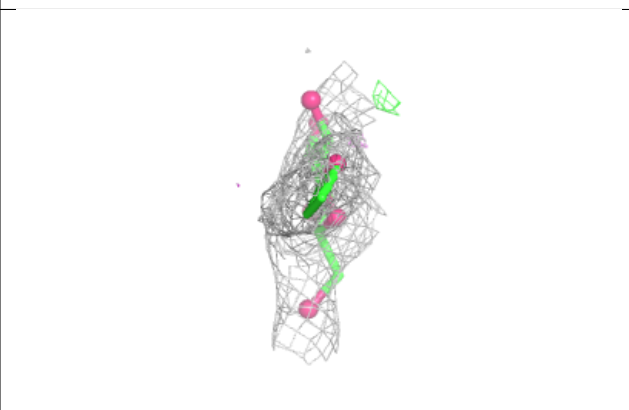
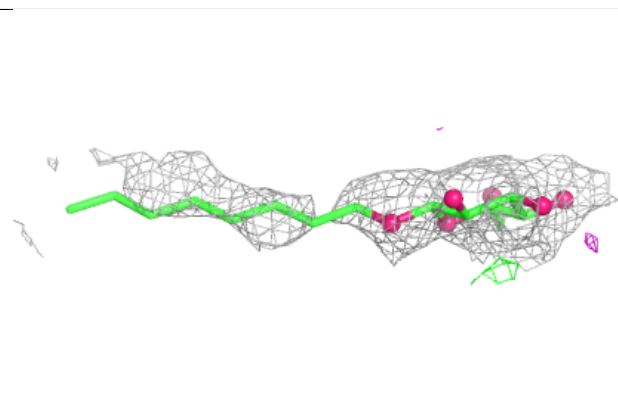
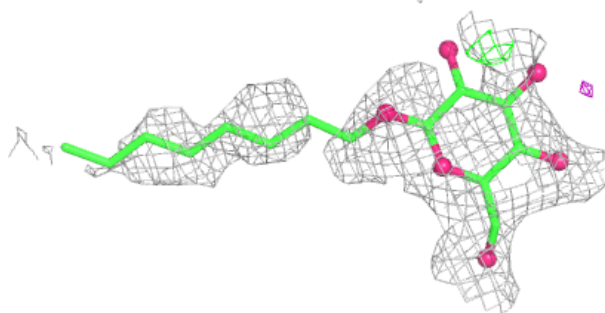
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BOG	D	3702	20/20	0.70	0.18	46,53,59,62	0
5	PGX	B	1701	25/26	0.73	0.34	72,78,84,85	0
3	NAG	B	1671	14/15	0.87	0.13	5,10,25,26	0
3	NAG	A	671	14/15	0.88	0.10	2,9,25,27	0
3	NAG	C	2671	14/15	0.88	0.12	7,10,25,28	0
3	NAG	D	3671	14/15	0.90	0.10	2,9,23,25	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

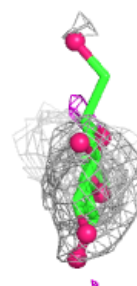
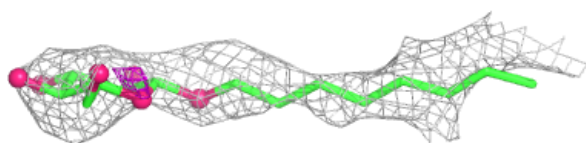
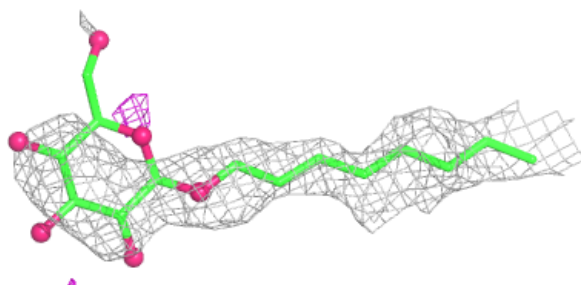
Electron density around BOG B 1702:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

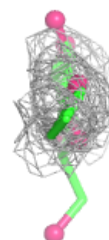
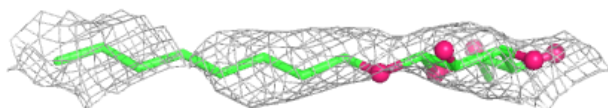
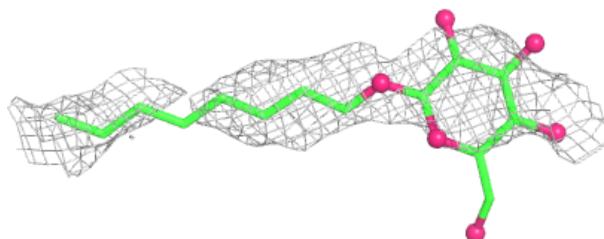


Electron density around BOG A 702:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

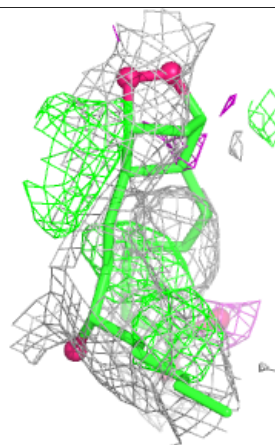
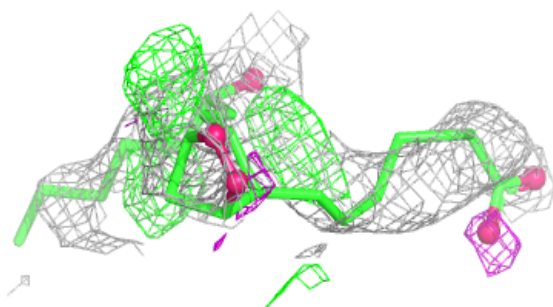
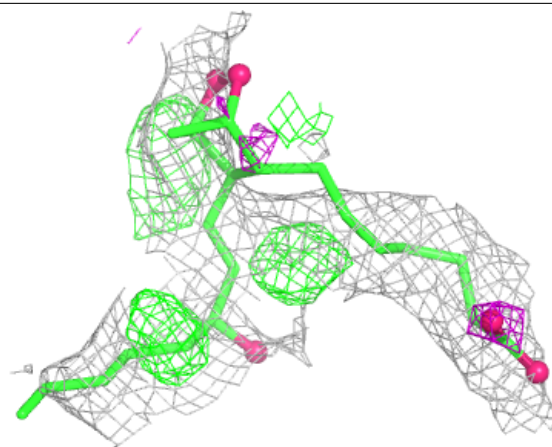
**Electron density around BOG C 2702:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



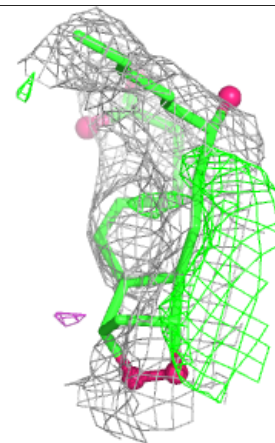
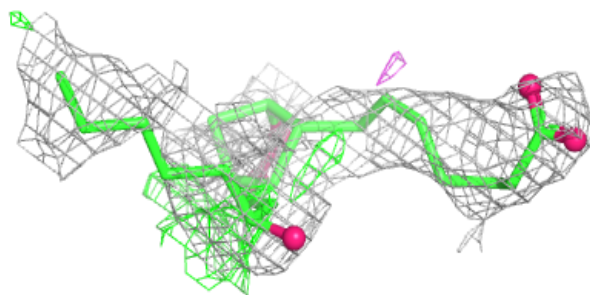
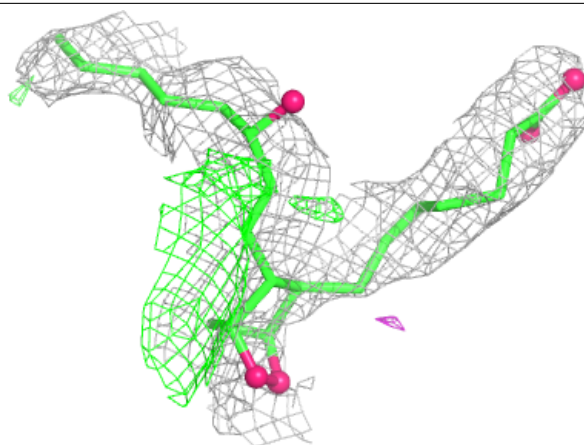
Electron density around PGX C 2701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



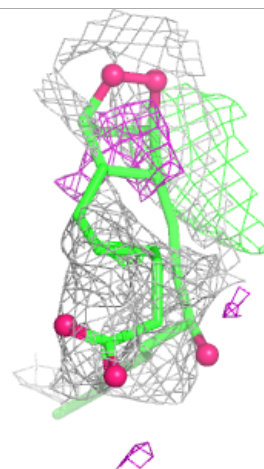
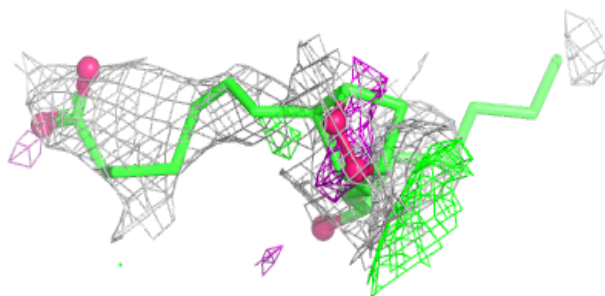
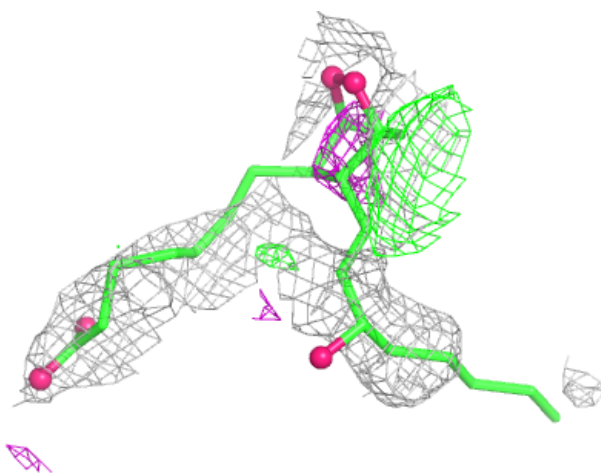
Electron density around PGX A 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



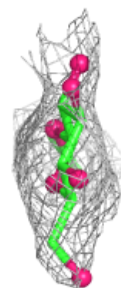
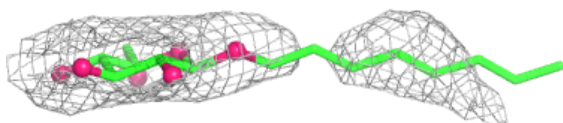
Electron density around PGX D 3701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

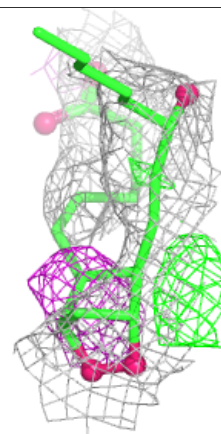
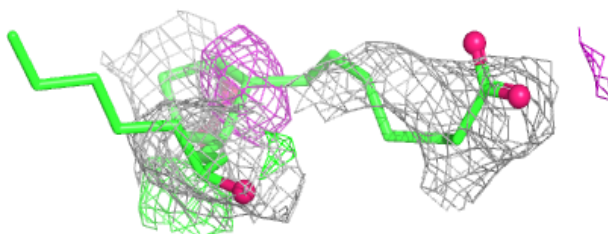
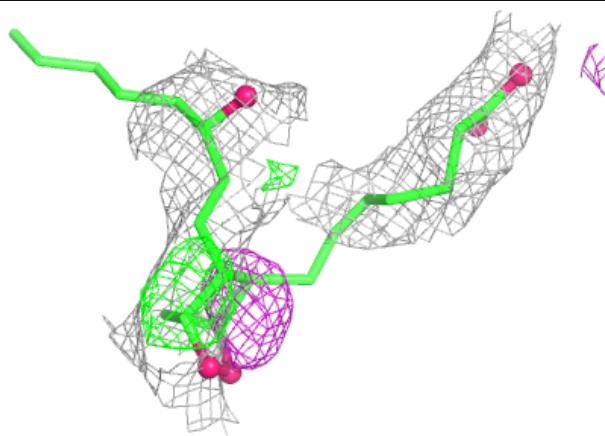


Electron density around BOG D 3702:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around PGX B 1701:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.