



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:56 AM UTC

PDB ID : 9PZL / pdb_00009pzl
Title : Pyruvate phosphate dikinase in complex with AMP-PNP and sulfate ions
Authors : Lim, K.; Herzberg, O.
Deposited on : 2025-08-11
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)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

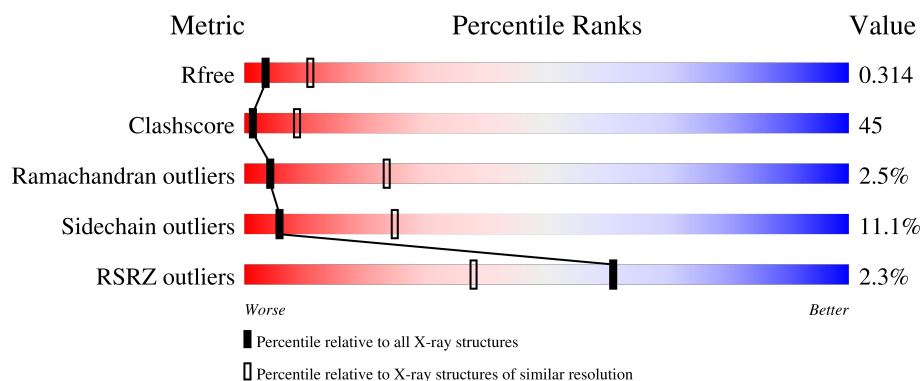
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

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)
Sidechain outliers	187428	2880 (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	874	3% 35% 55% 9%
1	B	874	% 36% 54% 9%
1	C	874	3% 32% 59% 9%
1	D	874	2% 37% 54% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

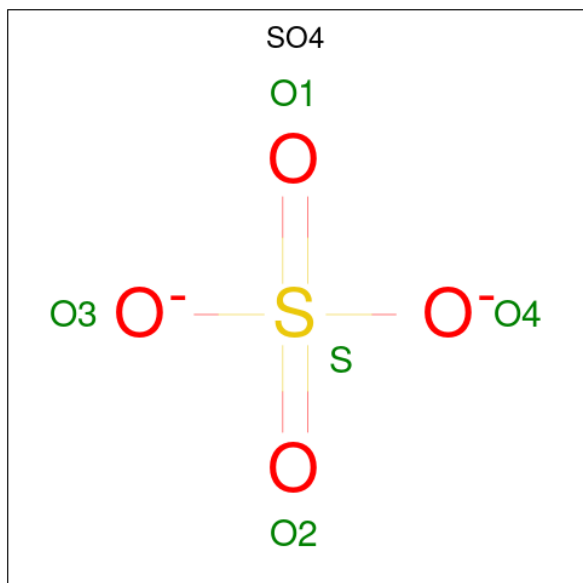
residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ANP	B	901	-	-	X	-
2	ANP	C	901	-	-	X	-
3	SO4	A	4004	-	-	X	-
3	SO4	C	902	-	-	X	-
3	SO4	D	903	-	-	X	-

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

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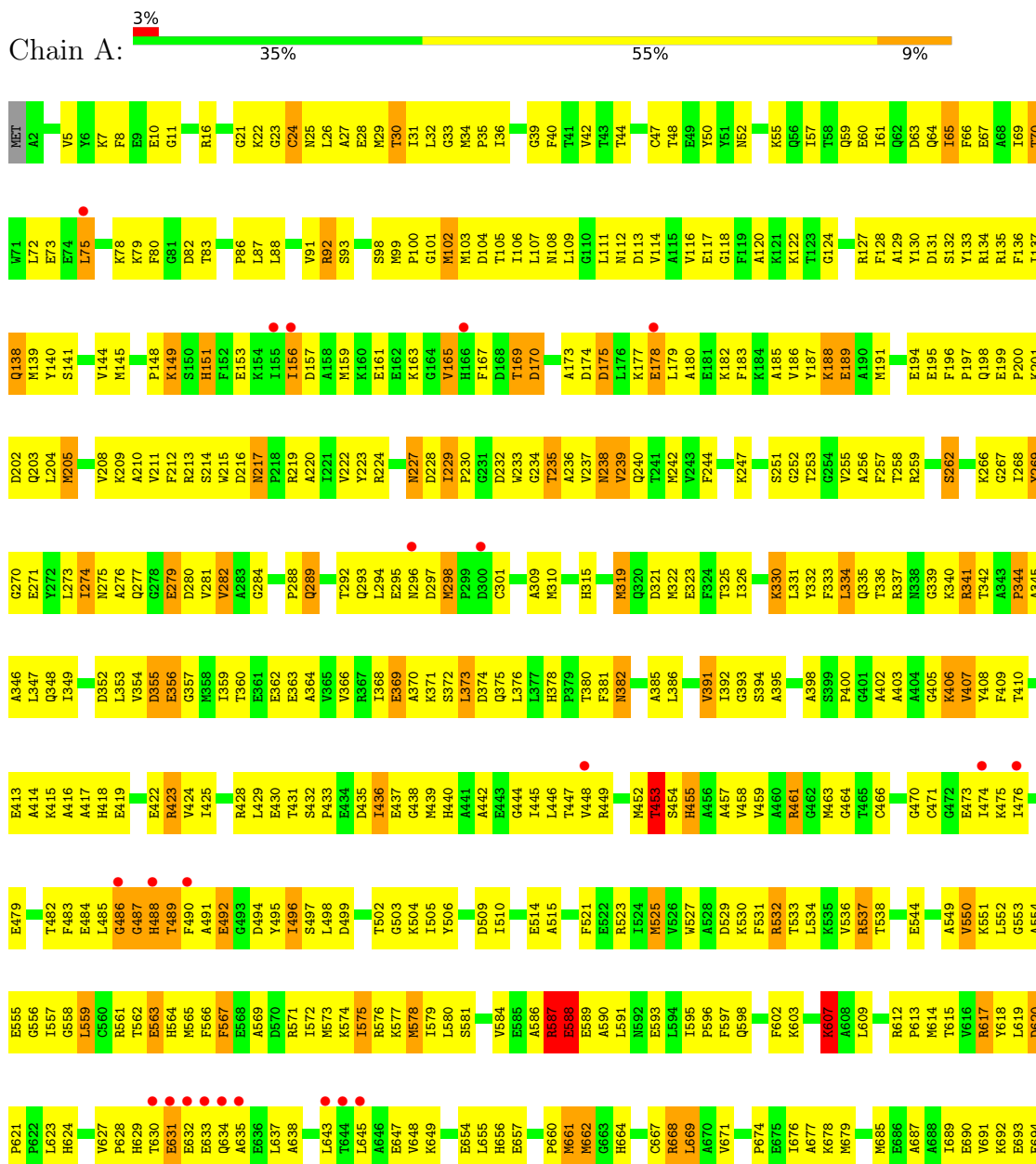
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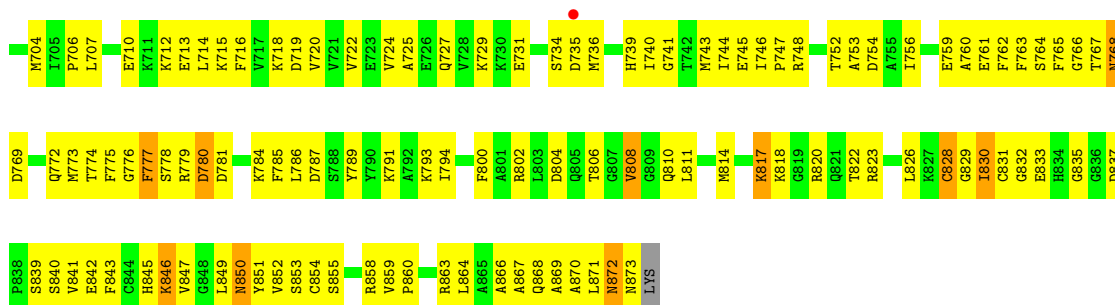
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

3 Residue-property plots

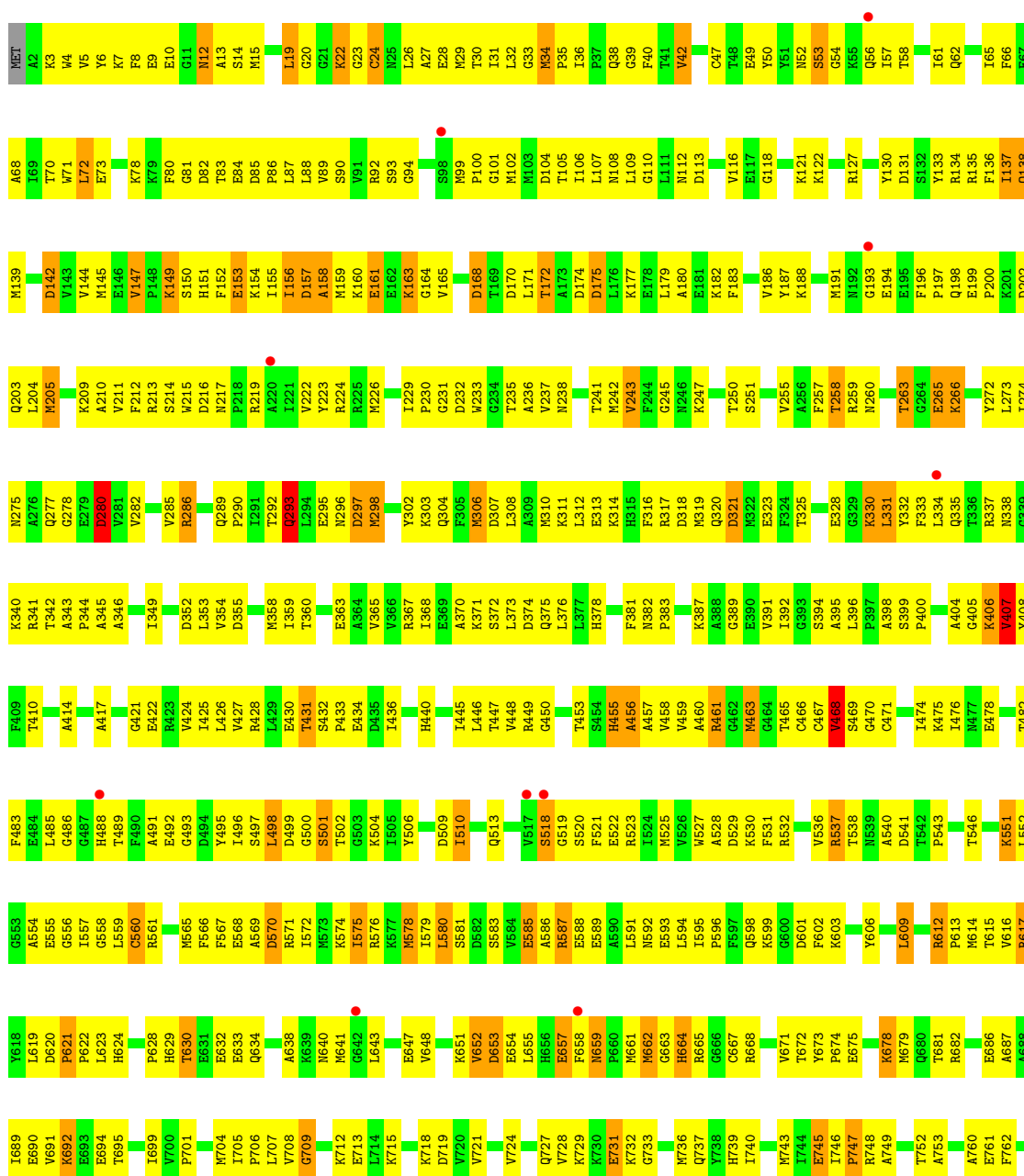
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Pyruvate, phosphate dikinase



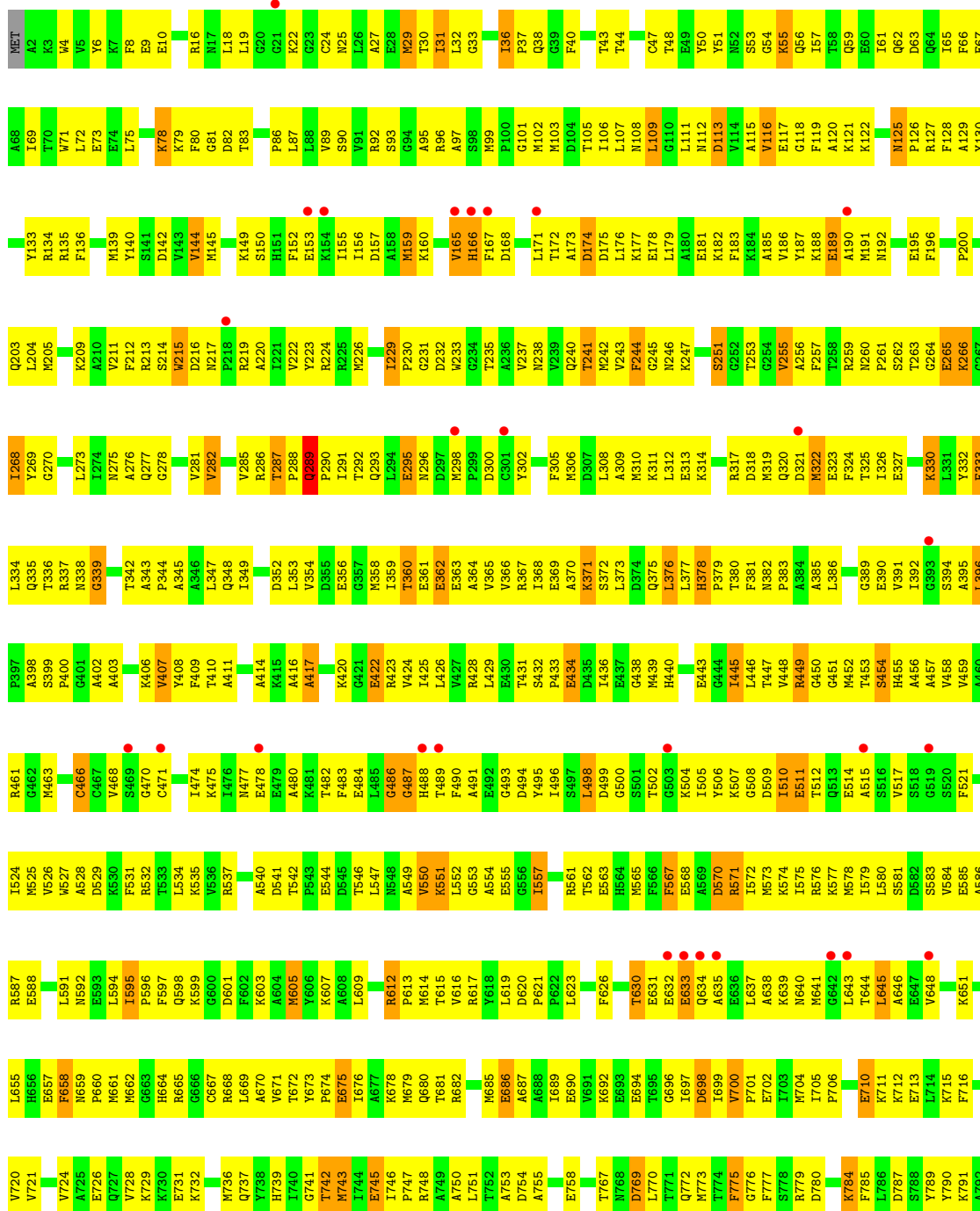


• Molecule 1: Pyruvate, phosphate dikinase





● Molecule 1: Pyruvate, phosphate dikinase



S839	S840	V841	E842	F843	C844	H845	K846	L849	N850	Y851	V852	S853	C854	P856	F857	R858	V859	P860	I861	A862	R863	L864	A865	A866	A867	Q868	N872	K873	LYS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	108.69Å 118.47Å 170.81Å 90.00° 90.40° 90.00°	Depositor
Resolution (Å)	47.53 – 3.00 47.53 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (47.53-3.00) 94.7 (47.53-3.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.219 , 0.302 0.229 , 0.314	Depositor DCC
R_{free} test set	4322 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.574	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 61.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	27192	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.57 % 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 4.8965e-04. 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: ANP, SO4

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	0.57	0/6876	0.97	11/9269 (0.1%)
1	B	0.63	0/6876	1.02	17/9269 (0.2%)
1	C	0.61	2/6876 (0.0%)	1.00	23/9269 (0.2%)
1	D	0.63	0/6876	0.99	13/9269 (0.1%)
All	All	0.61	2/27504 (0.0%)	1.00	64/37076 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	215	TRP	NE1-CE2	10.61	1.49	1.37
1	C	215	TRP	CD2-CE2	-5.27	1.32	1.41

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	215	TRP	CD2-CE2-CZ2	9.10	131.50	122.40
1	A	102	MET	N-CA-C	-7.29	104.38	113.28
1	D	104	ASP	N-CA-C	7.24	121.36	110.14
1	C	215	TRP	CE2-CD2-CG	7.23	115.88	107.20
1	C	289	GLN	CA-C-N	7.19	127.62	119.93
1	C	289	GLN	C-N-CA	7.19	127.62	119.93
1	C	378	HIS	CA-C-N	7.05	128.65	119.84
1	C	378	HIS	C-N-CA	7.05	128.65	119.84
1	B	407	VAL	N-CA-C	7.04	118.11	109.30
1	B	468	VAL	CB-CA-C	-6.96	102.48	110.41
1	B	823	ARG	CA-C-N	6.92	126.89	119.28
1	B	823	ARG	C-N-CA	6.92	126.89	119.28
1	D	229	ILE	CA-C-N	6.92	127.48	120.14
1	D	229	ILE	C-N-CA	6.92	127.48	120.14
1	C	742	THR	N-CA-C	6.82	119.77	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	MET	CA-C-N	6.67	127.25	120.04
1	A	298	MET	C-N-CA	6.67	127.25	120.04
1	C	700	VAL	CA-C-N	6.65	128.15	119.84
1	C	700	VAL	C-N-CA	6.65	128.15	119.84
1	C	837	ASP	CA-C-N	6.65	126.43	119.05
1	C	837	ASP	C-N-CA	6.65	126.43	119.05
1	D	12	ASN	N-CA-C	6.52	117.07	107.88
1	C	775	PHE	N-CA-C	-6.41	104.94	112.89
1	C	833	GLU	N-CA-C	-6.41	104.29	111.28
1	C	116	VAL	CB-CA-C	-6.02	104.16	112.04
1	C	278	GLY	N-CA-C	5.99	119.45	112.50
1	D	382	ASN	CA-C-N	5.99	125.69	119.05
1	D	382	ASN	C-N-CA	5.99	125.69	119.05
1	D	196	PHE	CA-C-N	5.96	125.89	119.76
1	D	196	PHE	C-N-CA	5.96	125.89	119.76
1	C	244	PHE	N-CA-C	5.88	118.80	107.44
1	B	53	SER	N-CA-C	-5.83	106.50	113.21
1	B	659	ASN	CA-C-N	5.79	125.47	119.05
1	B	659	ASN	C-N-CA	5.79	125.47	119.05
1	B	833	GLU	N-CA-C	-5.76	106.08	113.23
1	B	621	PRO	CA-C-N	5.73	126.18	119.99
1	B	621	PRO	C-N-CA	5.73	126.18	119.99
1	C	270	GLY	N-CA-C	5.55	119.65	110.55
1	C	389	GLY	N-CA-C	5.44	118.32	112.33
1	A	488	HIS	N-CA-C	5.44	115.47	108.34
1	A	559	LEU	N-CA-C	5.39	116.37	107.20
1	D	527	TRP	N-CA-C	-5.37	106.24	112.89
1	A	777	PHE	N-CA-C	5.34	117.19	109.07
1	C	215	TRP	CG-CD2-CE3	-5.33	128.57	133.90
1	C	595	ILE	CA-C-N	-5.32	113.19	119.84
1	C	595	ILE	C-N-CA	-5.32	113.19	119.84
1	C	229	ILE	N-CA-C	5.31	113.68	107.89
1	A	563	GLU	N-CA-C	5.25	116.69	111.07
1	D	675	GLU	N-CA-C	-5.23	105.75	111.82
1	A	607	LYS	N-CA-C	-5.18	106.96	113.28
1	B	851	TYR	N-CA-C	5.15	116.67	108.79
1	B	612	ARG	CA-C-N	5.14	125.05	119.85
1	B	612	ARG	C-N-CA	5.14	125.05	119.85
1	D	270	GLY	N-CA-C	5.14	118.25	110.75
1	C	417	ALA	N-CA-C	5.13	116.87	111.28
1	B	657	GLU	N-CA-C	5.13	117.76	108.69
1	B	506	TYR	N-CA-C	5.12	117.76	108.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	382	ASN	CA-C-N	5.12	124.30	118.97
1	A	382	ASN	C-N-CA	5.12	124.30	118.97
1	B	34	MET	CA-C-N	5.10	126.22	119.84
1	B	34	MET	C-N-CA	5.10	126.22	119.84
1	D	601	ASP	N-CA-C	-5.07	105.75	111.28
1	D	536	VAL	N-CA-C	5.04	115.29	107.28
1	A	453	THR	N-CA-C	-5.03	104.07	111.81

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6752	0	6668	586	0
1	B	6752	0	6668	608	0
1	C	6752	0	6668	700	0
1	D	6752	0	6668	592	0
2	A	31	0	13	7	0
2	B	31	0	13	17	0
2	C	31	0	13	16	0
2	D	31	0	12	7	0
3	A	15	0	0	3	0
3	B	15	0	0	1	0
3	C	15	0	0	3	0
3	D	15	0	0	3	0
All	All	27192	0	26723	2419	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 45.

All (2419) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:635:ALA:HB2	1:C:645:LEU:HD22	1.22	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:VAL:HG13	1:A:872:ASN:HD21	1.13	1.13
1:D:682:ARG:HH11	1:D:682:ARG:HG3	1.01	1.11
1:C:255:VAL:HB	1:C:453:THR:HG21	1.27	1.09
1:C:777:PHE:HA	1:D:662:MET:HB2	1.13	1.09
1:C:295:GLU:HG3	1:C:302:TYR:CD2	1.90	1.07
1:B:558:GLY:O	1:B:615:THR:HB	1.55	1.06
1:D:108:ASN:HB2	1:D:136:PHE:HB2	1.32	1.06
1:A:564:HIS:HA	1:A:567:PHE:HB2	1.36	1.03
1:A:842:GLU:HG2	1:A:846:LYS:HD3	1.43	1.00
1:A:289:GLN:NE2	1:A:293:GLN:HG2	1.77	0.99
1:C:172:THR:HG22	1:C:174:ASP:H	1.24	0.99
1:D:29:MET:HB3	1:D:36:ILE:HD11	1.46	0.97
1:D:802:ARG:HG3	1:D:802:ARG:HH11	1.29	0.96
1:C:373:LEU:HD11	1:C:864:LEU:HD23	1.48	0.96
1:A:255:VAL:HB	1:A:453:THR:CG2	1.95	0.96
1:A:628:PRO:HB2	1:A:633:GLU:HB3	1.48	0.96
1:D:255:VAL:HB	1:D:453:THR:HG21	1.45	0.96
1:B:425:ILE:HG21	1:B:496:ILE:HD11	1.48	0.96
1:A:102:MET:HE2	1:A:223:TYR:HB2	1.48	0.95
1:D:173:ALA:O	1:D:177:LYS:HG3	1.67	0.94
1:B:102:MET:HE3	1:B:219:ARG:HG3	1.46	0.94
1:C:255:VAL:HB	1:C:453:THR:CG2	1.96	0.94
1:A:80:PHE:HA	1:A:87:LEU:HB3	1.48	0.94
1:A:428:ARG:HB2	1:A:447:THR:HG22	1.47	0.93
1:A:537:ARG:HH12	1:A:613:PRO:HG2	1.34	0.93
1:C:637:LEU:HD12	1:C:640:ASN:HB2	1.50	0.92
1:B:9:GLU:HA	1:B:31:ILE:HD11	1.48	0.92
1:D:448:VAL:HG22	1:D:474:ILE:HB	1.51	0.92
1:D:395:ALA:HB3	1:D:468:VAL:HG12	1.49	0.92
1:D:219:ARG:HH11	1:D:219:ARG:HG3	1.35	0.92
1:D:699:ILE:HG22	1:D:701:PRO:HD3	1.48	0.91
1:A:112:ASN:O	1:A:116:VAL:HG23	1.69	0.91
1:C:27:ALA:O	1:C:31:ILE:HD13	1.71	0.91
1:A:92:ARG:HG2	1:A:238:ASN:HB2	1.52	0.91
1:B:255:VAL:HB	1:B:453:THR:CG2	2.00	0.91
1:B:661:MET:HE1	1:B:778:SER:HB2	1.51	0.91
1:C:690:GLU:HG3	1:C:732:LYS:HE3	1.53	0.91
1:C:317:ARG:HH21	1:C:359:ILE:HA	1.33	0.90
1:D:255:VAL:HB	1:D:453:THR:CG2	2.01	0.90
1:D:317:ARG:HA	1:D:358:MET:HE3	1.51	0.90
1:D:373:LEU:HB2	1:D:861:ILE:HG12	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:572:ILE:HG13	1:D:576:ARG:HE	1.36	0.89
1:B:93:SER:HB3	1:B:211:VAL:HG13	1.55	0.89
1:A:667:CYS:HB2	1:A:706:PRO:O	1.71	0.89
1:B:528:ALA:HB1	1:B:867:ALA:HB2	1.54	0.89
1:C:803:LEU:HD23	1:C:804:ASP:O	1.73	0.89
1:D:570:ASP:HB2	1:D:597:PHE:CE2	2.08	0.89
1:D:28:GLU:HG3	1:D:32:LEU:HD11	1.55	0.89
1:B:692:LYS:HB2	1:B:699:ILE:HD12	1.55	0.89
1:C:414:ALA:HB1	1:C:424:VAL:HG11	1.55	0.88
1:A:671:VAL:HG11	1:B:789:TYR:CE1	2.09	0.88
1:D:689:ILE:O	1:D:693:GLU:HG3	1.73	0.88
1:D:858:ARG:HD2	1:D:861:ILE:HD12	1.56	0.88
1:C:343:ALA:HB3	1:C:344:PRO:HD3	1.57	0.87
1:A:284:GLY:O	1:A:430:GLU:HB2	1.74	0.87
1:A:459:VAL:O	1:A:463:MET:HG3	1.74	0.87
1:B:674:PRO:O	1:B:678:LYS:HG3	1.75	0.87
1:C:95:ALA:HB2	1:C:103:MET:HE1	1.57	0.86
1:B:205:MET:HE2	1:B:205:MET:HA	1.55	0.86
1:D:634:GLN:HE22	1:D:649:LYS:HG3	1.41	0.86
1:A:525:MET:HE2	1:A:525:MET:HA	1.56	0.86
1:B:182:LYS:O	1:B:186:VAL:HG23	1.74	0.86
1:D:635:ALA:HB2	1:D:645:LEU:HD22	1.54	0.86
1:A:375:GLN:HG2	1:A:464:GLY:HA3	1.58	0.85
1:C:386:LEU:HD12	1:C:510:ILE:HG21	1.59	0.85
1:A:182:LYS:O	1:A:186:VAL:HG23	1.77	0.85
1:C:692:LYS:HE2	1:C:698:ASP:HA	1.59	0.85
1:B:798:ASP:HB3	1:B:801:ALA:HB3	1.59	0.85
1:C:777:PHE:HB3	1:D:668:ARG:NH1	1.92	0.85
1:A:753:ALA:HB3	1:A:818:LYS:HB2	1.56	0.85
1:C:454:SER:O	1:C:458:VAL:HG23	1.76	0.85
1:D:682:ARG:HG3	1:D:682:ARG:NH1	1.78	0.84
1:A:116:VAL:HG21	1:A:133:TYR:CD2	2.12	0.84
1:A:439:MET:HA	1:A:445:ILE:HD11	1.60	0.84
1:B:83:THR:HG23	1:B:84:GLU:HG2	1.59	0.84
1:D:572:ILE:O	1:D:576:ARG:HG3	1.78	0.84
1:D:827:LYS:HE3	1:D:850:ASN:HD22	1.41	0.84
1:B:317:ARG:HA	1:B:358:MET:HE3	1.58	0.83
1:B:102:MET:CE	1:B:219:ARG:HG3	2.07	0.83
1:B:22:LYS:HD3	1:B:92:ARG:HH21	1.43	0.83
1:C:309:ALA:HA	1:C:312:LEU:HD12	1.57	0.83
1:C:323:GLU:OE2	1:C:335:GLN:NE2	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:LYS:NZ	1:A:593:GLU:OE1	2.11	0.83
1:B:541:ASP:OD2	1:B:561:ARG:HD3	1.77	0.83
1:B:32:LEU:HD22	1:B:311:LYS:NZ	1.93	0.83
1:B:151:HIS:O	1:B:155:ILE:HG13	1.79	0.83
1:C:746:ILE:HD13	1:C:773:MET:HE1	1.59	0.82
1:C:226:MET:HE1	1:C:463:MET:HE3	1.61	0.82
1:A:258:THR:O	1:A:259:ARG:HG3	1.78	0.82
1:A:255:VAL:HG13	1:A:322:MET:O	1.80	0.81
1:C:109:LEU:HD12	1:C:136:PHE:HE1	1.42	0.81
1:C:491:ALA:N	1:C:494:ASP:OD2	2.12	0.81
1:C:843:PHE:O	1:C:847:VAL:HG22	1.80	0.81
1:A:80:PHE:HE2	1:A:200:PRO:O	1.64	0.81
1:A:382:ASN:HD22	1:A:385:ALA:HB2	1.43	0.81
1:C:745:GLU:HB2	1:C:769:ASP:HB2	1.61	0.81
1:D:62:GLN:HG3	1:D:205:MET:HE3	1.63	0.81
1:D:310:MET:HA	1:D:310:MET:HE2	1.62	0.80
1:D:623:LEU:HB2	1:D:655:LEU:HD22	1.60	0.80
1:B:12:ASN:ND2	1:B:14:SER:OG	2.14	0.80
1:C:78:LYS:HD3	1:C:86:PRO:O	1.81	0.80
1:C:844:CYS:HB3	1:C:849:LEU:HD22	1.62	0.80
1:C:382:ASN:HD22	1:C:385:ALA:CB	1.94	0.80
1:C:118:GLY:O	1:C:122:LYS:HG2	1.82	0.80
1:C:369:GLU:HG2	1:C:372:SER:HB3	1.63	0.80
1:B:785:PHE:CE1	1:B:786:LEU:HD13	2.16	0.80
1:D:29:MET:CB	1:D:36:ILE:HD11	2.11	0.80
1:D:837:ASP:HB3	1:D:840:SER:HB2	1.61	0.80
1:C:662:MET:HB3	1:D:777:PHE:HA	1.63	0.80
1:A:289:GLN:HE21	1:A:293:GLN:HG2	1.45	0.80
1:C:572:ILE:HG13	1:C:576:ARG:HE	1.46	0.80
1:C:306:MET:HE1	1:C:310:MET:HE2	1.63	0.79
1:C:777:PHE:HA	1:D:662:MET:CB	2.06	0.79
1:B:528:ALA:CB	1:B:867:ALA:HB2	2.12	0.79
1:D:172:THR:HG22	1:D:174:ASP:H	1.47	0.79
1:B:651:LYS:HD3	1:B:654:GLU:OE1	1.83	0.79
1:A:323:GLU:CD	1:A:335:GLN:HE21	1.91	0.79
1:B:675:GLU:HA	1:B:678:LYS:HD2	1.64	0.79
1:C:6:TYR:O	1:C:40:PHE:HB2	1.82	0.79
1:C:256:ALA:O	1:C:322:MET:HE2	1.83	0.79
1:A:453:THR:O	1:A:453:THR:HG22	1.81	0.78
1:C:386:LEU:HD12	1:C:510:ILE:HD12	1.65	0.78
1:C:337:ARG:NH1	2:C:901:ANP:OI1G	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:LYS:HA	1:B:194:GLU:O	1.83	0.78
1:A:57:ILE:HD12	1:A:61:ILE:HG21	1.66	0.78
1:A:482:THR:HB	1:A:489:THR:HG22	1.63	0.78
1:D:38:GLN:O	1:D:241:THR:HG22	1.83	0.78
1:A:255:VAL:HG22	1:A:323:GLU:HG2	1.65	0.78
1:C:594:LEU:HB2	1:C:679:MET:HE2	1.65	0.78
1:A:454:SER:O	1:A:458:VAL:HG23	1.84	0.78
1:A:435:ASP:O	1:A:439:MET:HG3	1.84	0.78
1:A:784:LYS:HD3	1:B:664:HIS:HB2	1.63	0.78
1:C:306:MET:HE1	1:C:310:MET:CE	2.13	0.78
1:A:690:GLU:O	1:A:694:GLU:HG3	1.84	0.78
1:A:73:GLU:HG2	1:A:79:LYS:HA	1.64	0.78
1:D:855:SER:OG	1:D:858:ARG:HG3	1.85	0.77
1:C:347:LEU:HD23	1:C:524:ILE:HG13	1.66	0.77
1:B:830:ILE:HG22	1:B:852:VAL:HG12	1.65	0.77
1:D:790:TYR:OH	1:D:798:ASP:HB2	1.84	0.77
1:C:102:MET:HE3	1:C:219:ARG:HG3	1.67	0.77
1:B:92:ARG:HD3	2:B:901:ANP:C8	2.13	0.77
1:D:638:ALA:HA	1:D:648:VAL:HG21	1.67	0.77
1:B:285:VAL:HG12	1:B:286:ARG:HD3	1.66	0.77
1:C:630:THR:O	1:C:634:GLN:HG3	1.85	0.76
1:B:152:PHE:O	1:B:156:ILE:HG22	1.85	0.76
1:C:746:ILE:HD12	1:D:776:GLY:HA3	1.67	0.76
1:D:406:LYS:HE2	1:D:493:GLY:O	1.84	0.76
1:A:216:ASP:OD1	1:A:793:LYS:HE3	1.84	0.76
1:A:685:MET:HE2	1:A:725:ALA:HB1	1.67	0.76
1:B:767:THR:OG1	1:B:834:HIS:ND1	2.17	0.76
1:C:635:ALA:O	1:C:638:ALA:HB3	1.84	0.76
1:D:134:ARG:HB3	1:D:180:ALA:HB2	1.67	0.76
1:B:323:GLU:OE1	1:B:335:GLN:NE2	2.19	0.76
1:B:407:VAL:HA	1:B:425:ILE:O	1.84	0.76
1:C:240:GLN:HG2	2:C:901:ANP:N6	2.00	0.76
1:D:381:PHE:CD2	1:D:386:LEU:HD13	2.21	0.76
1:C:159:MET:HE3	1:C:159:MET:HA	1.69	0.75
1:D:181:GLU:HA	1:D:184:LYS:HD3	1.68	0.75
1:C:615:THR:CG2	1:C:704:MET:HE2	2.17	0.75
1:C:674:PRO:O	1:C:678:LYS:HG3	1.86	0.75
1:D:119:PHE:O	1:D:123:THR:HG23	1.86	0.75
1:D:474:ILE:HG13	1:D:485:LEU:HD13	1.69	0.75
1:D:144:VAL:HG12	1:D:145:MET:HE3	1.68	0.75
1:D:373:LEU:HD11	1:D:864:LEU:HD22	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:ILE:HG21	1:D:507:LYS:HB2	1.68	0.75
1:A:255:VAL:HB	1:A:453:THR:HG23	1.68	0.75
1:C:103:MET:HB3	1:C:214:SER:HB3	1.67	0.75
1:C:552:LEU:O	1:C:863:ARG:NH1	2.20	0.75
1:C:584:VAL:HG22	1:C:588:GLU:OE2	1.87	0.75
1:D:435:ASP:O	1:D:439:MET:HG3	1.85	0.75
1:A:578:MET:HG2	1:A:587:ARG:HG3	1.68	0.75
1:B:20:GLY:O	1:B:24:CYS:HB3	1.86	0.75
1:D:149:LYS:O	1:D:152:PHE:N	2.20	0.75
1:A:845:HIS:CE1	1:A:870:ALA:HA	2.22	0.75
1:C:552:LEU:HD22	1:C:860:PRO:HG3	1.68	0.75
1:C:780:ASP:HB3	1:D:658:PHE:CE2	2.21	0.75
1:A:39:GLY:HA3	1:A:240:GLN:HA	1.68	0.75
1:C:780:ASP:HB3	1:D:658:PHE:HE2	1.52	0.74
1:A:763:PHE:HB2	1:A:828:CYS:HB3	1.69	0.74
1:C:448:VAL:HG22	1:C:474:ILE:HB	1.68	0.74
1:A:175:ASP:O	1:A:179:LEU:N	2.15	0.74
1:B:259:ARG:HB2	1:B:319:MET:HG3	1.69	0.74
1:A:739:HIS:ND1	1:A:761:GLU:OE1	2.19	0.74
1:D:188:LYS:HA	1:D:194:GLU:O	1.87	0.74
1:C:455:HIS:HE1	2:C:901:ANP:N3B	1.85	0.74
1:A:804:ASP:OD2	1:A:808:VAL:HG23	1.86	0.74
1:A:661:MET:HG2	1:A:662:MET:HG2	1.69	0.74
1:B:353:LEU:HD22	1:B:358:MET:HE2	1.70	0.74
1:B:578:MET:HG3	1:B:591:LEU:HG	1.70	0.74
1:D:496:ILE:HG22	1:D:507:LYS:HA	1.70	0.74
1:D:525:MET:HE2	1:D:525:MET:HA	1.68	0.74
1:B:661:MET:C	1:B:662:MET:HG2	2.13	0.73
1:C:92:ARG:HD2	2:C:901:ANP:O2A	1.86	0.73
1:C:153:GLU:HA	1:C:156:ILE:HB	1.69	0.73
1:D:827:LYS:HE3	1:D:850:ASN:ND2	2.03	0.73
1:B:785:PHE:HE1	1:B:786:LEU:HD13	1.51	0.73
1:A:360:THR:OG1	1:A:363:GLU:HG3	1.87	0.73
1:B:49:GLU:O	1:B:53:SER:N	2.19	0.73
1:B:205:MET:HA	1:B:205:MET:CE	2.18	0.73
1:C:215:TRP:NE1	1:C:231:GLY:O	2.15	0.73
1:C:312:LEU:HD11	1:C:333:PHE:CE2	2.24	0.73
1:D:153:GLU:O	1:D:156:ILE:HG22	1.88	0.73
1:B:92:ARG:HD3	2:B:901:ANP:N7	2.04	0.73
1:C:257:PHE:HB3	1:C:319:MET:SD	2.29	0.73
1:A:131:ASP:O	1:A:134:ARG:HG3	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:784:LYS:CD	1:B:664:HIS:HB2	2.18	0.73
1:A:323:GLU:OE1	1:A:335:GLN:NE2	2.20	0.73
1:B:779:ARG:HA	1:B:800:PHE:CE2	2.23	0.73
1:A:174:ASP:OD1	1:A:177:LYS:HD2	1.87	0.73
1:B:499:ASP:OD1	1:B:502:THR:HG23	1.89	0.73
1:D:104:ASP:H	1:D:214:SER:HB3	1.53	0.73
1:D:174:ASP:HA	1:D:177:LYS:HB2	1.69	0.72
1:C:305:PHE:CE1	1:C:324:PHE:CD1	2.78	0.72
1:D:717:VAL:O	1:D:721:VAL:HG23	1.89	0.72
1:A:230:PRO:HG2	1:A:233:TRP:CZ2	2.24	0.72
1:B:144:VAL:O	1:B:145:MET:HE2	1.89	0.72
1:C:455:HIS:HE1	2:C:901:ANP:PB	2.12	0.72
1:D:578:MET:HG2	1:D:587:ARG:HG3	1.71	0.72
1:A:91:VAL:HG22	1:A:239:VAL:HG13	1.71	0.72
1:A:107:LEU:HG	1:A:139:MET:HE1	1.70	0.72
1:A:370:ALA:HA	1:A:864:LEU:HD23	1.72	0.72
1:A:689:ILE:O	1:A:693:GLU:HG3	1.89	0.72
1:B:812:VAL:O	1:B:816:VAL:HG23	1.89	0.72
1:C:92:ARG:HD3	2:C:901:ANP:H8	1.70	0.72
1:A:430:GLU:HA	1:A:449:ARG:O	1.88	0.72
1:B:81:GLY:HA3	1:B:200:PRO:HG3	1.71	0.72
1:D:188:LYS:HE3	1:D:193:GLY:O	1.90	0.72
1:B:827:LYS:HD3	1:B:827:LYS:N	2.02	0.72
1:D:599:LYS:HE3	1:D:686:GLU:HB3	1.72	0.72
1:D:678:LYS:HA	1:D:724:VAL:HG21	1.72	0.72
1:C:573:MET:HE1	1:C:637:LEU:HD13	1.72	0.72
1:C:612:ARG:HH11	1:C:612:ARG:HG3	1.54	0.72
1:C:38:GLN:O	1:C:241:THR:HG22	1.90	0.71
1:A:255:VAL:HB	1:A:453:THR:HG21	1.71	0.71
1:B:396:LEU:O	1:B:468:VAL:HA	1.90	0.71
1:C:200:PRO:HA	1:C:203:GLN:OE1	1.90	0.71
1:C:142:ASP:OD2	1:C:149:LYS:HD3	1.90	0.71
1:C:592:ASN:HA	1:C:595:ILE:HG13	1.71	0.71
1:A:864:LEU:O	1:A:868:GLN:HG3	1.91	0.71
1:D:707:LEU:HD23	1:D:745:GLU:HG3	1.71	0.71
1:A:173:ALA:O	1:A:177:LYS:HG3	1.90	0.71
1:C:8:PHE:HB2	1:C:38:GLN:HE22	1.55	0.71
1:D:282:VAL:HB	1:D:455:HIS:CD2	2.26	0.71
1:A:99:MET:HE3	1:A:223:TYR:HD1	1.56	0.71
1:B:628:PRO:HG2	1:B:634:GLN:HG2	1.73	0.71
1:C:317:ARG:NH2	1:C:359:ILE:HA	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:HIS:CE1	2:C:901:ANP:N3B	2.58	0.71
1:D:808:VAL:O	1:D:812:VAL:HG23	1.91	0.71
1:A:167:PHE:HB3	1:A:169:THR:HG23	1.73	0.71
1:B:61:ILE:O	1:B:65:ILE:HG12	1.91	0.71
1:C:92:ARG:NH2	1:C:334:LEU:O	2.23	0.71
1:C:103:MET:HE2	1:C:215:TRP:HE3	1.55	0.71
1:D:727:GLN:O	1:D:731:GLU:HG3	1.91	0.71
1:A:282:VAL:HG11	2:A:4001:ANP:O2B	1.91	0.71
1:B:568:GLU:O	1:B:571:ARG:N	2.20	0.71
1:D:16:ARG:NH2	3:D:903:SO4:O2	2.24	0.71
1:A:108:ASN:OD1	1:A:242:MET:HE2	1.91	0.70
1:B:110:GLY:HA2	1:B:203:GLN:OE1	1.91	0.70
1:C:751:LEU:HD11	1:D:811:LEU:HG	1.72	0.70
1:C:806:THR:O	1:C:810:GLN:NE2	2.23	0.70
1:B:116:VAL:HG21	1:B:133:TYR:CD2	2.25	0.70
1:B:260:ASN:CG	1:B:263:THR:HG23	2.16	0.70
1:C:574:LYS:HB2	1:C:594:LEU:HD21	1.72	0.70
1:B:394:SER:HB3	1:B:504:LYS:HA	1.73	0.70
1:C:630:THR:HB	1:C:633:GLU:H	1.55	0.70
1:C:259:ARG:HB2	1:C:349:ILE:HD13	1.73	0.70
1:C:743:MET:HB3	1:C:745:GLU:OE2	1.91	0.70
1:D:835:GLY:O	1:D:854:CYS:HB3	1.92	0.70
1:A:159:MET:HE1	1:A:178:GLU:HB3	1.73	0.70
1:A:405:GLY:HA3	1:A:423:ARG:O	1.92	0.70
1:D:553:GLY:HA3	1:D:863:ARG:NH1	2.07	0.70
1:D:570:ASP:OD2	1:D:570:ASP:N	2.23	0.70
1:A:416:ALA:HA	1:A:419:GLU:OE2	1.91	0.70
1:B:9:GLU:HA	1:B:31:ILE:CD1	2.22	0.70
1:D:598:GLN:HA	1:D:601:ASP:OD2	1.92	0.70
1:B:22:LYS:HD3	1:B:92:ARG:NH2	2.05	0.69
1:D:553:GLY:HA3	1:D:863:ARG:HH11	1.57	0.69
1:A:256:ALA:HA	1:A:270:GLY:HA3	1.74	0.69
1:C:580:LEU:HD13	1:C:651:LYS:HG2	1.72	0.69
1:C:805:GLN:HG2	1:C:843:PHE:CD1	2.27	0.69
1:D:381:PHE:HZ	1:D:497:SER:HB3	1.57	0.69
1:B:112:ASN:O	1:B:116:VAL:HG23	1.92	0.69
1:D:343:ALA:HB2	1:D:372:SER:O	1.92	0.69
1:D:682:ARG:NH1	1:D:728:VAL:HG22	2.07	0.69
1:A:563:GLU:CD	1:A:617:ARG:HH12	2.00	0.69
1:A:777:PHE:HE1	1:A:800:PHE:CE2	2.10	0.69
1:C:305:PHE:HE1	1:C:324:PHE:CG	2.11	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:763:PHE:N	1:D:827:LYS:O	2.24	0.69
1:A:116:VAL:HG21	1:A:133:TYR:CG	2.27	0.69
1:A:334:LEU:HD13	2:A:4001:ANP:O2'	1.92	0.69
1:D:628:PRO:HB2	1:D:633:GLU:HB3	1.74	0.69
1:A:871:LEU:O	1:A:873:ASN:N	2.22	0.69
1:D:135:ARG:NH1	1:D:277:GLN:HB2	2.07	0.69
1:A:224:ARG:HG2	1:A:229:ILE:HB	1.75	0.69
1:A:255:VAL:CG2	1:A:323:GLU:HG2	2.22	0.69
1:C:186:VAL:O	1:C:189:GLU:HB3	1.92	0.69
1:C:615:THR:HG22	1:C:704:MET:HE2	1.75	0.69
1:D:674:PRO:O	1:D:678:LYS:HG3	1.93	0.69
1:A:556:GLY:HA2	1:A:612:ARG:HB3	1.74	0.69
1:B:440:HIS:HB2	1:B:463:MET:HE1	1.74	0.69
1:C:614:MET:O	1:C:702:GLU:HB2	1.93	0.69
1:C:637:LEU:HD21	1:C:641:MET:HE3	1.74	0.69
1:D:116:VAL:HG21	1:D:133:TYR:CG	2.28	0.69
1:A:482:THR:HA	1:A:490:PHE:O	1.92	0.69
1:A:674:PRO:O	1:A:678:LYS:HG3	1.93	0.69
1:A:409:PHE:CE2	1:A:476:ILE:HG23	2.28	0.68
1:A:778:SER:OG	1:A:781:ASP:HB2	1.92	0.68
1:A:843:PHE:HA	1:A:846:LYS:HE2	1.76	0.68
1:B:782:ALA:O	1:B:784:LYS:N	2.25	0.68
1:C:571:ARG:NH1	1:C:597:PHE:HB3	2.07	0.68
1:D:554:ALA:HB2	1:D:859:VAL:HG21	1.75	0.68
1:B:255:VAL:HB	1:B:453:THR:HG23	1.74	0.68
1:C:406:LYS:HB3	1:C:493:GLY:O	1.93	0.68
1:C:596:PRO:HG2	1:C:597:PHE:CD1	2.28	0.68
1:C:820:ARG:HA	1:C:823:ARG:O	1.93	0.68
1:A:341:ARG:HG3	1:A:346:ALA:HB2	1.74	0.68
1:B:392:ILE:HD12	1:B:485:LEU:HD23	1.73	0.68
1:D:102:MET:HB3	1:D:220:ALA:HA	1.73	0.68
1:D:481:LYS:HD3	1:D:492:GLU:OE2	1.93	0.68
1:B:258:THR:HB	1:B:310:MET:HE1	1.74	0.68
1:D:28:GLU:O	1:D:32:LEU:HD12	1.94	0.68
1:D:131:ASP:O	1:D:134:ARG:HG3	1.92	0.68
1:D:439:MET:O	1:D:465:THR:HG21	1.93	0.68
1:A:777:PHE:HA	1:B:662:MET:HB3	1.74	0.68
1:B:22:LYS:HE3	1:B:335:GLN:OE1	1.93	0.68
1:B:530:LYS:HE3	1:B:531:PHE:CE1	2.28	0.68
1:A:91:VAL:HG12	1:A:211:VAL:HG21	1.76	0.68
1:B:62:GLN:HG3	1:B:205:MET:SD	2.33	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:PRO:O	1:B:546:THR:HB	1.94	0.68
1:C:89:VAL:HG12	1:C:241:THR:HA	1.76	0.68
1:C:690:GLU:CG	1:C:732:LYS:HE3	2.21	0.68
1:B:387:LYS:HG2	1:B:387:LYS:O	1.93	0.68
1:B:578:MET:HG2	1:B:587:ARG:HA	1.76	0.68
1:D:439:MET:HE1	1:D:456:ALA:O	1.94	0.68
1:D:512:THR:HG23	1:D:513:GLN:N	2.08	0.68
1:C:54:GLY:O	1:C:56:GLN:HG3	1.94	0.68
1:B:80:PHE:CE2	1:B:200:PRO:HB2	2.29	0.68
1:B:374:ASP:OD1	1:B:375:GLN:N	2.26	0.68
1:C:482:THR:HG22	1:C:491:ALA:CB	2.24	0.68
1:D:116:VAL:HG21	1:D:133:TYR:CD2	2.28	0.68
1:B:293:GLN:HA	1:B:293:GLN:HE21	1.58	0.67
1:C:746:ILE:CD1	1:C:773:MET:HE1	2.24	0.67
1:C:823:ARG:HD2	1:C:826:LEU:HD13	1.77	0.67
1:A:83:THR:O	1:A:118:GLY:HA3	1.94	0.67
1:A:707:LEU:HD22	1:A:746:ILE:HD11	1.76	0.67
1:C:395:ALA:HB3	1:C:471:CYS:SG	2.33	0.67
1:A:455:HIS:NE2	2:A:4001:ANP:N3B	2.42	0.67
1:C:382:ASN:HD22	1:C:385:ALA:HB3	1.57	0.67
1:C:423:ARG:NH2	1:C:509:ASP:OD1	2.27	0.67
1:C:785:PHE:HB3	1:D:664:HIS:CD2	2.30	0.67
1:D:253:THR:HG21	1:D:278:GLY:HA2	1.76	0.67
1:B:406:LYS:HE3	1:B:493:GLY:O	1.93	0.67
1:B:591:LEU:O	1:B:594:LEU:HB2	1.94	0.67
1:C:173:ALA:O	1:C:177:LYS:HG3	1.94	0.67
1:C:266:LYS:NZ	1:C:356:GLU:OE2	2.28	0.67
1:A:496:ILE:HD12	1:A:497:SER:O	1.94	0.67
1:A:674:PRO:HB3	1:A:720:VAL:HG21	1.76	0.67
1:C:240:GLN:HG2	2:C:901:ANP:HN61	1.58	0.67
1:A:537:ARG:NH1	1:A:613:PRO:HG2	2.07	0.67
1:A:811:LEU:HD23	1:A:814:MET:HE3	1.76	0.67
1:B:399:SER:O	1:B:500:GLY:HA3	1.95	0.67
1:D:24:CYS:O	1:D:27:ALA:HB3	1.95	0.67
1:A:525:MET:HA	1:A:525:MET:CE	2.25	0.67
1:B:389:GLY:HA3	1:B:510:ILE:HD11	1.75	0.67
1:A:180:ALA:O	1:A:183:PHE:HB2	1.95	0.67
1:C:289:GLN:OE1	1:C:293:GLN:NE2	2.27	0.67
1:D:774:THR:HG21	1:D:808:VAL:HG22	1.76	0.67
1:C:92:ARG:HD3	2:C:901:ANP:C8	2.25	0.67
1:A:214:SER:HA	1:A:217:ASN:ND2	2.11	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ARG:HB2	1:A:319:MET:HG3	1.77	0.67
1:A:330:LYS:HD3	1:A:332:TYR:OH	1.95	0.67
1:A:453:THR:CG2	1:A:453:THR:O	2.43	0.67
1:B:255:VAL:HB	1:B:453:THR:HG21	1.75	0.67
1:D:572:ILE:HG13	1:D:576:ARG:NE	2.09	0.67
1:C:44:THR:O	1:C:47:CYS:HB3	1.95	0.66
1:A:718:LYS:HG3	1:A:740:ILE:HD13	1.76	0.66
1:B:92:ARG:CD	2:B:901:ANP:H8	2.25	0.66
1:B:833:GLU:HG3	1:B:858:ARG:HH22	1.60	0.66
1:B:321:ASP:OD1	1:B:337:ARG:HG2	1.95	0.66
1:B:365:VAL:HG11	1:B:867:ALA:HB1	1.76	0.66
1:D:369:GLU:HB3	1:D:372:SER:OG	1.95	0.66
1:A:44:THR:HG23	1:A:236:ALA:HB2	1.78	0.66
1:A:99:MET:HE1	1:A:224:ARG:HG3	1.77	0.66
1:C:9:GLU:O	1:C:31:ILE:HD11	1.96	0.66
1:C:711:LYS:HD3	1:C:755:ALA:O	1.95	0.66
1:A:382:ASN:HD22	1:A:385:ALA:CB	2.09	0.66
1:B:373:LEU:HD22	1:B:376:LEU:HD11	1.78	0.66
1:C:30:THR:HA	1:C:36:ILE:CD1	2.26	0.66
1:C:581:SER:HB2	1:C:587:ARG:HG3	1.78	0.66
1:D:321:ASP:HB3	1:D:337:ARG:HG3	1.77	0.66
1:A:223:TYR:O	1:A:227:ASN:ND2	2.29	0.66
1:C:117:GLU:O	1:C:121:LYS:HG3	1.96	0.66
1:C:424:VAL:O	1:C:443:GLU:HB2	1.95	0.66
1:D:704:MET:HA	1:D:741:GLY:O	1.95	0.66
1:A:145:MET:HG3	1:A:187:TYR:CE2	2.30	0.66
1:A:274:ILE:HD11	1:A:298:MET:HE1	1.78	0.66
1:D:782:ALA:O	1:D:786:LEU:HB2	1.95	0.66
1:A:704:MET:SD	1:A:743:MET:HG2	2.35	0.66
1:B:92:ARG:HA	1:B:105:THR:HG23	1.78	0.66
1:B:137:ILE:HG23	1:B:196:PHE:CD2	2.30	0.66
1:C:354:VAL:HG22	1:C:359:ILE:HG13	1.77	0.66
1:C:574:LYS:HD2	1:C:574:LYS:H	1.61	0.66
1:C:685:MET:O	1:C:689:ILE:HG13	1.95	0.66
1:B:32:LEU:HD22	1:B:311:LYS:HZ1	1.59	0.66
1:B:743:MET:HE3	1:B:745:GLU:CD	2.21	0.66
1:C:619:LEU:HD11	1:C:626:PHE:HZ	1.61	0.66
1:D:537:ARG:HD3	1:D:851:TYR:CD1	2.30	0.66
1:D:682:ARG:HH11	1:D:682:ARG:CG	1.93	0.66
1:C:692:LYS:O	1:C:696:GLY:N	2.27	0.65
1:D:546:THR:O	1:D:550:VAL:HG23	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:PHE:N	1:A:269:TYR:O	2.29	0.65
1:C:102:MET:O	1:C:219:ARG:NH2	2.29	0.65
1:D:395:ALA:HB3	1:D:468:VAL:CG1	2.22	0.65
1:A:112:ASN:HA	1:A:133:TYR:CE1	2.32	0.65
1:B:690:GLU:O	1:B:694:GLU:N	2.28	0.65
1:C:116:VAL:HG11	1:C:130:TYR:CE1	2.31	0.65
1:C:342:THR:HG23	1:C:461:ARG:HG3	1.79	0.65
1:C:406:LYS:HA	1:C:494:ASP:O	1.95	0.65
1:A:82:ASP:O	1:A:86:PRO:HB3	1.97	0.65
1:A:662:MET:HE1	1:A:773:MET:HG3	1.78	0.65
1:A:855:SER:OG	1:A:858:ARG:HG3	1.97	0.65
1:B:23:GLY:HA2	1:B:26:LEU:HB2	1.76	0.65
1:B:150:SER:O	1:B:154:LYS:N	2.20	0.65
1:D:12:ASN:O	1:D:24:CYS:HB2	1.96	0.65
1:A:366:VAL:HG13	1:A:872:ASN:ND2	1.99	0.65
1:A:398:ALA:HA	1:A:452:MET:HG2	1.79	0.65
1:C:689:ILE:CG2	1:C:732:LYS:HD2	2.26	0.65
1:D:534:LEU:HB2	1:D:866:ALA:HB1	1.78	0.65
1:B:727:GLN:OE1	1:B:731:GLU:HG3	1.95	0.65
1:D:102:MET:HE3	1:D:223:TYR:HB2	1.79	0.65
1:C:182:LYS:O	1:C:185:ALA:HB3	1.97	0.65
1:D:522:GLU:O	1:D:526:VAL:HG23	1.97	0.65
1:D:682:ARG:NH2	1:D:731:GLU:OE2	2.29	0.65
1:D:802:ARG:HG3	1:D:802:ARG:NH1	2.03	0.65
1:A:11:GLY:C	1:A:27:ALA:HB1	2.21	0.65
1:D:34:MET:HE1	1:D:312:LEU:HD11	1.79	0.65
1:A:297:ASP:HB3	1:A:298:MET:HE2	1.79	0.65
1:A:406:LYS:HD3	1:A:422:GLU:OE2	1.97	0.65
1:B:99:MET:HA	1:B:223:TYR:CE1	2.32	0.65
1:C:81:GLY:HA3	1:C:200:PRO:HG3	1.79	0.65
1:C:480:ALA:O	1:C:482:THR:HG23	1.96	0.65
1:B:343:ALA:HB3	1:B:344:PRO:HD3	1.79	0.65
1:B:353:LEU:HB3	1:B:359:ILE:HG12	1.79	0.65
1:C:16:ARG:HA	1:C:24:CYS:HB3	1.79	0.65
1:C:30:THR:HA	1:C:36:ILE:HD11	1.79	0.65
1:A:50:TYR:HE1	1:A:55:LYS:HZ1	1.43	0.64
1:A:289:GLN:HE22	1:A:293:GLN:HG2	1.62	0.64
1:C:188:LYS:HG3	1:C:195:GLU:HA	1.78	0.64
1:C:662:MET:HE3	1:C:773:MET:SD	2.37	0.64
1:A:79:LYS:O	1:A:82:ASP:HB2	1.96	0.64
1:C:644:THR:C	1:C:646:ALA:H	2.03	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:710:GLU:O	1:C:713:GLU:HB3	1.96	0.64
1:B:567:PHE:O	1:B:572:ILE:HB	1.97	0.64
1:C:553:GLY:HA3	1:C:863:ARG:CZ	2.27	0.64
1:D:408:TYR:OH	1:D:422:GLU:OE2	2.14	0.64
1:A:92:ARG:CG	1:A:238:ASN:HB2	2.26	0.64
1:C:581:SER:HB3	1:C:586:ALA:CB	2.27	0.64
1:A:662:MET:HE1	1:A:773:MET:CG	2.28	0.64
1:A:372:SER:HB2	1:A:375:GLN:NE2	2.13	0.64
1:B:398:ALA:O	1:B:461:ARG:HD3	1.97	0.64
1:C:664:HIS:HB2	1:D:784:LYS:HD2	1.80	0.64
1:C:4:TRP:CG	1:C:61:ILE:HG12	2.33	0.64
1:C:394:SER:HB3	1:C:504:LYS:HA	1.80	0.64
1:C:521:PHE:HZ	1:C:860:PRO:HB3	1.63	0.64
1:A:523:ARG:HG2	1:A:527:TRP:CZ2	2.33	0.64
1:C:103:MET:HB3	1:C:214:SER:CB	2.28	0.64
1:C:103:MET:HE2	1:C:215:TRP:CE3	2.33	0.64
1:C:166:HIS:HB3	1:C:167:PHE:CD2	2.33	0.64
1:C:285:VAL:HG12	1:C:286:ARG:HD3	1.80	0.64
1:C:659:ASN:OD1	1:D:661:MET:HB2	1.98	0.64
1:A:777:PHE:HB3	1:B:668:ARG:CZ	2.27	0.64
1:A:366:VAL:CG1	1:A:872:ASN:HD21	2.01	0.63
1:B:210:ALA:HA	1:B:213:ARG:HG3	1.81	0.63
1:B:797:SER:O	1:B:799:PRO:HD3	1.99	0.63
1:A:70:THR:HA	1:A:73:GLU:OE2	1.97	0.63
1:A:369:GLU:OE1	1:A:372:SER:HB3	1.98	0.63
1:B:580:LEU:HB2	1:B:641:MET:HE1	1.81	0.63
1:C:521:PHE:CZ	1:C:860:PRO:HB3	2.33	0.63
1:D:637:LEU:HG	1:D:641:MET:HE2	1.79	0.63
1:D:661:MET:HB3	1:D:662:MET:HE3	1.81	0.63
1:D:843:PHE:HA	1:D:846:LYS:HD3	1.79	0.63
1:A:428:ARG:O	1:A:447:THR:HA	1.99	0.63
1:C:495:TYR:CD2	1:C:509:ASP:HB2	2.34	0.63
1:C:612:ARG:HG3	1:C:612:ARG:NH1	2.12	0.63
1:C:672:THR:O	1:C:674:PRO:HD3	1.99	0.63
1:A:536:VAL:HG22	1:A:852:VAL:CG2	2.28	0.63
1:D:429:LEU:HG	1:D:430:GLU:HG3	1.81	0.63
1:D:842:GLU:HG2	1:D:846:LYS:HD2	1.81	0.63
1:A:16:ARG:NH1	1:A:21:GLY:HA2	2.14	0.63
1:B:678:LYS:HB3	1:B:724:VAL:HG21	1.80	0.63
1:C:330:LYS:HB2	1:C:330:LYS:NZ	2.14	0.63
1:C:555:GLU:O	1:C:612:ARG:HD2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ALA:O	1:A:461:ARG:HD3	1.98	0.63
1:A:746:ILE:HD12	1:B:776:GLY:HA3	1.80	0.63
1:C:574:LYS:HD2	1:C:574:LYS:N	2.13	0.63
1:D:218:PRO:O	1:D:222:VAL:HG23	1.99	0.63
1:A:98:SER:O	1:A:100:PRO:HD3	1.99	0.62
1:A:372:SER:C	1:A:374:ASP:H	2.07	0.62
1:B:38:GLN:O	1:B:241:THR:HG22	1.99	0.62
1:B:134:ARG:O	1:B:138:GLN:HB2	1.98	0.62
1:B:455:HIS:HE1	2:B:901:ANP:O2B	1.81	0.62
1:B:729:LYS:HE3	1:B:736:MET:H	1.64	0.62
1:C:205:MET:HA	1:C:205:MET:HE2	1.79	0.62
1:A:149:LYS:O	1:A:153:GLU:HB2	1.97	0.62
1:B:260:ASN:OD1	1:B:263:THR:HG23	1.98	0.62
1:B:395:ALA:HB1	1:B:469:SER:O	1.99	0.62
1:B:572:ILE:HG13	1:B:576:ARG:NE	2.13	0.62
1:B:657:GLU:OE2	1:B:663:GLY:HA3	2.00	0.62
1:B:34:MET:HB3	1:B:35:PRO:HD2	1.79	0.62
1:C:668:ARG:HG2	1:D:785:PHE:CE1	2.33	0.62
1:D:690:GLU:HA	1:D:693:GLU:OE1	1.98	0.62
1:A:628:PRO:CB	1:A:633:GLU:HB3	2.27	0.62
1:A:777:PHE:HE1	1:A:800:PHE:HE2	1.46	0.62
1:C:22:LYS:NZ	2:C:901:ANP:O2A	2.33	0.62
1:C:107:LEU:HB3	1:C:242:MET:HE1	1.81	0.62
1:C:724:VAL:O	1:C:728:VAL:HG23	2.00	0.62
1:D:474:ILE:CG1	1:D:485:LEU:HD13	2.29	0.62
1:A:767:THR:HG21	1:A:830:ILE:HD11	1.79	0.62
1:C:200:PRO:HA	1:C:203:GLN:CD	2.24	0.62
1:C:268:ILE:HG13	1:C:269:TYR:N	2.14	0.62
1:C:365:VAL:HG13	1:C:864:LEU:CD1	2.29	0.62
1:C:565:MET:HB3	1:C:598:GLN:HE21	1.63	0.62
1:D:282:VAL:HB	1:D:455:HIS:NE2	2.14	0.62
1:D:624:HIS:HB2	1:D:655:LEU:O	2.00	0.62
1:D:743:MET:HG2	1:D:764:SER:O	2.00	0.62
1:A:529:ASP:OD1	1:A:532:ARG:NH2	2.30	0.62
1:C:102:MET:HE3	1:C:219:ARG:CG	2.29	0.62
1:C:108:ASN:HB2	1:C:136:PHE:HB2	1.81	0.62
1:C:382:ASN:HB3	1:C:385:ALA:HB3	1.81	0.62
1:A:108:ASN:HB2	1:A:136:PHE:HB2	1.82	0.62
1:B:93:SER:HB3	1:B:211:VAL:CG1	2.25	0.62
1:B:448:VAL:C	1:B:449:ARG:HG2	2.24	0.62
1:D:102:MET:CE	1:D:223:TYR:HB2	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:VAL:HG13	1:A:494:ASP:O	2.00	0.62
1:A:871:LEU:C	1:A:873:ASN:H	2.07	0.62
1:B:92:ARG:HH11	2:B:901:ANP:H8	1.65	0.62
1:B:425:ILE:CG2	1:B:496:ILE:HD11	2.26	0.62
1:C:116:VAL:HG21	1:C:133:TYR:CD2	2.35	0.62
1:C:343:ALA:HB3	1:C:344:PRO:CD	2.29	0.62
1:C:567:PHE:HA	1:C:572:ILE:HD13	1.81	0.62
1:B:417:ALA:O	1:B:422:GLU:HB2	2.00	0.62
1:A:93:SER:HB3	1:A:211:VAL:HG13	1.81	0.62
1:A:373:LEU:HB3	1:A:376:LEU:HD12	1.81	0.62
1:A:448:VAL:HG22	1:A:474:ILE:HB	1.80	0.62
1:C:102:MET:HA	1:C:219:ARG:HE	1.64	0.62
1:D:252:GLY:HA3	1:D:272:TYR:OH	2.00	0.62
1:D:845:HIS:O	1:D:846:LYS:C	2.42	0.62
1:A:159:MET:HG3	1:A:163:LYS:HG3	1.80	0.61
1:A:409:PHE:O	1:A:428:ARG:NH1	2.32	0.61
1:B:90:SER:HB3	1:B:242:MET:SD	2.40	0.61
1:B:118:GLY:O	1:B:122:LYS:HG2	2.00	0.61
1:A:532:ARG:HB3	1:A:867:ALA:HA	1.82	0.61
1:B:794:ILE:O	1:B:795:TYR:HD1	1.84	0.61
1:C:637:LEU:HA	1:C:640:ASN:ND2	2.14	0.61
1:D:107:LEU:HD21	2:D:901:ANP:C8	2.30	0.61
1:D:543:PRO:O	1:D:547:LEU:HG	2.00	0.61
1:B:342:THR:HG23	1:B:461:ARG:HG2	1.83	0.61
1:B:572:ILE:HG13	1:B:576:ARG:HE	1.65	0.61
1:B:651:LYS:O	1:B:654:GLU:HB3	2.00	0.61
1:D:347:LEU:O	1:D:350:ALA:HB3	2.00	0.61
1:B:842:GLU:O	1:B:845:HIS:N	2.31	0.61
1:C:565:MET:CB	1:C:598:GLN:HE21	2.13	0.61
1:A:185:ALA:HA	1:A:188:LYS:HE2	1.80	0.61
1:A:352:ASP:O	1:A:356:GLU:HG3	2.00	0.61
1:A:521:PHE:HE1	1:A:860:PRO:HB3	1.64	0.61
1:B:160:LYS:HG2	1:B:171:LEU:HD21	1.82	0.61
1:B:557:ILE:HG21	1:B:560:CYS:HB2	1.80	0.61
1:C:127:ARG:NH1	1:C:246:ASN:O	2.29	0.61
1:C:305:PHE:CE1	1:C:324:PHE:CG	2.88	0.61
1:C:407:VAL:HG21	1:C:483:PHE:HE1	1.65	0.61
1:A:257:PHE:CZ	1:A:321:ASP:OD1	2.53	0.61
1:A:743:MET:HE1	1:A:766:GLY:HA3	1.83	0.61
1:B:289:GLN:HB3	1:B:290:PRO:HD2	1.81	0.61
1:C:440:HIS:HA	1:C:463:MET:HE1	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:ILE:HG12	1:D:224:ARG:NH2	2.15	0.61
1:A:455:HIS:CE1	2:A:4001:ANP:O2B	2.54	0.61
1:B:449:ARG:HA	1:B:470:GLY:HA2	1.82	0.61
1:C:282:VAL:HG21	1:C:323:GLU:OE1	2.00	0.61
1:D:32:LEU:HD21	1:D:315:HIS:CE1	2.35	0.61
1:A:534:LEU:HB2	1:A:866:ALA:HB1	1.83	0.61
1:C:362:GLU:HG3	1:C:531:PHE:CE1	2.35	0.61
1:C:386:LEU:CD1	1:C:510:ILE:HG21	2.30	0.61
1:C:682:ARG:O	1:C:686:GLU:HB2	2.01	0.61
1:D:149:LYS:O	1:D:150:SER:C	2.43	0.61
1:B:578:MET:SD	1:B:587:ARG:HG2	2.41	0.61
1:C:73:GLU:HG2	1:C:79:LYS:HA	1.83	0.61
1:C:216:ASP:OD1	1:C:793:LYS:HE3	2.01	0.61
1:A:603:LYS:HE2	1:A:691:VAL:HG23	1.82	0.61
1:A:635:ALA:HB2	1:A:645:LEU:HD13	1.82	0.61
1:B:830:ILE:CG2	1:B:852:VAL:HG12	2.30	0.61
1:C:575:ILE:O	1:C:579:ILE:HG13	2.01	0.61
1:C:639:LYS:HD2	1:C:640:ASN:OD1	2.00	0.61
1:D:342:THR:HG23	1:D:461:ARG:CG	2.31	0.61
1:A:134:ARG:HD2	1:A:134:ARG:C	2.25	0.60
1:B:518:SER:OG	1:B:519:GLY:N	2.33	0.60
1:A:196:PHE:O	1:A:198:GLN:NE2	2.34	0.60
1:B:159:MET:O	1:B:163:LYS:HB2	2.01	0.60
1:B:661:MET:HG2	1:B:662:MET:HE3	1.83	0.60
1:C:773:MET:SD	1:D:776:GLY:HA2	2.42	0.60
1:D:480:ALA:O	1:D:482:THR:HG23	2.01	0.60
1:A:409:PHE:HE2	1:A:476:ILE:HG23	1.65	0.60
1:A:488:HIS:CG	1:A:489:THR:H	2.19	0.60
1:C:746:ILE:HG22	1:C:748:ARG:H	1.65	0.60
1:D:473:GLU:HB2	1:D:485:LEU:HD11	1.84	0.60
1:A:587:ARG:O	1:A:588:GLU:C	2.44	0.60
1:B:102:MET:CE	1:B:219:ARG:O	2.49	0.60
1:B:606:TYR:CE1	1:B:614:MET:HE2	2.37	0.60
1:C:342:THR:HG23	1:C:461:ARG:CG	2.31	0.60
1:C:439:MET:HG2	1:C:445:ILE:HD13	1.82	0.60
1:C:599:LYS:HE3	1:C:686:GLU:HG2	1.81	0.60
1:C:635:ALA:HB2	1:C:645:LEU:CD2	2.15	0.60
1:A:88:LEU:HD21	1:A:111:LEU:HG	1.84	0.60
1:B:844:CYS:SG	1:B:849:LEU:HD22	2.41	0.60
1:D:271:GLU:OE1	1:D:453:THR:HB	2.01	0.60
1:D:772:GLN:OE1	1:D:779:ARG:N	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ALA:O	1:A:31:ILE:HD13	2.00	0.60
1:C:398:ALA:HB1	1:C:457:ALA:CB	2.32	0.60
1:C:658:PHE:O	1:C:660:PRO:HD3	2.00	0.60
1:B:304:GLN:O	1:B:308:LEU:HG	2.02	0.60
1:C:396:LEU:CD1	1:C:396:LEU:H	2.15	0.60
1:D:370:ALA:HA	1:D:864:LEU:HD23	1.84	0.60
1:A:108:ASN:HD21	1:A:277:GLN:HE22	1.50	0.60
1:B:406:LYS:HG2	1:B:495:TYR:CZ	2.36	0.60
1:B:528:ALA:O	1:B:532:ARG:HG2	2.02	0.60
1:C:282:VAL:HG13	1:C:455:HIS:NE2	2.17	0.60
1:A:8:PHE:CE2	1:A:26:LEU:HD13	2.37	0.60
1:B:455:HIS:CE1	2:B:901:ANP:O2B	2.55	0.60
1:B:820:ARG:HG2	1:B:824:PRO:HA	1.84	0.60
1:B:827:LYS:HD2	1:B:850:ASN:HD21	1.67	0.60
1:B:831:CYS:O	1:B:831:CYS:SG	2.60	0.60
1:B:833:GLU:CG	1:B:858:ARG:HH22	2.14	0.60
1:C:754:ASP:O	1:C:822:THR:HG21	2.01	0.60
1:D:395:ALA:HB2	1:D:471:CYS:HB2	1.83	0.60
1:D:745:GLU:HB2	1:D:769:ASP:HB3	1.83	0.60
1:B:6:TYR:O	1:B:40:PHE:HB2	2.02	0.60
1:B:205:MET:O	1:B:209:LYS:HG3	2.02	0.60
1:B:595:ILE:N	1:B:596:PRO:HD2	2.17	0.60
1:B:617:ARG:HG3	1:B:704:MET:HE3	1.83	0.60
1:C:537:ARG:HH22	1:C:613:PRO:HB2	1.67	0.60
1:A:34:MET:O	1:A:36:ILE:HD12	2.02	0.59
1:B:869:ALA:O	1:B:873:ASN:ND2	2.34	0.59
1:D:321:ASP:HB2	1:D:339:GLY:HA2	1.84	0.59
1:A:829:GLY:HA3	1:A:851:TYR:CZ	2.37	0.59
1:C:130:TYR:CE2	1:C:177:LYS:HE2	2.37	0.59
1:D:682:ARG:HH22	1:D:731:GLU:CD	2.10	0.59
1:D:782:ALA:HB1	1:D:786:LEU:HD22	1.84	0.59
1:C:392:ILE:HG13	1:C:505:ILE:HG22	1.84	0.59
1:C:580:LEU:HB2	1:C:641:MET:SD	2.41	0.59
1:C:689:ILE:HG21	1:C:732:LYS:HD2	1.83	0.59
1:A:714:LEU:HD21	1:A:760:ALA:HB2	1.83	0.59
1:C:312:LEU:HD11	1:C:333:PHE:HE2	1.67	0.59
1:C:630:THR:CG2	1:C:632:GLU:HB3	2.33	0.59
1:D:22:LYS:NZ	1:D:93:SER:O	2.30	0.59
1:B:406:LYS:HB3	1:B:493:GLY:O	2.02	0.59
1:C:108:ASN:HB3	1:C:111:LEU:HD12	1.83	0.59
1:C:803:LEU:O	1:C:804:ASP:C	2.45	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:LEU:HD21	1:A:474:ILE:HD11	1.84	0.59
1:B:457:ALA:HB1	1:B:461:ARG:NH1	2.18	0.59
1:A:538:THR:HG21	1:A:549:ALA:CB	2.33	0.59
1:B:260:ASN:HB3	1:B:265:GLU:H	1.68	0.59
1:C:55:LYS:NZ	1:C:213:ARG:HH11	2.01	0.59
1:D:174:ASP:HA	1:D:177:LYS:HD2	1.84	0.59
1:D:667:CYS:O	1:D:671:VAL:HG23	2.03	0.59
1:A:144:VAL:HG22	1:A:210:ALA:HB2	1.84	0.59
1:A:431:THR:HG23	1:A:447:THR:OG1	2.03	0.59
1:A:718:LYS:O	1:A:722:VAL:HG23	2.03	0.59
1:B:102:MET:HE2	1:B:223:TYR:HB2	1.84	0.59
1:B:603:LYS:HG2	1:B:691:VAL:HG23	1.85	0.59
1:C:29:MET:SD	1:C:336:THR:HG22	2.43	0.59
1:C:455:HIS:CE1	2:C:901:ANP:HNB1	2.21	0.59
1:A:153:GLU:C	1:A:156:ILE:HG22	2.27	0.59
1:A:557:ILE:HG13	1:A:609:LEU:HD21	1.85	0.59
1:B:296:ASN:HB2	1:B:297:ASP:OD1	2.02	0.59
1:B:579:ILE:HD13	1:B:623:LEU:HB3	1.84	0.59
1:B:609:LEU:HD22	1:B:612:ARG:HB2	1.83	0.59
1:C:664:HIS:HB2	1:D:784:LYS:CD	2.33	0.59
1:D:377:LEU:HD13	1:D:857:PHE:HD1	1.68	0.59
1:A:581:SER:HB2	1:A:587:ARG:HD3	1.84	0.58
1:A:829:GLY:HA3	1:A:851:TYR:CE2	2.38	0.58
1:C:109:LEU:HD21	1:C:204:LEU:HA	1.85	0.58
1:C:362:GLU:H	1:C:362:GLU:CD	2.11	0.58
1:D:226:MET:HE1	1:D:463:MET:HE3	1.85	0.58
1:A:631:GLU:OE1	1:C:821:GLN:NE2	2.35	0.58
1:C:527:TRP:O	1:C:531:PHE:CD2	2.56	0.58
1:A:55:LYS:NZ	1:A:213:ARG:HG2	2.18	0.58
1:C:317:ARG:HA	1:C:358:MET:HE3	1.85	0.58
1:C:667:CYS:SG	1:C:713:GLU:HG2	2.42	0.58
1:D:104:ASP:N	1:D:214:SER:HB3	2.18	0.58
1:C:369:GLU:O	1:C:372:SER:OG	2.12	0.58
1:C:637:LEU:CD1	1:C:640:ASN:HB2	2.31	0.58
1:D:690:GLU:HG3	1:D:732:LYS:HE3	1.84	0.58
1:C:406:LYS:HE2	1:C:493:GLY:O	2.03	0.58
1:D:757:ALA:O	1:D:823:ARG:NE	2.35	0.58
1:A:92:ARG:HA	1:A:105:THR:OG1	2.04	0.58
1:A:418:HIS:ND1	1:A:422:GLU:O	2.36	0.58
1:B:606:TYR:HB3	1:B:691:VAL:HG11	1.86	0.58
1:B:827:LYS:HD2	1:B:850:ASN:ND2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:459:VAL:O	1:C:463:MET:HG3	2.03	0.58
1:C:495:TYR:CE2	1:C:509:ASP:OD1	2.57	0.58
1:C:706:PRO:HA	1:C:743:MET:HB2	1.86	0.58
1:B:106:ILE:HA	1:B:139:MET:HE2	1.86	0.58
1:B:581:SER:HB3	1:B:586:ALA:CB	2.33	0.58
1:C:353:LEU:C	1:C:359:ILE:HG12	2.29	0.58
1:D:190:ALA:O	1:D:191:MET:HE2	2.03	0.58
1:B:109:LEU:HA	1:B:136:PHE:CE1	2.38	0.58
1:B:578:MET:HG2	1:B:587:ARG:CG	2.34	0.58
1:C:844:CYS:HB3	1:C:849:LEU:CD2	2.31	0.58
1:D:103:MET:SD	1:D:215:TRP:HA	2.42	0.58
1:D:219:ARG:HB3	1:D:436:ILE:CG2	2.33	0.58
1:D:224:ARG:HA	1:D:229:ILE:HD12	1.86	0.58
1:D:390:GLU:OE1	1:D:507:LYS:HD3	2.03	0.58
1:A:323:GLU:HB2	1:A:335:GLN:HB3	1.85	0.58
1:A:88:LEU:CD2	1:A:111:LEU:HG	2.33	0.58
1:A:380:THR:HG23	1:A:515:ALA:HB2	1.85	0.58
1:A:678:LYS:HA	1:A:724:VAL:HG21	1.85	0.58
1:A:763:PHE:O	1:A:828:CYS:HA	2.04	0.58
1:B:667:CYS:O	1:B:671:VAL:HG23	2.03	0.58
1:C:140:TYR:HB3	1:C:196:PHE:HZ	1.69	0.58
1:D:373:LEU:HD12	1:D:861:ILE:HA	1.84	0.58
1:D:374:ASP:HB3	1:D:861:ILE:HD11	1.86	0.58
1:D:410:THR:HA	1:D:428:ARG:HH11	1.67	0.58
1:B:92:ARG:HD2	2:B:901:ANP:O2A	2.04	0.57
1:C:212:PHE:CE1	1:C:237:VAL:HG23	2.38	0.57
1:C:619:LEU:HD12	1:C:621:PRO:HD2	1.85	0.57
1:D:219:ARG:HH11	1:D:219:ARG:CG	2.12	0.57
1:D:408:TYR:CD1	1:D:424:VAL:HG13	2.39	0.57
1:A:323:GLU:CD	1:A:335:GLN:NE2	2.62	0.57
1:A:372:SER:HB2	1:A:375:GLN:HE22	1.68	0.57
1:A:373:LEU:O	1:A:376:LEU:HB2	2.03	0.57
1:A:668:ARG:HH21	1:A:707:LEU:HD13	1.69	0.57
1:B:36:ILE:HG13	1:B:333:PHE:O	2.04	0.57
1:B:426:LEU:HD11	1:B:428:ARG:HD3	1.86	0.57
1:C:583:SER:HB3	1:C:586:ALA:HB2	1.86	0.57
1:D:168:ASP:O	1:D:171:LEU:HG	2.03	0.57
1:A:34:MET:HB3	1:A:35:PRO:HD2	1.85	0.57
1:A:321:ASP:HB3	1:A:337:ARG:HG3	1.86	0.57
1:A:499:ASP:OD1	1:A:502:THR:OG1	2.19	0.57
1:B:4:TRP:CD1	1:B:61:ILE:HG12	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:MET:HB2	1:B:19:LEU:HD11	1.85	0.57
1:B:748:ARG:O	1:B:752:THR:HG23	2.04	0.57
1:C:103:MET:CB	1:C:214:SER:HB3	2.35	0.57
1:C:268:ILE:HG13	1:C:269:TYR:H	1.69	0.57
1:C:396:LEU:N	1:C:396:LEU:HD12	2.19	0.57
1:C:635:ALA:N	1:C:645:LEU:HD13	2.19	0.57
1:D:104:ASP:H	1:D:214:SER:CB	2.17	0.57
1:D:535:LYS:O	1:D:851:TYR:HA	2.04	0.57
1:A:576:ARG:HD2	1:A:637:LEU:HD22	1.85	0.57
1:B:157:ASP:O	1:B:159:MET:N	2.37	0.57
1:B:712:LYS:O	1:B:715:LYS:HB3	2.04	0.57
1:D:126:PRO:O	1:D:130:TYR:HB2	2.05	0.57
1:D:785:PHE:HD1	1:D:789:TYR:CE1	2.22	0.57
1:A:22:LYS:HE2	1:A:335:GLN:OE1	2.03	0.57
1:A:144:VAL:HG12	1:A:145:MET:CE	2.34	0.57
1:A:506:TYR:CG	1:A:510:ILE:HD11	2.38	0.57
1:B:664:HIS:CE1	1:B:672:THR:OG1	2.58	0.57
1:C:803:LEU:C	1:C:804:ASP:O	2.47	0.57
1:D:224:ARG:HA	1:D:229:ILE:HB	1.86	0.57
1:A:375:GLN:HA	1:A:378:HIS:CE1	2.39	0.57
1:B:99:MET:O	1:B:102:MET:HG2	2.05	0.57
1:B:211:VAL:CG1	1:B:237:VAL:HG22	2.34	0.57
1:B:457:ALA:HB1	1:B:461:ARG:HH12	1.69	0.57
1:B:522:GLU:OE1	1:B:522:GLU:HA	2.03	0.57
1:C:777:PHE:HB3	1:D:668:ARG:HH11	1.64	0.57
1:D:82:ASP:H	1:D:86:PRO:HA	1.70	0.57
1:A:109:LEU:HD12	1:A:136:PHE:HE1	1.69	0.57
1:A:144:VAL:HG12	1:A:145:MET:HE3	1.86	0.57
1:B:289:GLN:HB3	1:B:290:PRO:CD	2.35	0.57
1:C:584:VAL:HA	1:C:587:ARG:CZ	2.35	0.57
1:D:219:ARG:HG3	1:D:219:ARG:NH1	2.11	0.57
1:D:843:PHE:O	1:D:846:LYS:HB2	2.05	0.57
1:A:5:VAL:HG22	1:A:42:VAL:HG22	1.86	0.57
1:C:614:MET:CG	1:C:615:THR:N	2.68	0.57
1:D:102:MET:HB3	1:D:220:ALA:CA	2.34	0.57
1:D:534:LEU:HD11	1:D:845:HIS:HB2	1.86	0.57
1:A:228:ASP:CG	1:A:802:ARG:NH1	2.62	0.57
1:A:668:ARG:NH2	1:A:707:LEU:HD13	2.20	0.57
1:A:837:ASP:O	1:A:841:VAL:HG23	2.05	0.57
1:B:537:ARG:NH2	1:B:613:PRO:HB2	2.19	0.57
1:C:257:PHE:CE1	1:C:321:ASP:HB2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:681:THR:HG21	1:C:721:VAL:O	2.05	0.57
1:C:19:LEU:HD23	1:C:43:THR:HG22	1.87	0.57
1:C:373:LEU:HD11	1:C:864:LEU:CD2	2.29	0.57
1:C:431:THR:HG23	1:C:447:THR:OG1	2.04	0.57
1:B:282:VAL:HG11	1:B:323:GLU:OE2	2.04	0.56
1:C:570:ASP:OD2	1:C:570:ASP:N	2.22	0.56
1:A:747:PRO:HD2	1:B:774:THR:O	2.05	0.56
1:B:701:PRO:HD2	1:B:737:GLN:O	2.04	0.56
1:C:155:ILE:HG21	1:C:182:LYS:HD3	1.87	0.56
1:C:224:ARG:O	1:C:229:ILE:N	2.31	0.56
1:C:777:PHE:HB3	1:D:668:ARG:HH12	1.69	0.56
1:D:103:MET:SD	1:D:215:TRP:HE3	2.27	0.56
1:D:603:LYS:HA	1:D:691:VAL:HG21	1.87	0.56
1:A:24:CYS:O	1:A:28:GLU:HB2	2.05	0.56
1:A:417:ALA:O	1:A:422:GLU:HB2	2.05	0.56
1:A:587:ARG:O	1:A:590:ALA:N	2.39	0.56
1:A:789:TYR:OH	1:B:668:ARG:HA	2.05	0.56
1:B:458:VAL:HA	1:B:461:ARG:NH2	2.21	0.56
1:B:572:ILE:O	1:B:576:ARG:HG3	2.05	0.56
1:B:609:LEU:HD11	1:B:614:MET:HB2	1.87	0.56
1:B:859:VAL:HG12	1:B:863:ARG:HD2	1.88	0.56
1:C:57:ILE:HG12	1:C:209:LYS:HE2	1.87	0.56
1:C:177:LYS:O	1:C:181:GLU:HG2	2.05	0.56
1:C:342:THR:CG2	1:C:461:ARG:HG3	2.35	0.56
1:C:366:VAL:HG23	1:C:871:LEU:HD13	1.88	0.56
1:C:726:GLU:OE1	1:C:726:GLU:HA	2.04	0.56
1:C:837:ASP:OD2	1:C:839:SER:HB3	2.04	0.56
1:D:167:PHE:HB3	1:D:169:THR:HG23	1.88	0.56
1:D:207:ALA:O	1:D:211:VAL:HG23	2.06	0.56
1:D:563:GLU:OE1	1:D:617:ARG:NH1	2.39	0.56
1:D:635:ALA:O	1:D:636:GLU:C	2.47	0.56
1:D:718:LYS:O	1:D:722:VAL:HG23	2.05	0.56
1:D:805:GLN:O	1:D:809:GLY:HA3	2.05	0.56
1:A:764:SER:HA	1:A:829:GLY:O	2.05	0.56
1:B:578:MET:HG2	1:B:587:ARG:CA	2.35	0.56
1:C:305:PHE:HE1	1:C:324:PHE:CD1	2.22	0.56
1:D:166:HIS:N	1:D:166:HIS:ND1	2.51	0.56
1:A:99:MET:CE	1:A:224:ARG:HG3	2.34	0.56
1:A:262:SER:O	1:A:342:THR:OG1	2.23	0.56
1:A:355:ASP:O	1:A:357:GLY:N	2.39	0.56
1:B:32:LEU:HD22	1:B:311:LYS:HZ3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:ASN:O	1:C:29:MET:HG2	2.05	0.56
1:C:396:LEU:HD22	1:C:451:GLY:HA2	1.88	0.56
1:C:398:ALA:HB1	1:C:457:ALA:HB1	1.85	0.56
1:C:490:PHE:HZ	1:C:507:LYS:HG3	1.70	0.56
1:D:446:LEU:HB2	1:D:498:LEU:HD11	1.86	0.56
1:A:34:MET:HB2	1:A:36:ILE:HD11	1.86	0.56
1:A:417:ALA:HB3	1:A:424:VAL:HG21	1.87	0.56
1:C:537:ARG:HD3	1:C:851:TYR:CD1	2.40	0.56
1:C:844:CYS:CB	1:C:849:LEU:HD22	2.33	0.56
1:D:188:LYS:HD2	1:D:195:GLU:HB3	1.88	0.56
1:D:408:TYR:HD1	1:D:424:VAL:HG13	1.71	0.56
1:A:573:MET:O	1:A:577:LYS:N	2.33	0.56
1:B:278:GLY:O	1:B:282:VAL:HG22	2.05	0.56
1:B:772:GLN:HG2	1:B:778:SER:HA	1.88	0.56
1:C:223:TYR:HD2	1:C:436:ILE:HD11	1.70	0.56
1:C:532:ARG:NH2	1:C:555:GLU:OE2	2.21	0.56
1:C:630:THR:HG22	1:C:632:GLU:H	1.70	0.56
1:D:4:TRP:HE1	1:D:60:GLU:CD	2.13	0.56
1:D:40:PHE:CD1	1:D:68:ALA:HB1	2.41	0.56
1:D:91:VAL:HG13	1:D:237:VAL:HG13	1.87	0.56
1:B:154:LYS:HA	1:B:157:ASP:HB2	1.86	0.56
1:B:257:PHE:CZ	1:B:321:ASP:HB2	2.41	0.56
1:B:263:THR:OG1	1:B:265:GLU:HB3	2.06	0.56
1:B:689:ILE:CG2	1:B:732:LYS:HD2	2.36	0.56
1:B:715:LYS:HE3	1:B:719:ASP:OD2	2.06	0.56
1:C:97:ALA:HB2	1:C:233:TRP:HZ3	1.70	0.56
1:C:178:GLU:CD	1:C:182:LYS:HE3	2.31	0.56
1:D:440:HIS:N	1:D:463:MET:HE1	2.21	0.56
1:A:321:ASP:N	1:A:337:ARG:O	2.36	0.56
1:A:634:GLN:HB3	1:A:648:VAL:HG11	1.88	0.56
1:B:476:ILE:CG2	1:B:478:GLU:HG3	2.36	0.56
1:C:403:ALA:HB2	1:C:466:CYS:HB3	1.88	0.56
1:D:224:ARG:NH2	1:D:793:LYS:HE3	2.21	0.56
1:A:321:ASP:OD2	1:A:337:ARG:NE	2.35	0.56
1:B:570:ASP:OD2	1:B:570:ASP:N	2.38	0.56
1:C:661:MET:O	1:C:661:MET:HG2	2.04	0.56
1:D:555:GLU:O	1:D:612:ARG:HB3	2.05	0.56
1:A:578:MET:HE3	1:A:591:LEU:HD21	1.89	0.55
1:B:211:VAL:HG12	1:B:237:VAL:HG22	1.86	0.55
1:B:219:ARG:HD2	1:B:433:PRO:O	2.06	0.55
1:B:621:PRO:HB2	1:B:622:PRO:HD2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:ILE:HG23	1:C:292:THR:N	2.22	0.55
1:D:50:TYR:HD2	1:D:57:ILE:HD11	1.71	0.55
1:A:536:VAL:HG22	1:A:852:VAL:HG22	1.87	0.55
1:C:343:ALA:O	1:C:347:LEU:HD12	2.05	0.55
1:C:414:ALA:CB	1:C:424:VAL:HG11	2.30	0.55
1:D:111:LEU:HB3	1:D:116:VAL:CG2	2.37	0.55
1:D:517:VAL:HG23	1:D:517:VAL:O	2.06	0.55
1:A:271:GLU:HB3	1:A:289:GLN:O	2.06	0.55
1:B:38:GLN:O	1:B:72:LEU:HD21	2.06	0.55
1:C:668:ARG:CZ	1:D:777:PHE:HB3	2.37	0.55
1:A:159:MET:SD	1:A:175:ASP:HB3	2.46	0.55
1:A:617:ARG:NH1	1:A:620:ASP:HB2	2.21	0.55
1:C:257:PHE:HA	1:C:320:GLN:O	2.06	0.55
1:C:321:ASP:O	1:C:336:THR:HA	2.06	0.55
1:C:395:ALA:CB	1:C:471:CYS:SG	2.94	0.55
1:A:50:TYR:HE1	1:A:55:LYS:NZ	2.04	0.55
1:A:153:GLU:O	1:A:157:ASP:OD2	2.25	0.55
1:A:196:PHE:HE1	1:A:203:GLN:NE2	2.04	0.55
1:A:219:ARG:HG2	1:A:219:ARG:HH11	1.71	0.55
1:B:337:ARG:NH1	3:B:902:SO4:O3	2.38	0.55
1:C:429:LEU:HD12	1:C:448:VAL:HB	1.89	0.55
1:D:619:LEU:HG	1:D:621:PRO:HD2	1.89	0.55
1:A:714:LEU:CD2	1:A:760:ALA:HB2	2.37	0.55
1:B:68:ALA:O	1:B:71:TRP:HB3	2.06	0.55
1:B:373:LEU:HD22	1:B:376:LEU:CD1	2.36	0.55
1:C:619:LEU:HD11	1:C:626:PHE:CZ	2.39	0.55
1:C:645:LEU:HA	1:C:648:VAL:HB	1.88	0.55
1:D:88:LEU:HD22	1:D:111:LEU:HG	1.89	0.55
1:A:284:GLY:HA3	1:A:431:THR:O	2.06	0.55
1:C:711:LYS:HE2	1:C:758:GLU:CD	2.32	0.55
1:D:89:VAL:O	1:D:109:LEU:N	2.40	0.55
1:D:342:THR:HB	1:D:344:PRO:HD2	1.89	0.55
1:A:111:LEU:HD22	1:A:116:VAL:HG22	1.88	0.55
1:A:712:LYS:HE3	1:B:794:ILE:HA	1.88	0.55
1:B:92:ARG:HD2	2:B:901:ANP:H8	1.88	0.55
1:C:446:LEU:HD12	1:C:468:VAL:O	2.06	0.55
1:D:359:ILE:HD11	1:D:364:ALA:HA	1.89	0.55
1:C:109:LEU:HD12	1:C:136:PHE:CE1	2.31	0.55
1:C:615:THR:HG21	1:C:704:MET:HE2	1.89	0.55
1:D:373:LEU:HB2	1:D:861:ILE:CG1	2.33	0.55
1:A:627:VAL:HB	1:A:628:PRO:HD2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:VAL:HA	1:B:359:ILE:O	2.07	0.55
1:B:558:GLY:O	1:B:615:THR:CB	2.44	0.55
1:B:689:ILE:HG21	1:B:732:LYS:HD2	1.88	0.55
1:C:396:LEU:H	1:C:396:LEU:HD12	1.71	0.55
1:C:431:THR:HB	1:C:456:ALA:HB3	1.88	0.55
1:C:746:ILE:O	1:C:747:PRO:C	2.50	0.55
1:D:13:ALA:O	1:D:15:MET:N	2.40	0.55
1:A:553:GLY:HA3	1:A:863:ARG:HD2	1.88	0.54
1:B:581:SER:HB3	1:B:586:ALA:HB1	1.87	0.54
1:D:131:ASP:HB2	1:D:176:LEU:HD13	1.89	0.54
1:D:161:GLU:C	1:D:163:LYS:H	2.15	0.54
1:D:215:TRP:CD1	1:D:234:GLY:HA2	2.42	0.54
1:A:785:PHE:HB3	1:B:664:HIS:CD2	2.42	0.54
1:B:854:CYS:SG	1:B:859:VAL:HA	2.46	0.54
1:C:361:GLU:C	1:C:363:GLU:H	2.14	0.54
1:C:408:TYR:HB2	1:C:414:ALA:HB2	1.88	0.54
1:C:753:ALA:HB3	1:C:815:ALA:HA	1.88	0.54
1:A:188:LYS:HA	1:A:194:GLU:O	2.07	0.54
1:A:259:ARG:HG2	1:A:266:LYS:HA	1.89	0.54
1:A:620:ASP:H	1:A:621:PRO:HD2	1.71	0.54
1:B:777:PHE:O	1:B:777:PHE:HD1	1.90	0.54
1:C:102:MET:O	1:C:219:ARG:CZ	2.55	0.54
1:C:598:GLN:OE1	1:C:679:MET:HE1	2.07	0.54
1:B:615:THR:CG2	1:B:704:MET:HB2	2.38	0.54
1:B:663:GLY:C	1:B:665:ARG:H	2.15	0.54
1:C:306:MET:HE1	1:C:310:MET:HE3	1.89	0.54
1:C:375:GLN:HA	1:C:378:HIS:ND1	2.23	0.54
1:C:662:MET:HE2	1:D:776:GLY:C	2.32	0.54
1:A:48:THR:HG22	1:A:52:ASN:ND2	2.23	0.54
1:A:354:VAL:HG21	1:A:364:ALA:HB2	1.88	0.54
1:A:581:SER:HB3	1:A:586:ALA:HB3	1.88	0.54
1:A:780:ASP:HB3	1:B:658:PHE:CD2	2.43	0.54
1:B:340:LYS:HB2	1:B:458:VAL:HG12	1.88	0.54
1:B:715:LYS:C	1:B:715:LYS:HD3	2.33	0.54
1:C:425:ILE:HG13	1:C:496:ILE:HG13	1.88	0.54
1:C:528:ALA:O	1:C:532:ARG:HG2	2.07	0.54
1:D:260:ASN:O	1:D:264:GLY:N	2.40	0.54
1:D:554:ALA:N	1:D:859:VAL:HG11	2.23	0.54
1:D:673:TYR:O	1:D:676:ILE:HG13	2.08	0.54
1:A:769:ASP:HB3	1:A:773:MET:CE	2.38	0.54
1:B:191:MET:HE2	1:B:191:MET:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:VAL:HG22	1:B:446:LEU:HB3	1.90	0.54
1:C:57:ILE:HD11	1:C:209:LYS:HG2	1.90	0.54
1:C:230:PRO:HG2	1:C:233:TRP:CZ2	2.42	0.54
1:C:789:TYR:CE1	1:D:671:VAL:HG11	2.42	0.54
1:C:829:GLY:HA2	1:C:851:TYR:O	2.07	0.54
1:D:12:ASN:ND2	1:D:14:SER:OG	2.40	0.54
1:D:165:VAL:HB	1:D:170:ASP:HB2	1.89	0.54
1:D:371:LYS:HB3	1:D:838:PRO:HG2	1.90	0.54
1:D:617:ARG:NH2	3:D:904:SO4:O3	2.29	0.54
1:A:196:PHE:HE1	1:A:203:GLN:HE21	1.54	0.54
1:B:323:GLU:OE1	2:B:901:ANP:O1B	2.26	0.54
1:B:667:CYS:SG	1:B:713:GLU:HG2	2.48	0.54
1:C:475:LYS:O	1:C:484:GLU:N	2.40	0.54
1:D:704:MET:SD	1:D:743:MET:HE2	2.47	0.54
1:A:349:ILE:HG22	1:A:353:LEU:HG	1.90	0.54
1:B:293:GLN:HA	1:B:293:GLN:NE2	2.20	0.54
1:B:383:PRO:HD3	1:B:513:GLN:HE22	1.73	0.54
1:C:674:PRO:HB3	1:C:720:VAL:HG21	1.90	0.54
1:C:754:ASP:HB3	1:C:818:LYS:HB3	1.89	0.54
1:D:406:LYS:HG2	1:D:495:TYR:CE1	2.42	0.54
1:D:856:PRO:C	1:D:858:ARG:H	2.16	0.54
1:A:257:PHE:CE1	1:A:321:ASP:HB2	2.43	0.54
1:A:624:HIS:O	1:A:629:HIS:NE2	2.36	0.54
1:A:715:LYS:HB2	1:A:759:GLU:HG3	1.90	0.54
1:C:92:ARG:HA	1:C:105:THR:HG23	1.89	0.54
1:C:259:ARG:HB2	1:C:319:MET:HG3	1.90	0.54
1:C:482:THR:HG22	1:C:491:ALA:HB2	1.90	0.54
1:C:772:GLN:HG2	1:C:800:PHE:CE1	2.42	0.54
1:D:92:ARG:NH2	1:D:334:LEU:O	2.39	0.54
1:D:724:VAL:O	1:D:728:VAL:HG23	2.07	0.54
1:A:7:LYS:HB2	1:A:10:GLU:HG3	1.89	0.54
1:A:369:GLU:CD	1:A:372:SER:HB3	2.33	0.54
1:A:563:GLU:OE2	1:A:617:ARG:NH1	2.39	0.54
1:B:555:GLU:O	1:B:612:ARG:HB3	2.08	0.54
1:B:739:HIS:ND1	1:B:761:GLU:OE1	2.31	0.54
1:C:440:HIS:HA	1:C:463:MET:CE	2.38	0.54
1:C:581:SER:HB3	1:C:586:ALA:HB3	1.89	0.54
1:D:91:VAL:HG22	1:D:239:VAL:HG22	1.90	0.54
1:B:12:ASN:ND2	1:B:15:MET:HG3	2.23	0.53
1:B:536:VAL:HG21	1:B:863:ARG:HG3	1.90	0.53
1:C:216:ASP:OD1	1:C:793:LYS:CE	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:857:PHE:N	1:C:857:PHE:CD1	2.75	0.53
1:D:134:ARG:HD2	1:D:135:ARG:N	2.23	0.53
1:D:558:GLY:HA3	1:D:853:SER:HB2	1.90	0.53
1:D:814:MET:CG	1:D:818:LYS:HE3	2.39	0.53
1:D:837:ASP:HB3	1:D:840:SER:CB	2.34	0.53
1:B:773:MET:N	1:B:773:MET:HE3	2.24	0.53
1:D:317:ARG:HA	1:D:358:MET:CE	2.32	0.53
1:D:454:SER:O	1:D:458:VAL:HG23	2.08	0.53
1:A:214:SER:O	1:A:217:ASN:N	2.42	0.53
1:A:391:VAL:HA	1:A:505:ILE:O	2.08	0.53
1:A:571:ARG:NE	1:A:597:PHE:HB3	2.23	0.53
1:A:638:ALA:HB1	1:A:643:LEU:C	2.33	0.53
1:A:794:ILE:O	1:B:712:LYS:HE3	2.09	0.53
1:B:643:LEU:HD22	1:B:647:GLU:OE2	2.09	0.53
1:C:609:LEU:O	1:C:612:ARG:NH1	2.41	0.53
1:A:403:ALA:CB	1:A:444:GLY:HA3	2.38	0.53
1:A:444:GLY:HA2	1:A:466:CYS:O	2.07	0.53
1:B:353:LEU:CB	1:B:359:ILE:HG12	2.38	0.53
1:B:538:THR:HG22	1:B:556:GLY:O	2.08	0.53
1:A:112:ASN:HA	1:A:133:TYR:CZ	2.44	0.53
1:A:403:ALA:HB3	1:A:498:LEU:HB2	1.90	0.53
1:B:708:VAL:HG12	1:B:709:GLY:N	2.24	0.53
1:C:245:GLY:O	1:C:276:ALA:N	2.40	0.53
1:C:510:ILE:HG22	1:C:511:GLU:N	2.23	0.53
1:C:540:ALA:HB3	1:C:557:ILE:HD11	1.90	0.53
1:C:573:MET:HE1	1:C:637:LEU:CD1	2.38	0.53
1:C:710:GLU:OE2	1:C:712:LYS:N	2.34	0.53
1:D:103:MET:HB3	1:D:214:SER:CB	2.39	0.53
1:D:199:GLU:O	1:D:203:GLN:HG3	2.08	0.53
1:A:134:ARG:HD2	1:A:135:ARG:N	2.23	0.53
1:B:318:ASP:HB3	1:B:338:ASN:OD1	2.09	0.53
1:B:375:GLN:HA	1:B:378:HIS:CE1	2.44	0.53
1:B:404:ALA:HB1	1:B:509:ASP:OD2	2.09	0.53
1:C:59:GLN:NE2	1:C:63:ASP:OD2	2.42	0.53
1:C:382:ASN:OD1	1:C:383:PRO:HD2	2.08	0.53
1:C:407:VAL:HB	1:C:496:ILE:HD11	1.90	0.53
1:C:823:ARG:O	1:C:823:ARG:HG2	2.08	0.53
1:D:38:GLN:OE1	1:D:38:GLN:HA	2.07	0.53
1:D:225:ARG:HG3	1:D:796:GLU:O	2.08	0.53
1:D:689:ILE:HG21	1:D:732:LYS:HD3	1.89	0.53
1:A:205:MET:O	1:A:209:LYS:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:TRP:CD2	1:A:234:GLY:HA2	2.43	0.53
1:A:657:GLU:HG2	1:B:781:ASP:HB3	1.91	0.53
1:A:833:GLU:HG2	1:A:833:GLU:O	2.08	0.53
1:B:81:GLY:HA2	1:B:110:GLY:O	2.08	0.53
1:B:142:ASP:OD1	1:B:149:LYS:HG2	2.09	0.53
1:B:147:VAL:HG11	1:B:186:VAL:HG12	1.91	0.53
1:B:216:ASP:OD1	1:B:793:LYS:HE3	2.09	0.53
1:C:79:LYS:HB2	1:C:82:ASP:HB2	1.90	0.53
1:C:701:PRO:HD2	1:C:737:GLN:O	2.09	0.53
1:D:346:ALA:O	1:D:350:ALA:N	2.37	0.53
1:B:92:ARG:HH11	2:B:901:ANP:C8	2.21	0.53
1:B:319:MET:HE3	1:B:341:ARG:NH2	2.24	0.53
1:C:22:LYS:HG2	1:C:335:GLN:OE1	2.08	0.53
1:C:80:PHE:CD2	1:C:200:PRO:HB2	2.44	0.53
1:D:317:ARG:O	1:D:318:ASP:HB2	2.07	0.53
1:D:617:ARG:HB2	1:D:704:MET:HE3	1.89	0.53
1:A:120:ALA:O	1:A:124:GLY:HA2	2.09	0.53
1:A:537:ARG:HD3	1:A:851:TYR:CD1	2.43	0.53
1:B:258:THR:O	1:B:259:ARG:HG3	2.09	0.53
1:C:580:LEU:HB2	1:C:641:MET:HE1	1.90	0.53
1:D:62:GLN:O	1:D:63:ASP:C	2.52	0.53
1:A:197:PRO:O	1:A:203:GLN:NE2	2.42	0.53
1:A:767:THR:OG1	1:A:832:GLY:HA3	2.08	0.53
1:B:153:GLU:OE1	1:B:153:GLU:HA	2.07	0.53
1:C:488:HIS:CG	1:C:489:THR:H	2.27	0.53
1:D:5:VAL:C	1:D:6:TYR:CD1	2.87	0.53
1:B:116:VAL:HG21	1:B:133:TYR:CE2	2.44	0.52
1:D:567:PHE:O	1:D:572:ILE:HB	2.08	0.52
1:D:667:CYS:HB2	1:D:706:PRO:O	2.09	0.52
1:D:767:THR:OG1	1:D:830:ILE:HD11	2.09	0.52
1:A:429:LEU:O	1:A:449:ARG:HG2	2.09	0.52
1:B:27:ALA:O	1:B:31:ILE:HD13	2.09	0.52
1:B:211:VAL:O	1:B:214:SER:HB2	2.09	0.52
1:B:226:MET:HE1	1:B:463:MET:HE2	1.92	0.52
1:C:107:LEU:HB3	1:C:242:MET:CE	2.39	0.52
1:C:360:THR:HG23	1:C:363:GLU:OE2	2.09	0.52
1:C:657:GLU:HG2	1:D:784:LYS:NZ	2.25	0.52
1:A:297:ASP:HB3	1:A:298:MET:CE	2.39	0.52
1:A:767:THR:HG21	1:A:830:ILE:CD1	2.40	0.52
1:A:787:ASP:OD2	1:A:791:LYS:HE3	2.09	0.52
1:C:379:PRO:O	1:C:402:ALA:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:528:ALA:HB1	1:C:867:ALA:HB2	1.91	0.52
1:C:637:LEU:HD11	1:C:641:MET:HG3	1.91	0.52
1:D:576:ARG:O	1:D:580:LEU:HD23	2.09	0.52
1:A:108:ASN:ND2	1:A:277:GLN:HE22	2.07	0.52
1:A:692:LYS:CB	1:A:736:MET:HE1	2.39	0.52
1:B:57:ILE:HG12	1:B:209:LYS:HE2	1.92	0.52
1:B:257:PHE:C	1:B:259:ARG:H	2.17	0.52
1:B:551:LYS:HD2	1:B:551:LYS:C	2.35	0.52
1:C:772:GLN:HG2	1:C:800:PHE:HE1	1.74	0.52
1:D:369:GLU:OE1	1:D:369:GLU:HA	2.09	0.52
1:A:330:LYS:HG2	1:A:332:TYR:CE2	2.45	0.52
1:B:137:ILE:HA	1:B:196:PHE:CE2	2.45	0.52
1:B:199:GLU:O	1:B:202:ASP:HB2	2.09	0.52
1:B:566:PHE:CZ	1:B:679:MET:HE1	2.45	0.52
1:B:844:CYS:O	1:B:849:LEU:HB2	2.09	0.52
1:C:119:PHE:CD2	1:C:129:ALA:HB1	2.44	0.52
1:A:331:LEU:HD21	1:A:333:PHE:HE1	1.74	0.52
1:C:156:ILE:HG13	1:C:179:LEU:HD11	1.92	0.52
1:C:547:LEU:O	1:C:550:VAL:HG23	2.10	0.52
1:C:715:LYS:O	1:C:715:LYS:HD3	2.08	0.52
1:D:38:GLN:O	1:D:241:THR:CG2	2.55	0.52
1:D:595:ILE:N	1:D:596:PRO:HD2	2.24	0.52
1:A:527:TRP:O	1:A:531:PHE:CD2	2.62	0.52
1:A:561:ARG:NH2	3:A:4004:SO4:O1	2.42	0.52
1:B:343:ALA:N	1:B:344:PRO:HD2	2.25	0.52
1:B:786:LEU:O	1:B:789:TYR:HB2	2.09	0.52
1:C:40:PHE:HE1	1:C:69:ILE:HD13	1.74	0.52
1:C:262:SER:C	1:C:345:ALA:HB2	2.34	0.52
1:C:584:VAL:HG13	1:C:585:GLU:N	2.25	0.52
1:C:859:VAL:N	1:C:860:PRO:CD	2.73	0.52
1:D:226:MET:SD	1:D:440:HIS:HD2	2.32	0.52
1:D:820:ARG:O	1:D:821:GLN:C	2.52	0.52
1:A:134:ARG:O	1:A:138:GLN:HB2	2.10	0.52
1:A:230:PRO:HG2	1:A:233:TRP:CE2	2.44	0.52
1:A:537:ARG:O	1:A:853:SER:HA	2.09	0.52
1:B:275:ASN:C	1:B:275:ASN:OD1	2.52	0.52
1:B:529:ASP:HA	1:B:532:ARG:HE	1.75	0.52
1:B:565:MET:O	1:B:571:ARG:HD2	2.10	0.52
1:C:31:ILE:CD1	1:C:31:ILE:H	2.23	0.52
1:C:111:LEU:HD13	1:C:133:TYR:HA	1.90	0.52
1:C:118:GLY:HA2	1:C:121:LYS:NZ	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:MET:CE	1:C:463:MET:HE3	2.38	0.52
1:C:581:SER:HB3	1:C:586:ALA:HB1	1.91	0.52
1:C:614:MET:HG3	1:C:615:THR:H	1.74	0.52
1:D:377:LEU:HD13	1:D:857:PHE:CD1	2.44	0.52
1:D:395:ALA:HB1	1:D:469:SER:O	2.10	0.52
1:A:82:ASP:H	1:A:86:PRO:HA	1.75	0.52
1:B:222:VAL:HG11	1:B:436:ILE:HG23	1.92	0.52
1:C:165:VAL:HG21	1:C:171:LEU:HD23	1.92	0.52
1:C:446:LEU:HB2	1:C:498:LEU:HD21	1.91	0.52
1:C:661:MET:HE3	1:D:659:ASN:ND2	2.25	0.52
1:D:521:PHE:CE1	1:D:525:MET:HG3	2.44	0.52
1:A:394:SER:HB2	1:A:503:GLY:O	2.09	0.52
1:B:12:ASN:HD22	1:B:14:SER:H	1.57	0.52
1:B:408:TYR:HD1	1:B:424:VAL:HG13	1.75	0.52
1:B:410:THR:O	1:B:426:LEU:HD13	2.10	0.52
1:B:561:ARG:HB3	1:B:617:ARG:NH1	2.25	0.52
1:C:353:LEU:HD12	1:C:367:ARG:NH1	2.25	0.52
1:D:512:THR:CG2	1:D:513:GLN:N	2.73	0.52
1:A:506:TYR:CB	1:A:510:ILE:HD11	2.40	0.51
1:B:13:ALA:HA	1:B:24:CYS:SG	2.50	0.51
1:B:131:ASP:O	1:B:135:ARG:HG3	2.09	0.51
1:B:661:MET:CE	1:B:778:SER:HB2	2.32	0.51
1:C:144:VAL:HG12	1:C:145:MET:HE2	1.91	0.51
1:C:575:ILE:CD1	1:C:578:MET:HE3	2.39	0.51
1:C:804:ASP:OD2	1:D:748:ARG:NE	2.38	0.51
1:D:142:ASP:OD2	1:D:149:LYS:HE3	2.09	0.51
1:A:354:VAL:CG2	1:A:364:ALA:HB2	2.41	0.51
1:B:142:ASP:HA	1:B:147:VAL:O	2.09	0.51
1:B:395:ALA:HB3	1:B:468:VAL:HG12	1.92	0.51
1:C:120:ALA:HB1	1:C:126:PRO:HB3	1.92	0.51
1:C:592:ASN:HA	1:C:595:ILE:CG1	2.38	0.51
1:D:20:GLY:HA3	1:D:94:GLY:O	2.09	0.51
1:D:50:TYR:CD1	1:D:50:TYR:C	2.88	0.51
1:D:126:PRO:HA	1:D:129:ALA:HB3	1.92	0.51
1:D:174:ASP:CA	1:D:177:LYS:HB2	2.40	0.51
1:D:321:ASP:HB2	1:D:339:GLY:CA	2.40	0.51
1:D:661:MET:SD	1:D:662:MET:CE	2.97	0.51
1:D:754:ASP:O	1:D:822:THR:HG21	2.10	0.51
1:A:842:GLU:HG3	1:A:869:ALA:HB1	1.92	0.51
1:D:634:GLN:NE2	1:D:649:LYS:HG3	2.18	0.51
1:A:73:GLU:HG2	1:A:79:LYS:CA	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:PHE:HE2	1:A:203:GLN:NE2	2.08	0.51
1:A:174:ASP:O	1:A:178:GLU:N	2.42	0.51
1:A:309:ALA:HA	1:A:322:MET:SD	2.51	0.51
1:A:398:ALA:CA	1:A:452:MET:HG2	2.41	0.51
1:A:837:ASP:OD2	1:A:840:SER:OG	2.25	0.51
1:B:137:ILE:HG23	1:B:196:PHE:CE2	2.46	0.51
1:B:302:TYR:O	1:B:306:MET:HB2	2.11	0.51
1:C:219:ARG:HD2	1:C:433:PRO:HB2	1.93	0.51
1:C:282:VAL:HG13	1:C:455:HIS:CE1	2.45	0.51
1:C:409:PHE:CZ	1:C:483:PHE:HD1	2.29	0.51
1:C:455:HIS:CE1	2:C:901:ANP:PB	3.00	0.51
1:D:255:VAL:HB	1:D:453:THR:HG23	1.91	0.51
1:D:532:ARG:HB3	1:D:867:ALA:HB2	1.91	0.51
1:D:537:ARG:NH2	1:D:702:GLU:OE1	2.43	0.51
1:D:557:ILE:HB	1:D:614:MET:HA	1.93	0.51
1:B:743:MET:HB3	1:B:745:GLU:HG2	1.92	0.51
1:D:318:ASP:HA	1:D:353:LEU:HD11	1.91	0.51
1:D:639:LYS:O	1:D:641:MET:N	2.43	0.51
1:A:63:ASP:O	1:A:67:GLU:HG3	2.11	0.51
1:A:262:SER:HB3	1:A:400:PRO:HD3	1.91	0.51
1:A:532:ARG:NH1	1:A:555:GLU:OE2	2.39	0.51
1:C:63:ASP:O	1:C:67:GLU:HG3	2.10	0.51
1:C:89:VAL:HG12	1:C:240:GLN:C	2.36	0.51
1:C:153:GLU:O	1:C:157:ASP:N	2.44	0.51
1:C:406:LYS:HG2	1:C:495:TYR:CE1	2.46	0.51
1:C:603:LYS:NZ	1:C:694:GLU:OE1	2.44	0.51
1:A:116:VAL:CG2	1:A:133:TYR:CG	2.94	0.51
1:A:565:MET:HE1	1:A:602:PHE:CE1	2.46	0.51
1:A:776:GLY:O	1:B:668:ARG:NH2	2.40	0.51
1:A:784:LYS:CG	1:B:664:HIS:HB2	2.39	0.51
1:A:806:THR:O	1:A:810:GLN:HG3	2.10	0.51
1:B:107:LEU:HG	1:B:139:MET:HE1	1.93	0.51
1:B:188:LYS:HG3	1:B:193:GLY:O	2.11	0.51
1:B:414:ALA:CB	1:B:424:VAL:HG11	2.40	0.51
1:B:414:ALA:HB1	1:B:424:VAL:HG11	1.93	0.51
1:C:596:PRO:HG2	1:C:597:PHE:HD1	1.71	0.51
1:D:627:VAL:HG21	1:D:652:VAL:HG13	1.91	0.51
1:B:53:SER:HB2	1:B:56:GLN:O	2.11	0.51
1:C:673:TYR:HB2	1:C:676:ILE:CD1	2.40	0.51
1:D:221:ILE:HG12	1:D:224:ARG:HH21	1.74	0.51
1:D:262:SER:O	1:D:342:THR:OG1	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:ALA:O	1:D:344:PRO:C	2.52	0.51
1:D:377:LEU:HD13	1:D:857:PHE:HB3	1.93	0.51
1:D:406:LYS:O	1:D:425:ILE:N	2.39	0.51
1:A:294:LEU:HD11	1:A:301:CYS:HB2	1.93	0.51
1:B:310:MET:HE2	1:B:310:MET:HA	1.93	0.51
1:B:540:ALA:HB3	1:B:557:ILE:HG12	1.93	0.51
1:B:575:ILE:HD11	1:B:579:ILE:HD11	1.92	0.51
1:C:101:GLY:O	1:C:433:PRO:HG3	2.10	0.51
1:C:390:GLU:OE1	1:C:507:LYS:HB3	2.11	0.51
1:C:692:LYS:HG2	1:C:697:ILE:O	2.10	0.51
1:A:106:ILE:HD13	1:A:140:TYR:HA	1.93	0.51
1:A:454:SER:OG	1:A:457:ALA:HB2	2.11	0.51
1:B:52:ASN:C	1:B:54:GLY:H	2.18	0.51
1:B:226:MET:HE1	1:B:463:MET:CE	2.41	0.51
1:C:282:VAL:CG1	1:C:455:HIS:CE1	2.94	0.51
1:C:599:LYS:O	1:C:603:LYS:HG3	2.10	0.51
1:C:750:ALA:HA	1:C:815:ALA:HB2	1.93	0.51
1:C:785:PHE:HB3	1:D:664:HIS:NE2	2.26	0.51
1:D:165:VAL:HB	1:D:170:ASP:CB	2.41	0.51
1:A:488:HIS:CG	1:A:489:THR:N	2.79	0.50
1:A:671:VAL:HG21	1:B:789:TYR:OH	2.10	0.50
1:B:368:ILE:HB	1:B:864:LEU:HD21	1.93	0.50
1:B:561:ARG:HG2	1:B:617:ARG:NH1	2.26	0.50
1:B:830:ILE:HG22	1:B:852:VAL:HA	1.93	0.50
1:D:511:GLU:HG2	1:D:512:THR:N	2.25	0.50
1:A:80:PHE:HA	1:A:87:LEU:CB	2.33	0.50
1:A:80:PHE:CE2	1:A:200:PRO:O	2.55	0.50
1:A:174:ASP:HA	1:A:177:LYS:HG3	1.93	0.50
1:A:370:ALA:HB2	1:A:868:GLN:OE1	2.10	0.50
1:A:678:LYS:HB3	1:A:724:VAL:HG21	1.93	0.50
1:B:53:SER:O	1:B:56:GLN:HB2	2.10	0.50
1:B:652:VAL:O	1:B:653:ASP:C	2.54	0.50
1:B:765:PHE:CZ	1:B:815:ALA:HB3	2.46	0.50
1:C:116:VAL:HG11	1:C:130:TYR:CD1	2.46	0.50
1:D:103:MET:HB3	1:D:214:SER:HB2	1.93	0.50
1:B:797:SER:O	1:B:799:PRO:CD	2.59	0.50
1:C:255:VAL:CB	1:C:453:THR:HG21	2.20	0.50
1:D:80:PHE:HD1	1:D:87:LEU:O	1.94	0.50
1:D:112:ASN:H	1:D:115:ALA:HB3	1.76	0.50
1:B:196:PHE:CG	1:B:197:PRO:HD2	2.47	0.50
1:B:583:SER:HB3	1:B:586:ALA:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:GLU:C	1:D:163:LYS:N	2.69	0.50
1:D:330:LYS:HD2	1:D:332:TYR:CE2	2.46	0.50
1:D:512:THR:HG23	1:D:513:GLN:H	1.77	0.50
1:D:816:VAL:HG21	1:D:849:LEU:HD11	1.94	0.50
1:A:440:HIS:HA	1:A:463:MET:HE1	1.92	0.50
1:B:163:LYS:HE2	1:B:163:LYS:O	2.11	0.50
1:B:760:ALA:HB1	1:B:762:PHE:O	2.12	0.50
1:C:160:LYS:HG2	1:C:171:LEU:HD21	1.94	0.50
1:C:644:THR:C	1:C:646:ALA:N	2.69	0.50
1:D:330:LYS:HE2	1:D:332:TYR:OH	2.11	0.50
1:D:525:MET:HA	1:D:525:MET:CE	2.40	0.50
1:A:199:GLU:HB2	1:A:202:ASP:HB2	1.94	0.50
1:B:57:ILE:HG22	1:B:61:ILE:HB	1.92	0.50
1:B:80:PHE:CZ	1:B:200:PRO:HB2	2.47	0.50
1:B:317:ARG:CA	1:B:358:MET:HE3	2.37	0.50
1:B:371:LYS:HG2	1:B:838:PRO:HG2	1.92	0.50
1:C:314:LYS:HA	1:C:358:MET:SD	2.52	0.50
1:C:630:THR:HG22	1:C:632:GLU:HB3	1.94	0.50
1:D:86:PRO:HG3	1:D:115:ALA:O	2.11	0.50
1:A:117:GLU:HA	1:A:117:GLU:OE2	2.11	0.50
1:A:689:ILE:HD13	1:A:734:SER:CB	2.42	0.50
1:A:774:THR:HG22	1:B:748:ARG:HB2	1.93	0.50
1:B:177:LYS:O	1:B:180:ALA:HB3	2.12	0.50
1:B:303:LYS:NZ	1:B:307:ASP:OD1	2.44	0.50
1:B:782:ALA:C	1:B:784:LYS:N	2.69	0.50
1:C:8:PHE:HB2	1:C:38:GLN:NE2	2.26	0.50
1:C:446:LEU:HD22	1:C:498:LEU:HD21	1.94	0.50
1:C:671:VAL:HG11	1:D:789:TYR:CE1	2.47	0.50
1:C:704:MET:HA	1:C:741:GLY:O	2.11	0.50
1:A:208:VAL:O	1:A:209:LYS:C	2.53	0.50
1:A:242:MET:HA	2:A:4001:ANP:HN62	1.77	0.50
1:A:767:THR:HG23	1:A:830:ILE:HG13	1.94	0.50
1:B:686:GLU:O	1:B:690:GLU:HG3	2.12	0.50
1:C:99:MET:HE3	1:C:220:ALA:HB1	1.94	0.50
1:C:255:VAL:HG12	1:C:256:ALA:H	1.76	0.50
1:C:392:ILE:CG1	1:C:505:ILE:HG22	2.41	0.50
1:C:748:ARG:NH2	1:D:804:ASP:OD1	2.37	0.50
1:D:572:ILE:HG12	1:D:576:ARG:HH21	1.77	0.50
1:A:716:PHE:CD1	1:A:716:PHE:C	2.89	0.50
1:B:431:THR:OG1	1:B:450:GLY:HA3	2.12	0.50
1:C:337:ARG:HD3	3:C:902:SO4:O2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:399:SER:O	1:C:500:GLY:HA3	2.11	0.50
1:C:787:ASP:OD2	1:C:791:LYS:HE3	2.10	0.50
1:D:30:THR:N	1:D:36:ILE:HD12	2.27	0.50
1:D:295:GLU:HA	1:D:302:TYR:CG	2.47	0.50
1:B:7:LYS:O	1:B:10:GLU:N	2.44	0.49
1:C:89:VAL:HG12	1:C:241:THR:CA	2.42	0.49
1:C:537:ARG:NH2	1:C:613:PRO:HB2	2.27	0.49
1:C:563:GLU:HG2	1:C:621:PRO:HD3	1.94	0.49
1:D:32:LEU:HD21	1:D:315:HIS:NE2	2.27	0.49
1:D:352:ASP:C	1:D:354:VAL:H	2.20	0.49
1:D:382:ASN:HB3	1:D:385:ALA:HB3	1.93	0.49
1:A:309:ALA:HB1	1:A:322:MET:HE1	1.93	0.49
1:B:243:VAL:O	2:B:901:ANP:H2	2.12	0.49
1:B:709:GLY:HA2	1:B:749:ALA:HB2	1.94	0.49
1:C:18:LEU:HG	1:C:43:THR:CG2	2.42	0.49
1:C:29:MET:HE1	1:C:333:PHE:HD2	1.76	0.49
1:C:406:LYS:HB2	1:C:408:TYR:HE1	1.77	0.49
1:D:563:GLU:OE2	1:D:621:PRO:HD3	2.12	0.49
1:A:102:MET:HB3	1:A:220:ALA:HA	1.95	0.49
1:B:576:ARG:HH12	1:B:628:PRO:N	2.10	0.49
1:B:782:ALA:C	1:B:784:LYS:H	2.20	0.49
1:C:62:GLN:NE2	1:C:66:PHE:HE2	2.11	0.49
1:C:306:MET:O	1:C:310:MET:HG2	2.12	0.49
1:C:458:VAL:HA	1:C:461:ARG:NH2	2.28	0.49
1:C:612:ARG:HH11	1:C:612:ARG:CG	2.23	0.49
1:C:620:ASP:N	1:C:621:PRO:HD2	2.26	0.49
1:C:775:PHE:HB3	1:C:777:PHE:CE2	2.47	0.49
1:D:69:ILE:HD11	1:D:204:LEU:HD22	1.94	0.49
1:A:634:GLN:CD	1:A:649:LYS:HE2	2.37	0.49
1:B:496:ILE:HD12	1:B:498:LEU:HD21	1.95	0.49
1:D:637:LEU:HA	1:D:640:ASN:HB2	1.94	0.49
1:A:109:LEU:HA	1:A:136:PHE:CE1	2.48	0.49
1:B:131:ASP:O	1:B:134:ARG:HG3	2.12	0.49
1:B:859:VAL:N	1:B:860:PRO:CD	2.76	0.49
1:C:216:ASP:CG	1:C:793:LYS:HE3	2.38	0.49
1:C:382:ASN:HD22	1:C:385:ALA:HB2	1.77	0.49
1:C:638:ALA:HB1	1:C:643:LEU:O	2.13	0.49
1:C:668:ARG:NH1	1:D:777:PHE:HB3	2.28	0.49
1:D:407:VAL:HG22	1:D:494:ASP:O	2.12	0.49
1:A:108:ASN:HD21	1:A:277:GLN:NE2	2.10	0.49
1:A:558:GLY:O	1:A:615:THR:HB	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:777:PHE:HB3	1:B:668:ARG:NH2	2.27	0.49
1:B:820:ARG:HA	1:B:823:ARG:O	2.12	0.49
1:C:65:ILE:O	1:C:69:ILE:HG12	2.12	0.49
1:C:134:ARG:HG3	1:C:135:ARG:H	1.77	0.49
1:C:453:THR:O	1:C:453:THR:HG22	2.13	0.49
1:C:790:TYR:OH	1:C:798:ASP:HB2	2.12	0.49
1:D:219:ARG:HB3	1:D:436:ILE:HG21	1.94	0.49
1:D:354:VAL:O	1:D:357:GLY:N	2.44	0.49
1:D:390:GLU:O	1:D:392:ILE:HG23	2.12	0.49
1:D:639:LYS:C	1:D:641:MET:H	2.20	0.49
1:A:276:ALA:HB1	1:A:280:ASP:OD1	2.13	0.49
1:A:564:HIS:CD2	1:A:565:MET:N	2.80	0.49
1:B:47:CYS:O	1:B:50:TYR:HB3	2.13	0.49
1:C:171:LEU:HB3	1:C:175:ASP:HB2	1.95	0.49
1:C:191:MET:O	1:C:192:ASN:HB2	2.13	0.49
1:C:449:ARG:HA	1:C:470:GLY:HA2	1.94	0.49
1:C:784:LYS:HD2	1:D:664:HIS:HB2	1.94	0.49
1:D:127:ARG:HG2	1:D:176:LEU:CD1	2.43	0.49
1:D:134:ARG:HD2	1:D:134:ARG:C	2.38	0.49
1:D:135:ARG:HH11	1:D:277:GLN:HB2	1.78	0.49
1:D:310:MET:HE2	1:D:310:MET:CA	2.39	0.49
1:A:8:PHE:CD1	1:A:40:PHE:HA	2.48	0.49
1:A:394:SER:HB2	1:A:504:LYS:HA	1.93	0.49
1:C:787:ASP:O	1:C:791:LYS:HG3	2.13	0.49
1:D:320:GLN:HA	1:D:337:ARG:O	2.13	0.49
1:D:636:GLU:O	1:D:640:ASN:CG	2.56	0.49
1:D:812:VAL:O	1:D:815:ALA:HB3	2.13	0.49
1:A:564:HIS:CD2	1:A:565:MET:HG3	2.47	0.49
1:B:628:PRO:HG2	1:B:634:GLN:CG	2.41	0.49
1:B:681:THR:HG21	1:B:724:VAL:HB	1.95	0.49
1:C:323:GLU:CD	1:C:335:GLN:NE2	2.71	0.49
1:D:90:SER:HB3	1:D:242:MET:SD	2.53	0.49
1:D:352:ASP:C	1:D:354:VAL:N	2.69	0.49
1:A:91:VAL:HG22	1:A:239:VAL:CG1	2.41	0.49
1:A:217:ASN:O	1:A:220:ALA:HB3	2.13	0.49
1:A:258:THR:O	1:A:259:ARG:CG	2.57	0.49
1:A:370:ALA:HA	1:A:864:LEU:CD2	2.41	0.49
1:A:572:ILE:O	1:A:576:ARG:HG3	2.13	0.49
1:B:9:GLU:CA	1:B:31:ILE:HD11	2.31	0.49
1:B:219:ARG:HD2	1:B:433:PRO:HB2	1.93	0.49
1:B:321:ASP:OD1	1:B:321:ASP:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:665:ARG:HG3	1:B:707:LEU:HD13	1.94	0.49
1:C:115:ALA:O	1:C:119:PHE:N	2.46	0.49
1:C:156:ILE:HD11	1:C:183:PHE:HZ	1.78	0.49
1:C:527:TRP:N	1:C:527:TRP:CD1	2.80	0.49
1:C:834:HIS:C	1:C:836:GLY:N	2.71	0.49
1:A:330:LYS:HD3	1:A:332:TYR:CZ	2.48	0.48
1:B:7:LYS:HB2	1:B:10:GLU:HG3	1.94	0.48
1:B:782:ALA:HA	1:B:785:PHE:CE2	2.48	0.48
1:D:215:TRP:CE2	1:D:224:ARG:NH1	2.81	0.48
1:A:331:LEU:HD21	1:A:333:PHE:CE1	2.48	0.48
1:A:395:ALA:HB1	1:A:470:GLY:O	2.12	0.48
1:A:527:TRP:N	1:A:527:TRP:CD1	2.79	0.48
1:A:781:ASP:OD1	1:B:657:GLU:HG2	2.13	0.48
1:B:259:ARG:HG2	1:B:266:LYS:HA	1.95	0.48
1:B:691:VAL:O	1:B:691:VAL:CG1	2.61	0.48
1:C:348:GLN:HA	1:C:348:GLN:OE1	2.13	0.48
1:C:532:ARG:NH1	1:C:534:LEU:O	2.46	0.48
1:D:26:LEU:O	1:D:30:THR:HB	2.13	0.48
1:D:92:ARG:HA	1:D:105:THR:HG23	1.95	0.48
1:A:8:PHE:O	1:A:27:ALA:HA	2.13	0.48
1:B:330:LYS:HD2	1:B:332:TYR:OH	2.13	0.48
1:C:80:PHE:CE2	1:C:200:PRO:HB2	2.48	0.48
1:C:369:GLU:HG2	1:C:372:SER:CB	2.40	0.48
1:C:563:GLU:CG	1:C:621:PRO:HD3	2.43	0.48
1:C:856:PRO:C	1:C:858:ARG:H	2.21	0.48
1:A:22:LYS:O	1:A:26:LEU:HG	2.14	0.48
1:A:564:HIS:C	1:A:566:PHE:H	2.20	0.48
1:B:168:ASP:OD1	1:B:168:ASP:N	2.46	0.48
1:B:448:VAL:C	1:B:449:ARG:CG	2.86	0.48
1:B:765:PHE:HZ	1:B:815:ALA:HB3	1.78	0.48
1:C:29:MET:HE1	1:C:333:PHE:CD2	2.48	0.48
1:D:80:PHE:CE1	1:D:89:VAL:HG22	2.48	0.48
1:D:323:GLU:HG2	1:D:335:GLN:HB3	1.95	0.48
1:D:628:PRO:HG3	1:D:637:LEU:HD23	1.95	0.48
1:A:109:LEU:HD12	1:A:136:PHE:CE1	2.47	0.48
1:A:835:GLY:O	1:A:854:CYS:HB3	2.12	0.48
1:C:273:LEU:HD12	1:C:281:VAL:HG23	1.95	0.48
1:D:708:VAL:HG11	1:D:714:LEU:HB2	1.95	0.48
1:D:792:ALA:O	1:D:793:LYS:HB2	2.13	0.48
1:A:144:VAL:HG22	1:A:210:ALA:CB	2.43	0.48
1:A:309:ALA:CB	1:A:322:MET:HE1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:SER:OG	1:A:433:PRO:HD2	2.13	0.48
1:A:704:MET:HE2	1:A:704:MET:HB3	1.76	0.48
1:A:859:VAL:O	1:A:863:ARG:HG3	2.13	0.48
1:B:743:MET:HE3	1:B:745:GLU:OE2	2.13	0.48
1:B:753:ALA:CB	1:B:815:ALA:HA	2.43	0.48
1:C:630:THR:HG21	1:C:632:GLU:HB3	1.96	0.48
1:D:128:PHE:HE1	1:D:244:PHE:CG	2.32	0.48
1:D:134:ARG:CZ	1:D:135:ARG:HG2	2.44	0.48
1:D:716:PHE:O	1:D:720:VAL:HG23	2.13	0.48
1:A:120:ALA:O	1:A:124:GLY:CA	2.62	0.48
1:B:187:TYR:CD1	1:B:187:TYR:C	2.91	0.48
1:C:30:THR:HA	1:C:36:ILE:HD13	1.96	0.48
1:C:375:GLN:O	1:C:377:LEU:N	2.46	0.48
1:C:580:LEU:HB3	1:C:643:LEU:CD1	2.44	0.48
1:C:676:ILE:O	1:C:680:GLN:HG3	2.13	0.48
1:C:833:GLU:HG3	1:C:858:ARG:NH2	2.28	0.48
1:D:17:ASN:ND2	1:D:96:ARG:NH2	2.61	0.48
1:D:28:GLU:C	1:D:32:LEU:HD12	2.38	0.48
1:A:634:GLN:NE2	1:A:649:LYS:HE2	2.29	0.48
1:A:671:VAL:HG11	1:B:789:TYR:CD1	2.49	0.48
1:B:144:VAL:HG12	1:B:145:MET:HE3	1.95	0.48
1:B:275:ASN:OD1	1:B:275:ASN:O	2.32	0.48
1:B:518:SER:O	1:B:521:PHE:HB3	2.14	0.48
1:B:565:MET:HE1	1:B:602:PHE:CE1	2.48	0.48
1:C:323:GLU:OE1	2:C:901:ANP:H3'	2.13	0.48
1:C:831:CYS:HA	1:C:853:SER:HB3	1.96	0.48
1:D:219:ARG:HB3	1:D:436:ILE:HG22	1.94	0.48
1:D:219:ARG:CG	1:D:219:ARG:NH1	2.71	0.48
1:D:772:GLN:HG3	1:D:800:PHE:HE1	1.78	0.48
1:A:580:LEU:N	1:A:580:LEU:HD22	2.29	0.48
1:B:42:VAL:O	1:B:236:ALA:HB1	2.14	0.48
1:B:588:GLU:HG2	1:B:675:GLU:HG2	1.95	0.48
1:B:846:LYS:HB3	1:B:846:LYS:HE3	1.72	0.48
1:C:37:PRO:HG3	1:C:332:TYR:CD1	2.48	0.48
1:C:103:MET:CE	1:C:215:TRP:HE3	2.26	0.48
1:C:342:THR:HG22	1:C:461:ARG:O	2.14	0.48
1:C:347:LEU:HD11	1:C:376:LEU:HD11	1.96	0.48
1:C:396:LEU:CD1	1:C:396:LEU:N	2.77	0.48
1:D:88:LEU:HD21	1:D:111:LEU:CD2	2.43	0.48
1:A:73:GLU:OE1	1:A:80:PHE:N	2.25	0.48
1:A:410:THR:OG1	1:A:413:GLU:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:GLU:H	1:A:473:GLU:CD	2.22	0.48
1:A:549:ALA:C	1:A:554:ALA:HB3	2.39	0.48
1:A:664:HIS:CD2	1:B:785:PHE:HB3	2.48	0.48
1:B:70:THR:HA	1:B:73:GLU:OE2	2.14	0.48
1:B:250:THR:HA	1:B:298:MET:HE1	1.95	0.48
1:B:585:GLU:H	1:B:585:GLU:HG2	1.41	0.48
1:C:448:VAL:HG13	1:C:471:CYS:O	2.14	0.48
1:D:174:ASP:HA	1:D:177:LYS:CB	2.41	0.48
1:D:288:PRO:C	1:D:289:GLN:HG3	2.39	0.48
1:D:381:PHE:CD1	1:D:402:ALA:HB1	2.48	0.48
1:A:92:ARG:HA	1:A:105:THR:HG23	1.95	0.47
1:A:552:LEU:O	1:A:863:ARG:NH1	2.47	0.47
1:B:22:LYS:HE2	1:B:92:ARG:CZ	2.44	0.47
1:B:455:HIS:O	1:B:456:ALA:C	2.57	0.47
1:B:519:GLY:O	1:B:522:GLU:N	2.47	0.47
1:B:772:GLN:HG3	1:B:800:PHE:CE1	2.49	0.47
1:C:400:PRO:HA	1:C:500:GLY:C	2.39	0.47
1:D:30:THR:HG22	1:D:31:ILE:HD13	1.96	0.47
1:D:385:ALA:CB	1:D:511:GLU:HB3	2.43	0.47
1:D:771:THR:HG21	1:D:799:PRO:O	2.13	0.47
1:B:154:LYS:O	1:B:158:ALA:N	2.45	0.47
1:C:343:ALA:HB2	1:C:375:GLN:NE2	2.29	0.47
1:C:767:THR:HA	1:C:770:LEU:HB3	1.97	0.47
1:A:282:VAL:CG1	1:A:455:HIS:CE1	2.98	0.47
1:A:630:THR:O	1:A:634:GLN:HG3	2.14	0.47
1:A:784:LYS:HD3	1:B:664:HIS:CB	2.39	0.47
1:B:529:ASP:HA	1:B:532:ARG:NE	2.30	0.47
1:C:583:SER:HB3	1:C:586:ALA:CB	2.45	0.47
1:C:634:GLN:HB3	1:C:645:LEU:HD11	1.95	0.47
1:D:427:VAL:HG22	1:D:446:LEU:HB3	1.95	0.47
1:A:282:VAL:HG13	1:A:455:HIS:CE1	2.50	0.47
1:A:415:LYS:HD2	1:A:437:GLU:HB3	1.96	0.47
1:A:525:MET:HB3	1:A:863:ARG:NH2	2.29	0.47
1:A:575:ILE:O	1:A:579:ILE:HG13	2.14	0.47
1:A:854:CYS:SG	1:A:859:VAL:HA	2.55	0.47
1:B:30:THR:O	1:B:33:GLY:N	2.34	0.47
1:C:286:ARG:O	1:C:288:PRO:HD3	2.14	0.47
1:D:552:LEU:O	1:D:863:ARG:NH1	2.47	0.47
1:D:630:THR:O	1:D:634:GLN:HG3	2.14	0.47
1:D:754:ASP:HA	1:D:818:LYS:O	2.15	0.47
1:B:72:LEU:HD22	1:B:241:THR:HB	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:LYS:C	1:B:551:LYS:CD	2.87	0.47
1:B:578:MET:HG2	1:B:587:ARG:CB	2.45	0.47
1:B:844:CYS:HB3	1:B:849:LEU:HD22	1.96	0.47
1:C:575:ILE:O	1:C:578:MET:HB3	2.14	0.47
1:C:716:PHE:CD1	1:C:716:PHE:C	2.92	0.47
1:D:109:LEU:HD11	1:D:207:ALA:CB	2.44	0.47
1:A:25:ASN:O	1:A:29:MET:HG3	2.14	0.47
1:A:342:THR:HB	1:A:344:PRO:HD2	1.97	0.47
1:B:456:ALA:O	1:B:460:ALA:N	2.44	0.47
1:B:578:MET:HG3	1:B:587:ARG:O	2.14	0.47
1:C:253:THR:HG21	1:C:277:GLN:O	2.13	0.47
1:D:31:ILE:HD12	1:D:31:ILE:HA	1.52	0.47
1:D:77:GLY:C	1:D:78:LYS:HG2	2.39	0.47
1:D:252:GLY:HA3	1:D:272:TYR:CZ	2.50	0.47
1:D:427:VAL:HA	1:D:446:LEU:O	2.14	0.47
1:A:743:MET:CE	1:A:766:GLY:HA3	2.44	0.47
1:A:831:CYS:O	1:A:831:CYS:SG	2.72	0.47
1:B:22:LYS:NZ	1:B:93:SER:O	2.47	0.47
1:B:127:ARG:NH1	1:B:127:ARG:HG2	2.30	0.47
1:B:149:LYS:O	1:B:150:SER:C	2.57	0.47
1:B:245:GLY:O	1:B:275:ASN:HA	2.15	0.47
1:B:355:ASP:CG	1:B:523:ARG:HH12	2.23	0.47
1:B:785:PHE:CE1	1:B:786:LEU:CD1	2.95	0.47
1:B:844:CYS:CB	1:B:849:LEU:HD22	2.44	0.47
1:C:222:VAL:HG11	1:C:436:ILE:HG23	1.96	0.47
1:C:273:LEU:HG	1:C:288:PRO:HB3	1.97	0.47
1:C:409:PHE:CE2	1:C:483:PHE:HD1	2.33	0.47
1:C:502:THR:C	1:C:504:LYS:H	2.23	0.47
1:C:637:LEU:HA	1:C:640:ASN:HD22	1.80	0.47
1:D:88:LEU:CD2	1:D:111:LEU:HG	2.44	0.47
1:D:259:ARG:HD3	1:D:266:LYS:HA	1.95	0.47
1:D:342:THR:HG23	1:D:461:ARG:HG3	1.97	0.47
1:D:549:ALA:HB1	1:D:554:ALA:CB	2.44	0.47
1:A:211:VAL:HG12	1:A:237:VAL:HG22	1.97	0.47
1:A:341:ARG:HB2	1:A:345:ALA:HB3	1.96	0.47
1:B:142:ASP:OD2	1:B:142:ASP:C	2.58	0.47
1:B:371:LYS:HA	1:B:861:ILE:HD13	1.97	0.47
1:B:620:ASP:HB3	1:B:621:PRO:HD3	1.95	0.47
1:C:22:LYS:HG3	3:C:902:SO4:O4	2.15	0.47
1:C:93:SER:HB3	1:C:211:VAL:HG13	1.97	0.47
1:C:482:THR:HA	1:C:491:ALA:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:TYR:CE1	1:D:191:MET:HG3	2.50	0.47
1:D:219:ARG:HG2	1:D:434:GLU:HA	1.96	0.47
1:D:282:VAL:HB	1:D:455:HIS:HE2	1.78	0.47
1:D:304:GLN:HB2	1:D:331:LEU:HD23	1.96	0.47
1:D:361:GLU:O	1:D:362:GLU:C	2.58	0.47
1:D:722:VAL:O	1:D:726:GLU:HG2	2.14	0.47
1:B:100:PRO:O	1:B:102:MET:HG2	2.14	0.47
1:B:343:ALA:HB3	1:B:344:PRO:CD	2.44	0.47
1:C:353:LEU:HB2	1:C:359:ILE:CD1	2.45	0.47
1:C:408:TYR:CD1	1:C:424:VAL:HG13	2.50	0.47
1:C:440:HIS:C	1:C:440:HIS:ND1	2.72	0.47
1:C:532:ARG:HB3	1:C:867:ALA:HA	1.97	0.47
1:C:584:VAL:HG13	1:C:585:GLU:H	1.79	0.47
1:D:255:VAL:CB	1:D:453:THR:CG2	2.86	0.47
1:D:569:ALA:O	1:D:572:ILE:HG22	2.15	0.47
1:D:814:MET:SD	1:D:818:LYS:HE3	2.55	0.47
1:A:156:ILE:HG23	1:A:157:ASP:N	2.30	0.47
1:B:214:SER:O	1:B:215:TRP:C	2.57	0.47
1:B:255:VAL:HG22	1:B:323:GLU:HA	1.97	0.47
1:B:619:LEU:HD12	1:B:621:PRO:HD2	1.97	0.47
1:C:244:PHE:H	1:C:327:GLU:HB2	1.80	0.47
1:C:398:ALA:HA	1:C:452:MET:HG2	1.97	0.47
1:C:546:THR:O	1:C:550:VAL:HG22	2.14	0.47
1:C:794:ILE:O	1:D:712:LYS:HE3	2.16	0.47
1:A:561:ARG:NH2	3:A:4004:SO4:S	2.89	0.46
1:A:576:ARG:O	1:A:580:LEU:HD23	2.15	0.46
1:A:595:ILE:HG13	1:A:679:MET:HG2	1.96	0.46
1:A:667:CYS:O	1:A:671:VAL:HG23	2.15	0.46
1:A:725:ALA:O	1:A:729:LYS:HG3	2.15	0.46
1:B:272:TYR:HE1	1:B:274:ILE:HD13	1.80	0.46
1:B:303:LYS:NZ	1:B:307:ASP:OD2	2.44	0.46
1:C:426:LEU:HG	1:C:428:ARG:HG2	1.97	0.46
1:C:662:MET:CE	1:C:773:MET:SD	3.03	0.46
1:C:729:LYS:HE3	1:C:736:MET:H	1.79	0.46
1:D:29:MET:HG2	1:D:312:LEU:HD21	1.96	0.46
1:D:127:ARG:NH2	1:D:246:ASN:O	2.48	0.46
1:D:630:THR:O	1:D:634:GLN:N	2.36	0.46
1:D:778:SER:OG	1:D:781:ASP:HB2	2.14	0.46
1:A:403:ALA:HB1	1:A:425:ILE:HD11	1.97	0.46
1:A:624:HIS:HB2	1:A:655:LEU:HB3	1.97	0.46
1:B:308:LEU:O	1:B:312:LEU:HG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:PRO:HD3	1:B:376:LEU:HD23	1.98	0.46
1:B:537:ARG:HG2	1:B:558:GLY:CA	2.45	0.46
1:B:843:PHE:O	1:B:847:VAL:HG22	2.16	0.46
1:C:102:MET:HE3	1:C:219:ARG:CB	2.45	0.46
1:C:186:VAL:C	1:C:189:GLU:HB3	2.40	0.46
1:C:263:THR:OG1	1:C:265:GLU:HB3	2.14	0.46
1:C:268:ILE:HG21	1:C:302:TYR:OH	2.15	0.46
1:C:343:ALA:HB2	1:C:375:GLN:HB2	1.96	0.46
1:C:662:MET:SD	1:D:662:MET:HE1	2.55	0.46
1:D:175:ASP:O	1:D:179:LEU:HB2	2.15	0.46
1:D:498:LEU:CD2	1:D:505:ILE:HG23	2.45	0.46
1:D:557:ILE:HG13	1:D:609:LEU:HD21	1.97	0.46
1:A:91:VAL:O	1:A:105:THR:HG23	2.15	0.46
1:A:136:PHE:CE2	1:A:203:GLN:NE2	2.83	0.46
1:A:603:LYS:CE	1:A:691:VAL:HG23	2.45	0.46
1:C:338:ASN:O	1:C:339:GLY:O	2.34	0.46
1:C:667:CYS:O	1:C:670:ALA:HB3	2.14	0.46
1:C:673:TYR:HB2	1:C:676:ILE:HD12	1.97	0.46
1:C:747:PRO:O	1:C:750:ALA:HB3	2.15	0.46
1:D:102:MET:O	1:D:220:ALA:HB2	2.15	0.46
1:D:414:ALA:HB1	1:D:424:VAL:HG11	1.97	0.46
1:D:541:ASP:OD1	1:D:541:ASP:N	2.48	0.46
1:A:220:ALA:O	1:A:223:TYR:N	2.48	0.46
1:A:440:HIS:CA	1:A:463:MET:HE1	2.46	0.46
1:A:780:ASP:HB3	1:B:658:PHE:HD2	1.80	0.46
1:B:82:ASP:O	1:B:86:PRO:HB3	2.16	0.46
1:B:391:VAL:HG21	1:B:504:LYS:HD3	1.98	0.46
1:B:568:GLU:O	1:B:571:ARG:HB2	2.16	0.46
1:C:89:VAL:HG12	1:C:241:THR:N	2.31	0.46
1:C:103:MET:HA	1:C:217:ASN:OD1	2.15	0.46
1:C:495:TYR:HB3	1:C:508:GLY:C	2.40	0.46
1:C:857:PHE:N	1:C:857:PHE:HD1	2.14	0.46
1:D:334:LEU:O	1:D:335:GLN:HB2	2.15	0.46
1:A:767:THR:CG2	1:A:830:ILE:HD11	2.45	0.46
1:B:528:ALA:CA	1:B:867:ALA:HB2	2.45	0.46
1:C:32:LEU:O	1:C:33:GLY:C	2.58	0.46
1:C:223:TYR:HD2	1:C:436:ILE:CD1	2.28	0.46
1:C:609:LEU:HD11	1:C:614:MET:HE2	1.98	0.46
1:D:32:LEU:HD21	1:D:315:HIS:CD2	2.50	0.46
1:D:172:THR:HG22	1:D:173:ALA:N	2.29	0.46
1:D:301:CYS:SG	1:D:329:GLY:O	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:635:ALA:CB	1:D:645:LEU:HD22	2.35	0.46
1:D:814:MET:HG3	1:D:818:LYS:HE3	1.96	0.46
1:A:495:TYR:CD2	1:A:509:ASP:HB2	2.50	0.46
1:A:669:LEU:HD12	1:A:669:LEU:HA	1.66	0.46
1:B:5:VAL:C	1:B:6:TYR:CD1	2.94	0.46
1:B:92:ARG:HD3	2:B:901:ANP:H8	1.84	0.46
1:B:92:ARG:CD	2:B:901:ANP:C8	2.84	0.46
1:B:331:LEU:HD12	1:B:332:TYR:N	2.31	0.46
1:C:16:ARG:HA	1:C:24:CYS:CB	2.46	0.46
1:C:135:ARG:O	1:C:139:MET:HG3	2.16	0.46
1:C:142:ASP:OD1	1:C:142:ASP:O	2.33	0.46
1:C:432:SER:OG	1:C:434:GLU:OE1	2.34	0.46
1:D:77:GLY:O	1:D:78:LYS:HG2	2.16	0.46
1:D:92:ARG:HD3	2:D:901:ANP:H8	1.97	0.46
1:D:180:ALA:O	1:D:183:PHE:N	2.48	0.46
1:D:253:THR:CG2	1:D:278:GLY:HA2	2.44	0.46
1:D:465:THR:O	1:D:466:CYS:C	2.58	0.46
1:D:498:LEU:HD21	1:D:505:ILE:HG23	1.98	0.46
1:A:16:ARG:NH2	3:A:4003:SO4:O3	2.49	0.46
1:B:321:ASP:OD1	1:B:321:ASP:O	2.34	0.46
1:B:578:MET:O	1:B:587:ARG:HG3	2.15	0.46
1:D:191:MET:HB2	1:D:194:GLU:O	2.16	0.46
1:D:257:PHE:HB3	1:D:259:ARG:O	2.16	0.46
1:A:139:MET:HE3	1:A:279:GLU:HG3	1.96	0.46
1:A:372:SER:C	1:A:374:ASP:N	2.69	0.46
1:A:784:LYS:HG3	1:B:664:HIS:HB2	1.97	0.46
1:B:92:ARG:HB2	1:B:238:ASN:HB2	1.97	0.46
1:B:100:PRO:O	1:B:102:MET:N	2.49	0.46
1:B:354:VAL:HG22	1:B:360:THR:O	2.16	0.46
1:B:554:ALA:HB2	1:B:859:VAL:HG21	1.97	0.46
1:B:574:LYS:CG	1:B:593:GLU:HB2	2.46	0.46
1:C:308:LEU:O	1:C:311:LYS:HB3	2.15	0.46
1:C:599:LYS:CE	1:C:686:GLU:HG2	2.46	0.46
1:D:5:VAL:HA	1:D:41:THR:O	2.14	0.46
1:D:710:GLU:OE2	1:D:712:LYS:HE2	2.16	0.46
1:D:765:PHE:CD2	1:D:765:PHE:N	2.84	0.46
1:D:767:THR:HA	1:D:770:LEU:HB3	1.98	0.46
1:D:837:ASP:OD1	1:D:838:PRO:HD2	2.16	0.46
1:A:120:ALA:HB2	1:A:129:ALA:CB	2.45	0.46
1:A:565:MET:HB3	1:A:598:GLN:NE2	2.31	0.46
1:B:56:GLN:C	1:B:57:ILE:HD13	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:GLU:HA	1:B:87:LEU:HD22	1.97	0.46
1:B:342:THR:HG21	1:B:400:PRO:HG3	1.96	0.46
1:B:630:THR:CG2	1:B:633:GLU:H	2.28	0.46
1:C:73:GLU:HA	1:C:87:LEU:HD22	1.97	0.46
1:C:353:LEU:CB	1:C:359:ILE:HG12	2.46	0.46
1:C:364:ALA:HA	1:C:367:ARG:HG2	1.97	0.46
1:C:540:ALA:HB3	1:C:557:ILE:CD1	2.46	0.46
1:C:574:LYS:HB2	1:C:594:LEU:CD2	2.44	0.46
1:C:804:ASP:CG	1:D:748:ARG:HH21	2.23	0.46
1:D:98:SER:HB2	3:D:903:SO4:O1	2.15	0.46
1:D:205:MET:O	1:D:209:LYS:HG3	2.16	0.46
1:B:292:THR:O	1:B:296:ASN:OD1	2.34	0.46
1:B:615:THR:HG22	1:B:704:MET:HB2	1.98	0.46
1:C:562:THR:HG21	1:C:616:VAL:HG13	1.98	0.46
1:C:672:THR:C	1:C:674:PRO:HD3	2.41	0.46
1:D:91:VAL:CG1	1:D:237:VAL:HG13	2.46	0.46
1:A:128:PHE:O	1:A:129:ALA:C	2.59	0.45
1:A:525:MET:HB3	1:A:863:ARG:CZ	2.45	0.45
1:A:607:LYS:HD3	1:A:691:VAL:HG22	1.98	0.45
1:A:775:PHE:C	1:B:746:ILE:HG21	2.41	0.45
1:B:345:ALA:O	1:B:346:ALA:C	2.59	0.45
1:C:50:TYR:HD2	1:C:57:ILE:HD13	1.81	0.45
1:C:95:ALA:HB2	1:C:103:MET:CE	2.37	0.45
1:C:289:GLN:HB3	1:C:290:PRO:HD2	1.97	0.45
1:C:483:PHE:N	1:C:490:PHE:O	2.43	0.45
1:C:700:VAL:HG22	1:C:737:GLN:HB2	1.98	0.45
1:C:824:PRO:C	1:C:826:LEU:H	2.24	0.45
1:D:359:ILE:CD1	1:D:364:ALA:HA	2.45	0.45
1:D:623:LEU:C	1:D:625:GLU:N	2.74	0.45
1:B:230:PRO:HG2	1:B:233:TRP:NE1	2.31	0.45
1:B:278:GLY:HA3	2:B:901:ANP:O3'	2.16	0.45
1:B:320:GLN:HA	1:B:337:ARG:O	2.15	0.45
1:B:383:PRO:HD3	1:B:513:GLN:NE2	2.30	0.45
1:B:483:PHE:C	1:B:483:PHE:CD2	2.94	0.45
1:B:552:LEU:HD12	1:B:856:PRO:O	2.15	0.45
1:B:773:MET:HE3	1:B:773:MET:CA	2.45	0.45
1:C:168:ASP:OD1	1:C:286:ARG:NH2	2.49	0.45
1:C:330:LYS:HG2	1:C:332:TYR:CE2	2.51	0.45
1:C:361:GLU:C	1:C:363:GLU:N	2.75	0.45
1:D:137:ILE:HG22	1:D:138:GLN:N	2.31	0.45
1:D:191:MET:HB3	1:D:194:GLU:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:LEU:CD1	1:D:857:PHE:O	2.64	0.45
1:D:855:SER:O	1:D:858:ARG:HB2	2.16	0.45
1:A:73:GLU:HG2	1:A:78:LYS:O	2.16	0.45
1:A:584:VAL:O	1:A:587:ARG:HB2	2.16	0.45
1:A:689:ILE:HD13	1:A:734:SER:HB2	1.97	0.45
1:B:49:GLU:HG2	1:B:61:ILE:HD11	1.99	0.45
1:B:280:ASP:OD2	1:B:280:ASP:N	2.37	0.45
1:B:708:VAL:CG1	1:B:709:GLY:N	2.79	0.45
1:C:371:LYS:H	1:C:371:LYS:HG2	1.59	0.45
1:C:562:THR:CG2	1:C:616:VAL:HG13	2.47	0.45
1:C:661:MET:HA	1:C:665:ARG:NH1	2.30	0.45
1:D:111:LEU:HD22	1:D:116:VAL:HG22	1.98	0.45
1:D:342:THR:CB	1:D:344:PRO:HD2	2.45	0.45
1:D:652:VAL:HG12	1:D:652:VAL:O	2.16	0.45
1:D:685:MET:HB3	1:D:728:VAL:HG11	1.97	0.45
1:A:620:ASP:H	1:A:621:PRO:CD	2.30	0.45
1:A:620:ASP:N	1:A:621:PRO:HD2	2.31	0.45
1:B:432:SER:OG	1:B:434:GLU:HB2	2.16	0.45
1:C:112:ASN:O	1:C:113:ASP:C	2.59	0.45
1:C:380:THR:HG23	1:C:515:ALA:HB2	1.97	0.45
1:C:408:TYR:HD1	1:C:424:VAL:HG13	1.81	0.45
1:C:657:GLU:HG2	1:D:784:LYS:HZ1	1.81	0.45
1:D:116:VAL:O	1:D:119:PHE:HB3	2.16	0.45
1:D:191:MET:CB	1:D:194:GLU:O	2.64	0.45
1:A:136:PHE:HE2	1:A:203:GLN:HE22	1.64	0.45
1:A:182:LYS:O	1:A:185:ALA:HB3	2.16	0.45
1:A:484:GLU:HG2	1:A:489:THR:OG1	2.17	0.45
1:B:31:ILE:N	1:B:31:ILE:HD12	2.31	0.45
1:B:157:ASP:O	1:B:158:ALA:C	2.60	0.45
1:B:311:LYS:O	1:B:314:LYS:N	2.49	0.45
1:B:525:MET:O	1:B:529:ASP:HB2	2.16	0.45
1:B:552:LEU:HD23	1:B:552:LEU:HA	1.77	0.45
1:B:643:LEU:HD13	1:B:647:GLU:OE2	2.16	0.45
1:C:90:SER:HB3	1:C:107:LEU:HD23	1.98	0.45
1:C:243:VAL:HG23	1:C:325:THR:HG21	1.97	0.45
1:C:259:ARG:HB2	1:C:349:ILE:CD1	2.46	0.45
1:C:287:THR:HG23	1:C:450:GLY:O	2.17	0.45
1:C:541:ASP:OD1	1:C:561:ARG:HD3	2.17	0.45
1:C:550:VAL:C	1:C:552:LEU:N	2.72	0.45
1:C:785:PHE:CD1	1:D:668:ARG:HG2	2.52	0.45
1:D:148:PRO:HB2	1:D:150:SER:OG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:334:LEU:HD22	2:D:901:ANP:C2	2.47	0.45
1:A:442:ALA:HB1	1:A:444:GLY:O	2.16	0.45
1:A:768:ASN:OD1	1:A:832:GLY:CA	2.64	0.45
1:B:8:PHE:O	1:B:27:ALA:HB1	2.17	0.45
1:C:318:ASP:OD1	1:C:367:ARG:NH1	2.49	0.45
1:C:571:ARG:CD	1:C:571:ARG:N	2.79	0.45
1:D:321:ASP:N	1:D:337:ARG:O	2.43	0.45
1:A:47:CYS:HB2	1:A:235:THR:O	2.17	0.45
1:A:259:ARG:HA	1:A:267:GLY:O	2.16	0.45
1:B:133:TYR:O	1:B:137:ILE:HG13	2.17	0.45
1:B:842:GLU:HA	1:B:869:ALA:HB2	1.98	0.45
1:C:50:TYR:CE2	1:C:55:LYS:C	2.95	0.45
1:C:305:PHE:CZ	1:C:324:PHE:CD1	3.04	0.45
1:C:588:GLU:HG3	1:C:675:GLU:HG2	1.99	0.45
1:C:635:ALA:CA	1:C:645:LEU:HD13	2.47	0.45
1:D:666:GLY:O	1:D:667:CYS:C	2.59	0.45
1:A:331:LEU:HG	1:A:332:TYR:N	2.31	0.45
1:A:339:GLY:O	1:A:340:LYS:C	2.58	0.45
1:A:609:LEU:O	1:A:612:ARG:HG3	2.16	0.45
1:A:741:GLY:HA3	1:A:762:PHE:CE1	2.51	0.45
1:B:7:LYS:O	1:B:8:PHE:C	2.60	0.45
1:B:50:TYR:HA	1:B:56:GLN:O	2.17	0.45
1:B:84:GLU:O	1:B:86:PRO:HD3	2.16	0.45
1:B:838:PRO:HA	1:B:841:VAL:HB	1.98	0.45
1:C:9:GLU:HG3	1:C:10:GLU:H	1.81	0.45
1:C:689:ILE:HA	1:C:736:MET:CE	2.46	0.45
1:C:710:GLU:HG3	1:C:713:GLU:H	1.82	0.45
1:D:664:HIS:CE1	1:D:672:THR:OG1	2.69	0.45
1:A:111:LEU:HB3	1:A:133:TYR:CD1	2.52	0.45
1:A:617:ARG:HD2	1:A:618:TYR:O	2.17	0.45
1:B:519:GLY:O	1:B:520:SER:C	2.57	0.45
1:C:577:LYS:O	1:C:581:SER:OG	2.16	0.45
1:C:855:SER:HB2	1:C:858:ARG:HG3	1.99	0.45
1:D:137:ILE:HG21	1:D:183:PHE:CB	2.47	0.45
1:D:634:GLN:CD	1:D:649:LYS:HE2	2.42	0.45
1:A:310:MET:HE2	1:A:310:MET:HA	1.99	0.45
1:A:381:PHE:CZ	1:A:497:SER:HB3	2.51	0.45
1:A:603:LYS:HE3	1:A:690:GLU:HB2	1.99	0.45
1:A:741:GLY:HA3	1:A:762:PHE:CZ	2.51	0.45
1:A:748:ARG:HB2	1:B:774:THR:HG22	1.97	0.45
1:B:395:ALA:HB2	1:B:471:CYS:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:MET:HG3	1:C:187:TYR:CE2	2.52	0.45
1:C:251:SER:HA	1:C:326:ILE:O	2.17	0.45
1:C:381:PHE:CE2	1:C:402:ALA:HA	2.52	0.45
1:C:603:LYS:HG2	1:C:687:ALA:HA	1.98	0.45
1:C:858:ARG:C	1:C:860:PRO:HD2	2.41	0.45
1:D:317:ARG:NH2	1:D:363:GLU:OE2	2.49	0.45
1:D:603:LYS:O	1:D:607:LYS:HG3	2.16	0.45
1:A:130:TYR:CE2	1:A:177:LYS:HE2	2.52	0.44
1:A:269:TYR:CD1	1:A:269:TYR:C	2.95	0.44
1:A:372:SER:O	1:A:374:ASP:N	2.50	0.44
1:B:100:PRO:HB2	1:B:459:VAL:HG23	1.99	0.44
1:B:257:PHE:C	1:B:259:ARG:N	2.75	0.44
1:C:136:PHE:CE2	1:C:196:PHE:HE1	2.35	0.44
1:C:142:ASP:CG	1:C:149:LYS:HD3	2.41	0.44
1:C:232:ASP:OD1	1:C:232:ASP:N	2.47	0.44
1:C:746:ILE:O	1:C:748:ARG:N	2.49	0.44
1:D:82:ASP:N	1:D:86:PRO:HA	2.30	0.44
1:D:128:PHE:CD2	1:D:128:PHE:C	2.94	0.44
1:D:288:PRO:CD	1:D:451:GLY:HA3	2.46	0.44
1:D:312:LEU:HD22	1:D:336:THR:HG21	1.99	0.44
1:A:55:LYS:HZ1	1:A:213:ARG:HG2	1.81	0.44
1:A:381:PHE:CE1	1:A:402:ALA:HB1	2.52	0.44
1:B:6:TYR:CD1	1:B:6:TYR:N	2.85	0.44
1:B:209:LYS:O	1:B:212:PHE:HB2	2.17	0.44
1:C:108:ASN:ND2	1:C:135:ARG:HB2	2.32	0.44
1:C:382:ASN:O	1:C:386:LEU:N	2.46	0.44
1:C:407:VAL:HG21	1:C:483:PHE:CE1	2.47	0.44
1:C:754:ASP:HA	1:C:818:LYS:O	2.18	0.44
1:D:590:ALA:HA	1:D:593:GLU:OE2	2.17	0.44
1:A:354:VAL:HG23	1:A:359:ILE:HG13	1.99	0.44
1:A:485:LEU:O	1:A:487:GLY:N	2.51	0.44
1:A:566:PHE:N	1:A:566:PHE:CD1	2.83	0.44
1:B:468:VAL:HG21	1:B:498:LEU:HB3	1.99	0.44
1:C:313:GLU:OE2	1:C:319:MET:HA	2.17	0.44
1:C:639:LYS:HE3	1:C:639:LYS:HB3	1.80	0.44
1:A:82:ASP:OD2	1:A:83:THR:N	2.46	0.44
1:A:536:VAL:N	1:A:555:GLU:OE1	2.31	0.44
1:A:559:LEU:HD12	1:A:704:MET:HE1	1.98	0.44
1:A:678:LYS:CB	1:A:724:VAL:HG21	2.47	0.44
1:A:710:GLU:HG3	1:A:713:GLU:H	1.82	0.44
1:B:107:LEU:HD12	1:B:277:GLN:HE21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:THR:HB	1:B:174:ASP:HB2	1.99	0.44
1:B:175:ASP:OD1	1:B:175:ASP:N	2.51	0.44
1:B:485:LEU:HG	1:B:486:GLY:N	2.31	0.44
1:B:583:SER:HB3	1:B:586:ALA:CB	2.47	0.44
1:C:549:ALA:C	1:C:554:ALA:HB3	2.42	0.44
1:C:580:LEU:HB2	1:C:641:MET:CE	2.47	0.44
1:C:591:LEU:HB3	1:C:679:MET:HG3	1.99	0.44
1:D:669:LEU:HG	1:D:673:TYR:HD2	1.81	0.44
1:A:244:PHE:HB2	1:A:247:LYS:HG3	2.00	0.44
1:A:403:ALA:O	1:A:498:LEU:N	2.47	0.44
1:A:769:ASP:O	1:A:773:MET:HE3	2.17	0.44
1:B:5:VAL:C	1:B:6:TYR:HD1	2.25	0.44
1:B:88:LEU:HD23	1:B:88:LEU:HA	1.83	0.44
1:C:29:MET:HB2	1:C:36:ILE:HG12	2.00	0.44
1:C:312:LEU:O	1:C:313:GLU:C	2.59	0.44
1:C:407:VAL:HG12	1:C:496:ILE:HG12	1.98	0.44
1:C:575:ILE:HD12	1:C:578:MET:HE3	1.98	0.44
1:C:681:THR:HG23	1:C:721:VAL:HG13	1.99	0.44
1:D:107:LEU:HD11	2:D:901:ANP:O4'	2.16	0.44
1:D:704:MET:HB3	1:D:762:PHE:HE1	1.82	0.44
1:A:8:PHE:CE1	1:A:40:PHE:CA	3.00	0.44
1:A:561:ARG:HH11	1:A:563:GLU:CG	2.31	0.44
1:A:660:PRO:HD2	1:B:659:ASN:OD1	2.17	0.44
1:B:320:GLN:NE2	1:B:338:ASN:OD1	2.46	0.44
1:B:833:GLU:HG3	1:B:858:ARG:NH2	2.31	0.44
1:C:322:MET:HB2	1:C:322:MET:HE3	1.45	0.44
1:C:510:ILE:HG22	1:C:511:GLU:H	1.82	0.44
1:C:527:TRP:O	1:C:531:PHE:HD2	2.00	0.44
1:D:174:ASP:HA	1:D:177:LYS:CG	2.48	0.44
1:D:623:LEU:HB2	1:D:655:LEU:CD2	2.40	0.44
1:A:93:SER:OG	1:A:104:ASP:O	2.27	0.44
1:A:141:SER:O	1:A:145:MET:HB2	2.16	0.44
1:B:856:PRO:O	1:B:859:VAL:HG23	2.17	0.44
1:C:526:VAL:HG12	1:C:527:TRP:HD1	1.83	0.44
1:C:635:ALA:HA	1:C:645:LEU:HD13	2.00	0.44
1:C:794:ILE:HG22	1:C:795:TYR:CD1	2.52	0.44
1:C:830:ILE:HG21	1:C:844:CYS:SG	2.58	0.44
1:D:585:GLU:H	1:D:585:GLU:HG2	1.63	0.44
1:D:726:GLU:OE2	1:D:726:GLU:HA	2.17	0.44
1:D:741:GLY:HA3	1:D:762:PHE:CD1	2.53	0.44
1:A:139:MET:CE	1:A:279:GLU:HG3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ARG:CG	1:A:229:ILE:HB	2.46	0.44
1:B:127:ARG:HG2	1:B:127:ARG:HH11	1.82	0.44
1:B:342:THR:HG21	1:B:400:PRO:CG	2.48	0.44
1:B:561:ARG:HB3	1:B:617:ARG:HH12	1.82	0.44
1:B:630:THR:HG23	1:B:632:GLU:HB3	1.99	0.44
1:C:571:ARG:NH2	1:C:601:ASP:OD2	2.51	0.44
1:D:537:ARG:NH2	1:D:613:PRO:HB2	2.32	0.44
1:D:634:GLN:HB3	1:D:645:LEU:HD11	2.00	0.44
1:D:690:GLU:HG3	1:D:732:LYS:CE	2.48	0.44
1:A:148:PRO:HG2	1:A:151:HIS:ND1	2.33	0.44
1:A:603:LYS:CG	1:A:687:ALA:HB1	2.48	0.44
1:A:847:VAL:HG23	1:A:849:LEU:HD13	2.00	0.44
1:B:349:ILE:O	1:B:352:ASP:HB2	2.18	0.44
1:B:400:PRO:O	1:B:466:CYS:HA	2.18	0.44
1:B:482:THR:HB	1:B:489:THR:CG2	2.48	0.44
1:B:537:ARG:HH21	1:B:613:PRO:HB2	1.82	0.44
1:B:747:PRO:HD3	1:B:770:LEU:HD12	2.00	0.44
1:C:22:LYS:HZ1	2:C:901:ANP:PA	2.41	0.44
1:C:365:VAL:HG13	1:C:864:LEU:HD13	1.99	0.44
1:C:417:ALA:HB1	1:C:422:GLU:OE2	2.18	0.44
1:C:490:PHE:CZ	1:C:507:LYS:HG3	2.51	0.44
1:C:541:ASP:OD2	1:C:561:ARG:HB2	2.17	0.44
1:C:615:THR:HA	1:C:702:GLU:O	2.17	0.44
1:D:99:MET:HG2	1:D:223:TYR:CD1	2.53	0.44
1:D:427:VAL:HG12	1:D:476:ILE:HD13	1.99	0.44
1:D:440:HIS:CA	1:D:463:MET:HE1	2.48	0.44
1:D:525:MET:HB3	1:D:863:ARG:NH2	2.32	0.44
1:D:751:LEU:HA	1:D:814:MET:SD	2.58	0.44
1:D:844:CYS:O	1:D:845:HIS:C	2.61	0.44
1:A:99:MET:HA	1:A:223:TYR:CE1	2.53	0.43
1:A:393:GLY:C	1:A:505:ILE:HD12	2.43	0.43
1:A:823:ARG:O	1:A:826:LEU:HB3	2.18	0.43
1:B:527:TRP:N	1:B:527:TRP:CD1	2.85	0.43
1:B:614:MET:HE3	1:B:616:VAL:CG2	2.48	0.43
1:B:802:ARG:HG3	1:B:837:ASP:OD2	2.18	0.43
1:C:614:MET:CG	1:C:615:THR:H	2.31	0.43
1:C:621:PRO:HG2	1:C:626:PHE:HZ	1.82	0.43
1:D:351:CYS:O	1:D:354:VAL:HB	2.18	0.43
1:D:753:ALA:HB3	1:D:818:LYS:HB2	1.99	0.43
1:D:804:ASP:OD2	1:D:808:VAL:HG23	2.18	0.43
1:A:66:PHE:HA	1:A:69:ILE:HB	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:PHE:HE1	1:A:235:THR:O	2.01	0.43
1:A:455:HIS:HE1	2:A:4001:ANP:O2B	1.97	0.43
1:A:715:LYS:O	1:A:719:ASP:N	2.41	0.43
1:B:373:LEU:HB2	1:B:861:ILE:HG12	2.00	0.43
1:B:540:ALA:O	1:B:557:ILE:HD13	2.18	0.43
1:B:682:ARG:NH1	1:B:728:VAL:HG22	2.34	0.43
1:C:411:ALA:HA	1:C:438:GLY:HA3	2.00	0.43
1:C:704:MET:SD	1:C:743:MET:HG2	2.57	0.43
1:C:753:ALA:CB	1:C:815:ALA:HA	2.48	0.43
1:D:224:ARG:HH22	1:D:793:LYS:HE3	1.83	0.43
1:D:360:THR:OG1	1:D:363:GLU:HG3	2.18	0.43
1:D:406:LYS:HD3	1:D:422:GLU:OE2	2.18	0.43
1:D:580:LEU:HG	1:D:641:MET:HE1	1.99	0.43
1:A:32:LEU:HD11	1:A:315:HIS:CD2	2.53	0.43
1:A:65:ILE:HG21	1:A:205:MET:HE1	1.99	0.43
1:A:112:ASN:O	1:A:113:ASP:C	2.62	0.43
1:A:145:MET:SD	1:A:191:MET:SD	3.16	0.43
1:A:748:ARG:O	1:A:748:ARG:HG2	2.17	0.43
1:B:222:VAL:O	1:B:226:MET:HG3	2.18	0.43
1:B:381:PHE:HE2	1:B:498:LEU:O	2.01	0.43
1:B:406:LYS:HE3	1:B:406:LYS:HB3	1.72	0.43
1:B:406:LYS:HG2	1:B:495:TYR:CE1	2.54	0.43
1:B:580:LEU:CB	1:B:641:MET:HE1	2.48	0.43
1:B:681:THR:HG21	1:B:721:VAL:O	2.19	0.43
1:B:718:LYS:HG3	1:B:740:ILE:HG21	2.00	0.43
1:B:829:GLY:HA3	1:B:851:TYR:CE1	2.53	0.43
1:C:31:ILE:HD12	1:C:31:ILE:N	2.33	0.43
1:C:118:GLY:HA2	1:C:121:LYS:HZ3	1.84	0.43
1:C:171:LEU:HB3	1:C:175:ASP:CB	2.48	0.43
1:C:182:LYS:O	1:C:186:VAL:HG23	2.18	0.43
1:C:362:GLU:O	1:C:366:VAL:HG23	2.17	0.43
1:C:466:CYS:SG	1:C:498:LEU:HB2	2.59	0.43
1:C:804:ASP:HB2	1:C:808:VAL:HG23	2.00	0.43
1:C:807:GLY:O	1:C:810:GLN:HB2	2.18	0.43
1:D:111:LEU:HD23	1:D:111:LEU:HA	1.81	0.43
1:D:119:PHE:CZ	1:D:128:PHE:CE2	3.06	0.43
1:D:243:VAL:HG23	2:D:901:ANP:H2	2.00	0.43
1:D:439:MET:HE3	1:D:445:ILE:HD13	1.99	0.43
1:D:531:PHE:HB2	1:D:867:ALA:HB1	1.99	0.43
1:D:570:ASP:CB	1:D:597:PHE:CE2	2.92	0.43
1:A:73:GLU:CD	1:A:80:PHE:H	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LEU:N	1:A:75:LEU:HD23	2.32	0.43
1:A:92:ARG:HB3	1:A:105:THR:HG21	2.00	0.43
1:A:259:ARG:HB2	1:A:319:MET:CG	2.46	0.43
1:A:869:ALA:O	1:A:873:ASN:HB2	2.17	0.43
1:B:823:ARG:HD2	1:B:826:LEU:HD13	2.00	0.43
2:B:901:ANP:O1B	2:B:901:ANP:O1A	2.36	0.43
1:C:615:THR:OG1	1:C:702:GLU:OE1	2.37	0.43
1:D:188:LYS:HA	1:D:191:MET:HB2	1.99	0.43
1:A:363:GLU:O	1:A:364:ALA:C	2.62	0.43
1:A:391:VAL:HG22	1:A:506:TYR:CE1	2.53	0.43
1:A:474:ILE:HG23	1:A:483:PHE:CD2	2.53	0.43
1:A:536:VAL:HA	1:A:852:VAL:O	2.19	0.43
1:B:363:GLU:O	1:B:367:ARG:HG2	2.18	0.43
1:B:374:ASP:OD1	1:B:375:GLN:HG3	2.19	0.43
1:B:782:ALA:O	1:B:783:GLY:C	2.61	0.43
1:C:96:ARG:HD2	1:C:233:TRP:CH2	2.53	0.43
1:C:96:ARG:HD2	1:C:233:TRP:CZ3	2.54	0.43
1:C:99:MET:HG2	1:C:223:TYR:CD1	2.53	0.43
1:C:150:SER:C	1:C:152:PHE:H	2.26	0.43
1:C:188:LYS:HE3	1:C:195:GLU:HB3	2.01	0.43
1:C:486:GLY:O	1:C:487:GLY:C	2.60	0.43
1:D:174:ASP:O	1:D:178:GLU:N	2.43	0.43
1:D:271:GLU:OE1	1:D:288:PRO:HG3	2.18	0.43
1:D:300:ASP:O	1:D:304:GLN:HG3	2.17	0.43
1:D:341:ARG:HB2	1:D:345:ALA:HB3	2.00	0.43
1:D:377:LEU:HD12	1:D:857:PHE:O	2.18	0.43
1:D:396:LEU:HB3	1:D:452:MET:SD	2.59	0.43
1:D:496:ILE:HG22	1:D:506:TYR:O	2.18	0.43
1:A:79:LYS:HE2	1:A:79:LYS:HB3	1.76	0.43
1:A:137:ILE:HA	1:A:196:PHE:CE2	2.54	0.43
1:A:395:ALA:HB2	1:A:471:CYS:HA	2.00	0.43
1:A:564:HIS:C	1:A:566:PHE:N	2.77	0.43
1:A:727:GLN:O	1:A:731:GLU:HG3	2.19	0.43
1:B:112:ASN:HB3	1:B:198:GLN:O	2.18	0.43
1:B:488:HIS:CG	1:B:489:THR:H	2.36	0.43
1:B:537:ARG:HB3	1:B:853:SER:OG	2.18	0.43
1:B:753:ALA:HB3	1:B:818:LYS:HB2	2.01	0.43
1:C:30:THR:O	1:C:32:LEU:N	2.51	0.43
1:C:130:TYR:CD2	1:C:177:LYS:HE2	2.53	0.43
1:C:830:ILE:O	1:C:853:SER:N	2.51	0.43
1:D:179:LEU:HG	1:D:183:PHE:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:381:PHE:HD1	1:D:381:PHE:HA	1.73	0.43
1:D:592:ASN:HA	1:D:595:ILE:HG13	2.00	0.43
1:D:765:PHE:HD2	1:D:829:GLY:O	2.01	0.43
1:B:134:ARG:HD2	1:B:138:GLN:OE1	2.19	0.43
1:B:295:GLU:HG3	1:B:302:TYR:CD2	2.54	0.43
1:B:583:SER:O	1:B:586:ALA:HB3	2.19	0.43
1:C:102:MET:O	1:C:219:ARG:NE	2.51	0.43
1:C:789:TYR:OH	1:D:671:VAL:HG21	2.19	0.43
1:D:90:SER:HB2	1:D:107:LEU:HD23	2.00	0.43
1:D:187:TYR:CE1	1:D:196:PHE:HA	2.54	0.43
1:D:306:MET:O	1:D:310:MET:HG2	2.19	0.43
1:D:557:ILE:HG22	1:D:559:LEU:H	1.84	0.43
1:D:599:LYS:O	1:D:603:LYS:HG3	2.19	0.43
1:D:644:THR:C	1:D:646:ALA:H	2.27	0.43
1:D:682:ARG:NH2	1:D:731:GLU:CD	2.73	0.43
1:D:738:TYR:HE1	1:D:740:ILE:HD11	1.83	0.43
1:A:386:LEU:HD11	1:A:506:TYR:CZ	2.54	0.43
1:A:521:PHE:O	1:A:525:MET:HG2	2.19	0.43
1:A:549:ALA:O	1:A:550:VAL:C	2.62	0.43
1:A:779:ARG:C	1:A:781:ASP:H	2.26	0.43
1:B:50:TYR:HD2	1:B:57:ILE:HD13	1.83	0.43
1:B:94:GLY:C	1:B:235:THR:OG1	2.62	0.43
1:B:229:ILE:HA	1:B:230:PRO:HD3	1.93	0.43
1:C:37:PRO:HD3	1:C:332:TYR:HB3	2.01	0.43
1:C:550:VAL:HG11	1:C:612:ARG:CZ	2.49	0.43
1:D:73:GLU:HG2	1:D:80:PHE:H	1.83	0.43
1:D:399:SER:HB3	1:D:467:CYS:N	2.34	0.43
1:A:30:THR:HA	1:A:36:ILE:HD13	2.01	0.43
1:A:386:LEU:HD11	1:A:506:TYR:CE2	2.54	0.43
1:A:407:VAL:C	1:A:408:TYR:CD1	2.97	0.43
1:A:448:VAL:O	1:A:470:GLY:HA2	2.19	0.43
1:A:561:ARG:HH11	1:A:563:GLU:HB2	1.83	0.43
1:B:109:LEU:C	1:B:109:LEU:HD23	2.43	0.43
1:B:530:LYS:HE3	1:B:531:PHE:HE1	1.77	0.43
1:C:111:LEU:HD13	1:C:133:TYR:CA	2.48	0.43
1:C:772:GLN:OE1	1:C:779:ARG:N	2.33	0.43
1:C:869:ALA:O	1:C:873:ASN:HB2	2.17	0.43
1:D:127:ARG:HG2	1:D:176:LEU:HD12	2.00	0.43
1:D:182:LYS:O	1:D:186:VAL:HG23	2.19	0.43
1:D:518:SER:OG	1:D:519:GLY:N	2.51	0.43
1:D:637:LEU:HG	1:D:641:MET:CE	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:704:MET:HB3	1:D:762:PHE:CE1	2.54	0.43
1:A:215:TRP:CG	1:A:234:GLY:HA2	2.54	0.43
1:B:34:MET:HB2	1:B:36:ILE:HD13	2.01	0.43
1:B:161:GLU:O	1:B:164:GLY:N	2.39	0.43
1:B:400:PRO:HA	1:B:500:GLY:O	2.18	0.43
1:B:499:ASP:C	1:B:501:SER:H	2.27	0.43
1:C:31:ILE:CD1	1:C:31:ILE:N	2.82	0.43
1:C:291:ILE:CG2	1:C:292:THR:N	2.81	0.43
1:C:391:VAL:HA	1:C:505:ILE:O	2.19	0.43
1:C:416:ALA:O	1:C:420:LYS:N	2.49	0.43
1:C:495:TYR:HB3	1:C:508:GLY:O	2.18	0.43
1:C:621:PRO:HG2	1:C:626:PHE:CZ	2.54	0.43
1:D:225:ARG:HG3	1:D:797:SER:HA	2.01	0.43
1:D:229:ILE:HA	1:D:230:PRO:HD3	1.72	0.43
1:A:93:SER:OG	1:A:103:MET:HB3	2.19	0.42
1:A:440:HIS:HA	1:A:463:MET:CE	2.48	0.42
1:A:609:LEU:CD1	1:A:614:MET:HB2	2.49	0.42
1:A:729:LYS:HE2	1:A:729:LYS:HB3	1.67	0.42
2:A:4001:ANP:O1B	2:A:4001:ANP:O1A	2.37	0.42
1:B:230:PRO:C	1:B:232:ASP:H	2.26	0.42
1:B:568:GLU:O	1:B:569:ALA:C	2.62	0.42
1:B:578:MET:HG2	1:B:587:ARG:HG2	2.01	0.42
1:B:602:PHE:HB2	1:B:687:ALA:CB	2.48	0.42
1:B:794:ILE:C	1:B:795:TYR:HD1	2.27	0.42
1:C:455:HIS:HE1	2:C:901:ANP:O2B	2.01	0.42
1:C:529:ASP:C	1:C:531:PHE:H	2.27	0.42
1:D:62:GLN:CG	1:D:66:PHE:CE2	3.02	0.42
1:D:571:ARG:HA	1:D:594:LEU:HD21	2.01	0.42
1:A:382:ASN:HB3	1:A:385:ALA:HB3	2.00	0.42
1:A:566:PHE:O	1:A:567:PHE:C	2.62	0.42
1:B:121:LYS:HE2	1:B:121:LYS:HB2	1.87	0.42
1:B:137:ILE:HG13	1:B:137:ILE:H	1.60	0.42
1:B:168:ASP:C	1:B:170:ASP:H	2.27	0.42
1:B:431:THR:HG23	1:B:447:THR:OG1	2.19	0.42
1:C:30:THR:C	1:C:32:LEU:N	2.77	0.42
1:C:871:LEU:C	1:C:873:ASN:H	2.27	0.42
1:A:23:GLY:O	1:A:25:ASN:N	2.53	0.42
1:A:355:ASP:O	1:A:356:GLU:C	2.61	0.42
1:A:533:THR:OG1	1:A:845:HIS:CE1	2.72	0.42
1:A:722:VAL:O	1:A:722:VAL:HG12	2.19	0.42
1:A:722:VAL:HG22	1:A:740:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:772:GLN:HG3	1:A:800:PHE:HE1	1.82	0.42
1:B:82:ASP:CG	1:B:83:THR:N	2.77	0.42
1:B:793:LYS:NZ	1:B:793:LYS:HB3	2.34	0.42
1:C:125:ASN:HD21	1:C:128:PHE:HB3	1.85	0.42
1:C:576:ARG:O	1:C:580:LEU:HD23	2.20	0.42
1:C:639:LYS:C	1:C:641:MET:H	2.27	0.42
1:D:259:ARG:NH2	1:D:353:LEU:HD23	2.34	0.42
1:D:345:ALA:O	1:D:349:ILE:HG13	2.19	0.42
1:A:630:THR:HG22	1:A:632:GLU:H	1.84	0.42
1:A:707:LEU:HD23	1:A:745:GLU:HG3	2.01	0.42
1:A:843:PHE:CD2	1:A:843:PHE:C	2.98	0.42
1:B:257:PHE:O	1:B:259:ARG:N	2.52	0.42
1:B:375:GLN:HA	1:B:378:HIS:ND1	2.35	0.42
1:B:729:LYS:O	1:B:733:GLY:N	2.47	0.42
1:C:128:PHE:CE2	1:C:247:LYS:HE2	2.55	0.42
1:C:352:ASP:O	1:C:356:GLU:N	2.42	0.42
1:D:301:CYS:HA	1:D:304:GLN:HG3	2.01	0.42
1:D:367:ARG:HE	1:D:367:ARG:HB3	1.37	0.42
1:D:463:MET:HB2	1:D:465:THR:OG1	2.18	0.42
1:A:230:PRO:HB2	1:A:233:TRP:NE1	2.35	0.42
1:A:677:ALA:HB3	1:A:720:VAL:HG11	2.02	0.42
1:A:752:THR:O	1:A:753:ALA:C	2.62	0.42
1:B:150:SER:HA	1:B:153:GLU:HB2	2.01	0.42
1:B:706:PRO:HA	1:B:743:MET:HG3	2.01	0.42
1:B:858:ARG:C	1:B:860:PRO:CD	2.92	0.42
1:C:322:MET:HG2	1:C:333:PHE:HE2	1.85	0.42
1:C:361:GLU:O	1:C:363:GLU:N	2.52	0.42
1:C:368:ILE:CG2	1:C:369:GLU:N	2.82	0.42
1:C:580:LEU:HD23	1:C:641:MET:HE1	2.02	0.42
1:C:587:ARG:O	1:C:591:LEU:HG	2.20	0.42
1:C:705:ILE:O	1:C:743:MET:HB2	2.19	0.42
1:D:424:VAL:O	1:D:425:ILE:HD13	2.20	0.42
1:D:805:GLN:HG2	1:D:843:PHE:CD1	2.53	0.42
1:A:72:LEU:HA	1:A:72:LEU:HD23	1.83	0.42
1:A:219:ARG:HG2	1:A:219:ARG:NH1	2.35	0.42
1:A:242:MET:HE3	1:A:242:MET:HB3	1.91	0.42
1:B:34:MET:SD	1:B:312:LEU:HD21	2.59	0.42
1:B:78:LYS:HB3	1:B:85:ASP:O	2.20	0.42
1:B:779:ARG:O	1:B:782:ALA:HB3	2.18	0.42
1:B:842:GLU:O	1:B:844:CYS:N	2.52	0.42
1:C:103:MET:SD	1:C:235:THR:HB	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:553:GLY:HA3	1:C:863:ARG:NH1	2.35	0.42
1:C:571:ARG:NH1	1:C:597:PHE:CB	2.80	0.42
1:C:597:PHE:HD1	1:C:597:PHE:H	1.68	0.42
1:C:623:LEU:CB	1:C:655:LEU:HD13	2.50	0.42
1:C:784:LYS:H	1:C:784:LYS:HG2	1.41	0.42
2:C:901:ANP:O1A	2:C:901:ANP:O1B	2.37	0.42
1:D:103:MET:HB3	1:D:214:SER:HB3	2.01	0.42
1:D:224:ARG:CA	1:D:229:ILE:HB	2.47	0.42
1:D:268:ILE:HG21	1:D:302:TYR:OH	2.19	0.42
1:D:463:MET:H	1:D:463:MET:HG3	1.58	0.42
1:D:537:ARG:HD3	1:D:851:TYR:CG	2.55	0.42
1:D:598:GLN:O	1:D:601:ASP:HB2	2.20	0.42
1:D:676:ILE:O	1:D:680:GLN:HG3	2.19	0.42
1:A:188:LYS:HG2	1:A:189:GLU:N	2.34	0.42
1:A:595:ILE:N	1:A:596:PRO:HD2	2.35	0.42
1:A:746:ILE:HG22	1:A:748:ARG:H	1.84	0.42
1:B:29:MET:HB3	1:B:36:ILE:HG12	2.01	0.42
1:B:66:PHE:CE1	1:B:204:LEU:HD23	2.55	0.42
1:B:214:SER:HA	1:B:217:ASN:OD1	2.19	0.42
1:B:341:ARG:CD	1:B:346:ALA:HA	2.50	0.42
1:B:624:HIS:O	1:B:624:HIS:ND1	2.53	0.42
1:C:353:LEU:HB2	1:C:359:ILE:HG12	2.02	0.42
1:C:506:TYR:CD2	1:C:506:TYR:N	2.87	0.42
1:D:50:TYR:CE1	1:D:55:LYS:HA	2.54	0.42
1:D:246:ASN:CG	1:D:277:GLN:HG3	2.45	0.42
1:D:270:GLY:O	1:D:291:ILE:HG22	2.19	0.42
1:D:571:ARG:HD3	1:D:594:LEU:CD2	2.49	0.42
1:D:573:MET:HA	1:D:573:MET:HE3	2.01	0.42
1:D:623:LEU:C	1:D:625:GLU:H	2.27	0.42
1:D:818:LYS:O	1:D:821:GLN:HB2	2.19	0.42
1:A:678:LYS:CA	1:A:724:VAL:HG21	2.49	0.42
1:B:219:ARG:CD	1:B:433:PRO:O	2.67	0.42
1:B:399:SER:OG	1:B:465:THR:O	2.36	0.42
1:B:537:ARG:HB3	1:B:853:SER:CB	2.50	0.42
1:C:309:ALA:O	1:C:312:LEU:HB2	2.19	0.42
1:C:352:ASP:C	1:C:354:VAL:N	2.75	0.42
1:C:706:PRO:HA	1:C:743:MET:CB	2.50	0.42
1:C:837:ASP:HA	1:C:838:PRO:HD3	1.82	0.42
1:D:224:ARG:CB	1:D:229:ILE:HB	2.50	0.42
1:D:478:GLU:C	1:D:481:LYS:H	2.28	0.42
1:D:537:ARG:HG2	1:D:556:GLY:CA	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:627:VAL:HB	1:D:628:PRO:HD2	2.02	0.42
1:D:751:LEU:HD23	1:D:814:MET:SD	2.60	0.42
1:A:259:ARG:HH12	1:A:352:ASP:CB	2.32	0.42
1:A:820:ARG:NH2	1:A:850:ASN:OD1	2.53	0.42
1:B:138:GLN:HG3	1:B:183:PHE:CE2	2.54	0.42
1:B:777:PHE:CD1	1:B:777:PHE:C	2.98	0.42
1:C:191:MET:HE2	1:C:191:MET:HA	2.01	0.42
1:C:257:PHE:CD1	1:C:321:ASP:HB2	2.55	0.42
1:C:260:ASN:HA	1:C:261:PRO:HD3	1.77	0.42
1:C:568:GLU:O	1:C:572:ILE:HB	2.20	0.42
1:C:659:ASN:CG	1:D:661:MET:HB2	2.44	0.42
1:D:257:PHE:N	1:D:269:TYR:O	2.45	0.42
1:D:473:GLU:CB	1:D:485:LEU:HD11	2.50	0.42
1:A:624:HIS:O	1:A:624:HIS:ND1	2.53	0.42
1:A:765:PHE:N	1:A:829:GLY:O	2.42	0.42
1:A:772:GLN:CG	1:A:800:PHE:HE1	2.33	0.42
1:A:823:ARG:O	1:A:826:LEU:CB	2.68	0.42
1:B:652:VAL:O	1:B:655:LEU:N	2.52	0.42
1:C:381:PHE:HZ	1:C:498:LEU:O	2.02	0.42
1:C:577:LYS:HA	1:C:641:MET:CE	2.49	0.42
1:C:645:LEU:O	1:C:645:LEU:HG	2.20	0.42
1:D:92:ARG:NH1	2:D:901:ANP:H2'	2.33	0.42
1:D:423:ARG:HH22	1:D:509:ASP:CG	2.26	0.42
1:D:523:ARG:O	1:D:526:VAL:HB	2.20	0.42
1:D:524:ILE:HD13	1:D:524:ILE:HA	1.89	0.42
1:A:60:GLU:O	1:A:64:GLN:CG	2.68	0.41
1:A:212:PHE:CE1	1:A:237:VAL:HG23	2.54	0.41
1:A:215:TRP:CH2	1:A:224:ARG:HD3	2.55	0.41
1:A:491:ALA:O	1:A:492:GLU:C	2.62	0.41
1:A:654:GLU:C	1:A:656:HIS:H	2.26	0.41
1:B:325:THR:O	1:B:332:TYR:N	2.51	0.41
1:B:343:ALA:N	1:B:344:PRO:CD	2.83	0.41
1:B:467:CYS:SG	1:B:468:VAL:N	2.93	0.41
1:B:497:SER:OG	1:B:509:ASP:HA	2.19	0.41
1:B:614:MET:HE3	1:B:616:VAL:HG23	2.00	0.41
1:B:704:MET:C	1:B:705:ILE:HD12	2.45	0.41
1:B:830:ILE:HG22	1:B:852:VAL:CG1	2.43	0.41
1:C:127:ARG:O	1:C:176:LEU:HD13	2.20	0.41
1:C:475:LYS:O	1:C:483:PHE:HB2	2.20	0.41
1:C:793:LYS:O	1:D:712:LYS:HD2	2.20	0.41
1:C:842:GLU:O	1:C:846:LYS:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:LEU:HG	1:D:136:PHE:CE1	2.55	0.41
1:D:204:LEU:O	1:D:208:VAL:HG23	2.20	0.41
1:A:92:ARG:HA	1:A:105:THR:CG2	2.50	0.41
1:A:566:PHE:CE1	1:A:619:LEU:HD13	2.56	0.41
1:A:648:VAL:HG12	1:A:649:LYS:N	2.35	0.41
1:B:104:ASP:OD1	1:B:219:ARG:NH2	2.47	0.41
1:B:224:ARG:HE	1:B:231:GLY:HA2	1.85	0.41
1:B:455:HIS:CE1	2:B:901:ANP:PB	3.13	0.41
1:B:715:LYS:C	1:B:715:LYS:CD	2.93	0.41
1:C:16:ARG:NH2	3:C:903:SO4:O2	2.53	0.41
1:C:29:MET:HE3	1:C:29:MET:HB3	1.85	0.41
1:C:71:TRP:O	1:C:75:LEU:HB2	2.20	0.41
1:C:370:ALA:O	1:C:861:ILE:HG23	2.19	0.41
1:C:510:ILE:CG2	1:C:511:GLU:N	2.83	0.41
1:C:525:MET:HE2	1:C:525:MET:HA	2.03	0.41
1:D:317:ARG:HH22	1:D:363:GLU:CD	2.28	0.41
1:D:692:LYS:HD2	1:D:698:ASP:HA	2.02	0.41
1:D:745:GLU:HA	1:D:770:LEU:HB2	2.01	0.41
1:D:774:THR:CG2	1:D:808:VAL:HG22	2.47	0.41
1:A:348:GLN:O	1:A:352:ASP:OD2	2.37	0.41
1:B:303:LYS:NZ	1:B:307:ASP:CG	2.78	0.41
1:B:673:TYR:C	1:B:675:GLU:N	2.78	0.41
1:B:786:LEU:HD12	1:B:786:LEU:HA	1.82	0.41
1:C:343:ALA:CB	1:C:375:GLN:HB2	2.51	0.41
1:C:424:VAL:HG12	1:C:425:ILE:N	2.33	0.41
1:C:428:ARG:O	1:C:447:THR:HA	2.21	0.41
1:C:541:ASP:O	1:C:605:MET:HE2	2.21	0.41
1:D:18:LEU:HG	1:D:43:THR:CG2	2.50	0.41
1:D:321:ASP:HB3	1:D:337:ARG:CG	2.47	0.41
1:D:762:PHE:CD1	1:D:762:PHE:C	2.98	0.41
1:A:156:ILE:CG2	1:A:157:ASP:N	2.83	0.41
1:A:395:ALA:O	1:A:503:GLY:HA3	2.21	0.41
1:B:491:ALA:O	1:B:492:GLU:C	2.64	0.41
1:B:574:LYS:HG2	1:B:593:GLU:HB2	2.02	0.41
1:B:575:ILE:O	1:B:579:ILE:HG13	2.21	0.41
1:B:595:ILE:HG12	1:B:679:MET:HG2	2.02	0.41
1:B:691:VAL:O	1:B:695:THR:OG1	2.24	0.41
1:C:189:GLU:HG3	1:C:190:ALA:N	2.36	0.41
1:D:28:GLU:O	1:D:29:MET:C	2.64	0.41
1:D:30:THR:CA	1:D:36:ILE:HD12	2.51	0.41
1:D:119:PHE:CE1	1:D:123:THR:HG21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:ILE:CG2	1:D:183:PHE:HB3	2.50	0.41
1:D:139:MET:CE	1:D:279:GLU:HG3	2.50	0.41
1:A:39:GLY:CA	1:A:240:GLN:HA	2.42	0.41
1:A:274:ILE:HG22	1:A:275:ASN:HB2	2.02	0.41
1:A:382:ASN:ND2	1:A:385:ALA:CB	2.82	0.41
1:A:532:ARG:HB3	1:A:867:ALA:CA	2.47	0.41
1:A:789:TYR:CE1	1:B:671:VAL:HG11	2.56	0.41
1:B:318:ASP:O	1:B:320:GLN:HG2	2.20	0.41
1:B:525:MET:HA	1:B:525:MET:HE2	2.03	0.41
1:B:528:ALA:HA	1:B:867:ALA:CB	2.50	0.41
1:C:159:MET:HA	1:C:159:MET:CE	2.45	0.41
1:C:477:ASN:O	1:C:478:GLU:C	2.63	0.41
1:D:62:GLN:HG2	1:D:66:PHE:CD2	2.56	0.41
1:D:455:HIS:NE2	2:D:901:ANP:O2B	2.54	0.41
1:D:594:LEU:HD23	1:D:594:LEU:HA	1.88	0.41
1:D:602:PHE:O	1:D:605:MET:N	2.54	0.41
1:D:867:ALA:O	1:D:868:GLN:C	2.61	0.41
1:A:137:ILE:CG2	1:A:183:PHE:HB3	2.51	0.41
1:A:165:VAL:HB	1:A:170:ASP:CB	2.51	0.41
1:A:347:LEU:HD11	1:A:376:LEU:HD11	2.03	0.41
1:A:859:VAL:HB	1:A:860:PRO:HD3	2.02	0.41
1:B:22:LYS:HE2	1:B:92:ARG:NH2	2.36	0.41
1:B:108:ASN:OD1	1:B:242:MET:HE2	2.21	0.41
1:B:638:ALA:O	1:B:643:LEU:N	2.36	0.41
1:B:777:PHE:HD1	1:B:777:PHE:C	2.29	0.41
1:B:859:VAL:N	1:B:860:PRO:HD3	2.36	0.41
1:C:108:ASN:HD22	1:C:135:ARG:HB2	1.86	0.41
1:C:264:GLY:HA2	1:C:349:ILE:CG1	2.51	0.41
1:C:392:ILE:HG13	1:C:505:ILE:CG2	2.50	0.41
1:C:597:PHE:CD1	1:C:597:PHE:N	2.89	0.41
1:C:751:LEU:CD1	1:D:811:LEU:HG	2.44	0.41
1:D:163:LYS:HE2	1:D:163:LYS:HB3	1.91	0.41
1:D:317:ARG:HH21	1:D:359:ILE:HA	1.85	0.41
1:D:369:GLU:CB	1:D:372:SER:OG	2.66	0.41
1:A:82:ASP:OD2	1:A:83:THR:HG22	2.20	0.41
1:A:211:VAL:HG11	1:A:237:VAL:HG13	2.01	0.41
1:A:222:VAL:HG11	1:A:437:GLU:OE2	2.20	0.41
1:A:382:ASN:ND2	1:A:385:ALA:HB2	2.22	0.41
1:A:485:LEU:O	1:A:486:GLY:C	2.64	0.41
1:A:572:ILE:HG13	1:A:576:ARG:HG3	2.02	0.41
1:A:689:ILE:O	1:A:690:GLU:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ASP:C	1:B:159:MET:N	2.76	0.41
1:B:767:THR:HA	1:B:770:LEU:HB3	2.02	0.41
1:B:777:PHE:HE2	1:B:795:TYR:HE2	1.69	0.41
1:C:99:MET:HG2	1:C:223:TYR:HD1	1.85	0.41
1:C:321:ASP:C	1:C:322:MET:HG3	2.46	0.41
1:C:698:ASP:OD1	1:C:699:ILE:N	2.54	0.41
1:D:343:ALA:CB	1:D:372:SER:O	2.65	0.41
1:D:495:TYR:CD2	1:D:509:ASP:HB2	2.55	0.41
1:D:536:VAL:O	1:D:536:VAL:HG12	2.21	0.41
1:D:618:TYR:CE1	1:D:703:ILE:HG23	2.56	0.41
1:A:29:MET:HE2	1:A:336:THR:HG22	2.03	0.41
1:A:107:LEU:H	1:A:139:MET:HE2	1.86	0.41
1:A:282:VAL:O	1:A:455:HIS:HB2	2.20	0.41
1:A:375:GLN:HA	1:A:378:HIS:ND1	2.36	0.41
1:A:414:ALA:HB1	1:A:424:VAL:HG11	2.02	0.41
1:A:837:ASP:HB3	1:A:840:SER:OG	2.21	0.41
1:B:448:VAL:HG22	1:B:474:ILE:HB	2.02	0.41
1:B:495:TYR:HB3	1:B:509:ASP:HB2	2.02	0.41
1:B:538:THR:HA	1:B:854:CYS:O	2.20	0.41
1:C:378:HIS:HA	1:C:379:PRO:HD3	1.75	0.41
1:C:638:ALA:HB2	1:C:648:VAL:HG21	2.02	0.41
1:C:671:VAL:HG21	1:D:789:TYR:CZ	2.55	0.41
1:C:833:GLU:O	1:C:858:ARG:NH2	2.53	0.41
1:D:73:GLU:HG2	1:D:79:LYS:HA	2.03	0.41
1:D:377:LEU:HD13	1:D:857:PHE:CB	2.51	0.41
1:D:525:MET:HE2	1:D:528:ALA:HB3	2.03	0.41
1:A:59:GLN:OE1	1:A:63:ASP:OD1	2.39	0.41
1:A:204:LEU:O	1:A:208:VAL:HG23	2.21	0.41
1:A:484:GLU:HG2	1:A:489:THR:HG23	2.03	0.41
1:A:575:ILE:HD12	1:A:578:MET:HB3	2.02	0.41
1:A:753:ALA:HB3	1:A:818:LYS:CB	2.39	0.41
1:A:794:ILE:HD13	1:B:713:GLU:HA	2.03	0.41
1:B:24:CYS:O	1:B:28:GLU:HB2	2.21	0.41
1:B:130:TYR:CZ	1:B:177:LYS:HG2	2.55	0.41
1:B:172:THR:HG21	1:B:174:ASP:OD2	2.21	0.41
1:B:372:SER:HB2	1:B:375:GLN:NE2	2.34	0.41
1:B:606:TYR:HA	1:B:609:LEU:HB2	2.02	0.41
1:B:673:TYR:C	1:B:675:GLU:H	2.29	0.41
1:C:101:GLY:HA3	1:C:455:HIS:ND1	2.36	0.41
1:C:156:ILE:O	1:C:156:ILE:CG2	2.67	0.41
1:C:323:GLU:CD	1:C:335:GLN:HE21	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:446:LEU:HD21	1:C:474:ILE:HD11	2.03	0.41
1:C:449:ARG:CA	1:C:470:GLY:HA2	2.51	0.41
1:C:541:ASP:C	1:C:605:MET:HE2	2.46	0.41
1:C:711:LYS:HE3	1:C:755:ALA:HB1	2.03	0.41
1:C:811:LEU:HA	1:C:811:LEU:HD23	1.65	0.41
1:D:26:LEU:HD21	1:D:334:LEU:O	2.21	0.41
1:D:58:THR:O	1:D:59:GLN:C	2.63	0.41
1:D:99:MET:CE	1:D:215:TRP:CZ3	3.04	0.41
1:D:120:ALA:HB1	1:D:126:PRO:HB3	2.03	0.41
1:D:142:ASP:CG	1:D:149:LYS:HE3	2.46	0.41
1:D:373:LEU:HD11	1:D:864:LEU:CD2	2.44	0.41
1:D:571:ARG:NE	1:D:597:PHE:HB3	2.35	0.41
1:B:150:SER:O	1:B:151:HIS:C	2.64	0.41
1:B:179:LEU:HG	1:B:183:PHE:CE1	2.56	0.41
1:B:343:ALA:O	1:B:346:ALA:HB3	2.21	0.41
1:B:382:ASN:HA	1:B:383:PRO:HD3	1.91	0.41
1:B:489:THR:HG21	1:D:31:ILE:HG13	2.03	0.41
1:C:396:LEU:HB3	1:C:452:MET:HG3	2.03	0.41
1:C:681:THR:CG2	1:C:721:VAL:HG13	2.51	0.41
1:D:22:LYS:HE3	1:D:335:GLN:NE2	2.36	0.41
1:D:134:ARG:O	1:D:135:ARG:C	2.63	0.41
1:D:301:CYS:O	1:D:302:TYR:C	2.63	0.41
1:D:430:GLU:OE2	1:D:449:ARG:NH2	2.54	0.41
1:D:842:GLU:O	1:D:843:PHE:C	2.63	0.41
1:A:101:GLY:CA	1:A:455:HIS:CE1	3.04	0.40
1:A:281:VAL:HG13	1:A:288:PRO:HG3	2.03	0.40
1:A:292:THR:O	1:A:295:GLU:HB3	2.20	0.40
1:A:347:LEU:HD23	1:A:368:ILE:HD13	2.02	0.40
1:A:375:GLN:CG	1:A:464:GLY:HA3	2.41	0.40
1:A:529:ASP:O	1:A:530:LYS:C	2.62	0.40
1:A:754:ASP:HA	1:A:818:LYS:O	2.20	0.40
1:B:247:LYS:HD3	1:B:328:GLU:OE1	2.21	0.40
1:B:405:GLY:O	1:B:495:TYR:HA	2.21	0.40
1:B:474:ILE:C	1:B:475:LYS:HD3	2.46	0.40
1:B:778:SER:O	1:B:782:ALA:HB2	2.21	0.40
1:C:92:ARG:HB2	1:C:238:ASN:HB2	2.03	0.40
1:D:152:PHE:C	1:D:154:LYS:H	2.29	0.40
1:D:174:ASP:O	1:D:177:LYS:HB2	2.22	0.40
1:D:366:VAL:CG2	1:D:872:ASN:OD1	2.69	0.40
1:A:31:ILE:C	1:A:33:GLY:N	2.78	0.40
1:A:251:SER:O	1:A:274:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:GLY:HA3	1:A:274:ILE:HA	2.03	0.40
1:A:252:GLY:O	1:A:326:ILE:N	2.51	0.40
1:A:253:THR:HA	1:A:325:THR:HA	2.03	0.40
1:A:341:ARG:HD3	1:A:349:ILE:HD12	2.03	0.40
1:A:603:LYS:O	1:A:607:LYS:HG2	2.21	0.40
1:A:859:VAL:N	1:A:860:PRO:CD	2.84	0.40
1:B:47:CYS:HA	1:B:212:PHE:CD1	2.56	0.40
1:B:134:ARG:NH1	1:B:138:GLN:HE22	2.19	0.40
1:B:334:LEU:HD22	2:B:901:ANP:C5	2.51	0.40
1:B:373:LEU:CD2	1:B:376:LEU:HD11	2.49	0.40
1:B:598:GLN:O	1:B:601:ASP:HB2	2.21	0.40
1:C:29:MET:CB	1:C:36:ILE:HG12	2.50	0.40
1:C:48:THR:HA	1:C:51:TYR:HB2	2.03	0.40
1:C:90:SER:HB3	1:C:107:LEU:CD2	2.50	0.40
1:C:140:TYR:CD1	1:C:196:PHE:CZ	3.09	0.40
1:C:409:PHE:CE2	1:C:483:PHE:CD1	3.08	0.40
1:C:644:THR:O	1:C:646:ALA:N	2.54	0.40
1:C:767:THR:O	1:C:834:HIS:CE1	2.74	0.40
1:C:776:GLY:HA3	1:D:773:MET:HE3	2.03	0.40
1:D:36:ILE:O	1:D:37:PRO:C	2.63	0.40
1:D:83:THR:CG2	1:D:84:GLU:N	2.84	0.40
1:D:859:VAL:N	1:D:860:PRO:CD	2.84	0.40
1:A:371:LYS:O	1:A:371:LYS:HG3	2.19	0.40
1:A:436:ILE:C	1:A:438:GLY:N	2.77	0.40
1:A:619:LEU:HD12	1:A:619:LEU:HA	1.96	0.40
1:B:224:ARG:NE	1:B:231:GLY:HA2	2.36	0.40
1:B:312:LEU:O	1:B:316:PHE:HD2	2.04	0.40
1:B:540:ALA:HB3	1:B:557:ILE:CG1	2.51	0.40
1:B:609:LEU:HD23	1:B:609:LEU:HA	1.71	0.40
1:C:342:THR:HG23	1:C:461:ARG:HG2	2.03	0.40
1:C:550:VAL:C	1:C:552:LEU:H	2.30	0.40
1:C:595:ILE:HG12	1:C:679:MET:HG2	2.04	0.40
1:C:620:ASP:N	1:C:621:PRO:CD	2.85	0.40
1:C:794:ILE:O	1:C:795:TYR:HD1	2.04	0.40
1:C:808:VAL:O	1:C:809:GLY:C	2.63	0.40
1:D:534:LEU:CD1	1:D:845:HIS:HB2	2.49	0.40
1:D:536:VAL:HG22	1:D:852:VAL:HG22	2.04	0.40
1:D:627:VAL:HB	1:D:652:VAL:HG22	2.02	0.40
1:A:578:MET:HE1	1:A:676:ILE:HG12	2.03	0.40
1:A:579:ILE:HG12	1:A:623:LEU:HD13	2.03	0.40
1:A:779:ARG:C	1:A:781:ASP:N	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:GLY:HA2	1:B:72:LEU:HD11	2.02	0.40
1:B:90:SER:HB2	1:B:107:LEU:HD22	2.04	0.40
1:B:112:ASN:O	1:B:116:VAL:CG2	2.66	0.40
1:B:343:ALA:HB2	1:B:372:SER:OG	2.22	0.40
1:B:344:PRO:HD3	1:B:376:LEU:CD2	2.51	0.40
1:B:448:VAL:O	1:B:449:ARG:HG2	2.22	0.40
1:B:592:ASN:C	1:B:594:LEU:N	2.78	0.40
1:B:657:GLU:OE2	1:B:663:GLY:CA	2.68	0.40
1:B:771:THR:O	1:B:775:PHE:HB2	2.22	0.40
1:C:398:ALA:HB1	1:C:457:ALA:HB2	2.01	0.40
1:C:499:ASP:HB3	1:C:502:THR:OG1	2.21	0.40
1:C:634:GLN:HB3	1:C:645:LEU:CD1	2.51	0.40
1:C:811:LEU:HD11	1:D:751:LEU:HD11	2.02	0.40
1:D:50:TYR:HD2	1:D:57:ILE:CD1	2.34	0.40
1:D:580:LEU:HG	1:D:641:MET:CE	2.51	0.40
1:D:636:GLU:O	1:D:640:ASN:ND2	2.55	0.40
1:D:644:THR:C	1:D:646:ALA:N	2.78	0.40
1:D:675:GLU:CD	1:D:675:GLU:H	2.30	0.40
1:D:856:PRO:C	1:D:858:ARG:N	2.79	0.40
1:A:199:GLU:C	1:A:201:LYS:N	2.77	0.40
1:A:368:ILE:O	1:A:370:ALA:N	2.54	0.40
1:A:768:ASN:HD21	1:A:832:GLY:HA2	1.85	0.40
1:B:31:ILE:CD1	1:B:31:ILE:N	2.85	0.40
1:B:151:HIS:CD2	1:B:151:HIS:H	2.40	0.40
1:B:154:LYS:O	1:B:157:ASP:HB2	2.21	0.40
1:B:527:TRP:HB3	1:B:531:PHE:CE2	2.57	0.40
1:B:559:LEU:HB2	1:B:831:CYS:SG	2.61	0.40
1:B:599:LYS:HD2	1:B:686:GLU:HB3	2.04	0.40
1:B:606:TYR:HE1	1:B:614:MET:HE2	1.83	0.40
1:B:864:LEU:O	1:B:867:ALA:HB3	2.21	0.40
1:C:400:PRO:O	1:C:466:CYS:HA	2.22	0.40
1:C:431:THR:HB	1:C:456:ALA:CB	2.50	0.40
1:D:30:THR:HA	1:D:36:ILE:HD12	2.04	0.40
1:D:39:GLY:HA2	1:D:72:LEU:HD11	2.03	0.40
1:D:219:ARG:CB	1:D:436:ILE:HG21	2.52	0.40
1:D:245:GLY:HA3	1:D:252:GLY:O	2.22	0.40
1:D:274:ILE:O	1:D:275:ASN:C	2.65	0.40
1:D:416:ALA:O	1:D:420:LYS:HG3	2.22	0.40
1:D:634:GLN:C	1:D:645:LEU:HD13	2.46	0.40
1:D:842:GLU:O	1:D:845:HIS:HB3	2.21	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	870/874 (100%)	750 (86%)	96 (11%)	24 (3%)	4	21
1	B	870/874 (100%)	738 (85%)	112 (13%)	20 (2%)	5	25
1	C	870/874 (100%)	736 (85%)	111 (13%)	23 (3%)	4	23
1	D	870/874 (100%)	748 (86%)	101 (12%)	21 (2%)	4	24
All	All	3480/3496 (100%)	2972 (85%)	420 (12%)	88 (2%)	4	23

All (88) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	355	ASP
1	A	356	GLU
1	A	872	ASN
1	B	783	GLY
1	C	658	PHE
1	C	857	PHE
1	D	14	SER
1	D	54	GLY
1	D	150	SER
1	A	486	GLY
1	A	492	GLU
1	A	550	VAL
1	A	850	ASN
1	B	101	GLY
1	B	158	ALA
1	B	731	GLU
1	C	31	ILE
1	C	189	GLU
1	C	339	GLY
1	C	376	LEU
1	C	454	SER
1	D	466	CYS

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Mol	Chain	Res	Type
1	D	640	ASN
1	A	24	CYS
1	A	138	GLN
1	A	319	MET
1	A	487	GLY
1	A	588	GLU
1	A	817	LYS
1	B	138	GLN
1	B	421	GLY
1	B	455	HIS
1	B	653	ASP
1	C	486	GLY
1	C	645	LEU
1	C	698	ASP
1	D	13	ALA
1	D	28	GLU
1	D	664	HIS
1	D	846	LYS
1	A	151	HIS
1	A	170	ASP
1	A	279	GLU
1	A	373	LEU
1	A	479	GLU
1	A	587	ARG
1	B	258	THR
1	B	589	GLU
1	C	78	LYS
1	C	113	ASP
1	C	362	GLU
1	C	605	MET
1	C	804	ASP
1	C	826	LEU
1	D	38	GLN
1	D	288	PRO
1	D	745	GLU
1	A	369	GLU
1	A	569	ALA
1	A	780	ASP
1	B	280	ASP
1	B	293	GLN
1	B	370	ALA
1	B	456	ALA

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Mol	Chain	Res	Type
1	B	664	HIS
1	B	709	GLY
1	B	843	PHE
1	C	144	VAL
1	C	551	LYS
1	C	872	ASN
1	D	162	GLU
1	D	318	ASP
1	D	518	SER
1	D	667	CYS
1	D	845	HIS
1	A	344	PRO
1	B	640	ASN
1	B	780	ASP
1	C	487	GLY
1	D	715	LYS
1	A	620	ASP
1	D	291	ILE
1	D	421	GLY
1	C	268	ILE
1	C	809	GLY
1	D	100	PRO
1	C	825	GLY
1	B	652	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	713/715 (100%)	629 (88%)	84 (12%)	5	22
1	B	713/715 (100%)	632 (89%)	81 (11%)	5	24
1	C	713/715 (100%)	636 (89%)	77 (11%)	6	26
1	D	713/715 (100%)	638 (90%)	75 (10%)	6	27
All	All	2852/2860 (100%)	2535 (89%)	317 (11%)	6	25

All (317) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	THR
1	A	65	ILE
1	A	70	THR
1	A	75	LEU
1	A	92	ARG
1	A	114	VAL
1	A	122	LYS
1	A	127	ARG
1	A	132	SER
1	A	149	LYS
1	A	156	ILE
1	A	161	GLU
1	A	165	VAL
1	A	169	THR
1	A	175	ASP
1	A	178	GLU
1	A	188	LYS
1	A	189	GLU
1	A	195	GLU
1	A	205	MET
1	A	217	ASN
1	A	227	ASN
1	A	229	ILE
1	A	232	ASP
1	A	235	THR
1	A	238	ASN
1	A	239	VAL
1	A	262	SER
1	A	268	ILE
1	A	269	TYR
1	A	273	LEU
1	A	274	ILE
1	A	282	VAL
1	A	289	GLN
1	A	296	ASN
1	A	330	LYS
1	A	334	LEU
1	A	341	ARG
1	A	362	GLU
1	A	391	VAL
1	A	392	ILE
1	A	406	LYS

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Mol	Chain	Res	Type
1	A	407	VAL
1	A	423	ARG
1	A	436	ILE
1	A	453	THR
1	A	455	HIS
1	A	461	ARG
1	A	475	LYS
1	A	489	THR
1	A	496	ILE
1	A	514	GLU
1	A	525	MET
1	A	532	ARG
1	A	537	ARG
1	A	544	GLU
1	A	551	LYS
1	A	562	THR
1	A	567	PHE
1	A	575	ILE
1	A	578	MET
1	A	587	ARG
1	A	588	GLU
1	A	589	GLU
1	A	607	LYS
1	A	617	ARG
1	A	631	GLU
1	A	647	GLU
1	A	661	MET
1	A	662	MET
1	A	668	ARG
1	A	669	LEU
1	A	735	ASP
1	A	744	ILE
1	A	756	ILE
1	A	768	ASN
1	A	786	LEU
1	A	808	VAL
1	A	817	LYS
1	A	822	THR
1	A	828	CYS
1	A	830	ILE
1	A	839	SER
1	A	846	LYS

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Mol	Chain	Res	Type
1	B	3	LYS
1	B	12	ASN
1	B	19	LEU
1	B	22	LYS
1	B	24	CYS
1	B	42	VAL
1	B	58	THR
1	B	72	LEU
1	B	89	VAL
1	B	113	ASP
1	B	137	ILE
1	B	142	ASP
1	B	147	VAL
1	B	149	LYS
1	B	153	GLU
1	B	156	ILE
1	B	157	ASP
1	B	161	GLU
1	B	163	LYS
1	B	165	VAL
1	B	168	ASP
1	B	172	THR
1	B	175	ASP
1	B	205	MET
1	B	243	VAL
1	B	251	SER
1	B	263	THR
1	B	265	GLU
1	B	266	LYS
1	B	273	LEU
1	B	280	ASP
1	B	286	ARG
1	B	293	GLN
1	B	297	ASP
1	B	298	MET
1	B	306	MET
1	B	313	GLU
1	B	321	ASP
1	B	330	LYS
1	B	331	LEU
1	B	406	LYS
1	B	407	VAL

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Mol	Chain	Res	Type
1	B	430	GLU
1	B	431	THR
1	B	445	ILE
1	B	461	ARG
1	B	463	MET
1	B	468	VAL
1	B	498	LEU
1	B	501	SER
1	B	510	ILE
1	B	518	SER
1	B	537	ARG
1	B	551	LYS
1	B	560	CYS
1	B	570	ASP
1	B	575	ILE
1	B	578	MET
1	B	580	LEU
1	B	585	GLU
1	B	587	ARG
1	B	609	LEU
1	B	617	ARG
1	B	629	HIS
1	B	630	THR
1	B	648	VAL
1	B	662	MET
1	B	678	LYS
1	B	692	LYS
1	B	745	GLU
1	B	747	PRO
1	B	769	ASP
1	B	773	MET
1	B	777	PHE
1	B	780	ASP
1	B	787	ASP
1	B	793	LYS
1	B	804	ASP
1	B	821	GLN
1	B	827	LYS
1	B	839	SER
1	C	29	MET
1	C	36	ILE
1	C	53	SER

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Mol	Chain	Res	Type
1	C	55	LYS
1	C	72	LEU
1	C	83	THR
1	C	106	ILE
1	C	109	LEU
1	C	125	ASN
1	C	159	MET
1	C	165	VAL
1	C	166	HIS
1	C	174	ASP
1	C	241	THR
1	C	251	SER
1	C	255	VAL
1	C	265	GLU
1	C	266	LYS
1	C	275	ASN
1	C	282	VAL
1	C	287	THR
1	C	289	GLN
1	C	295	GLU
1	C	296	ASN
1	C	298	MET
1	C	300	ASP
1	C	322	MET
1	C	330	LYS
1	C	333	PHE
1	C	360	THR
1	C	371	LYS
1	C	396	LEU
1	C	407	VAL
1	C	410	THR
1	C	422	GLU
1	C	434	GLU
1	C	445	ILE
1	C	449	ARG
1	C	466	CYS
1	C	498	LEU
1	C	510	ILE
1	C	511	GLU
1	C	512	THR
1	C	514	GLU
1	C	517	VAL

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Mol	Chain	Res	Type
1	C	535	LYS
1	C	542	THR
1	C	544	GLU
1	C	550	VAL
1	C	551	LYS
1	C	557	ILE
1	C	567	PHE
1	C	570	ASP
1	C	571	ARG
1	C	607	LYS
1	C	612	ARG
1	C	617	ARG
1	C	630	THR
1	C	631	GLU
1	C	633	GLU
1	C	669	LEU
1	C	675	GLU
1	C	686	GLU
1	C	710	GLU
1	C	731	GLU
1	C	739	HIS
1	C	742	THR
1	C	743	MET
1	C	745	GLU
1	C	769	ASP
1	C	784	LYS
1	C	797	SER
1	C	802	ARG
1	C	803	LEU
1	C	814	MET
1	C	821	GLN
1	C	841	VAL
1	D	16	ARG
1	D	30	THR
1	D	31	ILE
1	D	38	GLN
1	D	42	VAL
1	D	50	TYR
1	D	52	ASN
1	D	55	LYS
1	D	58	THR
1	D	109	LEU

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Mol	Chain	Res	Type
1	D	114	VAL
1	D	128	PHE
1	D	137	ILE
1	D	145	MET
1	D	150	SER
1	D	155	ILE
1	D	156	ILE
1	D	161	GLU
1	D	166	HIS
1	D	169	THR
1	D	178	GLU
1	D	181	GLU
1	D	202	ASP
1	D	219	ARG
1	D	241	THR
1	D	273	LEU
1	D	292	THR
1	D	304	GLN
1	D	306	MET
1	D	323	GLU
1	D	330	LYS
1	D	334	LEU
1	D	341	ARG
1	D	363	GLU
1	D	366	VAL
1	D	367	ARG
1	D	381	PHE
1	D	407	VAL
1	D	429	LEU
1	D	431	THR
1	D	434	GLU
1	D	453	THR
1	D	455	HIS
1	D	463	MET
1	D	488	HIS
1	D	496	ILE
1	D	512	THR
1	D	514	GLU
1	D	524	ILE
1	D	536	VAL
1	D	537	ARG
1	D	541	ASP

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Mol	Chain	Res	Type
1	D	548	ASN
1	D	551	LYS
1	D	570	ASP
1	D	584	VAL
1	D	615	THR
1	D	617	ARG
1	D	633	GLU
1	D	682	ARG
1	D	734	SER
1	D	769	ASP
1	D	777	PHE
1	D	781	ASP
1	D	786	LEU
1	D	797	SER
1	D	798	ASP
1	D	802	ARG
1	D	803	LEU
1	D	817	LYS
1	D	826	LEU
1	D	839	SER
1	D	846	LYS
1	D	849	LEU
1	D	868	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	108	ASN
1	A	203	GLN
1	A	275	ASN
1	A	277	GLN
1	A	289	GLN
1	A	296	ASN
1	A	315	HIS
1	A	320	GLN
1	A	335	GLN
1	A	382	ASN
1	A	440	HIS
1	A	488	HIS
1	A	564	HIS
1	A	664	HIS

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Mol	Chain	Res	Type
1	A	845	HIS
1	A	872	ASN
1	B	12	ASN
1	B	38	GLN
1	B	151	HIS
1	B	240	GLN
1	B	293	GLN
1	B	455	HIS
1	B	477	ASN
1	B	513	GLN
1	B	592	ASN
1	B	873	ASN
1	C	12	ASN
1	C	38	GLN
1	C	151	HIS
1	C	217	ASN
1	C	238	ASN
1	C	289	GLN
1	C	293	GLN
1	C	382	ASN
1	C	455	HIS
1	C	727	GLN
1	C	834	HIS
1	C	873	ASN
1	D	12	ASN
1	D	76	ASN
1	D	125	ASN
1	D	227	ASN
1	D	238	ASN
1	D	335	GLN
1	D	378	HIS
1	D	440	HIS
1	D	564	HIS
1	D	624	HIS
1	D	634	GLN
1	D	739	HIS
1	D	868	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
3	SO4	B	902	-	4,4,4	0.68	0	6,6,6	0.24	0
3	SO4	B	904	-	4,4,4	0.57	0	6,6,6	0.35	0
3	SO4	C	902	-	4,4,4	0.49	0	6,6,6	0.31	0
3	SO4	C	904	-	4,4,4	0.67	0	6,6,6	0.53	0
3	SO4	A	4004	-	4,4,4	0.65	0	6,6,6	0.23	0
3	SO4	D	902	-	4,4,4	0.58	0	6,6,6	0.36	0
3	SO4	A	4003	-	4,4,4	0.82	0	6,6,6	0.28	0
3	SO4	A	4002	-	4,4,4	0.61	0	6,6,6	0.25	0
2	ANP	B	901	-	33,33,33	2.47	10 (30%)	45,52,52	2.35	12 (26%)
3	SO4	D	904	-	4,4,4	0.49	0	6,6,6	0.17	0
2	ANP	C	901	-	33,33,33	2.49	5 (15%)	45,52,52	2.36	11 (24%)
2	ANP	A	4001	-	33,33,33	2.49	7 (21%)	45,52,52	2.36	13 (28%)
2	ANP	D	901	-	33,33,33	2.50	9 (27%)	45,52,52	2.38	13 (28%)
3	SO4	B	903	-	4,4,4	0.60	0	6,6,6	0.17	0
3	SO4	D	903	-	4,4,4	0.67	0	6,6,6	0.27	0
3	SO4	C	903	-	4,4,4	0.78	0	6,6,6	0.28	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	ANP	A	4001	-	-	3/18/38/38	0/3/3/3
2	ANP	D	901	-	-	7/18/38/38	0/3/3/3
2	ANP	B	901	-	-	7/18/38/38	0/3/3/3
2	ANP	C	901	-	-	6/18/38/38	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	901	ANP	PB-O1B	9.47	1.60	1.46
2	C	901	ANP	PB-O1B	8.99	1.59	1.46
2	A	4001	ANP	PB-O1B	8.93	1.59	1.46
2	B	901	ANP	PB-O1B	8.76	1.59	1.46
2	C	901	ANP	PG-O1G	6.59	1.56	1.46
2	A	4001	ANP	PG-O1G	6.56	1.56	1.46
2	B	901	ANP	PG-O1G	6.43	1.55	1.46
2	D	901	ANP	PG-O1G	5.47	1.54	1.46
2	C	901	ANP	C6-N6	5.24	1.47	1.34
2	A	4001	ANP	C6-N6	5.02	1.47	1.34
2	D	901	ANP	C6-N6	4.97	1.46	1.34
2	B	901	ANP	C6-N6	4.91	1.46	1.34
2	B	901	ANP	C5'-C4'	-2.97	1.42	1.51
2	D	901	ANP	C5'-C4'	-2.96	1.42	1.51
2	C	901	ANP	C5'-C4'	-2.76	1.43	1.51
2	D	901	ANP	PG-N3B	2.61	1.70	1.63
2	D	901	ANP	O3'-C3'	-2.53	1.36	1.43
2	A	4001	ANP	C5'-C4'	-2.46	1.44	1.51
2	C	901	ANP	PG-N3B	2.42	1.69	1.63
2	A	4001	ANP	PG-N3B	2.42	1.69	1.63
2	B	901	ANP	PG-N3B	2.31	1.69	1.63
2	A	4001	ANP	O3'-C3'	-2.27	1.37	1.43
2	A	4001	ANP	C3'-C4'	-2.25	1.47	1.53
2	D	901	ANP	C3'-C4'	-2.21	1.47	1.53
2	D	901	ANP	C5-N7	-2.20	1.35	1.39
2	B	901	ANP	PG-O3G	-2.14	1.51	1.56
2	B	901	ANP	C2'-C3'	-2.14	1.47	1.53
2	B	901	ANP	O3'-C3'	-2.10	1.37	1.43
2	D	901	ANP	PB-N3B	2.10	1.68	1.63
2	B	901	ANP	C3'-C4'	-2.02	1.47	1.53
2	B	901	ANP	C5-N7	-2.01	1.35	1.39

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	901	ANP	C4-N9-C8	6.11	112.16	105.74
2	B	901	ANP	C4-N9-C8	6.07	112.11	105.74
2	A	4001	ANP	N3-C4-N9	6.01	137.40	127.17
2	D	901	ANP	N3-C4-N9	5.75	136.95	127.17
2	A	4001	ANP	C5-C4-N3	-5.74	118.81	126.72
2	C	901	ANP	N9-C8-N7	-5.64	105.93	113.94
2	D	901	ANP	C4-N9-C8	5.63	111.65	105.74
2	B	901	ANP	N3-C4-N9	5.61	136.71	127.17
2	B	901	ANP	N9-C8-N7	-5.60	105.98	113.94
2	D	901	ANP	C5-C4-N3	-5.50	119.14	126.72
2	A	4001	ANP	C4-N9-C8	5.48	111.49	105.74
2	B	901	ANP	C5-C4-N3	-5.29	119.43	126.72
2	D	901	ANP	N9-C8-N7	-5.21	106.55	113.94
2	A	4001	ANP	N9-C8-N7	-5.20	106.56	113.94
2	C	901	ANP	N3-C4-N9	5.08	135.80	127.17
2	C	901	ANP	C5-C4-N3	-4.98	119.86	126.72
2	C	901	ANP	N3-C2-N1	-4.78	121.34	128.58
2	A	4001	ANP	N3-C2-N1	-4.77	121.36	128.58
2	B	901	ANP	N3-C2-N1	-4.58	121.65	128.58
2	C	901	ANP	C5-N7-C8	4.55	110.60	103.45
2	B	901	ANP	C5-N7-C8	4.45	110.45	103.45
2	C	901	ANP	C4-N9-C1'	-4.35	116.45	126.63
2	D	901	ANP	N3-C2-N1	-4.33	122.03	128.58
2	D	901	ANP	C5-N7-C8	4.22	110.08	103.45
2	A	4001	ANP	C5-N7-C8	4.20	110.05	103.45
2	D	901	ANP	O5'-C5'-C4'	3.72	121.67	108.99
2	B	901	ANP	O1G-PG-N3B	-3.57	106.51	111.77
2	D	901	ANP	O1G-PG-N3B	-3.57	106.52	111.77
2	A	4001	ANP	C2-N3-C4	3.56	120.53	111.83
2	B	901	ANP	C4-N9-C1'	-3.51	118.42	126.63
2	C	901	ANP	C2-N3-C4	3.42	120.19	111.83
2	B	901	ANP	C2-N3-C4	3.23	119.71	111.83
2	C	901	ANP	C4-C5-N7	-3.16	106.97	110.58
2	D	901	ANP	C4-N9-C1'	-3.12	119.34	126.63
2	A	4001	ANP	C4-N9-C1'	-3.08	119.43	126.63
2	D	901	ANP	C2-N3-C4	3.06	119.31	111.83
2	A	4001	ANP	O5'-C5'-C4'	3.03	119.30	108.99
2	D	901	ANP	C6-C5-C4	2.65	120.79	117.18
2	B	901	ANP	C4-C5-N7	-2.61	107.60	110.58
2	C	901	ANP	O5'-C5'-C4'	2.50	117.50	108.99
2	D	901	ANP	C4-C5-N7	-2.42	107.81	110.58
2	A	4001	ANP	O2G-PG-O1G	-2.40	107.42	113.45
2	B	901	ANP	O5'-C5'-C4'	2.37	117.06	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4001	ANP	C4-C5-N7	-2.16	108.11	110.58
2	D	901	ANP	N6-C6-N1	2.14	123.15	118.38
2	A	4001	ANP	C3'-C2'-C1'	2.10	105.43	101.46
2	B	901	ANP	C6-C5-C4	2.04	119.97	117.18
2	A	4001	ANP	N6-C6-N1	2.02	122.88	118.38
2	C	901	ANP	O3A-PB-N3B	2.00	112.14	106.59

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4001	ANP	PG-N3B-PB-O1B
2	A	4001	ANP	C5'-O5'-PA-O1A
2	B	901	ANP	PB-N3B-PG-O1G
2	B	901	ANP	PG-N3B-PB-O1B
2	B	901	ANP	PA-O3A-PB-O2B
2	C	901	ANP	PB-N3B-PG-O1G
2	C	901	ANP	PG-N3B-PB-O1B
2	C	901	ANP	PA-O3A-PB-O2B
2	D	901	ANP	PB-N3B-PG-O1G
2	D	901	ANP	C5'-O5'-PA-O1A
2	D	901	ANP	C5'-O5'-PA-O2A
2	D	901	ANP	C5'-O5'-PA-O3A
2	D	901	ANP	C3'-C4'-C5'-O5'
2	D	901	ANP	O4'-C4'-C5'-O5'
2	C	901	ANP	O4'-C4'-C5'-O5'
2	D	901	ANP	C4'-C5'-O5'-PA
2	B	901	ANP	C5'-O5'-PA-O1A
2	B	901	ANP	C5'-O5'-PA-O2A
2	B	901	ANP	C5'-O5'-PA-O3A
2	C	901	ANP	C5'-O5'-PA-O1A
2	A	4001	ANP	PA-O3A-PB-O1B
2	B	901	ANP	PA-O3A-PB-O1B
2	C	901	ANP	PA-O3A-PB-O1B

There are no ring outliers.

11 monomers are involved in 57 short contacts:

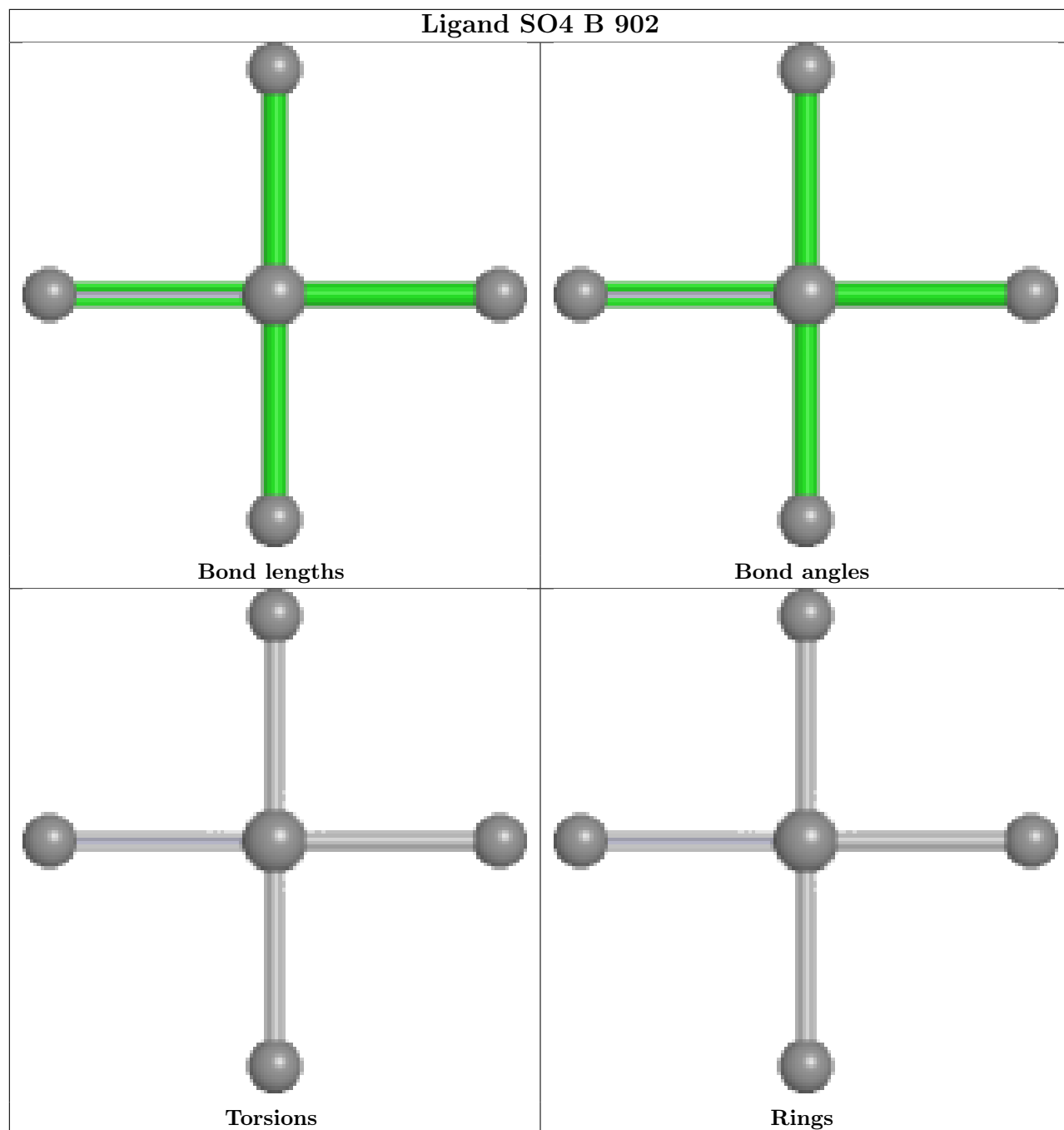
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	902	SO4	1	0
3	C	902	SO4	2	0

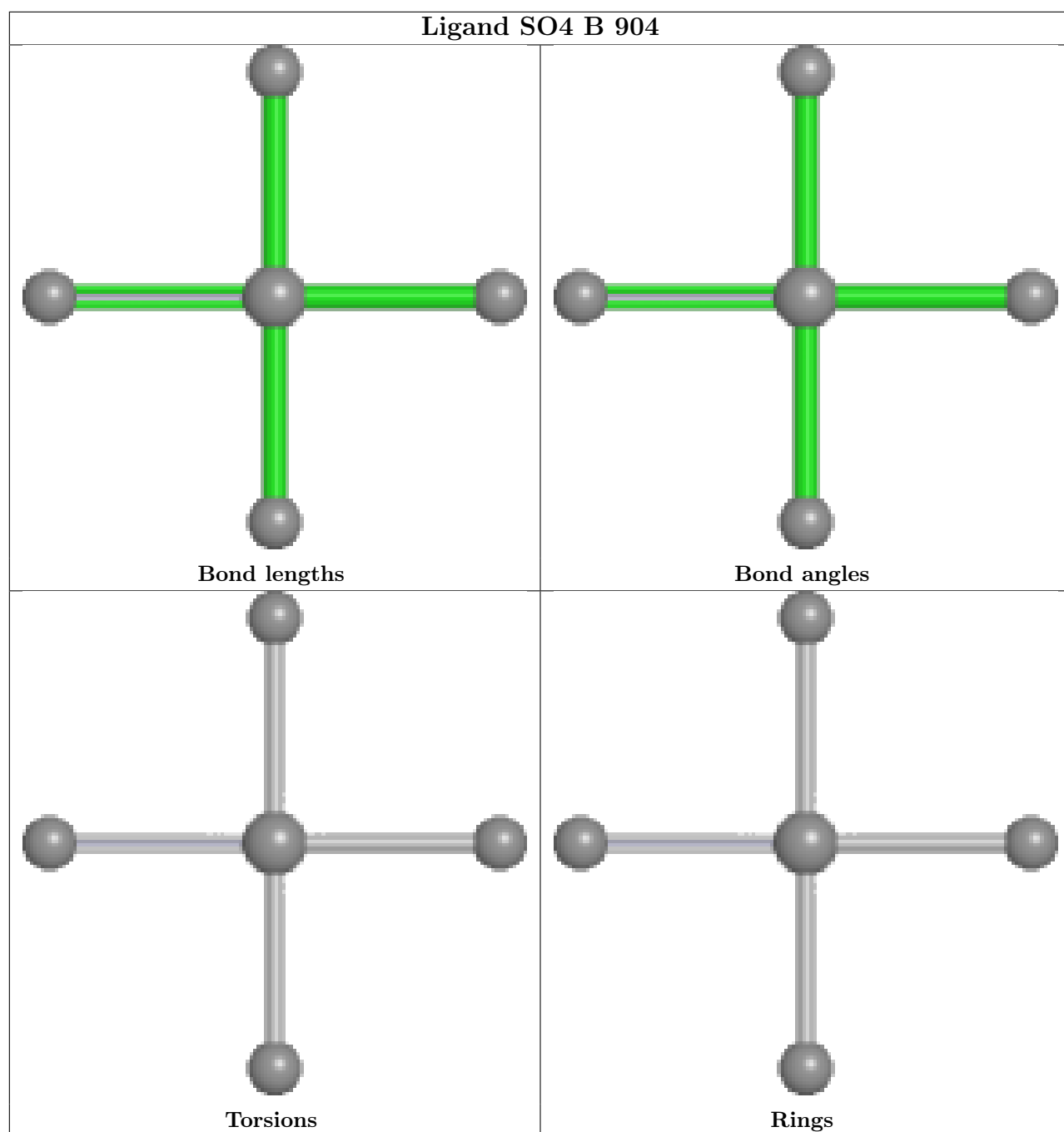
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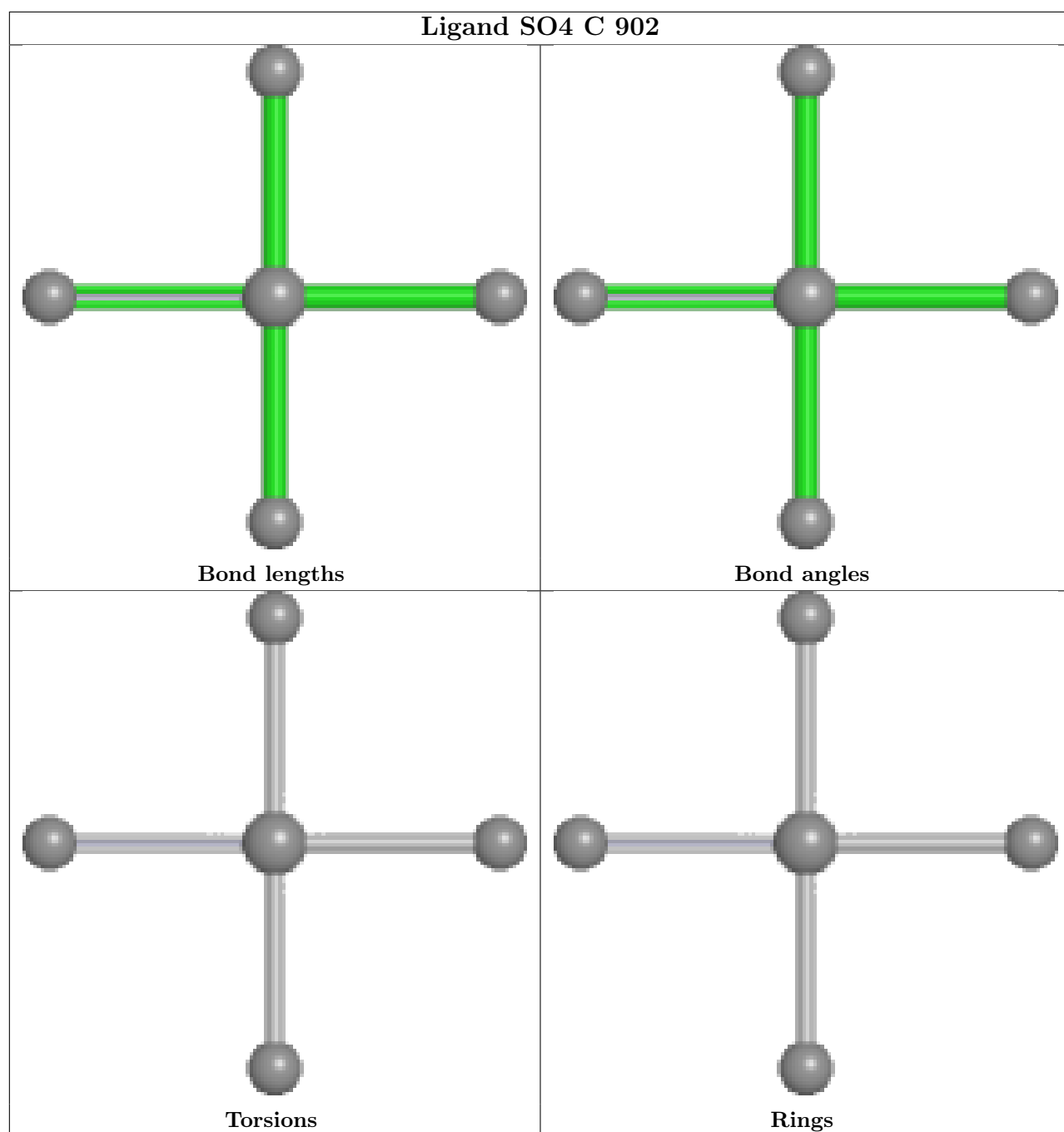
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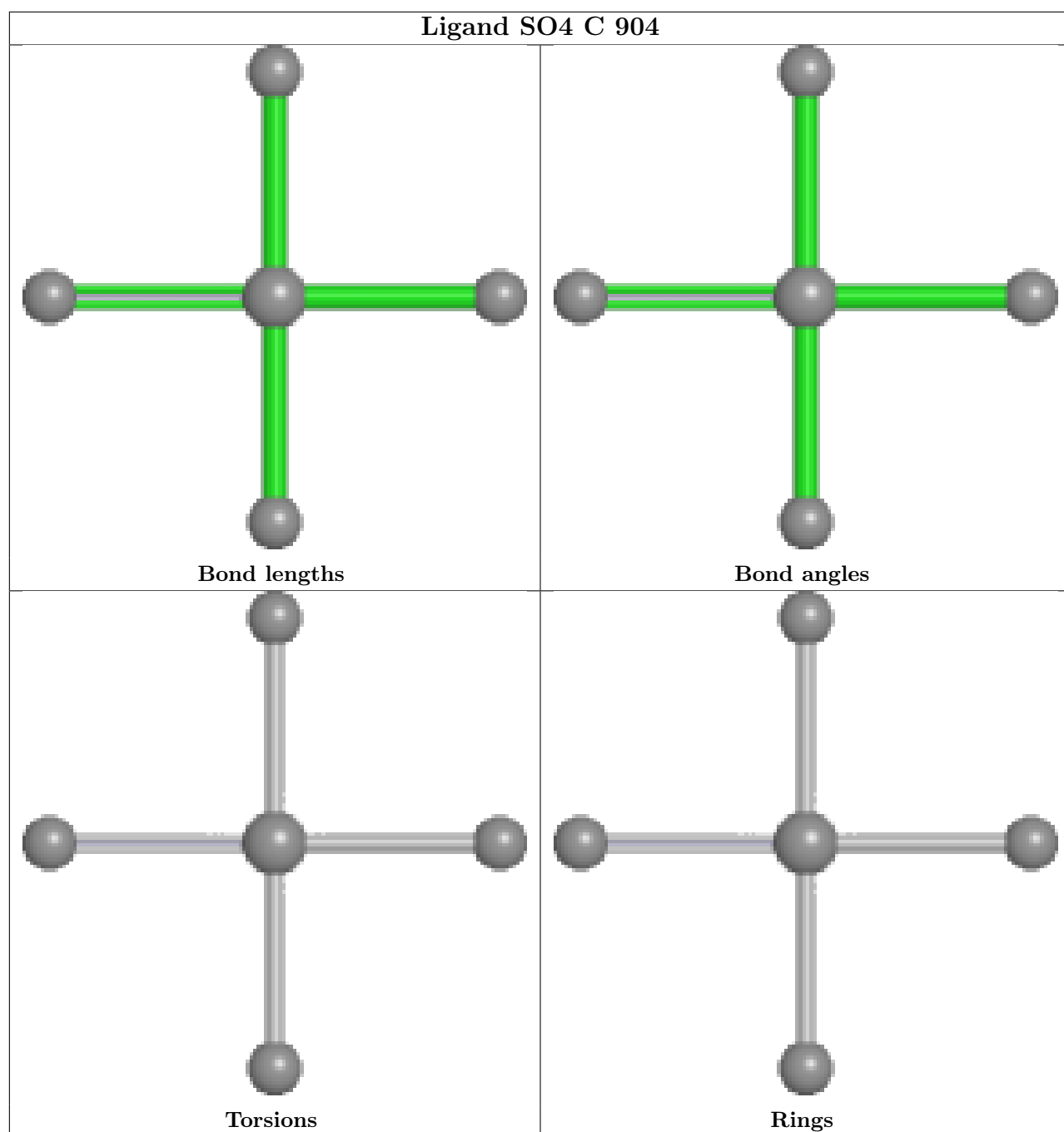
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4004	SO4	2	0
3	A	4003	SO4	1	0
2	B	901	ANP	17	0
3	D	904	SO4	1	0
2	C	901	ANP	16	0
2	A	4001	ANP	7	0
2	D	901	ANP	7	0
3	D	903	SO4	2	0
3	C	903	SO4	1	0

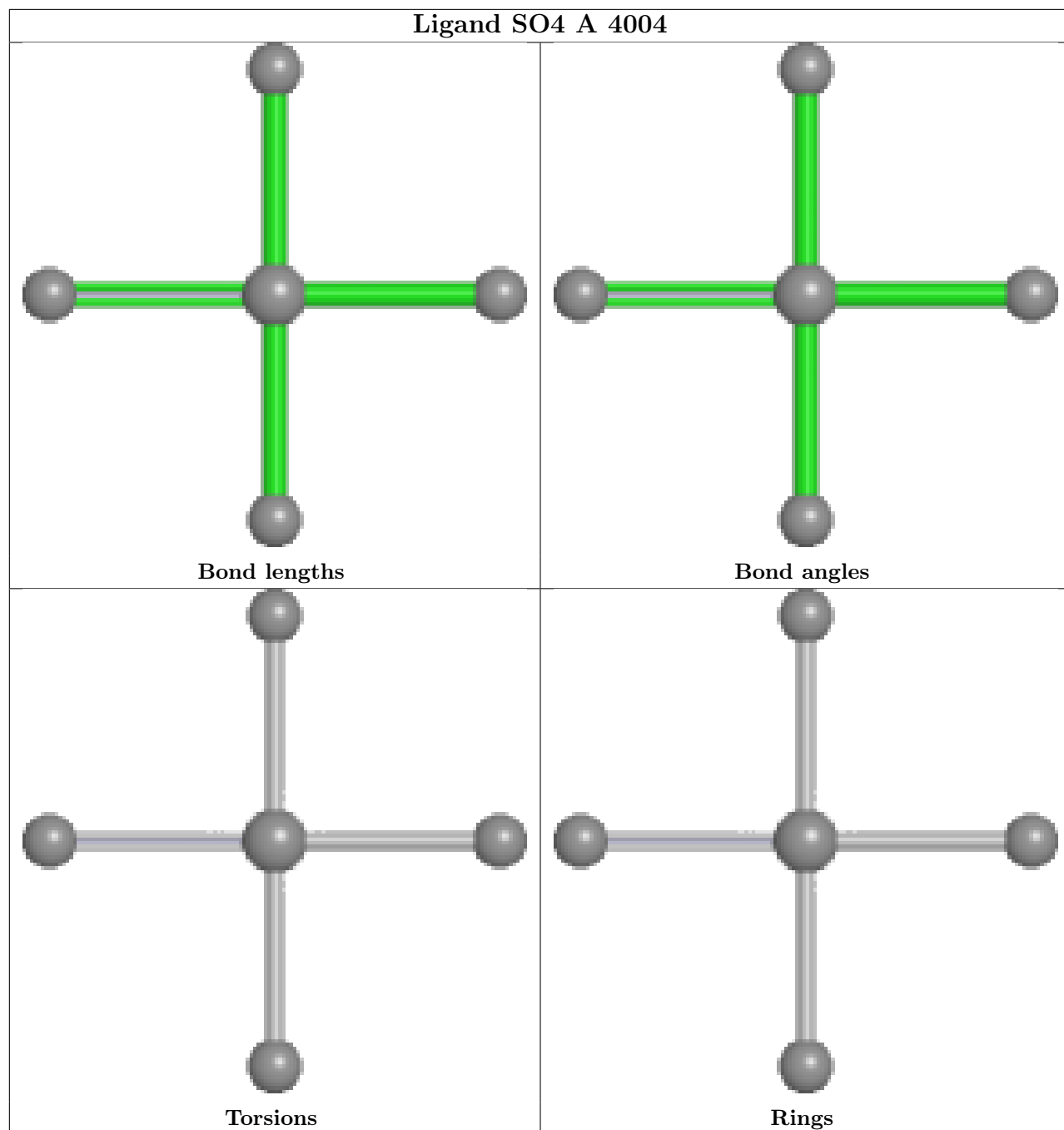
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

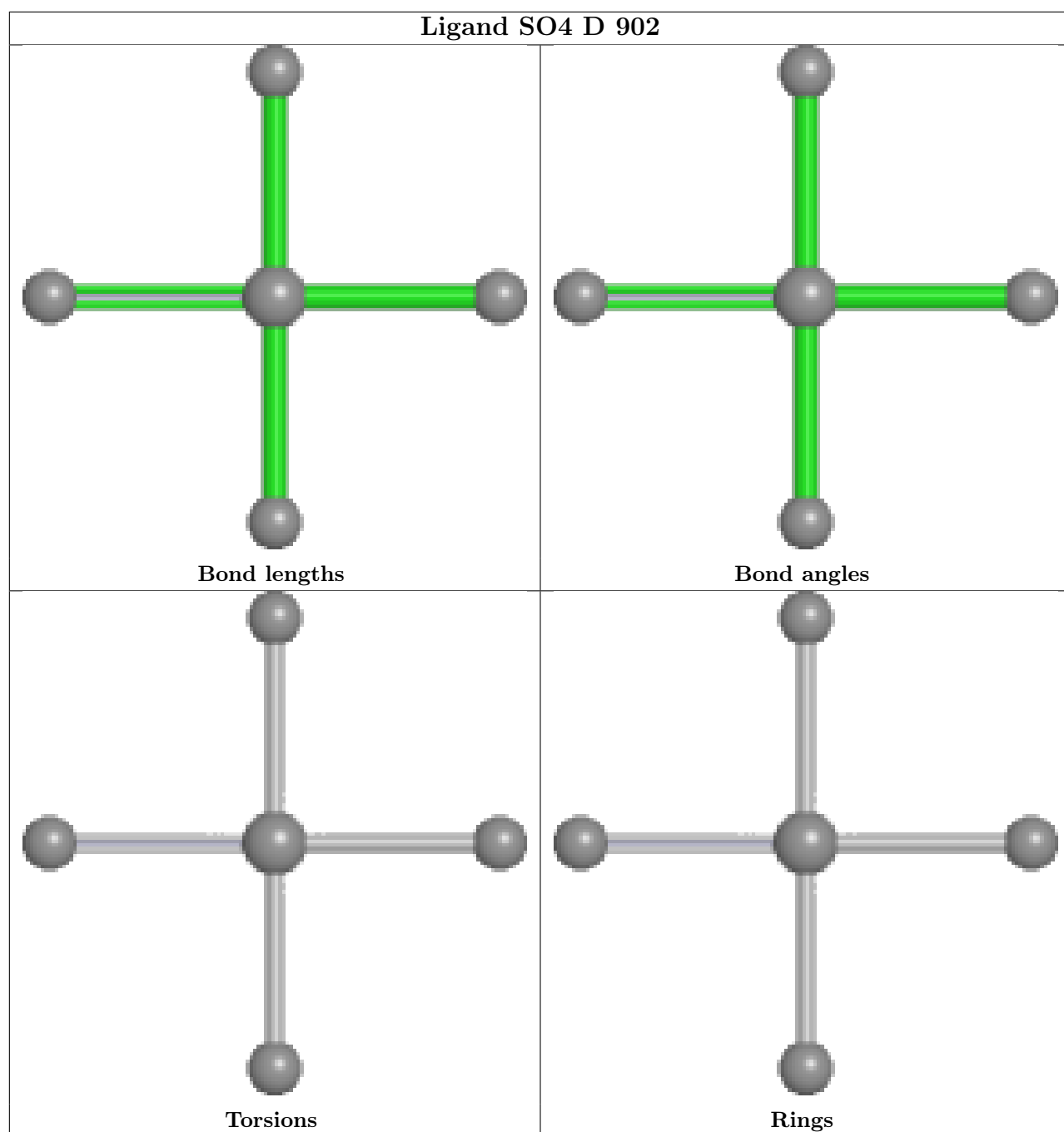


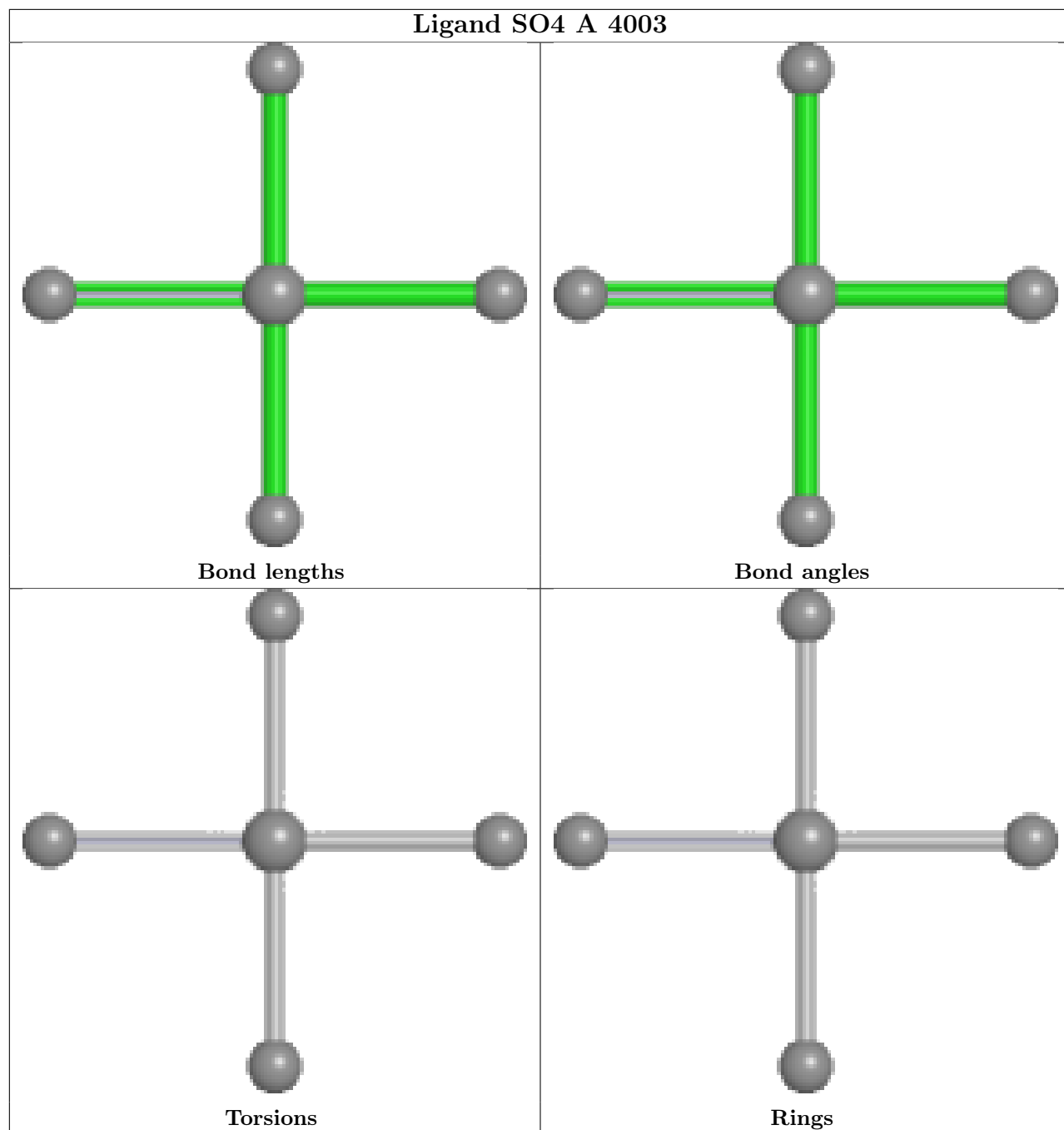


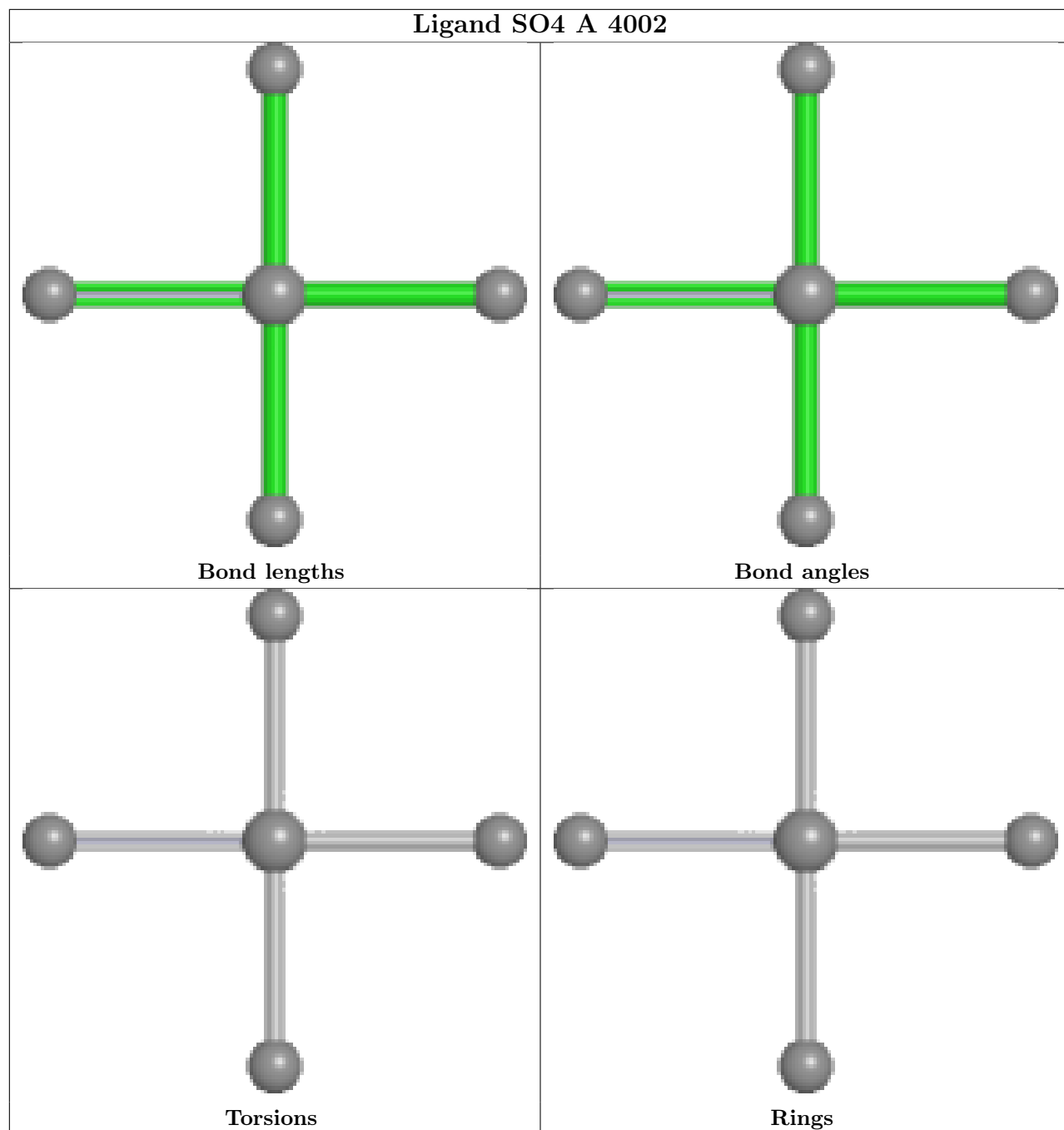


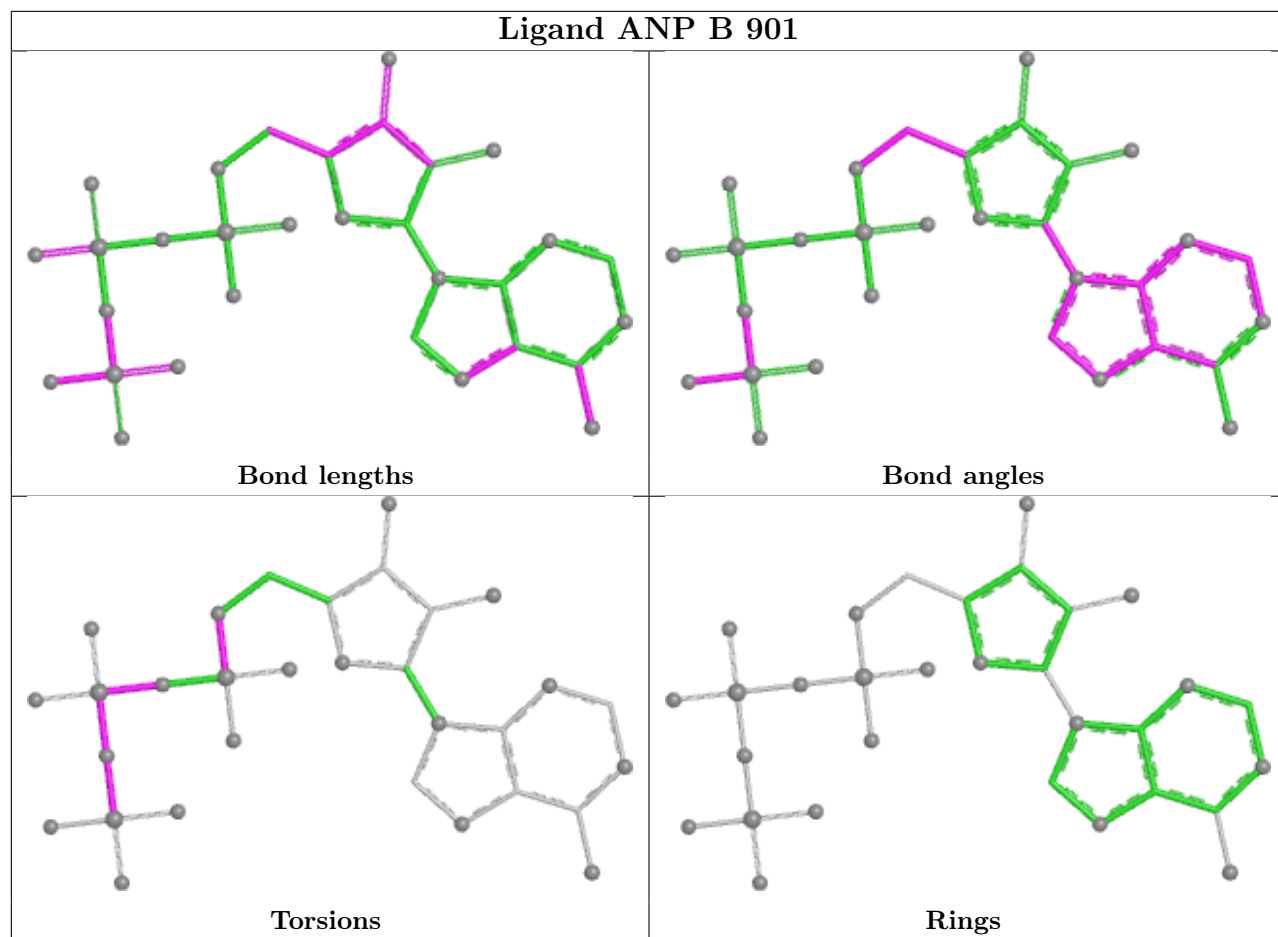


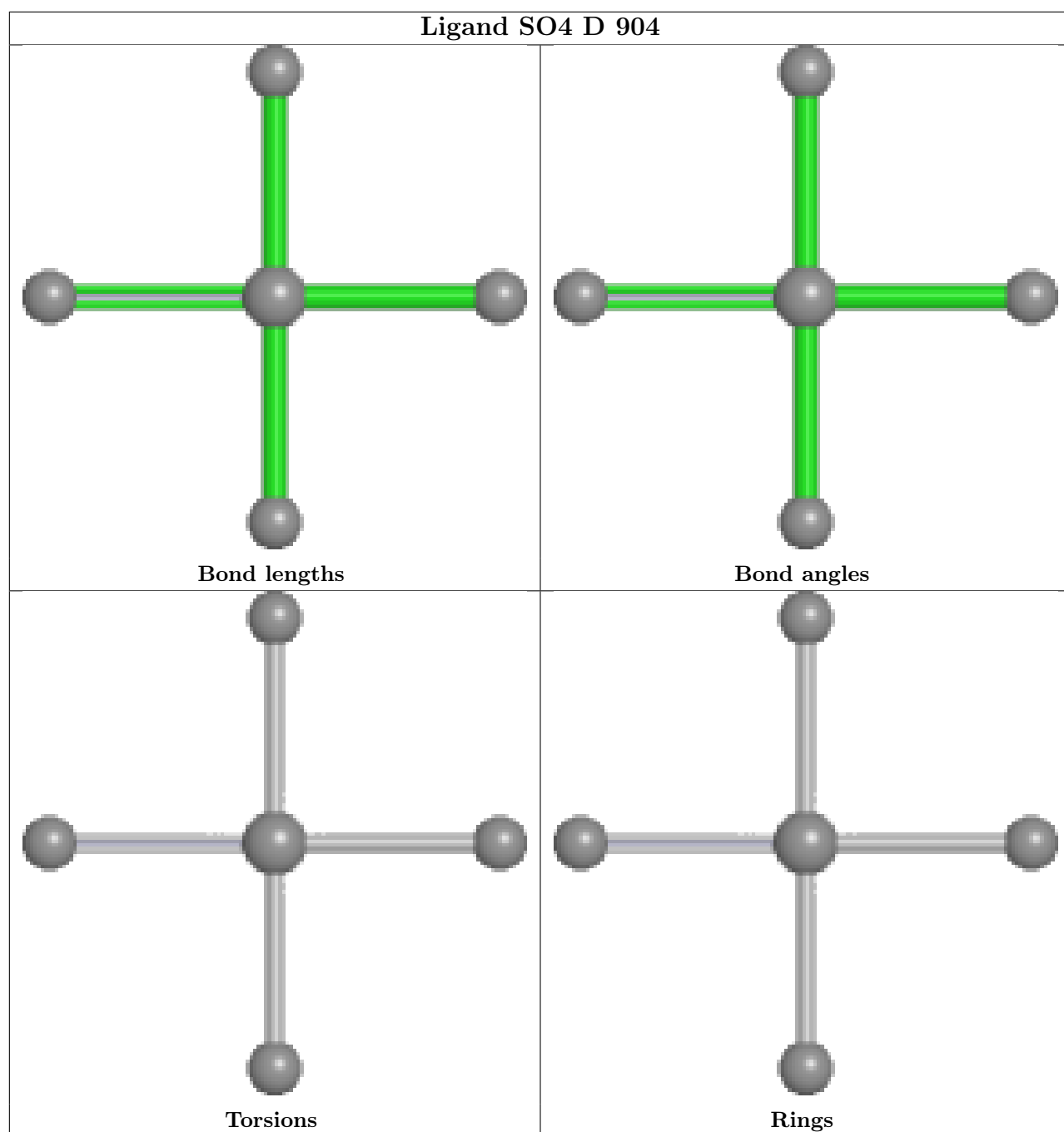


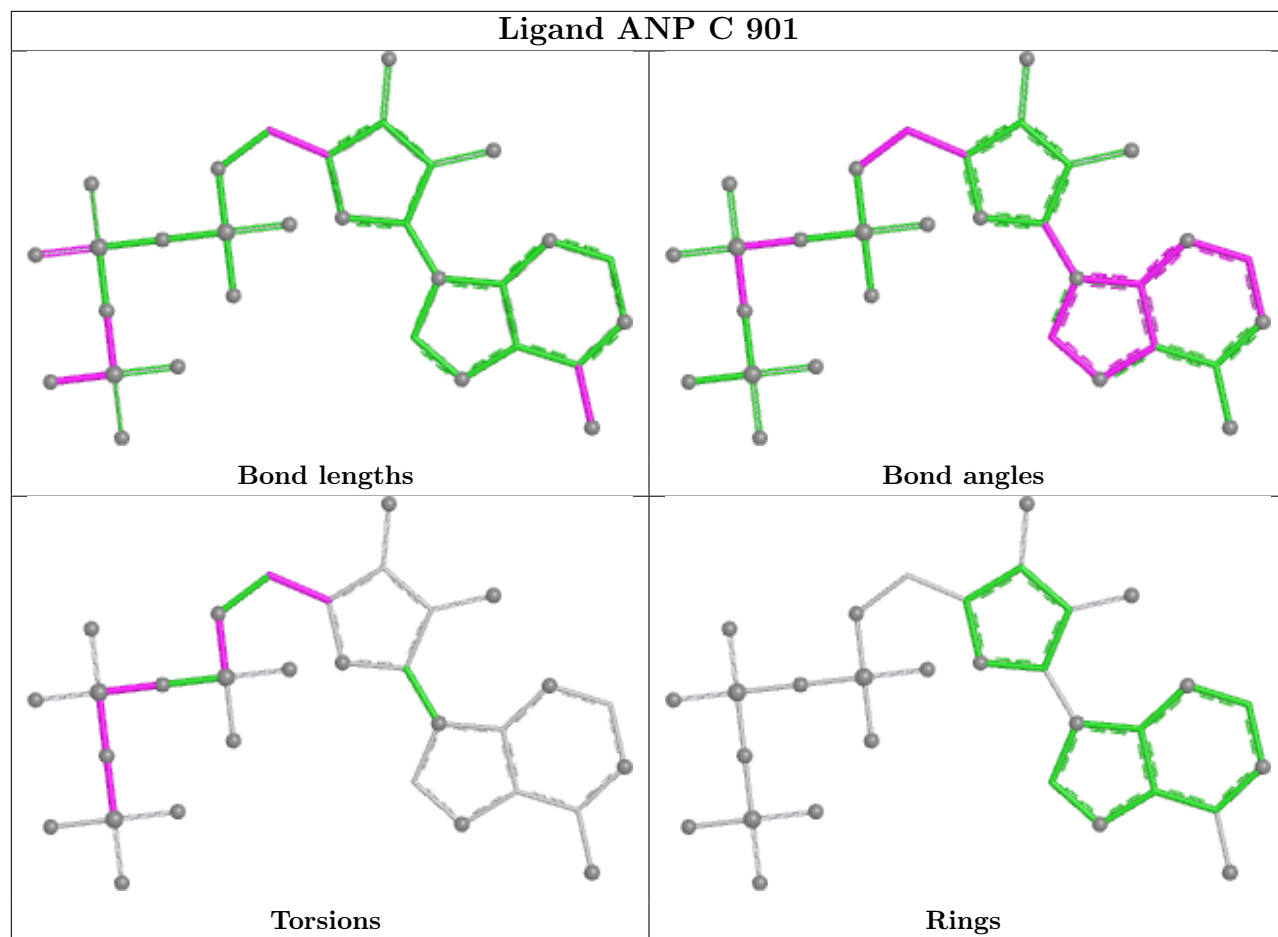


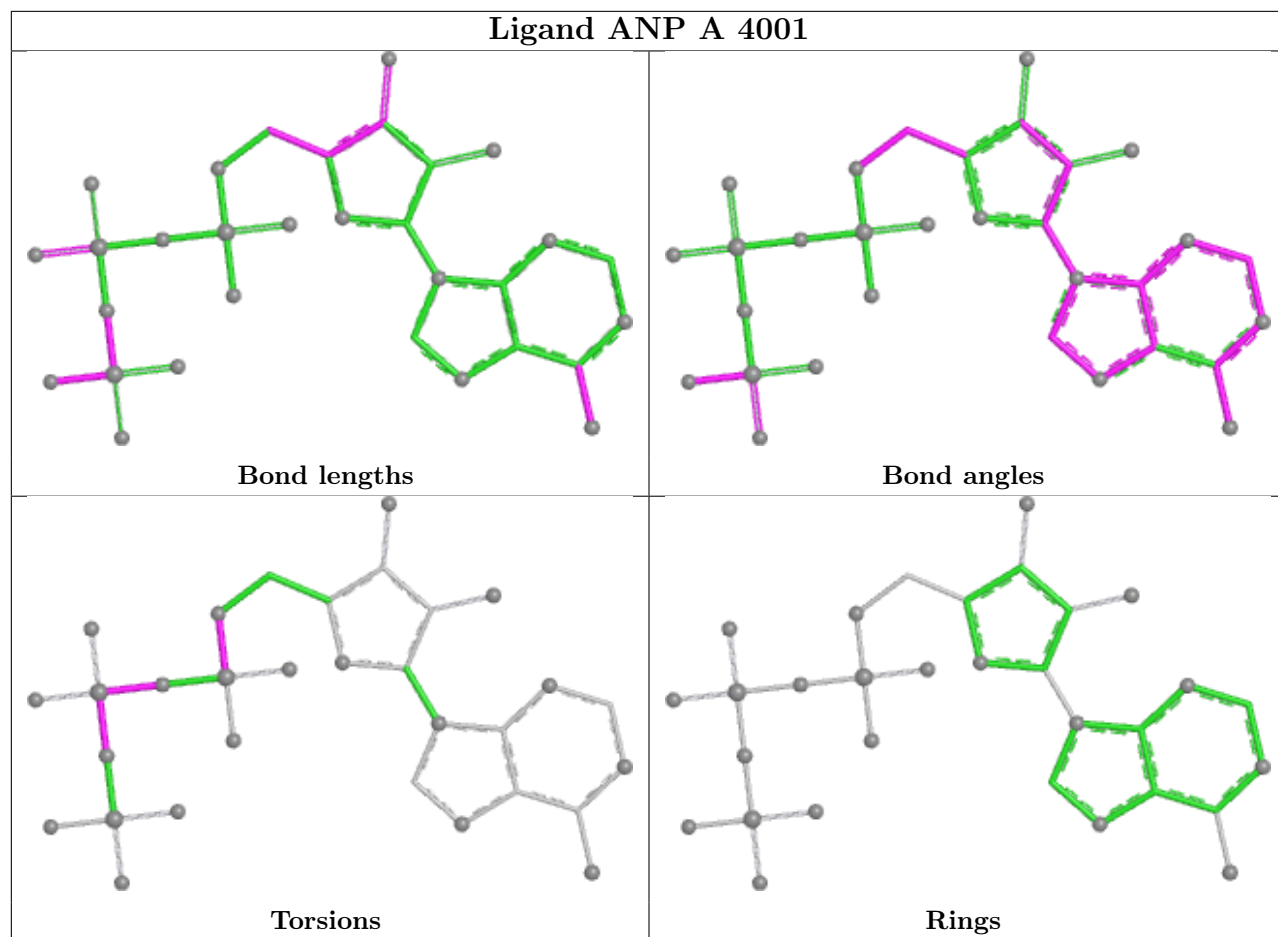


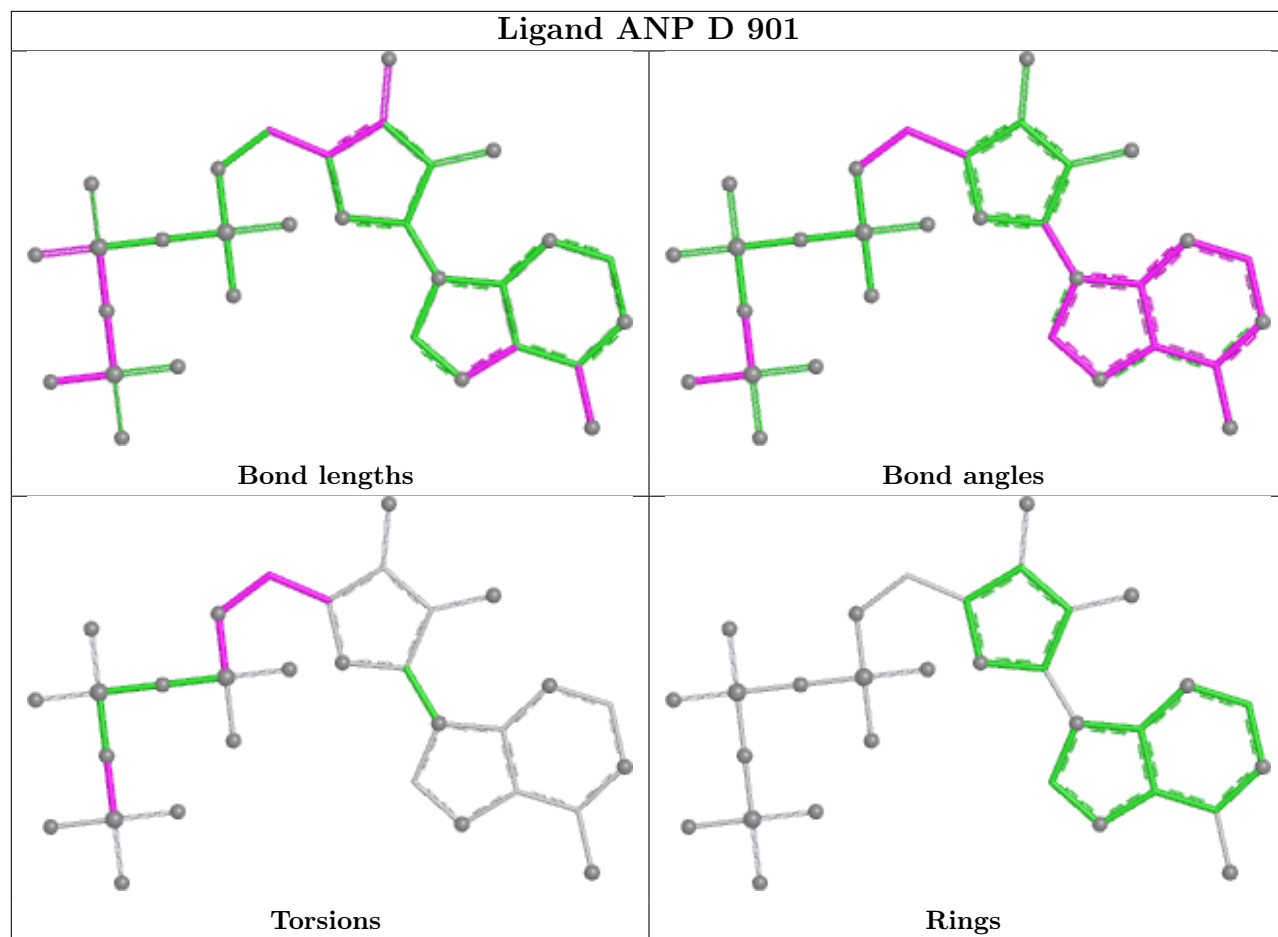


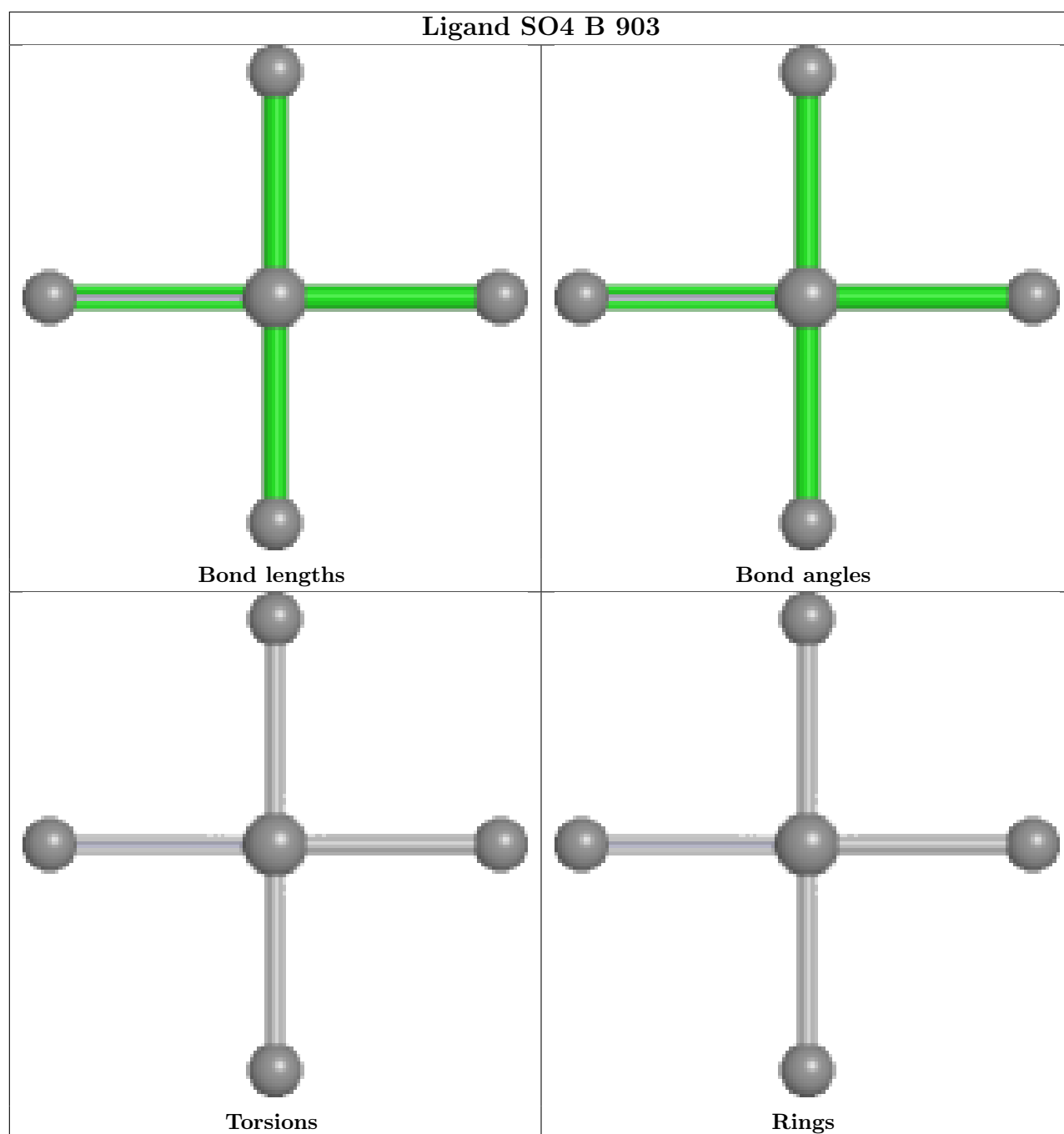


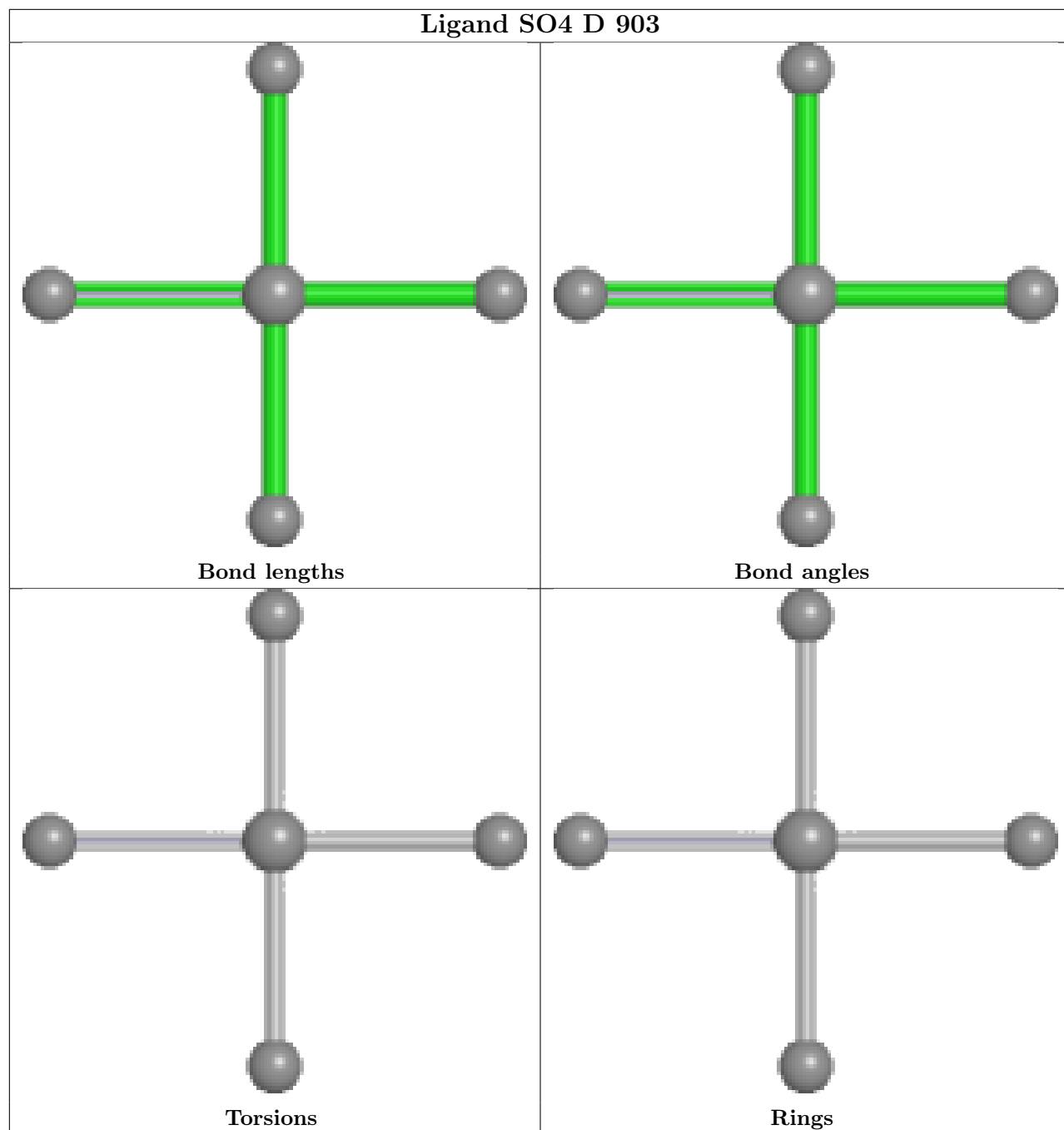


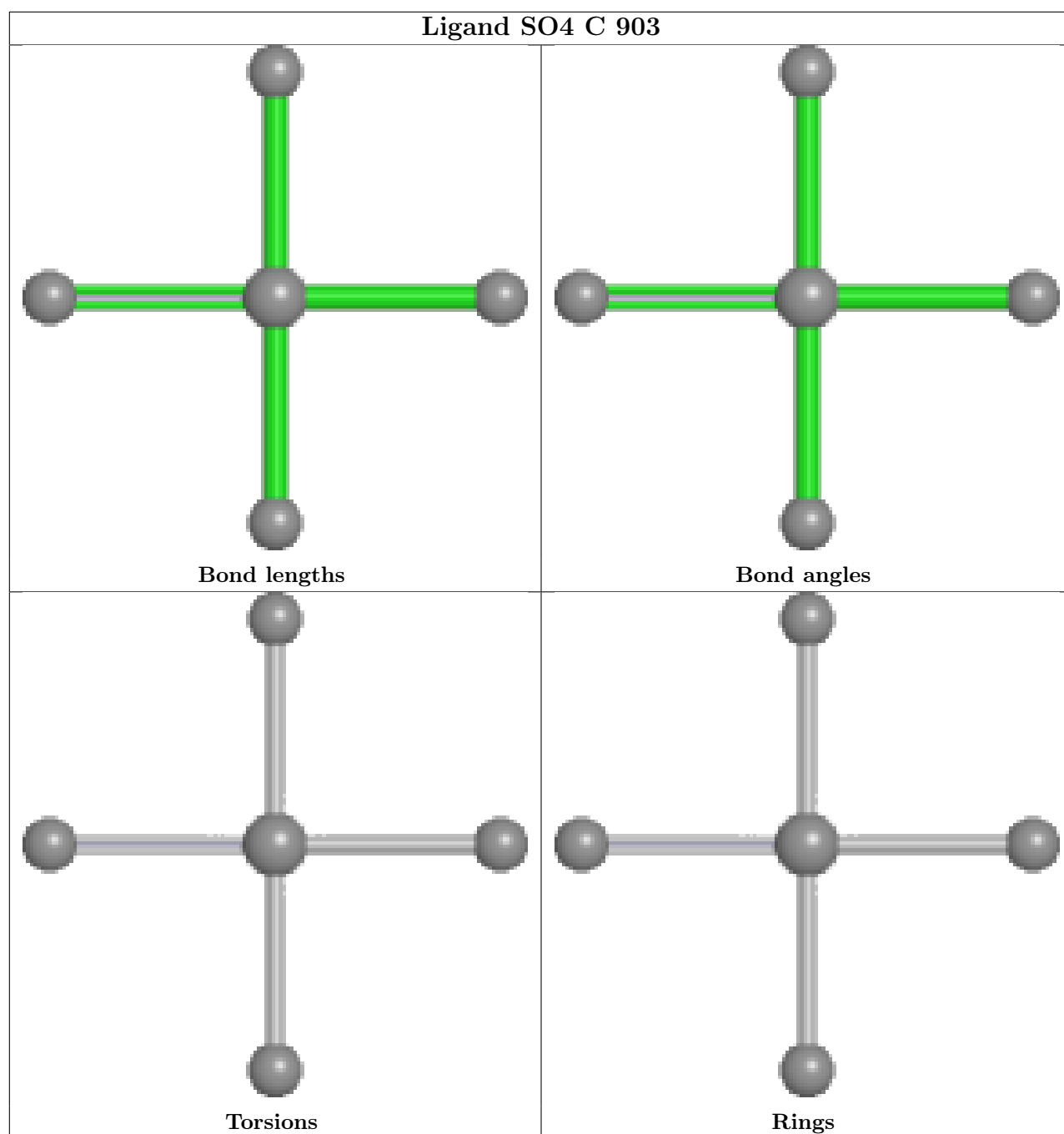












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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	872/874 (99%)	0.46	23 (2%) 57 34	16, 39, 68, 83	0
1	B	872/874 (99%)	0.24	12 (1%) 73 51	13, 30, 51, 76	0
1	C	872/874 (99%)	0.49	28 (3%) 50 29	16, 38, 68, 91	0
1	D	872/874 (99%)	0.31	18 (2%) 63 40	16, 30, 56, 76	0
All	All	3488/3496 (99%)	0.37	81 (2%) 61 38	13, 34, 63, 91	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	192	ASN	3.7
1	B	220	ALA	3.6
1	C	643	LEU	3.5
1	A	644	THR	3.5
1	A	448	VAL	3.3
1	C	635	ALA	3.2
1	D	517	VAL	3.1
1	A	643	LEU	3.1
1	C	634	GLN	2.9
1	A	296	ASN	2.9
1	D	518	SER	2.9
1	A	166	HIS	2.8
1	C	166	HIS	2.8
1	D	194	GLU	2.8
1	B	193	GLY	2.7
1	D	181	GLU	2.7
1	D	640	ASN	2.7
1	D	637	LEU	2.6
1	C	154	LYS	2.6
1	C	633	GLU	2.6
1	D	633	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	218	PRO	2.6
1	C	167	PHE	2.5
1	C	488	HIS	2.5
1	D	477	ASN	2.5
1	D	630	THR	2.5
1	C	519	GLY	2.5
1	A	155	ILE	2.4
1	D	631	GLU	2.4
1	D	647	GLU	2.4
1	C	642	GLY	2.4
1	D	642	GLY	2.4
1	C	301	CYS	2.4
1	A	488	HIS	2.4
1	A	632	GLU	2.4
1	B	334	LEU	2.4
1	C	489	THR	2.4
1	C	190	ALA	2.4
1	A	631	GLU	2.4
1	C	648	VAL	2.4
1	B	642	GLY	2.3
1	D	556	GLY	2.3
1	C	471	CYS	2.3
1	C	321	ASP	2.3
1	A	635	ALA	2.3
1	B	518	SER	2.3
1	B	844	CYS	2.3
1	B	658	PHE	2.3
1	A	630	THR	2.3
1	C	469	SER	2.3
1	D	768	ASN	2.3
1	B	517	VAL	2.3
1	B	98	SER	2.3
1	A	634	GLN	2.2
1	C	632	GLU	2.2
1	A	490	PHE	2.2
1	A	156	ILE	2.2
1	C	153	GLU	2.2
1	D	512	THR	2.2
1	C	165	VAL	2.2
1	A	645	LEU	2.2
1	B	488	HIS	2.2
1	B	821	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	478	GLU	2.2
1	A	486	GLY	2.2
1	C	393	GLY	2.2
1	A	476	ILE	2.1
1	D	478	GLU	2.1
1	A	474	ILE	2.1
1	A	633	GLU	2.1
1	C	171	LEU	2.1
1	A	178	GLU	2.1
1	B	56	GLN	2.1
1	C	503	GLY	2.1
1	A	75	LEU	2.0
1	A	735	ASP	2.0
1	C	21	GLY	2.0
1	C	298	MET	2.0
1	C	515	ALA	2.0
1	A	300	ASP	2.0
1	D	479	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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	SO4	A	4003	5/5	0.72	0.19	50,51,75,83	0
3	SO4	A	4004	5/5	0.75	0.20	51,56,67,67	0
3	SO4	C	904	5/5	0.80	0.14	39,41,50,70	0
3	SO4	C	903	5/5	0.81	0.15	46,50,53,72	0
3	SO4	D	903	5/5	0.83	0.20	45,45,52,65	0

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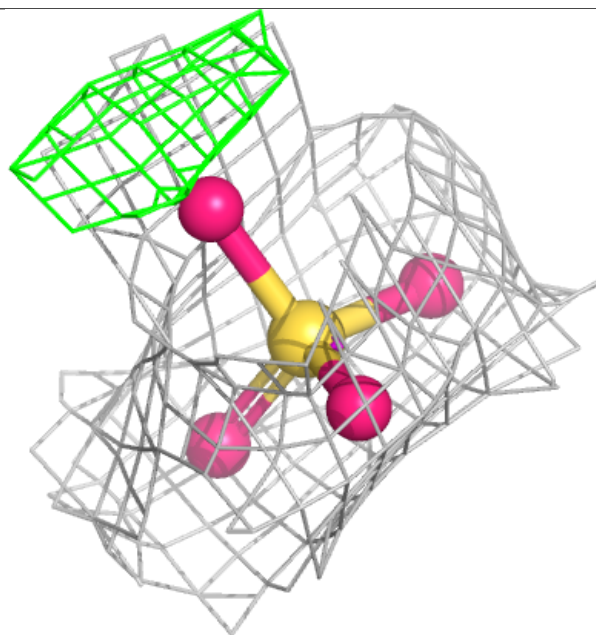
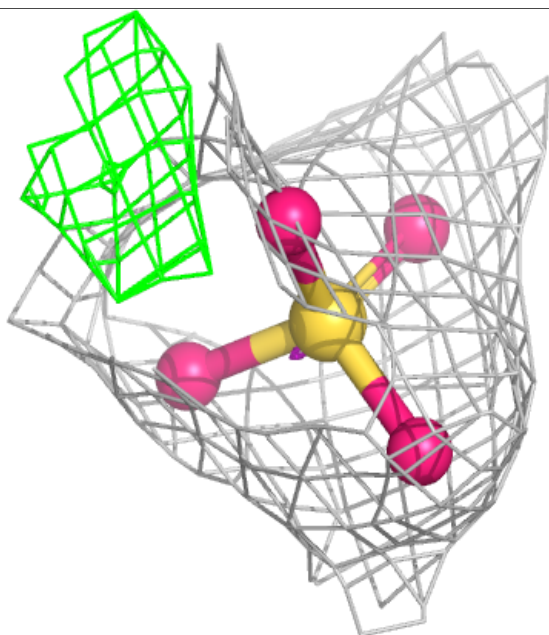
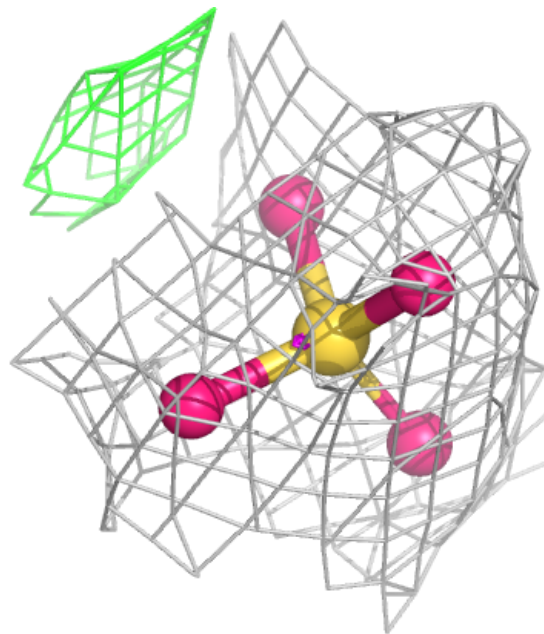
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	B	903	5/5	0.85	0.17	43,47,48,57	0
3	SO4	B	902	5/5	0.87	0.18	45,46,56,65	0
3	SO4	C	902	5/5	0.89	0.15	37,42,48,49	0
2	ANP	C	901	31/31	0.91	0.11	25,37,45,46	0
3	SO4	A	4002	5/5	0.91	0.20	43,47,52,61	0
3	SO4	B	904	5/5	0.92	0.09	40,45,58,58	0
3	SO4	D	902	5/5	0.93	0.20	32,37,41,52	0
2	ANP	A	4001	31/31	0.93	0.09	33,39,44,46	0
3	SO4	D	904	5/5	0.93	0.13	40,43,51,53	0
2	ANP	B	901	31/31	0.94	0.10	24,30,36,45	0
2	ANP	D	901	31/31	0.94	0.10	19,27,37,38	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.

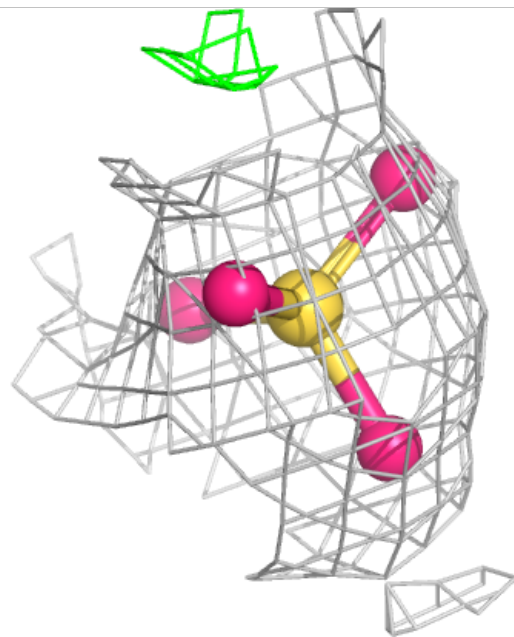
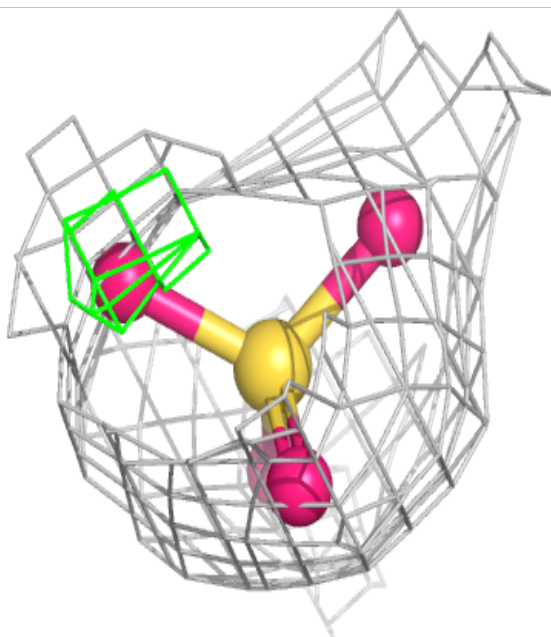
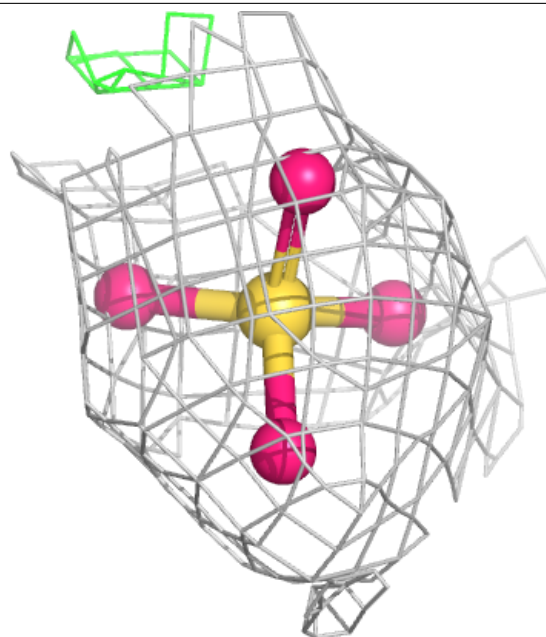
Electron density around SO4 A 4003:

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



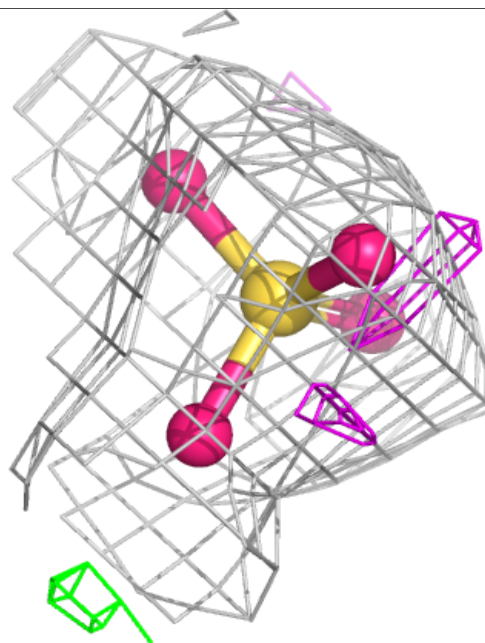
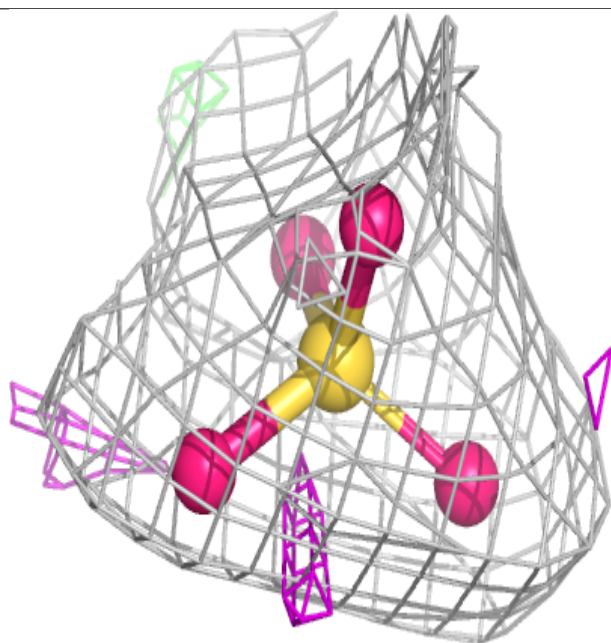
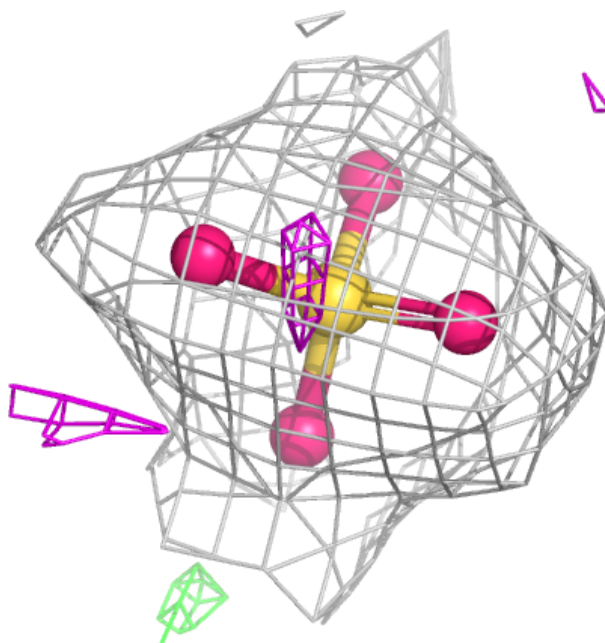
Electron density around SO4 A 4004:

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



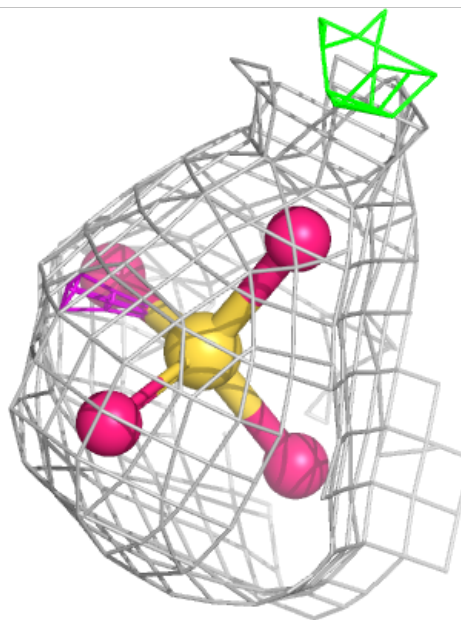
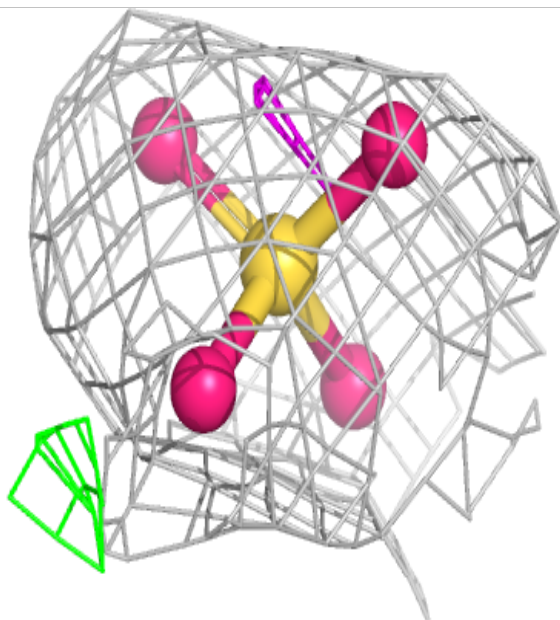
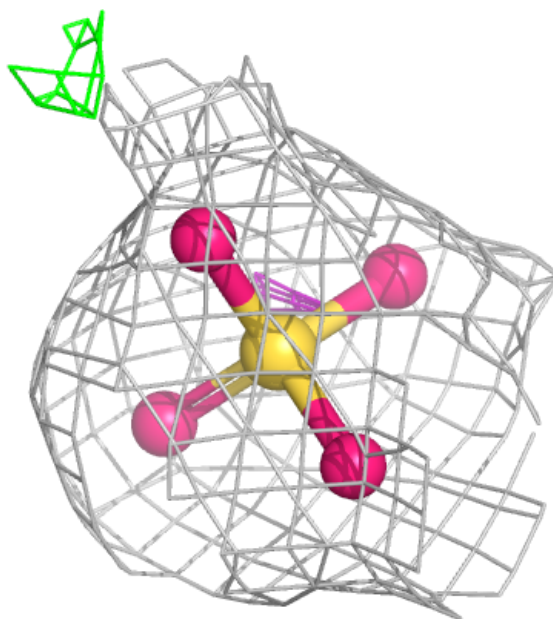
Electron density around SO4 C 904:

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



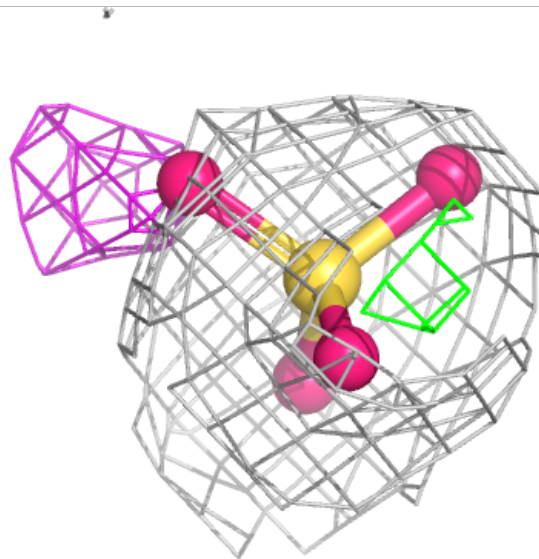
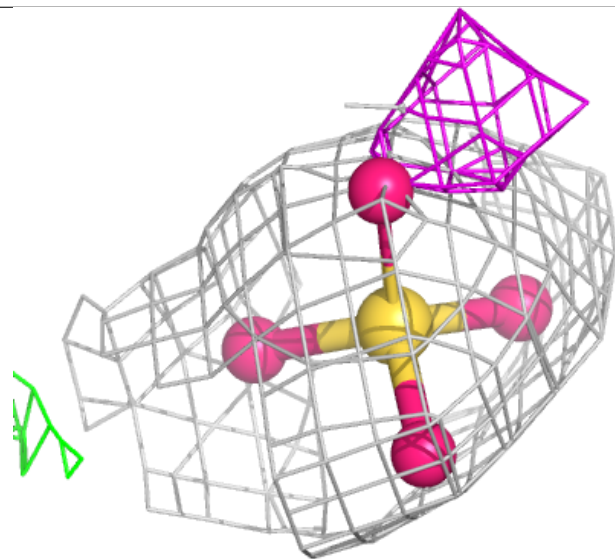
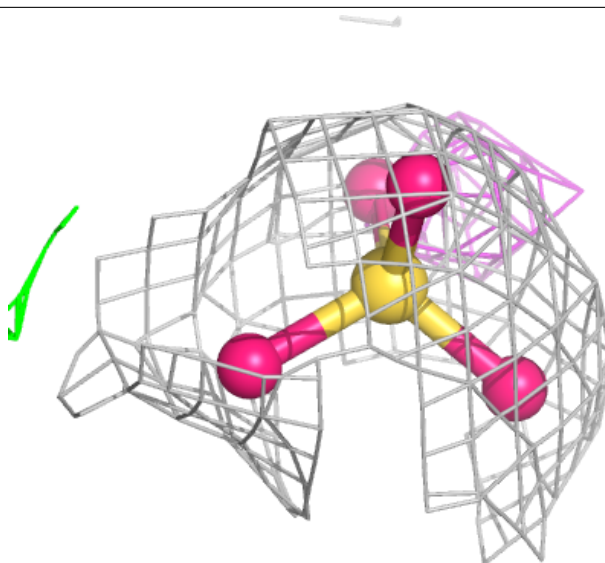
Electron density around SO4 C 903:

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



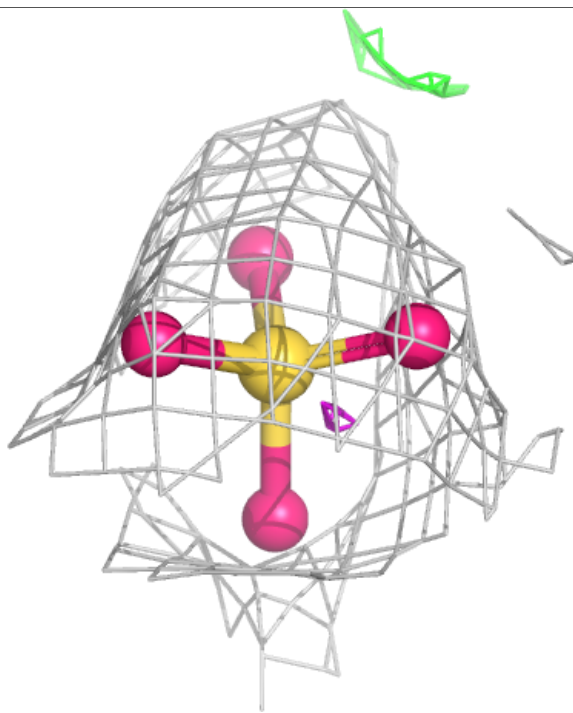
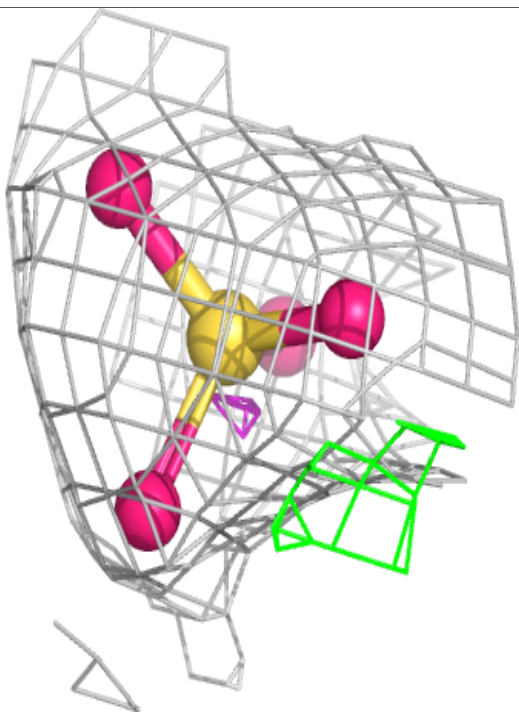
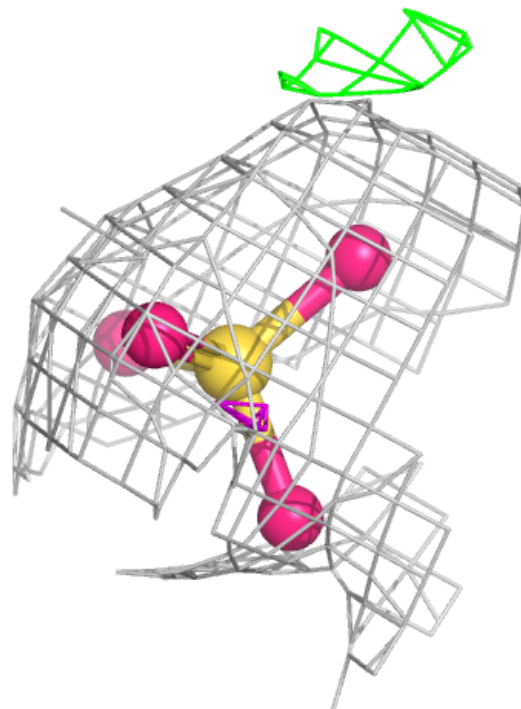
Electron density around SO4 D 903:

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



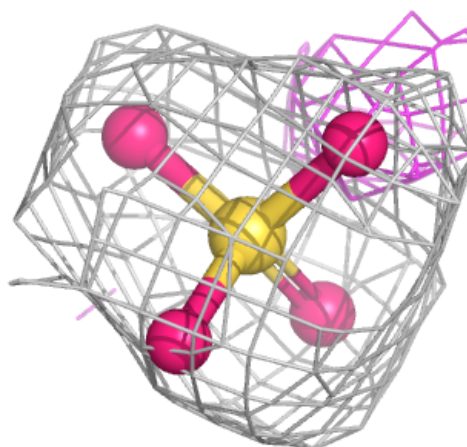
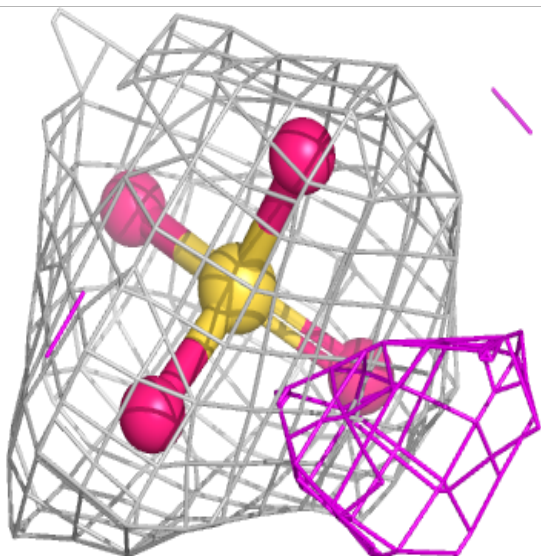
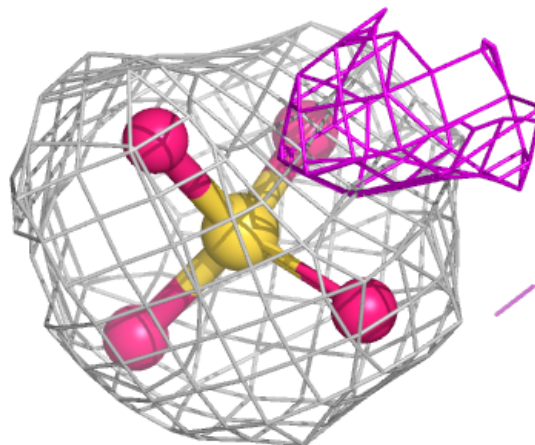
Electron density around SO4 B 903:

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



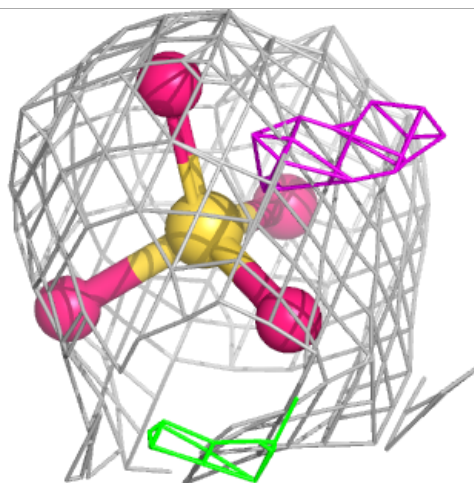
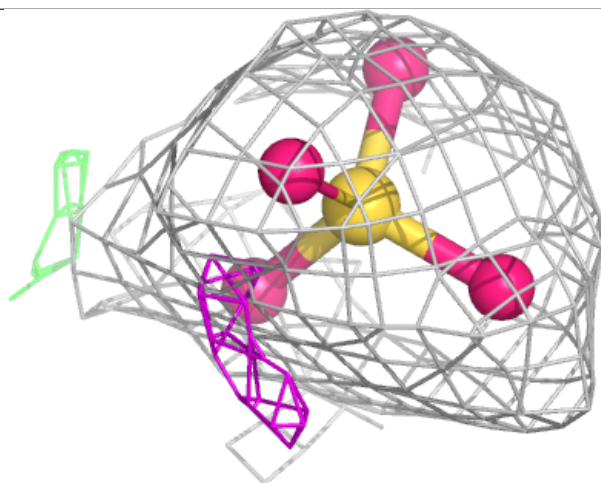
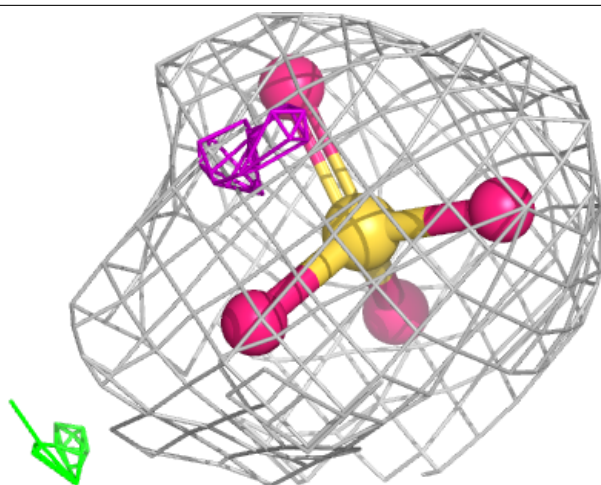
Electron density around SO4 B 902:

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



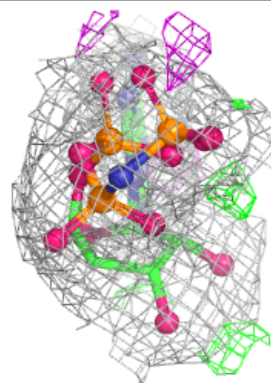
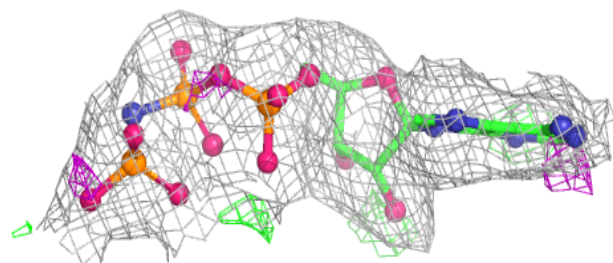
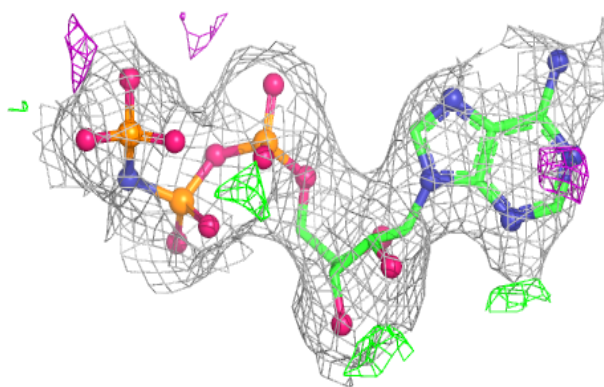
Electron density around SO4 C 902:

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



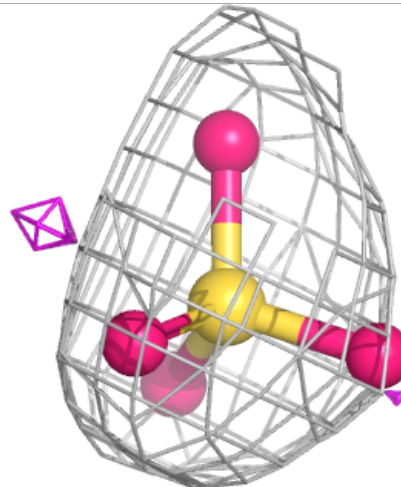
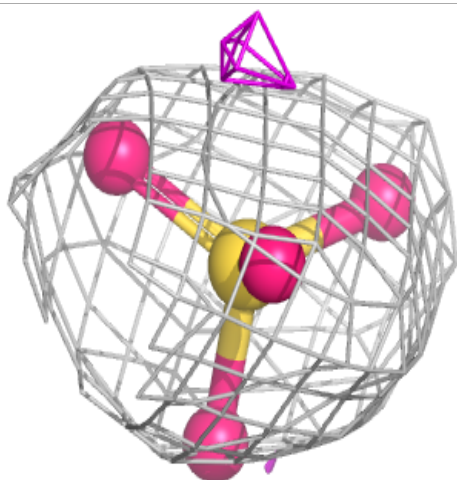
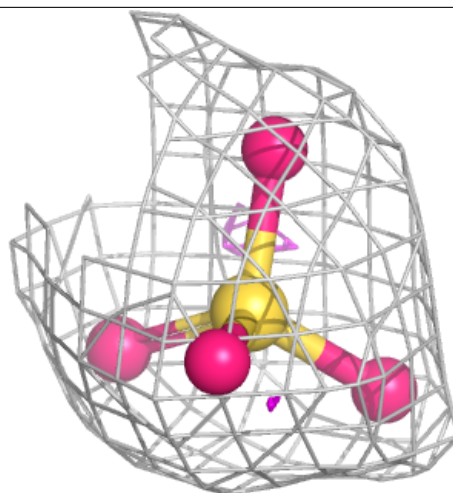
Electron density around ANP C 901:

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



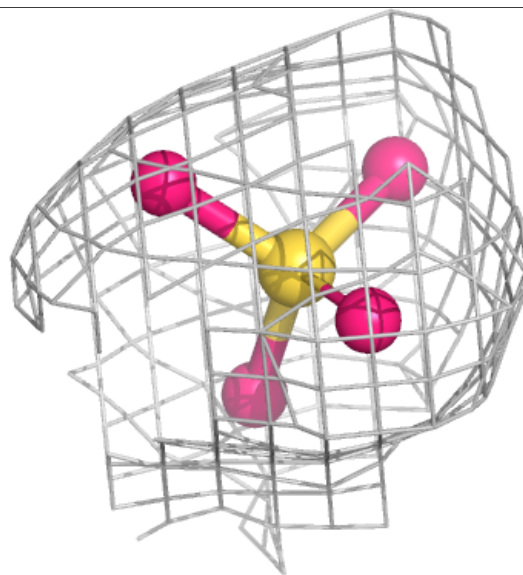
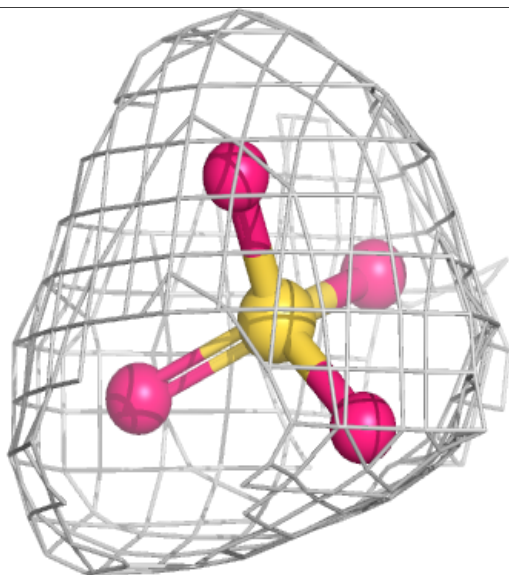
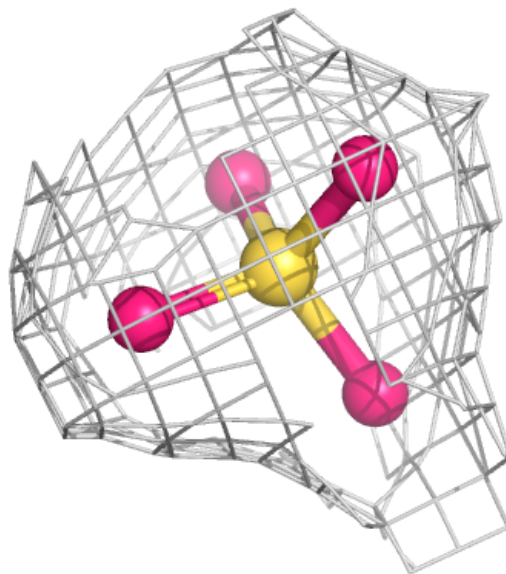
Electron density around SO4 A 4002:

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



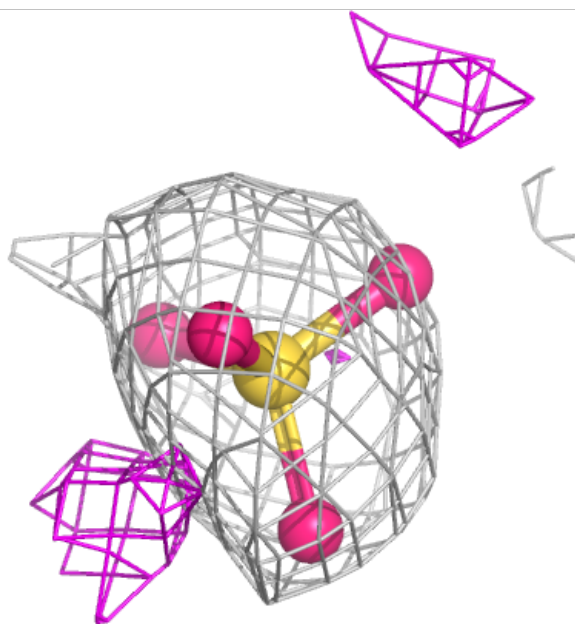
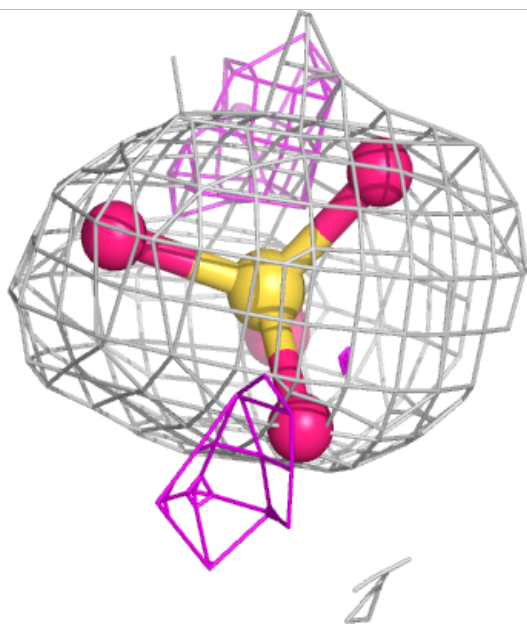
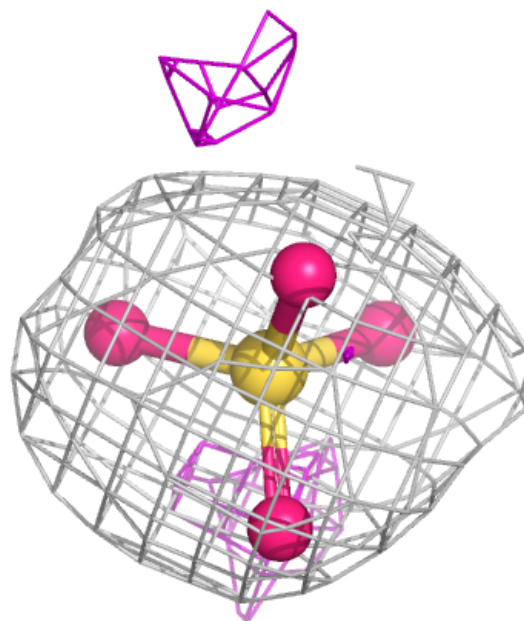
Electron density around SO4 B 904:

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



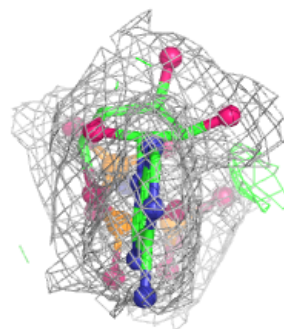
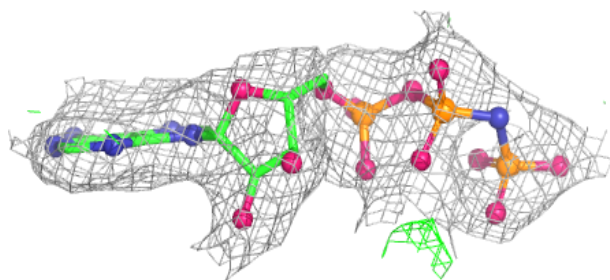
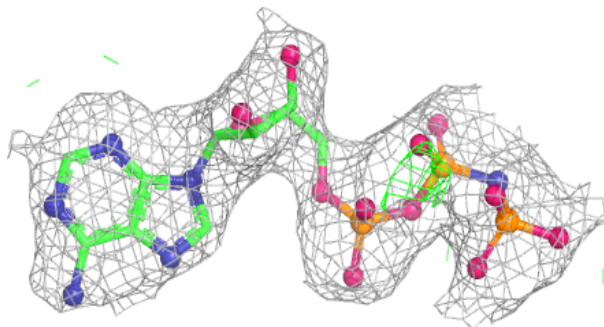
Electron density around SO4 D 902:

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



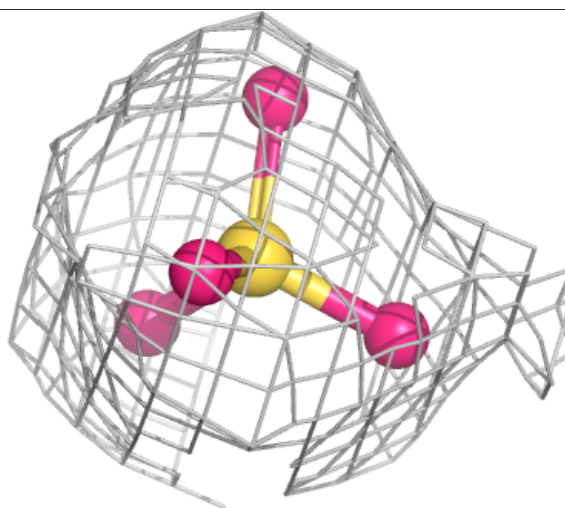
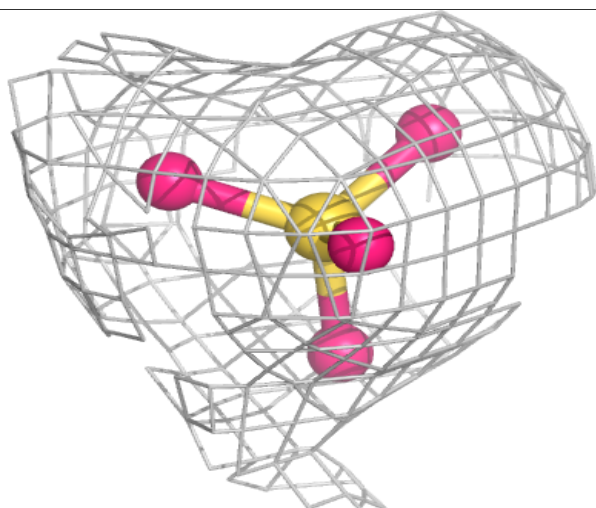
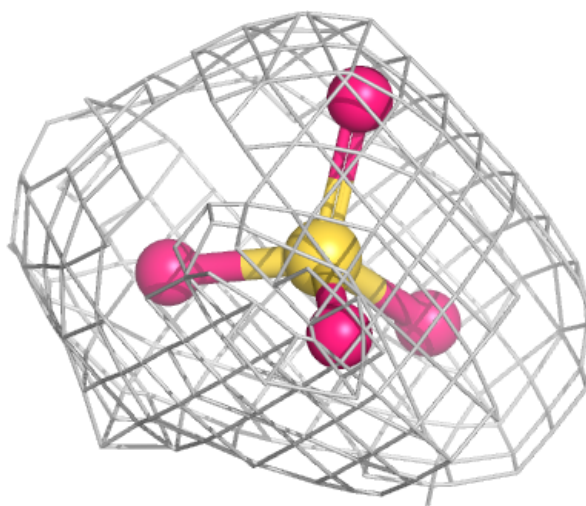
Electron density around ANP A 4001:

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



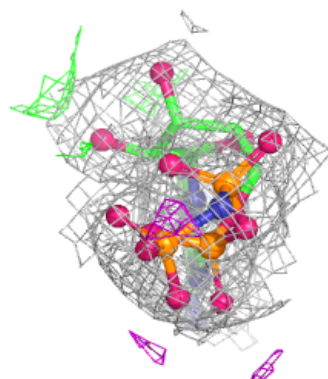
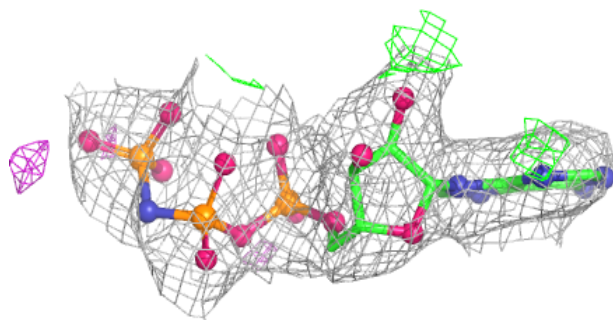
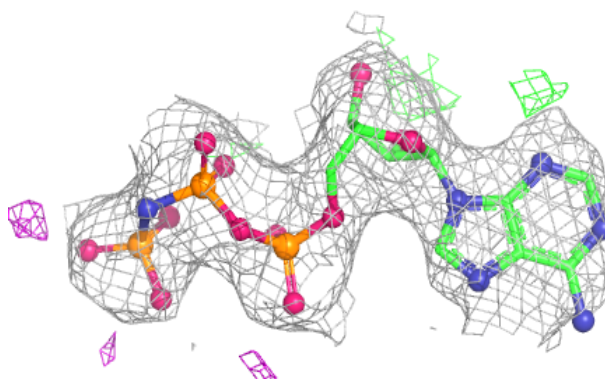
Electron density around SO4 D 904:

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

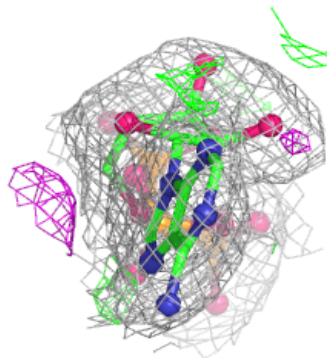
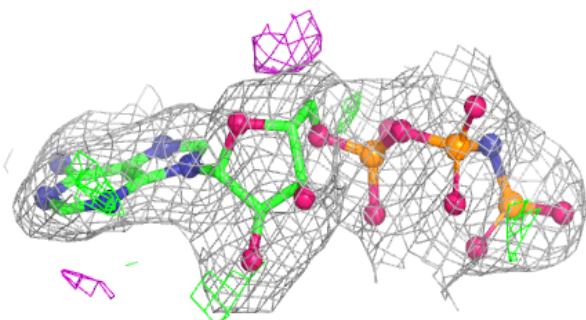
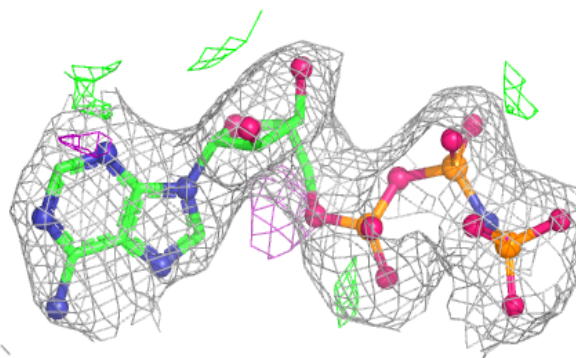


Electron density around ANP B 901:

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

**Electron density around ANP D 901:**

$2mF_o-DF_c$ (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.