



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:09 PM UTC

PDB ID : 1WPG / pdb_00001wpg
Title : Crystal structure of the SR CA2+-ATPase with MGF4
Authors : Toyoshima, C.; Nomura, H.; Tsuda, T.
Deposited on : 2004-09-02
Resolution : 2.30 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

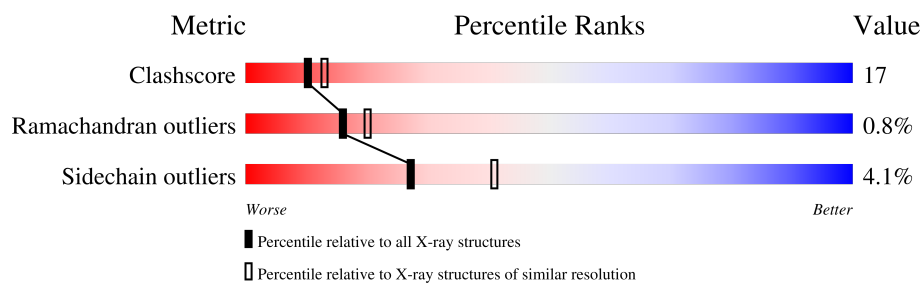
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	994	 66% 31% .
1	B	994	 66% 31% .
1	C	994	 66% 31% .
1	D	994	 65% 32% .

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 31698 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Sarcoplasmic/endoplasmic reticulum calcium ATPase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	994	Total	C	N	O	S	0	0	0
			7671	4876	1287	1451	57			
1	B	994	Total	C	N	O	S	0	0	0
			7671	4876	1287	1451	57			
1	C	994	Total	C	N	O	S	0	0	0
			7671	4876	1287	1451	57			
1	D	994	Total	C	N	O	S	0	0	0
			7671	4876	1287	1451	57			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	994	GLY	-	SEE REMARK 999	UNP P04191
B	994	GLY	-	SEE REMARK 999	UNP P04191
C	994	GLY	-	SEE REMARK 999	UNP P04191
D	994	GLY	-	SEE REMARK 999	UNP P04191

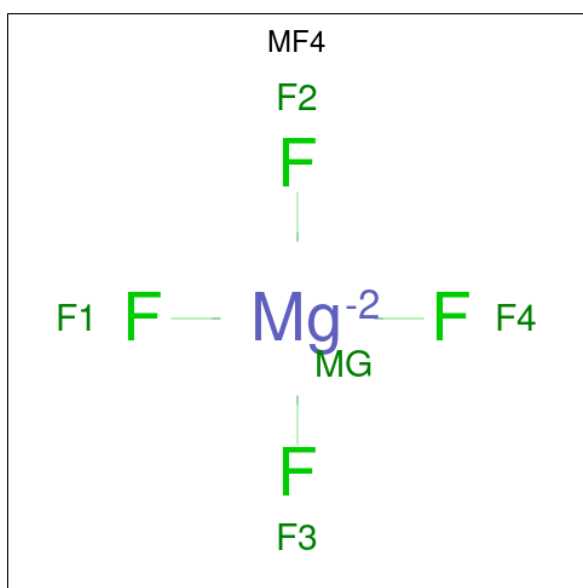
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	B	2	Total	Mg	0	0
			2	2		
2	C	2	Total	Mg	0	0
			2	2		
2	D	2	Total	Mg	0	0
			2	2		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

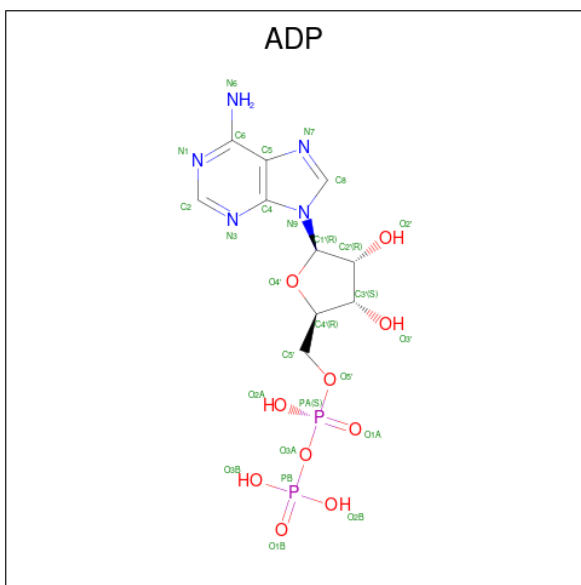
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Na 1	0	0
3	B	1	Total 1	Na 1	0	0
3	C	1	Total 1	Na 1	0	0
3	D	1	Total 1	Na 1	0	0

- Molecule 4 is TETRAFLUOROMAGNESATE(2-) (CCD ID: MF4) (formula: F_4Mg).



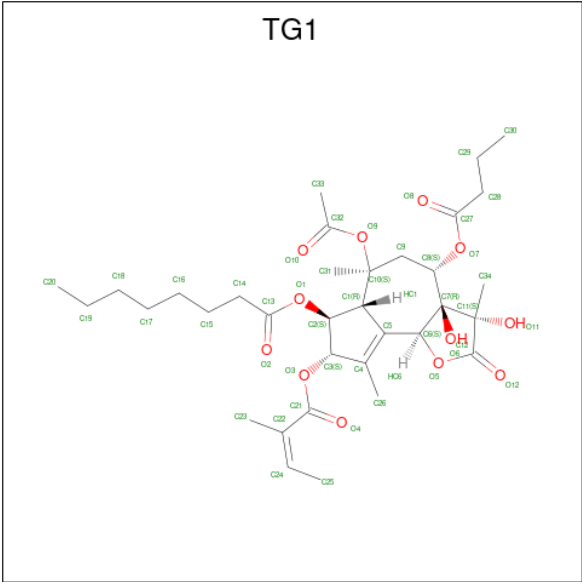
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 5	F 4	Mg 1	0	0
4	B	1	Total 5	F 4	Mg 1	0	0
4	C	1	Total 5	F 4	Mg 1	0	0
4	D	1	Total 5	F 4	Mg 1	0	0

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
5	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
5	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
5	D	1	Total 27	C 10	N 5	O 10	P 2	0	0

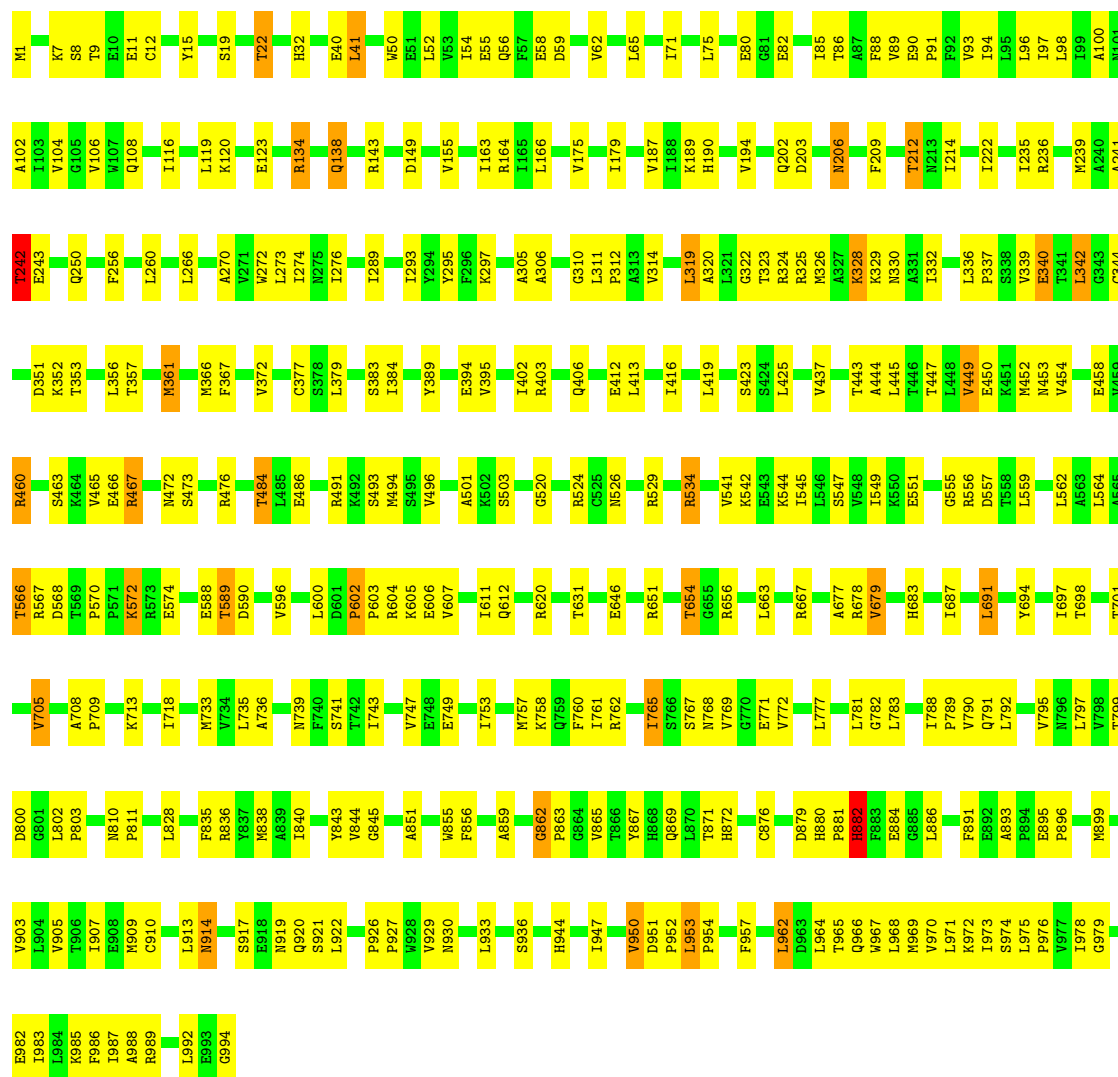
- Molecule 6 is OCTANOIC ACID [3S-[3ALPHA, 3ABETA, 4ALPHA, 6BETA, 6ABETA, 7BETA, 8ALPHA(Z), 9BALPHA]]-6-(ACETYLOXY)-2,3,-3A,4,5,6,6A,7,8,9B-DECAHYDRO-3,3A-DIHYDROXY-3,6,9-TRIMETHYL-8-[(2-METHYL-1-OXO-2-BUTENYL)OXY]-2-OXO-4-(1-OXOBUTOXY)-AZULENO[4,5-B]FURAN-7-YL ESTER (CCD ID: TG1) (formula: $C_{34}H_{50}O_{12}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			46	34	12		
6	B	1	Total	C	O	0	0
			46	34	12		
6	C	1	Total	C	O	0	0
			46	34	12		
6	D	1	Total	C	O	0	0
			46	34	12		

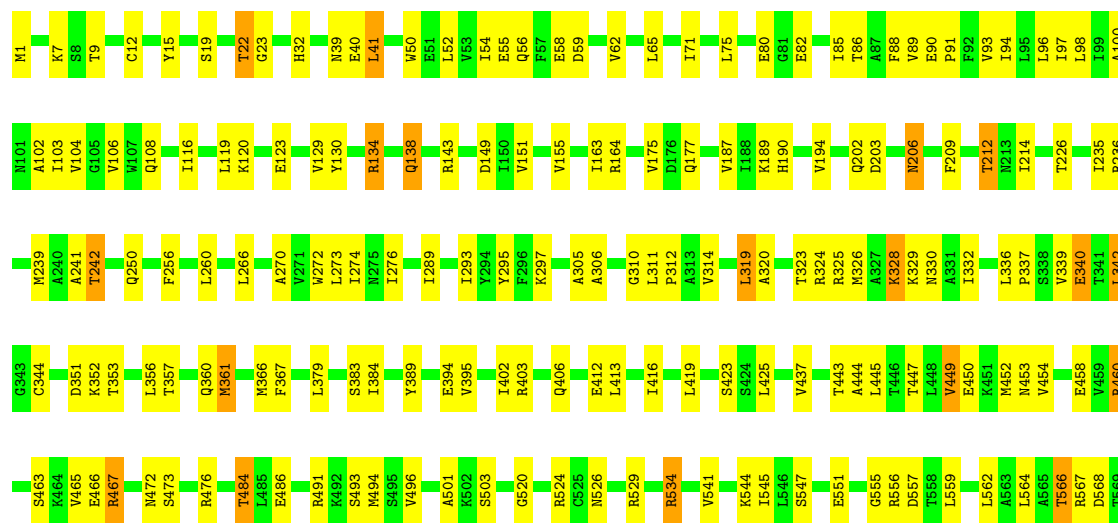
- Molecule 7 is water.

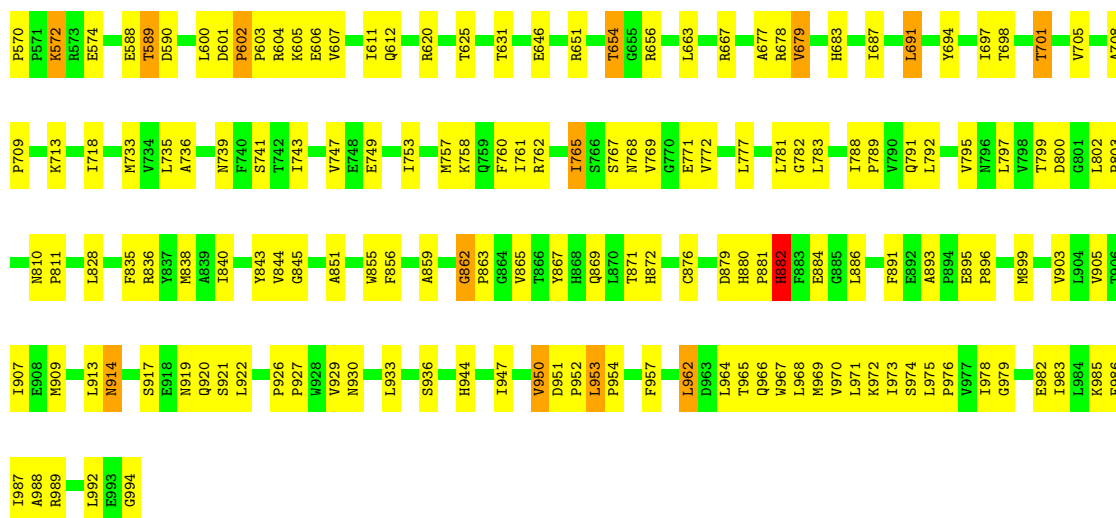
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	165	Total	O	0	0
			165	165		
7	B	180	Total	O	0	0
			180	180		
7	C	180	Total	O	0	0
			180	180		
7	D	165	Total	O	0	0
			165	165		



• Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1

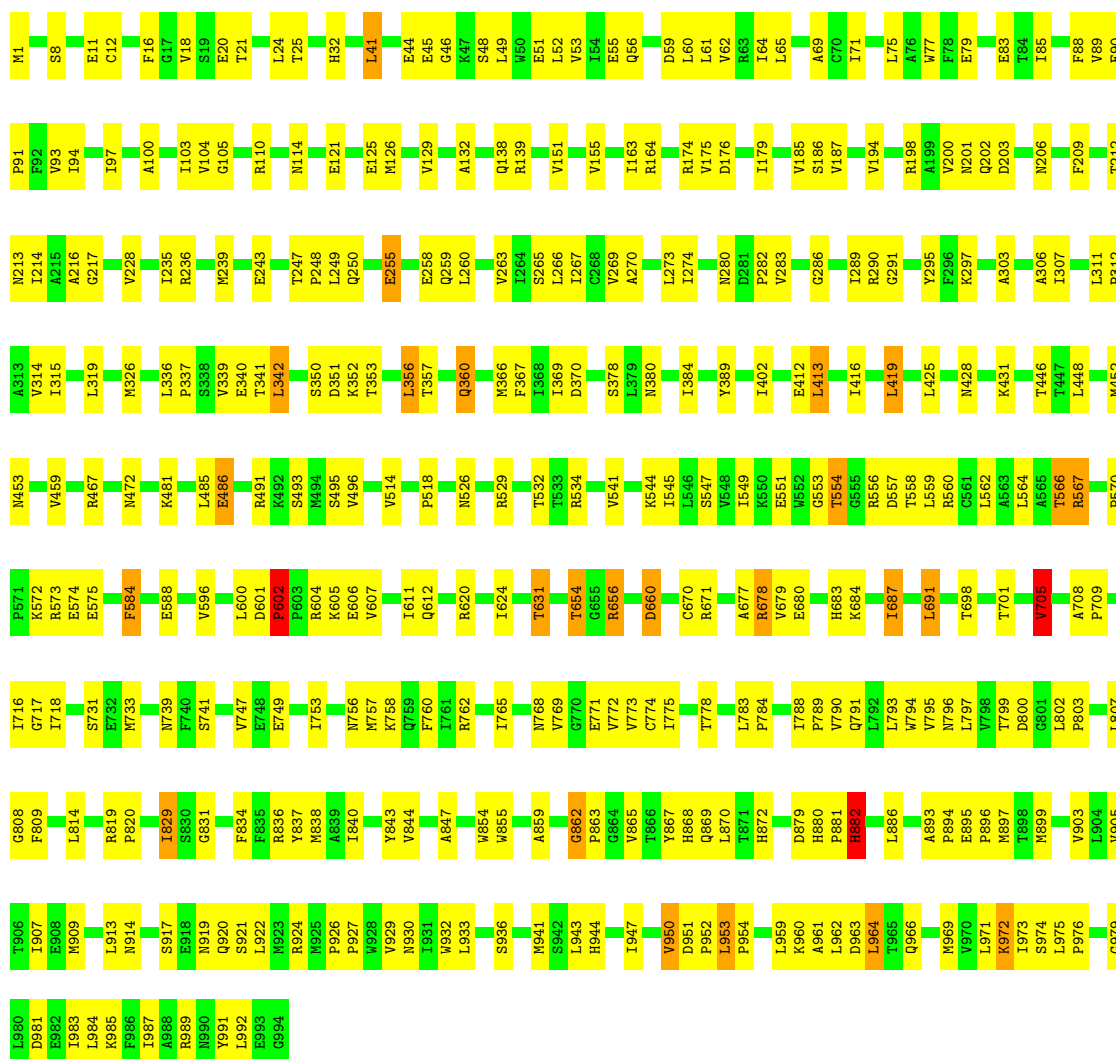
Chain C: 66% 31%





● Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1

Chain D: 65% 32% .



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.21Å 275.39Å 109.94Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	15.00 – 2.30	Depositor
% Data completeness (in resolution range)	93.4 (15.00-2.30)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.245	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	31698	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, TG1, ADP, MF4, MG

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	0.46	9/7812 (0.1%)	0.89	19/10592 (0.2%)
1	B	0.51	7/7812 (0.1%)	0.90	15/10592 (0.1%)
1	C	0.51	8/7812 (0.1%)	0.91	18/10592 (0.2%)
1	D	0.47	9/7812 (0.1%)	0.89	22/10592 (0.2%)
All	All	0.49	33/31248 (0.1%)	0.90	74/42368 (0.2%)

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	526	ASN	CG-OD1	5.54	1.34	1.23
1	C	32	HIS	ND1-CE1	5.41	1.38	1.32
1	C	526	ASN	CG-OD1	5.41	1.33	1.23
1	A	202	GLN	CD-OE1	5.40	1.33	1.23
1	B	32	HIS	ND1-CE1	5.34	1.37	1.32
1	B	872	HIS	ND1-CE1	5.33	1.37	1.32
1	D	872	HIS	ND1-CE1	5.33	1.37	1.32
1	B	250	GLN	CD-OE1	5.32	1.33	1.23
1	C	250	GLN	CD-OE1	5.29	1.33	1.23
1	D	612	GLN	CD-OE1	5.28	1.33	1.23
1	A	138	GLN	CD-OE1	5.28	1.33	1.23
1	A	612	GLN	CD-OE1	5.27	1.33	1.23
1	C	872	HIS	ND1-CE1	5.26	1.37	1.32
1	D	32	HIS	ND1-CE1	5.24	1.37	1.32
1	A	32	HIS	ND1-CE1	5.24	1.37	1.32
1	A	526	ASN	CG-OD1	5.20	1.33	1.23
1	A	360	GLN	CD-OE1	5.20	1.33	1.23
1	D	138	GLN	CD-OE1	5.18	1.33	1.23
1	C	612	GLN	CD-OE1	5.17	1.33	1.23
1	D	526	ASN	CG-OD1	5.16	1.33	1.23
1	B	138	GLN	CD-OE1	5.16	1.33	1.23
1	C	138	GLN	CD-OE1	5.15	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	206	ASN	CG-OD1	5.13	1.33	1.23
1	B	206	ASN	CG-OD1	5.13	1.33	1.23
1	B	612	GLN	CD-OE1	5.13	1.33	1.23
1	A	114	ASN	CG-OD1	5.11	1.33	1.23
1	D	114	ASN	CG-OD1	5.11	1.33	1.23
1	A	202	GLN	CD-NE2	-5.09	1.22	1.33
1	A	380	ASN	CG-OD1	5.08	1.33	1.23
1	D	206	ASN	CG-OD1	5.06	1.33	1.23
1	D	380	ASN	CG-OD1	5.06	1.33	1.23
1	C	360	GLN	CD-OE1	5.04	1.33	1.23
1	D	360	GLN	CD-OE1	5.04	1.33	1.23

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	556	ARG	N-CA-C	-8.97	102.35	113.20
1	C	556	ARG	N-CA-C	-8.85	102.49	113.20
1	D	602	PRO	N-CA-C	8.39	120.94	110.70
1	C	602	PRO	N-CA-C	8.37	119.54	110.58
1	A	602	PRO	N-CA-C	8.00	120.47	110.70
1	B	654	THR	N-CA-C	-7.74	99.06	110.52
1	C	654	THR	N-CA-C	-7.45	99.49	110.52
1	D	964	LEU	N-CA-C	-7.06	104.14	112.89
1	C	194	VAL	N-CA-C	-7.05	101.17	108.15
1	B	194	VAL	N-CA-C	-7.01	101.21	108.15
1	C	163	ILE	N-CA-C	7.00	118.57	108.48
1	A	964	LEU	N-CA-C	-6.97	104.25	112.89
1	B	163	ILE	N-CA-C	6.97	118.51	108.48
1	B	602	PRO	N-CA-C	6.89	119.10	110.70
1	D	601	ASP	CA-C-N	6.71	127.30	120.38
1	D	601	ASP	C-N-CA	6.71	127.30	120.38
1	A	32	HIS	CB-CG-CD2	-6.67	122.53	131.20
1	B	351	ASP	N-CA-C	-6.64	101.77	110.53
1	D	32	HIS	CB-CG-CD2	-6.63	122.58	131.20
1	D	194	VAL	CA-C-N	6.62	128.12	119.84
1	D	194	VAL	C-N-CA	6.62	128.12	119.84
1	C	351	ASP	N-CA-C	-6.61	101.80	110.53
1	A	194	VAL	CA-C-N	6.60	128.09	119.84
1	A	194	VAL	C-N-CA	6.60	128.09	119.84
1	B	32	HIS	CB-CG-CD2	-6.54	122.69	131.20
1	C	872	HIS	CB-CG-CD2	-6.50	122.75	131.20
1	D	872	HIS	CB-CG-CD2	-6.49	122.76	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	872	HIS	CB-CG-CD2	-6.48	122.77	131.20
1	C	32	HIS	CB-CG-CD2	-6.45	122.81	131.20
1	A	601	ASP	CA-C-N	6.23	126.79	120.38
1	A	601	ASP	C-N-CA	6.23	126.79	120.38
1	D	605	LYS	N-CA-C	6.20	118.54	111.11
1	A	605	LYS	N-CA-C	6.14	118.47	111.11
1	A	654	THR	N-CA-C	-6.04	101.83	110.59
1	C	601	ASP	CA-C-N	6.04	124.01	119.66
1	C	601	ASP	C-N-CA	6.04	124.01	119.66
1	C	605	LYS	N-CA-C	6.01	117.50	111.07
1	A	159	VAL	CA-C-N	5.96	125.66	119.64
1	A	159	VAL	C-N-CA	5.96	125.66	119.64
1	D	163	ILE	N-CA-C	5.93	117.01	108.48
1	C	419	LEU	N-CA-C	5.91	118.96	111.69
1	B	605	LYS	N-CA-C	5.89	117.38	111.07
1	A	556	ARG	N-CA-C	-5.88	105.37	112.54
1	A	163	ILE	N-CA-C	5.86	116.92	108.48
1	D	654	THR	N-CA-C	-5.78	102.21	110.59
1	A	32	HIS	CB-CG-ND1	5.77	131.36	122.70
1	D	32	HIS	CB-CG-ND1	5.75	131.32	122.70
1	D	556	ARG	N-CA-C	-5.74	105.54	112.54
1	D	872	HIS	CB-CG-ND1	5.64	131.16	122.70
1	B	419	LEU	N-CA-C	5.62	118.60	111.69
1	B	32	HIS	CB-CG-ND1	5.61	131.12	122.70
1	C	872	HIS	CB-CG-ND1	5.60	131.10	122.70
1	C	242	THR	CB-CA-C	-5.59	109.02	117.07
1	B	872	HIS	CB-CG-ND1	5.58	131.06	122.70
1	D	350	SER	N-CA-C	5.57	118.27	108.75
1	B	242	THR	CB-CA-C	-5.55	109.08	117.07
1	C	32	HIS	CB-CG-ND1	5.53	130.99	122.70
1	A	350	SER	N-CA-C	5.52	118.19	108.75
1	A	419	LEU	N-CA-C	5.50	118.45	111.69
1	D	419	LEU	N-CA-C	5.42	118.02	111.40
1	D	705	VAL	N-CA-C	-5.32	106.09	113.00
1	A	584	PHE	N-CA-C	5.31	118.55	111.75
1	A	351	ASP	N-CA-C	-5.31	103.52	110.53
1	D	351	ASP	N-CA-C	-5.29	103.54	110.53
1	C	625	THR	N-CA-C	5.29	117.85	109.50
1	B	242	THR	N-CA-C	5.28	113.11	108.78
1	D	584	PHE	N-CA-C	5.26	118.48	111.75
1	C	175	VAL	N-CA-C	5.23	116.01	108.48
1	C	242	THR	N-CA-C	5.20	113.05	108.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	705	VAL	N-CA-C	-5.14	106.32	113.00
1	D	41	LEU	CA-C-N	5.06	125.29	119.83
1	D	41	LEU	C-N-CA	5.06	125.29	119.83
1	B	175	VAL	N-CA-C	5.03	115.73	108.48
1	D	532	THR	N-CA-C	-5.02	106.58	113.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7671	0	7764	256	0
1	B	7671	0	7764	281	0
1	C	7671	0	7764	278	0
1	D	7671	0	7764	254	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	27	0	12	0	0
5	B	27	0	12	2	0
5	C	27	0	12	2	0
5	D	27	0	12	0	0
6	A	46	0	50	0	0
6	B	46	0	50	2	0
6	C	46	0	50	2	0
6	D	46	0	50	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	165	0	0	5	0
7	B	180	0	0	8	0
7	C	180	0	0	7	0
7	D	165	0	0	6	0
All	All	31698	0	31304	1065	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (1065) 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:460:ARG:H	1:C:460:ARG:HD3	1.09	1.15
1:B:460:ARG:HD3	1:B:460:ARG:H	1.10	1.13
1:B:1:MET:HE1	1:B:12:CYS:HA	1.38	1.03
1:C:1:MET:HE1	1:C:12:CYS:HA	1.37	1.02
1:D:679:VAL:HG13	1:D:683:HIS:HB2	1.47	0.96
1:C:921:SER:HB2	1:C:989:ARG:HH22	1.30	0.95
1:B:921:SER:HB2	1:B:989:ARG:HH22	1.31	0.94
1:A:679:VAL:HG13	1:A:683:HIS:HB2	1.49	0.93
1:C:366:MET:HE2	1:C:384:ILE:HD11	1.47	0.93
1:A:202:GLN:H	1:A:202:GLN:HE21	1.13	0.92
1:D:366:MET:HE2	1:D:384:ILE:HD11	1.50	0.91
1:B:342:LEU:HD12	1:B:733:MET:HE1	1.52	0.91
1:B:366:MET:HE2	1:B:384:ILE:HD11	1.50	0.91
1:D:448:LEU:HG	1:D:452:MET:HE2	1.53	0.90
1:A:366:MET:HE2	1:A:384:ILE:HD11	1.54	0.89
1:A:448:LEU:HG	1:A:452:MET:HE2	1.54	0.89
1:C:484:THR:HB	1:C:496:VAL:HG12	1.56	0.88
1:C:342:LEU:HD12	1:C:733:MET:HE1	1.56	0.88
1:B:484:THR:HB	1:B:496:VAL:HG12	1.57	0.87
1:B:494:MET:HE2	7:B:3036:HOH:O	1.75	0.86
1:B:319:LEU:HB3	1:B:336:LEU:HD12	1.58	0.85
1:C:494:MET:HE2	7:C:4036:HOH:O	1.77	0.85
1:C:319:LEU:HB3	1:C:336:LEU:HD12	1.59	0.84
1:C:460:ARG:HD3	1:C:460:ARG:N	1.93	0.81
1:A:289:ILE:HG22	1:A:290:ARG:HH11	1.46	0.80
1:D:289:ILE:HG22	1:D:290:ARG:HH11	1.46	0.80
1:B:460:ARG:HD3	1:B:460:ARG:N	1.94	0.80
1:D:174:ARG:HG3	1:D:216:ALA:HB3	1.63	0.79
1:A:260:LEU:HD11	1:A:306:ALA:HB1	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ARG:HG3	1:A:216:ALA:HB3	1.65	0.78
1:A:125:GLU:HG3	1:A:126:MET:HG2	1.65	0.77
1:D:125:GLU:HG3	1:D:126:MET:HG2	1.65	0.77
1:D:260:LEU:HD11	1:D:306:ALA:HB1	1.67	0.77
1:B:865:VAL:HG11	1:B:869:GLN:HB2	1.67	0.76
1:B:921:SER:H	1:B:989:ARG:HH12	1.29	0.76
1:D:413:LEU:HD22	1:D:564:LEU:HD12	1.66	0.76
1:A:247:THR:HB	1:A:248:PRO:HD2	1.68	0.76
1:C:865:VAL:HG11	1:C:869:GLN:HB2	1.68	0.76
1:C:921:SER:H	1:C:989:ARG:HH12	1.29	0.75
1:D:247:THR:HB	1:D:248:PRO:HD2	1.69	0.75
1:A:412:GLU:OE1	1:A:529:ARG:HD2	1.88	0.74
1:B:972:LYS:HE2	1:B:972:LYS:HA	1.69	0.74
1:C:972:LYS:HA	1:C:972:LYS:HE2	1.70	0.74
1:A:413:LEU:HD22	1:A:564:LEU:HD12	1.68	0.74
1:B:209:PHE:O	1:B:212:THR:HB	1.87	0.74
1:A:553:GLY:O	1:A:554:THR:CG2	2.37	0.73
1:D:412:GLU:OE1	1:D:529:ARG:HD2	1.88	0.73
1:B:80:GLU:HG3	1:B:82:GLU:HG2	1.70	0.73
1:C:80:GLU:HG3	1:C:82:GLU:HG2	1.70	0.73
1:C:458:GLU:HB2	1:C:460:ARG:HE	1.54	0.73
1:B:458:GLU:HB2	1:B:460:ARG:HE	1.54	0.72
1:C:212:THR:HG21	7:C:4082:HOH:O	1.87	0.72
1:B:844:VAL:HG22	1:B:907:ILE:HG21	1.71	0.72
1:C:844:VAL:HG22	1:C:907:ILE:HG21	1.71	0.72
1:B:235:ILE:HG22	1:B:239:MET:HE2	1.71	0.72
1:C:1:MET:HE2	1:C:7:LYS:HD2	1.69	0.71
1:B:567:ARG:HD3	1:B:570:PRO:HA	1.72	0.71
1:B:212:THR:HG21	7:B:3082:HOH:O	1.88	0.71
1:C:326:MET:HE1	1:C:339:VAL:HG22	1.72	0.71
1:B:922:LEU:HD23	1:B:927:PRO:HG3	1.72	0.71
1:C:567:ARG:HD3	1:C:570:PRO:HA	1.72	0.71
1:B:326:MET:HE1	1:B:339:VAL:HG22	1.72	0.71
1:B:260:LEU:HD11	1:B:306:ALA:HB1	1.72	0.71
1:C:260:LEU:HD11	1:C:306:ALA:HB1	1.73	0.71
1:D:319:LEU:HB3	1:D:336:LEU:HD12	1.71	0.71
1:C:235:ILE:HG22	1:C:239:MET:HE2	1.72	0.70
1:C:922:LEU:HD23	1:C:927:PRO:HG3	1.73	0.70
1:C:735:LEU:HD11	1:C:743:ILE:HD11	1.72	0.70
1:A:984:LEU:HA	1:A:987:ILE:HD12	1.73	0.70
1:B:1:MET:HE3	1:B:15:TYR:CB	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:LEU:HB3	1:A:336:LEU:HD12	1.72	0.70
1:C:735:LEU:HD21	1:C:743:ILE:HD13	1.74	0.69
1:D:90:GLU:HB3	1:D:91:PRO:HD3	1.72	0.69
1:A:90:GLU:HB3	1:A:91:PRO:HD3	1.72	0.69
1:B:735:LEU:HD21	1:B:743:ILE:HD13	1.74	0.69
1:B:1:MET:HE2	1:B:7:LYS:HD2	1.71	0.69
1:C:913:LEU:HD22	1:C:927:PRO:HB3	1.73	0.69
1:A:202:GLN:H	1:A:202:GLN:NE2	1.90	0.69
1:B:913:LEU:HD22	1:B:927:PRO:HB3	1.73	0.69
1:D:984:LEU:HA	1:D:987:ILE:HD12	1.75	0.69
1:B:735:LEU:HD11	1:B:743:ILE:HD11	1.74	0.68
1:D:176:ASP:O	1:D:212:THR:HG23	1.92	0.68
1:A:553:GLY:O	1:A:554:THR:HG23	1.93	0.68
1:C:90:GLU:HB3	1:C:91:PRO:HD3	1.76	0.68
1:C:209:PHE:O	1:C:212:THR:HB	1.94	0.68
1:D:369:ILE:HD11	1:D:545:ILE:HD11	1.75	0.67
1:D:749:GLU:O	1:D:753:ILE:HG12	1.94	0.67
1:A:61:LEU:HD22	1:A:307:ILE:HD12	1.75	0.67
1:A:749:GLU:O	1:A:753:ILE:HG12	1.94	0.67
1:B:782:GLY:HA3	1:B:871:THR:HG23	1.77	0.67
1:A:202:GLN:HE21	1:A:202:GLN:N	1.90	0.67
1:D:413:LEU:CD2	1:D:564:LEU:HD12	2.25	0.67
1:D:61:LEU:HD22	1:D:307:ILE:HD12	1.76	0.67
1:A:176:ASP:O	1:A:212:THR:HG23	1.94	0.67
1:B:90:GLU:HB3	1:B:91:PRO:HD3	1.76	0.67
1:C:1:MET:HE3	1:C:15:TYR:CB	2.25	0.67
1:A:369:ILE:HD11	1:A:545:ILE:HD11	1.76	0.67
1:D:412:GLU:OE2	1:D:566:THR:HG21	1.95	0.67
1:C:782:GLY:HA3	1:C:871:THR:HG23	1.77	0.67
1:D:756:ASN:HB3	1:D:808:GLY:HA2	1.75	0.66
1:A:567:ARG:HD2	1:A:570:PRO:HA	1.77	0.66
1:B:416:ILE:HD11	1:B:566:THR:HG22	1.77	0.66
1:B:412:GLU:OE1	1:B:529:ARG:HD2	1.94	0.66
1:D:567:ARG:HD2	1:D:570:PRO:HA	1.77	0.66
1:C:412:GLU:OE1	1:C:529:ARG:HD2	1.95	0.66
1:A:65:LEU:HD11	1:A:307:ILE:HG13	1.77	0.66
1:A:49:LEU:HD12	1:A:52:LEU:HD11	1.77	0.65
1:A:235:ILE:O	1:A:239:MET:HG2	1.96	0.65
1:C:979:GLY:O	1:C:983:ILE:HG12	1.96	0.65
1:D:708:ALA:HB3	1:D:709:PRO:HD3	1.78	0.65
1:A:413:LEU:CD2	1:A:564:LEU:HD12	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:819:ARG:HG2	1:A:820:PRO:HD2	1.76	0.65
1:C:412:GLU:OE2	1:C:566:THR:HG21	1.96	0.65
1:D:65:LEU:HD11	1:D:307:ILE:HG13	1.78	0.65
1:A:756:ASN:HB3	1:A:808:GLY:HA2	1.77	0.65
1:D:49:LEU:HD12	1:D:52:LEU:HD11	1.77	0.65
1:D:126:MET:HG3	1:D:139:ARG:NH1	2.12	0.65
1:D:235:ILE:O	1:D:239:MET:HG2	1.97	0.65
1:D:8:SER:OG	1:D:11:GLU:HG3	1.97	0.65
1:B:950:VAL:HG12	1:B:952:PRO:HD2	1.78	0.65
1:D:788:ILE:HG12	1:D:791:GLN:NE2	2.12	0.65
1:A:788:ILE:HG12	1:A:791:GLN:NE2	2.12	0.64
1:C:950:VAL:HG12	1:C:952:PRO:HD2	1.79	0.64
1:C:65:LEU:HD23	1:C:98:LEU:HD11	1.79	0.64
1:C:416:ILE:HD11	1:C:566:THR:HG22	1.79	0.64
1:A:412:GLU:OE2	1:A:566:THR:HG21	1.97	0.64
1:B:1:MET:HE2	1:B:7:LYS:CE	2.27	0.64
1:A:126:MET:HG3	1:A:139:ARG:NH1	2.13	0.64
1:B:41:LEU:HB2	1:B:123:GLU:OE1	1.98	0.64
1:A:708:ALA:HB3	1:A:709:PRO:HD3	1.79	0.64
1:B:384:ILE:HD12	1:B:395:VAL:HG22	1.80	0.64
1:B:718:ILE:HD13	1:B:743:ILE:HD12	1.80	0.64
1:B:979:GLY:O	1:B:983:ILE:HG12	1.98	0.63
1:C:1:MET:HE2	1:C:7:LYS:CE	2.27	0.63
1:C:384:ILE:HD12	1:C:395:VAL:HG22	1.80	0.63
1:D:174:ARG:CG	1:D:216:ALA:HB3	2.29	0.63
1:D:819:ARG:HG2	1:D:820:PRO:HD2	1.78	0.63
1:B:19:SER:HB3	1:B:22:THR:HG23	1.80	0.63
1:B:65:LEU:HD23	1:B:98:LEU:HD11	1.81	0.63
1:B:412:GLU:OE2	1:B:566:THR:HG21	1.98	0.63
1:D:963:ASP:H	1:D:966:GLN:HG3	1.63	0.62
1:C:342:LEU:HD22	1:C:747:VAL:HG22	1.82	0.62
1:C:988:ALA:HA	1:C:992:LEU:HD12	1.80	0.62
1:A:894:PRO:HB2	1:A:960:LYS:HB2	1.81	0.62
1:B:119:LEU:HD22	1:B:239:MET:CE	2.29	0.62
1:B:988:ALA:HA	1:B:992:LEU:HD12	1.80	0.62
1:D:342:LEU:HD22	1:D:747:VAL:HG22	1.80	0.62
1:D:894:PRO:HB2	1:D:960:LYS:HB2	1.82	0.62
1:A:963:ASP:H	1:A:966:GLN:HG3	1.63	0.62
1:A:553:GLY:C	1:A:554:THR:HG23	2.25	0.62
1:C:1:MET:HE2	1:C:7:LYS:CD	2.29	0.62
1:C:367:PHE:CE2	1:C:379:LEU:HD13	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:MET:HG2	1:B:749:GLU:HG2	1.81	0.62
1:B:367:PHE:CE2	1:B:379:LEU:HD13	2.35	0.62
1:C:19:SER:HB3	1:C:22:THR:HG23	1.81	0.62
1:A:802:LEU:HB2	1:A:803:PRO:HD3	1.81	0.61
1:C:933:LEU:O	1:C:936:SER:HB3	2.00	0.61
1:A:174:ARG:CG	1:A:216:ALA:HB3	2.30	0.61
1:C:119:LEU:HD22	1:C:239:MET:CE	2.29	0.61
1:C:326:MET:HG2	1:C:749:GLU:HG2	1.81	0.61
1:B:933:LEU:O	1:B:936:SER:HB3	2.00	0.61
1:B:986:PHE:HA	1:B:989:ARG:HE	1.65	0.61
1:B:342:LEU:HD12	1:B:733:MET:CE	2.28	0.61
1:A:8:SER:OG	1:A:11:GLU:HG3	2.01	0.61
1:D:802:LEU:HB2	1:D:803:PRO:HD3	1.82	0.61
1:B:679:VAL:HG13	1:B:683:HIS:HB2	1.83	0.61
1:C:41:LEU:HB2	1:C:123:GLU:OE1	2.01	0.61
1:B:1:MET:HE2	1:B:7:LYS:CD	2.30	0.61
1:B:449:VAL:CG2	1:B:472:ASN:ND2	2.64	0.61
1:C:810:ASN:HA	1:C:930:ASN:HD22	1.66	0.60
1:C:986:PHE:HA	1:C:989:ARG:HE	1.65	0.60
1:A:983:ILE:O	1:A:987:ILE:HG13	2.01	0.60
1:D:198:ARG:HH22	1:D:660:ASP:HA	1.64	0.60
1:D:983:ILE:O	1:D:987:ILE:HG13	2.01	0.60
1:C:272:TRP:HA	1:C:295:TYR:HE2	1.67	0.60
1:B:155:VAL:HA	1:B:214:ILE:HG22	1.83	0.60
1:B:691:LEU:HB3	1:B:698:THR:HG21	1.83	0.60
1:A:270:ALA:O	1:A:274:ILE:HG13	2.02	0.60
1:B:332:ILE:N	1:B:332:ILE:HD12	2.17	0.60
1:B:810:ASN:HA	1:B:930:ASN:HD22	1.66	0.60
1:C:975:LEU:N	1:C:976:PRO:HD2	2.15	0.60
1:A:198:ARG:HH22	1:A:660:ASP:HA	1.65	0.60
1:B:272:TRP:HA	1:B:295:TYR:HE2	1.67	0.60
1:C:449:VAL:CG2	1:C:472:ASN:ND2	2.65	0.60
1:B:802:LEU:HB2	1:B:803:PRO:HD3	1.83	0.60
1:B:951:ASP:HB3	1:B:952:PRO:HD3	1.84	0.60
1:B:975:LEU:N	1:B:976:PRO:HD2	2.15	0.60
1:C:951:ASP:HB3	1:C:952:PRO:HD3	1.84	0.59
1:C:802:LEU:HB2	1:C:803:PRO:HD3	1.83	0.59
1:D:270:ALA:O	1:D:274:ILE:HG13	2.02	0.59
1:A:416:ILE:HD11	1:A:566:THR:HG22	1.83	0.59
1:B:55:GLU:HA	1:B:58:GLU:HG3	1.84	0.59
1:B:342:LEU:HD22	1:B:747:VAL:HG22	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:ILE:HD12	1:C:332:ILE:N	2.17	0.59
1:D:953:LEU:HB2	1:D:954:PRO:HD3	1.85	0.59
1:D:963:ASP:H	1:D:966:GLN:CG	2.16	0.59
1:A:865:VAL:HG11	1:A:869:GLN:HB2	1.83	0.59
1:A:953:LEU:HB2	1:A:954:PRO:HD3	1.85	0.59
1:C:55:GLU:HA	1:C:58:GLU:HG3	1.85	0.59
1:D:865:VAL:HG11	1:D:869:GLN:HB2	1.83	0.59
1:A:342:LEU:HD22	1:A:747:VAL:HG22	1.83	0.59
1:B:879:ASP:O	1:B:882:HIS:HB2	2.02	0.59
1:D:691:LEU:HB3	1:D:698:THR:HG21	1.83	0.59
1:C:718:ILE:HD13	1:C:743:ILE:HD12	1.85	0.58
1:A:963:ASP:H	1:A:966:GLN:CG	2.17	0.58
1:C:342:LEU:HD12	1:C:733:MET:CE	2.31	0.58
1:A:829:ILE:HD12	1:A:837:TYR:HD1	1.68	0.58
1:C:879:ASP:O	1:C:882:HIS:HB2	2.03	0.58
1:D:979:GLY:O	1:D:983:ILE:HG12	2.04	0.58
1:B:323:THR:HA	1:B:326:MET:HE3	1.84	0.58
1:B:203:ASP:OD1	1:B:678:ARG:NH1	2.36	0.58
1:B:326:MET:HE1	1:B:339:VAL:CG2	2.33	0.58
1:C:491:ARG:HD2	1:C:588:GLU:OE2	2.02	0.58
1:D:416:ILE:HD11	1:D:566:THR:HG22	1.85	0.58
1:B:855:TRP:HA	1:B:859:ALA:HB2	1.86	0.58
1:C:323:THR:HA	1:C:326:MET:HE3	1.85	0.58
1:C:679:VAL:HG13	1:C:683:HIS:HB2	1.86	0.58
1:C:855:TRP:HA	1:C:859:ALA:HB2	1.86	0.58
1:D:829:ILE:HD12	1:D:837:TYR:HD1	1.69	0.58
1:C:691:LEU:HB3	1:C:698:THR:HG21	1.85	0.57
1:A:969:MET:HE3	1:A:969:MET:O	2.04	0.57
1:A:979:GLY:O	1:A:983:ILE:HG12	2.05	0.57
1:B:491:ARG:HD2	1:B:588:GLU:OE2	2.03	0.57
1:C:964:LEU:O	1:C:968:LEU:HG	2.04	0.57
1:D:969:MET:O	1:D:969:MET:HE3	2.04	0.57
1:C:155:VAL:HA	1:C:214:ILE:HG22	1.85	0.57
1:A:691:LEU:HB3	1:A:698:THR:HG21	1.85	0.57
1:D:340:GLU:HG3	1:D:341:THR:N	2.20	0.57
1:B:836:ARG:HH22	1:B:985:LYS:HE2	1.70	0.57
1:B:921:SER:H	1:B:989:ARG:NH1	2.02	0.57
1:C:256:PHE:CZ	1:C:765:ILE:HD11	2.40	0.57
1:C:326:MET:HE1	1:C:339:VAL:CG2	2.34	0.57
1:C:491:ARG:HG2	1:C:493:SER:OG	2.04	0.57
1:C:708:ALA:HB3	1:C:709:PRO:HD3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:844:VAL:HG22	1:D:907:ILE:HG21	1.86	0.57
1:C:656:ARG:HG3	7:C:4516:HOH:O	2.05	0.57
1:A:340:GLU:HG3	1:A:341:THR:N	2.20	0.56
1:A:844:VAL:HG22	1:A:907:ILE:HG21	1.86	0.56
1:B:718:ILE:HG21	1:B:743:ILE:CD1	2.35	0.56
1:B:953:LEU:H	1:B:954:PRO:HD2	1.69	0.56
1:B:964:LEU:O	1:B:968:LEU:HG	2.05	0.56
1:C:921:SER:H	1:C:989:ARG:NH1	2.02	0.56
1:C:953:LEU:H	1:C:954:PRO:HD2	1.69	0.56
1:A:879:ASP:O	1:A:882:HIS:HB2	2.04	0.56
1:B:256:PHE:CZ	1:B:765:ILE:HD11	2.40	0.56
1:B:491:ARG:HG2	1:B:493:SER:OG	2.04	0.56
1:A:90:GLU:HB2	1:A:790:VAL:HG22	1.86	0.56
1:A:491:ARG:HD2	1:A:588:GLU:OE2	2.05	0.56
1:B:572:LYS:H	1:B:572:LYS:HD2	1.71	0.56
1:B:944:HIS:O	1:B:947:ILE:HG22	2.04	0.56
1:C:944:HIS:O	1:C:947:ILE:HG22	2.04	0.56
1:D:879:ASP:O	1:D:882:HIS:HB2	2.04	0.56
1:B:656:ARG:HG3	7:B:3516:HOH:O	2.06	0.56
1:C:791:GLN:O	1:C:795:VAL:HG23	2.05	0.56
1:A:311:LEU:N	1:A:312:PRO:HD2	2.20	0.56
1:B:293:ILE:O	1:B:297:LYS:HB2	2.06	0.56
1:B:458:GLU:CB	1:B:460:ARG:HE	2.18	0.56
1:C:460:ARG:H	1:C:460:ARG:CD	1.96	0.56
1:C:572:LYS:H	1:C:572:LYS:HD2	1.71	0.56
1:D:975:LEU:N	1:D:976:PRO:HD2	2.21	0.56
1:C:458:GLU:CB	1:C:460:ARG:HE	2.18	0.56
1:D:90:GLU:HB2	1:D:790:VAL:HG22	1.87	0.56
1:B:1:MET:HE3	1:B:15:TYR:CG	2.41	0.56
1:B:357:THR:HA	1:B:603:PRO:HA	1.86	0.56
1:C:836:ARG:HH22	1:C:985:LYS:HE2	1.71	0.56
1:A:52:LEU:HD12	1:A:53:VAL:HG23	1.88	0.56
1:A:975:LEU:N	1:A:976:PRO:HD2	2.21	0.56
1:C:293:ILE:O	1:C:297:LYS:HB2	2.06	0.56
1:C:357:THR:HA	1:C:603:PRO:HA	1.87	0.56
1:C:607:VAL:O	1:C:611:ILE:HG12	2.06	0.56
1:D:865:VAL:HG12	1:D:867:TYR:H	1.70	0.56
1:A:247:THR:OG1	1:A:250:GLN:HG3	2.05	0.55
1:A:788:ILE:HG23	1:A:897:MET:HE1	1.87	0.55
1:A:865:VAL:HG12	1:A:867:TYR:H	1.69	0.55
1:C:270:ALA:O	1:C:274:ILE:HG12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:718:ILE:HG21	1:C:743:ILE:CD1	2.36	0.55
1:B:460:ARG:H	1:B:460:ARG:CD	1.97	0.55
1:D:972:LYS:HA	1:D:972:LYS:NZ	2.22	0.55
1:A:788:ILE:HB	1:A:789:PRO:HD2	1.89	0.55
1:D:52:LEU:HD12	1:D:53:VAL:HG23	1.88	0.55
1:A:60:LEU:O	1:A:64:ILE:HG12	2.06	0.55
1:B:895:GLU:N	1:B:896:PRO:HD2	2.22	0.55
1:B:962:LEU:HD23	1:B:962:LEU:N	2.22	0.55
1:D:247:THR:OG1	1:D:250:GLN:HG3	2.05	0.55
1:D:341:THR:HG22	1:D:716:ILE:HD11	1.87	0.55
1:A:972:LYS:HA	1:A:972:LYS:NZ	2.22	0.55
1:D:311:LEU:N	1:D:312:PRO:HD2	2.21	0.55
1:D:788:ILE:HG23	1:D:897:MET:HE1	1.88	0.55
1:A:794:TRP:NE1	1:A:947:ILE:HD11	2.22	0.55
1:D:788:ILE:HB	1:D:789:PRO:HD2	1.89	0.55
1:C:895:GLU:N	1:C:896:PRO:HD2	2.22	0.55
1:C:962:LEU:N	1:C:962:LEU:HD23	2.22	0.55
1:D:60:LEU:O	1:D:64:ILE:HG12	2.07	0.55
1:A:206:ASN:ND2	1:A:207:MET:HG2	2.22	0.54
1:B:270:ALA:O	1:B:274:ILE:HG12	2.07	0.54
1:B:791:GLN:O	1:B:795:VAL:HG23	2.06	0.54
1:D:326:MET:HE1	1:D:339:VAL:CG1	2.37	0.54
1:D:793:LEU:O	1:D:797:LEU:HB2	2.07	0.54
1:B:607:VAL:O	1:B:611:ILE:HG12	2.07	0.54
1:C:336:LEU:HB2	1:C:337:PRO:HD3	1.89	0.54
1:A:419:LEU:O	1:A:481:LYS:HE2	2.07	0.54
1:A:774:CYS:O	1:A:778:THR:HG22	2.06	0.54
1:A:793:LEU:O	1:A:797:LEU:HB2	2.08	0.54
1:A:966:GLN:HE21	1:A:966:GLN:HA	1.73	0.54
1:B:104:VAL:HG12	1:B:108:GLN:HE21	1.72	0.54
1:B:567:ARG:CD	1:B:570:PRO:HA	2.37	0.54
1:C:757:MET:HA	1:C:760:PHE:CE2	2.42	0.54
1:A:326:MET:HE1	1:A:339:VAL:CG1	2.37	0.54
1:B:336:LEU:HB2	1:B:337:PRO:HD3	1.89	0.54
1:D:794:TRP:NE1	1:D:947:ILE:HD11	2.23	0.54
1:B:757:MET:HA	1:B:760:PHE:CE2	2.42	0.54
1:C:104:VAL:HG12	1:C:108:GLN:HE21	1.72	0.54
1:A:93:VAL:O	1:A:97:ILE:HG12	2.07	0.54
1:C:914:ASN:HD22	1:C:922:LEU:HD11	1.72	0.54
1:D:966:GLN:HE21	1:D:966:GLN:HA	1.73	0.54
1:D:987:ILE:O	1:D:991:TYR:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:LEU:HG	1:B:564:LEU:HD12	1.90	0.54
1:C:458:GLU:HB3	1:C:460:ARG:HH21	1.73	0.54
1:D:93:VAL:O	1:D:97:ILE:HG12	2.07	0.54
1:D:353:THR:HA	1:D:357:THR:OG1	2.07	0.54
1:D:491:ARG:HD2	1:D:588:GLU:OE2	2.08	0.54
1:B:795:VAL:HG12	1:B:800:ASP:OD2	2.08	0.54
1:B:914:ASN:HD22	1:B:922:LEU:HD11	1.73	0.54
1:A:265:SER:O	1:A:269:VAL:HG23	2.08	0.53
1:A:557:ASP:HB3	1:A:559:LEU:HG	1.90	0.53
1:A:572:LYS:HB2	1:A:575:GLU:HG3	1.89	0.53
1:A:670:CYS:SG	1:A:687:ILE:HG22	2.48	0.53
1:A:987:ILE:O	1:A:991:TYR:HB2	2.09	0.53
1:B:917:SER:OG	1:B:920:GLN:HB2	2.07	0.53
1:C:325:ARG:HH12	1:C:753:ILE:HD11	1.71	0.53
1:C:567:ARG:CD	1:C:570:PRO:HA	2.38	0.53
1:D:265:SER:O	1:D:269:VAL:HG23	2.08	0.53
1:B:988:ALA:O	1:B:992:LEU:HB2	2.07	0.53
1:C:203:ASP:OD1	1:C:678:ARG:NH1	2.41	0.53
1:C:879:ASP:HB3	1:C:882:HIS:ND1	2.23	0.53
1:D:419:LEU:O	1:D:481:LYS:HE2	2.08	0.53
1:D:557:ASP:HB3	1:D:559:LEU:HG	1.90	0.53
1:C:1:MET:HE3	1:C:15:TYR:CG	2.44	0.53
1:C:795:VAL:HG12	1:C:800:ASP:OD2	2.09	0.53
1:D:549:ILE:HD11	1:D:596:VAL:HG21	1.90	0.53
1:B:962:LEU:HB2	1:B:966:GLN:CB	2.38	0.53
1:C:413:LEU:HG	1:C:564:LEU:HD12	1.91	0.53
1:C:800:ASP:C	1:C:803:PRO:HD2	2.33	0.53
1:C:988:ALA:O	1:C:992:LEU:HB2	2.08	0.53
1:B:402:ILE:C	1:B:402:ILE:HD12	2.33	0.53
1:B:449:VAL:HG22	1:B:472:ASN:HD21	1.74	0.53
1:C:962:LEU:HB2	1:C:966:GLN:CB	2.38	0.53
1:A:624:ILE:CG2	1:A:684:LYS:HG2	2.38	0.53
1:C:735:LEU:HD21	1:C:743:ILE:CD1	2.38	0.53
1:A:71:ILE:O	1:A:75:LEU:HD13	2.09	0.53
1:A:847:ALA:HA	1:A:973:ILE:HD11	1.90	0.53
1:B:458:GLU:HB3	1:B:460:ARG:HH21	1.74	0.53
1:B:879:ASP:HB3	1:B:882:HIS:ND1	2.24	0.53
1:C:328:LYS:NZ	1:C:328:LYS:HB3	2.24	0.53
1:A:547:SER:O	1:A:551:GLU:HG3	2.09	0.53
1:B:94:ILE:O	1:B:98:LEU:HD13	2.09	0.53
1:B:735:LEU:HD21	1:B:743:ILE:CD1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:774:CYS:O	1:D:778:THR:HG22	2.07	0.53
1:B:325:ARG:HH12	1:B:753:ILE:HD11	1.72	0.52
1:C:94:ILE:O	1:C:98:LEU:HD13	2.09	0.52
1:C:917:SER:OG	1:C:920:GLN:HB2	2.09	0.52
1:D:572:LYS:HB2	1:D:575:GLU:HG3	1.90	0.52
1:A:794:TRP:CE2	1:A:947:ILE:HD11	2.44	0.52
1:C:843:TYR:OH	1:C:976:PRO:HG2	2.09	0.52
1:D:794:TRP:CE2	1:D:947:ILE:HD11	2.44	0.52
1:A:129:VAL:HG12	1:A:151:VAL:HG12	1.91	0.52
1:A:341:THR:HG22	1:A:716:ILE:HD11	1.90	0.52
1:D:175:VAL:CG1	1:D:212:THR:HG21	2.40	0.52
1:D:847:ALA:HA	1:D:973:ILE:HD11	1.90	0.52
1:A:353:THR:HA	1:A:357:THR:OG1	2.08	0.52
1:D:739:ASN:OD1	1:D:741:SER:HB2	2.10	0.52
1:D:962:LEU:HB3	1:D:966:GLN:HB2	1.91	0.52
1:A:1:MET:HE2	1:A:16:PHE:HE1	1.74	0.52
1:A:175:VAL:CG1	1:A:212:THR:HG21	2.39	0.52
1:A:624:ILE:HG21	1:A:684:LYS:HG2	1.92	0.52
1:B:749:GLU:O	1:B:753:ILE:HG12	2.09	0.52
1:B:800:ASP:C	1:B:803:PRO:HD2	2.34	0.52
1:C:449:VAL:HG22	1:C:472:ASN:HD21	1.75	0.52
1:D:670:CYS:SG	1:D:687:ILE:HG22	2.50	0.52
1:D:800:ASP:C	1:D:803:PRO:HD2	2.34	0.52
1:A:89:VAL:O	1:A:93:VAL:HG23	2.09	0.52
1:A:962:LEU:HB3	1:A:966:GLN:HB2	1.91	0.52
1:B:843:TYR:OH	1:B:976:PRO:HG2	2.09	0.52
1:A:326:MET:HG3	1:A:749:GLU:HG2	1.91	0.52
1:D:71:ILE:O	1:D:75:LEU:HD13	2.09	0.52
1:D:212:THR:HG22	1:D:213:ASN:N	2.23	0.52
1:D:547:SER:O	1:D:551:GLU:HG3	2.10	0.52
1:D:972:LYS:HA	1:D:972:LYS:HZ3	1.75	0.52
1:A:739:ASN:OD1	1:A:741:SER:HB2	2.10	0.52
1:B:328:LYS:HB3	1:B:328:LYS:NZ	2.26	0.52
1:D:326:MET:HG3	1:D:749:GLU:HG2	1.92	0.52
1:C:749:GLU:O	1:C:753:ILE:HG12	2.10	0.51
1:C:926:PRO:O	1:C:929:VAL:HG23	2.08	0.51
1:A:541:VAL:O	1:A:545:ILE:HG12	2.10	0.51
1:B:718:ILE:HG21	1:B:743:ILE:HD11	1.90	0.51
1:D:838:MET:HE3	1:D:838:MET:HA	1.92	0.51
1:A:921:SER:H	1:A:989:ARG:HH12	1.58	0.51
1:B:926:PRO:O	1:B:929:VAL:HG23	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:962:LEU:HD23	1:B:962:LEU:H	1.75	0.51
1:C:85:ILE:HD13	1:D:110:ARG:CZ	2.40	0.51
1:B:572:LYS:HD2	1:B:572:LYS:N	2.26	0.51
1:B:739:ASN:OD1	1:B:741:SER:HB2	2.10	0.51
1:C:12:CYS:SG	1:C:164:ARG:HG3	2.51	0.51
1:C:273:LEU:O	1:C:276:ILE:HG13	2.09	0.51
1:D:369:ILE:CD1	1:D:545:ILE:HD11	2.40	0.51
1:D:921:SER:H	1:D:989:ARG:HH12	1.58	0.51
1:A:369:ILE:CD1	1:A:545:ILE:HD11	2.41	0.51
1:A:921:SER:H	1:A:989:ARG:NH1	2.08	0.51
1:A:795:VAL:HA	1:A:799:THR:HB	1.93	0.51
1:B:769:VAL:HG21	6:B:1103:TG1:H332	1.93	0.51
1:D:89:VAL:O	1:D:93:VAL:HG23	2.10	0.51
1:D:129:VAL:HG12	1:D:151:VAL:HG12	1.93	0.51
1:A:800:ASP:C	1:A:803:PRO:HD2	2.35	0.51
1:B:893:ALA:O	1:B:896:PRO:HD2	2.11	0.51
1:D:921:SER:H	1:D:989:ARG:NH1	2.08	0.51
1:A:947:ILE:O	1:A:954:PRO:HG3	2.10	0.51
1:B:12:CYS:SG	1:B:164:ARG:HG3	2.51	0.51
1:B:604:ARG:HB2	1:B:607:VAL:HG23	1.92	0.51
1:D:795:VAL:HA	1:D:799:THR:HB	1.93	0.51
1:C:572:LYS:HD2	1:C:572:LYS:N	2.26	0.51
1:C:589:THR:HG23	7:C:4006:HOH:O	2.11	0.51
1:A:48:SER:O	1:A:52:LEU:HG	2.11	0.51
1:B:950:VAL:O	1:B:954:PRO:HD2	2.10	0.51
1:C:589:THR:CG2	1:C:590:ASP:N	2.74	0.51
1:C:893:ALA:O	1:C:896:PRO:HD2	2.11	0.51
1:D:340:GLU:HG3	1:D:341:THR:H	1.76	0.51
1:D:947:ILE:O	1:D:954:PRO:HG3	2.10	0.51
1:B:332:ILE:HD13	1:B:736:ALA:HB2	1.93	0.50
1:B:520:GLY:O	1:B:524:ARG:HG3	2.11	0.50
1:C:962:LEU:HD23	1:C:962:LEU:H	1.76	0.50
1:D:974:SER:C	1:D:976:PRO:HD2	2.36	0.50
1:A:339:VAL:HG23	1:A:340:GLU:N	2.26	0.50
1:A:549:ILE:HD11	1:A:596:VAL:HG21	1.93	0.50
1:D:757:MET:HA	1:D:760:PHE:CE2	2.47	0.50
1:A:631:THR:HG21	7:A:2517:HOH:O	2.10	0.50
1:A:974:SER:C	1:A:976:PRO:HD2	2.36	0.50
1:B:557:ASP:HB3	1:B:559:LEU:HG	1.93	0.50
1:C:769:VAL:HG21	6:C:1203:TG1:H332	1.94	0.50
1:C:950:VAL:O	1:C:954:PRO:HD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:352:LYS:HE2	7:D:5068:HOH:O	2.11	0.50
1:A:249:LEU:HB3	1:A:340:GLU:OE2	2.12	0.50
1:A:838:MET:HE3	1:A:838:MET:HA	1.93	0.50
1:A:880:HIS:N	1:A:881:PRO:HD2	2.26	0.50
1:B:273:LEU:O	1:B:276:ILE:HG13	2.10	0.50
1:A:25:THR:HA	1:A:132:ALA:HB3	1.93	0.50
1:A:340:GLU:HG3	1:A:341:THR:H	1.77	0.50
1:B:969:MET:HE2	1:B:973:ILE:HD11	1.93	0.50
1:D:100:ALA:O	1:D:103:ILE:HG22	2.11	0.50
1:D:541:VAL:O	1:D:545:ILE:HG12	2.12	0.50
1:A:212:THR:HG22	1:A:213:ASN:N	2.25	0.50
1:A:757:MET:HA	1:A:760:PHE:CE2	2.47	0.50
1:A:895:GLU:OE2	1:A:960:LYS:HD3	2.12	0.50
1:A:903:VAL:O	1:A:907:ILE:HG13	2.10	0.50
1:B:326:MET:CG	1:B:749:GLU:HG2	2.42	0.50
1:B:761:ILE:HG21	1:B:828:LEU:HD13	1.93	0.50
1:D:48:SER:O	1:D:52:LEU:HG	2.12	0.50
1:B:449:VAL:HG21	1:B:472:ASN:CG	2.36	0.50
1:B:708:ALA:HB3	1:B:709:PRO:HD3	1.93	0.50
1:D:339:VAL:HG23	1:D:340:GLU:N	2.26	0.50
1:A:972:LYS:HA	1:A:972:LYS:HZ3	1.77	0.50
1:C:326:MET:CG	1:C:749:GLU:HG2	2.42	0.50
1:D:880:HIS:N	1:D:881:PRO:HD2	2.26	0.50
1:B:85:ILE:HG23	1:B:86:THR:HG23	1.94	0.50
1:C:795:VAL:HA	1:C:799:THR:HB	1.93	0.50
1:D:249:LEU:HB3	1:D:340:GLU:OE2	2.12	0.50
1:D:428:ASN:OD1	1:D:431:LYS:HG3	2.12	0.50
1:D:758:LYS:HE3	1:D:762:ARG:NH2	2.27	0.50
1:A:428:ASN:OD1	1:A:431:LYS:HG3	2.12	0.49
1:B:93:VAL:O	1:B:97:ILE:HG13	2.11	0.49
1:C:311:LEU:N	1:C:312:PRO:HD2	2.26	0.49
1:C:332:ILE:HD13	1:C:736:ALA:HB2	1.94	0.49
1:C:520:GLY:O	1:C:524:ARG:HG3	2.12	0.49
1:C:989:ARG:HA	1:C:994:GLY:HA2	1.93	0.49
1:A:88:PHE:C	1:A:91:PRO:HD2	2.37	0.49
1:A:854:TRP:CE3	1:A:899:MET:HE2	2.46	0.49
1:B:289:ILE:O	1:B:293:ILE:HG13	2.13	0.49
1:B:555:GLY:C	1:B:557:ASP:H	2.20	0.49
1:B:989:ARG:HA	1:B:994:GLY:HA2	1.93	0.49
1:C:557:ASP:HB3	1:C:559:LEU:HG	1.93	0.49
1:D:25:THR:HA	1:D:132:ALA:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:739:ASN:OD1	1:C:741:SER:HB2	2.12	0.49
1:D:311:LEU:O	1:D:314:VAL:HG12	2.13	0.49
1:D:402:ILE:C	1:D:402:ILE:HD12	2.36	0.49
1:A:56:GLN:OE1	1:A:105:GLY:HA3	2.12	0.49
1:A:110:ARG:CZ	1:B:85:ILE:HD13	2.42	0.49
1:A:260:LEU:HD21	1:A:307:ILE:HD13	1.94	0.49
1:C:402:ILE:HD12	1:C:402:ILE:C	2.36	0.49
1:C:463:SER:OG	1:C:465:VAL:HG22	2.12	0.49
1:D:1:MET:HE2	1:D:16:PHE:HE1	1.77	0.49
1:D:895:GLU:OE2	1:D:960:LYS:HD3	2.12	0.49
1:A:895:GLU:N	1:A:896:PRO:HD2	2.27	0.49
1:B:836:ARG:O	1:B:840:ILE:HG12	2.12	0.49
1:C:93:VAL:O	1:C:97:ILE:HG13	2.12	0.49
1:C:353:THR:HA	1:C:357:THR:OG1	2.13	0.49
1:B:880:HIS:N	1:B:881:PRO:HD2	2.27	0.49
1:C:880:HIS:N	1:C:881:PRO:HD2	2.27	0.49
1:C:969:MET:HE2	1:C:973:ILE:HD11	1.94	0.49
1:D:389:TYR:HB3	1:D:425:LEU:HD11	1.95	0.49
1:A:389:TYR:HB3	1:A:425:LEU:HD11	1.95	0.49
1:C:604:ARG:HB2	1:C:607:VAL:HG23	1.94	0.49
1:D:88:PHE:C	1:D:91:PRO:HD2	2.37	0.49
1:A:402:ILE:C	1:A:402:ILE:HD12	2.37	0.49
1:A:758:LYS:HE3	1:A:762:ARG:NH2	2.28	0.49
1:B:403:ARG:HG3	1:B:403:ARG:HH11	1.77	0.49
1:B:795:VAL:HA	1:B:799:THR:HB	1.94	0.49
1:C:85:ILE:HG23	1:C:86:THR:HG23	1.95	0.49
1:C:555:GLY:C	1:C:557:ASP:H	2.21	0.49
1:C:769:VAL:HA	6:C:1203:TG1:H231	1.95	0.49
1:D:125:GLU:HG3	1:D:126:MET:N	2.27	0.49
1:D:260:LEU:HD21	1:D:307:ILE:HD13	1.95	0.49
1:A:100:ALA:O	1:A:103:ILE:HG22	2.13	0.49
1:B:534:ARG:HH21	1:B:568:ASP:HB2	1.77	0.49
1:B:865:VAL:HG11	1:B:869:GLN:CB	2.41	0.49
1:C:781:LEU:HD23	1:C:783:LEU:CD1	2.43	0.49
1:D:854:TRP:CE3	1:D:899:MET:HE2	2.47	0.49
1:D:903:VAL:O	1:D:907:ILE:HG13	2.11	0.49
1:B:134:ARG:HG2	1:B:138:GLN:NE2	2.27	0.49
1:C:85:ILE:HD13	1:D:110:ARG:NH1	2.28	0.49
1:A:65:LEU:CD1	1:A:307:ILE:HG13	2.41	0.48
1:A:311:LEU:O	1:A:314:VAL:HG12	2.13	0.48
1:B:383:SER:O	1:B:384:ILE:HD13	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:769:VAL:HA	6:B:1103:TG1:H231	1.95	0.48
1:B:974:SER:C	1:B:976:PRO:HD2	2.37	0.48
1:C:761:ILE:HG21	1:C:828:LEU:HD13	1.94	0.48
1:D:56:GLN:OE1	1:D:105:GLY:HA3	2.12	0.48
1:D:560:ARG:HG2	1:D:560:ARG:HH11	1.76	0.48
1:A:553:GLY:C	1:A:554:THR:CG2	2.85	0.48
1:B:311:LEU:N	1:B:312:PRO:HD2	2.27	0.48
1:C:134:ARG:HG2	1:C:138:GLN:NE2	2.27	0.48
1:C:361:MET:HB3	1:C:444:ALA:HB2	1.94	0.48
1:D:203:ASP:OD1	1:D:678:ARG:NH1	2.46	0.48
1:D:553:GLY:O	1:D:554:THR:HG23	2.12	0.48
1:D:895:GLU:N	1:D:896:PRO:HD2	2.27	0.48
1:A:486:GLU:O	1:A:491:ARG:NH2	2.40	0.48
1:B:50:TRP:CD1	1:B:54:ILE:HD11	2.48	0.48
1:B:463:SER:OG	1:B:465:VAL:HG22	2.13	0.48
1:B:777:LEU:O	1:B:781:LEU:HB2	2.12	0.48
1:C:289:ILE:O	1:C:293:ILE:HG13	2.14	0.48
1:C:777:LEU:O	1:C:781:LEU:HB2	2.12	0.48
1:C:865:VAL:HG11	1:C:869:GLN:CB	2.41	0.48
1:B:606:GLU:HG3	1:B:739:ASN:OD1	2.14	0.48
1:C:383:SER:O	1:C:384:ILE:HD13	2.13	0.48
1:C:718:ILE:HG21	1:C:743:ILE:HD11	1.94	0.48
1:A:125:GLU:HG3	1:A:126:MET:N	2.27	0.48
1:A:893:ALA:HB1	1:A:895:GLU:OE1	2.13	0.48
1:B:40:GLU:CD	1:B:143:ARG:HE	2.21	0.48
1:B:452:MET:O	1:B:453:ASN:C	2.57	0.48
1:C:458:GLU:CB	1:C:460:ARG:HH21	2.26	0.48
1:C:494:MET:HE1	5:C:1202:ADP:HN62	1.78	0.48
1:C:899:MET:O	1:C:903:VAL:HG23	2.13	0.48
1:D:65:LEU:CD1	1:D:307:ILE:HG13	2.41	0.48
1:D:803:PRO:HG2	1:D:909:MET:HE1	1.95	0.48
1:A:560:ARG:HG2	1:A:560:ARG:HH11	1.77	0.48
1:B:449:VAL:HG22	1:B:472:ASN:ND2	2.29	0.48
1:C:836:ARG:O	1:C:840:ILE:HG12	2.14	0.48
1:C:974:SER:C	1:C:976:PRO:HD2	2.38	0.48
1:D:126:MET:HG3	1:D:139:ARG:HH12	1.77	0.48
1:A:769:VAL:O	1:A:773:VAL:HG23	2.14	0.48
1:A:917:SER:OG	1:A:920:GLN:HB2	2.14	0.48
1:B:600:LEU:O	1:B:602:PRO:HD3	2.14	0.48
1:C:50:TRP:CD1	1:C:54:ILE:HD11	2.49	0.48
1:C:119:LEU:HD22	1:C:239:MET:HE1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:486:GLU:O	1:C:491:ARG:NH2	2.41	0.48
1:A:51:GLU:O	1:A:55:GLU:HG3	2.13	0.48
1:A:203:ASP:OD1	1:A:678:ARG:NH1	2.46	0.48
1:C:403:ARG:HG3	1:C:403:ARG:HH11	1.78	0.48
1:B:589:THR:CG2	1:B:590:ASP:N	2.77	0.48
1:D:760:PHE:C	1:D:760:PHE:CD1	2.92	0.48
1:A:886:LEU:N	1:A:886:LEU:HD23	2.29	0.47
1:B:119:LEU:HD22	1:B:239:MET:HE1	1.96	0.47
1:D:917:SER:OG	1:D:920:GLN:HB2	2.14	0.47
1:A:52:LEU:HD12	1:A:53:VAL:N	2.29	0.47
1:B:190:HIS:O	1:B:206:ASN:HA	2.14	0.47
1:B:353:THR:HA	1:B:357:THR:OG1	2.15	0.47
1:B:758:LYS:HG3	1:B:828:LEU:HD22	1.95	0.47
1:C:914:ASN:ND2	1:C:922:LEU:HD11	2.30	0.47
1:D:52:LEU:HD12	1:D:53:VAL:N	2.29	0.47
1:D:606:GLU:CD	1:D:606:GLU:H	2.22	0.47
1:D:893:ALA:HB1	1:D:895:GLU:OE1	2.13	0.47
1:A:59:ASP:O	1:A:62:VAL:HG22	2.14	0.47
1:A:239:MET:CE	1:A:708:ALA:HB1	2.44	0.47
1:A:259:GLN:O	1:A:263:VAL:HG23	2.14	0.47
1:A:342:LEU:HD12	1:A:733:MET:HE1	1.96	0.47
1:B:494:MET:CE	5:B:1102:ADP:HN62	2.27	0.47
1:B:899:MET:O	1:B:903:VAL:HG23	2.14	0.47
1:B:914:ASN:ND2	1:B:922:LEU:HD11	2.30	0.47
1:D:624:ILE:CG2	1:D:684:LYS:HG2	2.44	0.47
1:A:452:MET:O	1:A:453:ASN:C	2.58	0.47
1:A:678:ARG:HB3	7:A:2069:HOH:O	2.13	0.47
1:B:486:GLU:O	1:B:491:ARG:NH2	2.41	0.47
1:B:494:MET:HE1	5:B:1102:ADP:HN62	1.79	0.47
1:B:547:SER:O	1:B:551:GLU:HG3	2.15	0.47
1:B:458:GLU:CB	1:B:460:ARG:HH21	2.27	0.47
1:B:781:LEU:HD23	1:B:783:LEU:CD1	2.44	0.47
1:B:803:PRO:HG2	1:B:909:MET:HE1	1.96	0.47
1:C:449:VAL:HG22	1:C:472:ASN:ND2	2.29	0.47
1:D:51:GLU:O	1:D:55:GLU:HG3	2.13	0.47
1:D:607:VAL:O	1:D:611:ILE:HG12	2.15	0.47
1:D:836:ARG:NH2	1:D:985:LYS:HE2	2.29	0.47
1:A:799:THR:HG21	1:A:905:VAL:HG22	1.96	0.47
1:A:926:PRO:O	1:A:929:VAL:HG23	2.15	0.47
1:B:242:THR:HB	1:B:243:GLU:H	1.54	0.47
1:B:361:MET:HB3	1:B:444:ALA:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:ILE:HD13	1:C:797:LEU:HD11	1.97	0.47
1:D:259:GLN:O	1:D:263:VAL:HG23	2.15	0.47
1:A:100:ALA:O	1:A:104:VAL:HG23	2.14	0.47
1:A:607:VAL:O	1:A:611:ILE:HG12	2.15	0.47
1:B:97:ILE:HD13	1:B:797:LEU:HD11	1.97	0.47
1:C:40:GLU:CD	1:C:143:ARG:HE	2.22	0.47
1:C:310:GLY:O	1:C:314:VAL:HG23	2.15	0.47
1:D:687:ILE:O	1:D:691:LEU:HD22	2.14	0.47
1:D:769:VAL:O	1:D:773:VAL:HG23	2.15	0.47
1:D:933:LEU:O	1:D:936:SER:HB3	2.15	0.47
1:A:962:LEU:HB3	1:A:966:GLN:CB	2.44	0.47
1:B:50:TRP:O	1:B:54:ILE:HG13	2.15	0.47
1:B:811:PRO:HG3	1:B:929:VAL:CG1	2.45	0.47
1:C:758:LYS:HG3	1:C:828:LEU:HD22	1.96	0.47
1:D:100:ALA:O	1:D:104:VAL:HG23	2.15	0.47
1:D:679:VAL:HG13	1:D:683:HIS:CB	2.33	0.47
1:B:589:THR:HG23	7:B:3006:HOH:O	2.15	0.47
1:B:836:ARG:NH2	1:B:985:LYS:HE2	2.28	0.47
1:C:449:VAL:HG21	1:C:472:ASN:CG	2.40	0.47
1:C:494:MET:CE	5:C:1202:ADP:HN62	2.27	0.47
1:D:486:GLU:O	1:D:491:ARG:NH2	2.41	0.47
1:D:631:THR:HG21	7:D:5517:HOH:O	2.13	0.47
1:D:962:LEU:HB3	1:D:966:GLN:CB	2.44	0.47
1:A:760:PHE:CD1	1:A:760:PHE:C	2.93	0.47
1:B:501:ALA:C	1:B:503:SER:H	2.23	0.47
1:B:667:ARG:HG2	1:B:694:TYR:CE1	2.49	0.47
1:C:534:ARG:HH21	1:C:568:ASP:HB2	1.79	0.47
1:C:781:LEU:HD23	1:C:783:LEU:HD11	1.96	0.47
1:D:452:MET:O	1:D:453:ASN:C	2.58	0.47
1:D:624:ILE:HG21	1:D:684:LYS:HG2	1.97	0.47
1:D:799:THR:HG21	1:D:905:VAL:HG22	1.97	0.47
1:A:553:GLY:O	1:A:554:THR:HG22	2.14	0.46
1:A:606:GLU:H	1:A:606:GLU:CD	2.23	0.46
1:A:803:PRO:HG2	1:A:909:MET:HE1	1.96	0.46
1:A:836:ARG:NH2	1:A:985:LYS:HE2	2.29	0.46
1:B:865:VAL:HG12	1:B:867:TYR:H	1.81	0.46
1:C:803:PRO:HG2	1:C:909:MET:HE1	1.97	0.46
1:D:59:ASP:O	1:D:62:VAL:HG22	2.15	0.46
1:D:239:MET:CE	1:D:708:ALA:HB1	2.45	0.46
1:A:933:LEU:O	1:A:936:SER:HB3	2.16	0.46
1:B:305:ALA:HB2	1:B:792:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:966:GLN:O	1:B:969:MET:HB3	2.14	0.46
1:C:541:VAL:O	1:C:545:ILE:HG12	2.16	0.46
1:C:683:HIS:O	1:C:687:ILE:HG13	2.15	0.46
1:C:811:PRO:HG3	1:C:929:VAL:CG1	2.46	0.46
1:C:865:VAL:HG12	1:C:867:TYR:H	1.81	0.46
1:C:947:ILE:HD11	1:C:957:PHE:CD2	2.50	0.46
1:A:126:MET:HG3	1:A:139:ARG:HH12	1.79	0.46
1:A:370:ASP:HB3	1:A:378:SER:OG	2.15	0.46
1:C:452:MET:O	1:C:453:ASN:C	2.58	0.46
1:D:315:ILE:HG23	1:D:757:MET:HE3	1.97	0.46
1:D:836:ARG:O	1:D:840:ILE:HG12	2.15	0.46
1:A:200:VAL:CG1	1:A:201:ASN:N	2.78	0.46
1:B:96:LEU:HD23	1:B:96:LEU:O	2.15	0.46
1:B:865:VAL:CG1	1:B:869:GLN:HB2	2.41	0.46
1:C:606:GLU:HG3	1:C:739:ASN:OD1	2.16	0.46
1:C:926:PRO:HA	1:C:927:PRO:HD3	1.86	0.46
1:D:428:ASN:CG	1:D:431:LYS:HG3	2.41	0.46
1:D:865:VAL:C	1:D:867:TYR:H	2.24	0.46
1:A:428:ASN:CG	1:A:431:LYS:HG3	2.41	0.46
1:A:701:THR:HA	1:A:718:ILE:O	2.15	0.46
1:A:829:ILE:HD12	1:A:837:TYR:CD1	2.50	0.46
1:A:836:ARG:O	1:A:840:ILE:HG12	2.15	0.46
1:B:344:CYS:SG	1:B:697:ILE:HG13	2.55	0.46
1:B:926:PRO:HA	1:B:927:PRO:HD3	1.86	0.46
1:C:667:ARG:HG2	1:C:694:TYR:CE1	2.50	0.46
1:C:966:GLN:O	1:C:969:MET:HB3	2.15	0.46
1:D:886:LEU:N	1:D:886:LEU:HD23	2.31	0.46
1:A:315:ILE:HG23	1:A:757:MET:HE3	1.97	0.46
1:A:352:LYS:HE2	7:A:2068:HOH:O	2.16	0.46
1:B:52:LEU:O	1:B:56:GLN:HG2	2.16	0.46
1:B:71:ILE:O	1:B:75:LEU:HD13	2.16	0.46
1:B:947:ILE:HD11	1:B:957:PHE:CD2	2.51	0.46
1:C:501:ALA:C	1:C:503:SER:H	2.23	0.46
1:C:965:THR:HA	1:C:968:LEU:HD12	1.97	0.46
1:A:110:ARG:NH1	1:B:85:ILE:HD13	2.31	0.46
1:A:495:SER:HB3	1:A:514:VAL:HG22	1.97	0.46
1:B:337:PRO:O	1:B:340:GLU:HG3	2.16	0.46
1:B:450:GLU:OE1	1:B:467:ARG:NH2	2.47	0.46
1:C:52:LEU:O	1:C:56:GLN:HG2	2.16	0.46
1:C:71:ILE:O	1:C:75:LEU:HD13	2.16	0.46
1:C:547:SER:O	1:C:551:GLU:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:865:VAL:C	1:A:867:TYR:H	2.24	0.46
1:B:310:GLY:O	1:B:314:VAL:HG23	2.16	0.46
1:B:810:ASN:HA	1:B:930:ASN:ND2	2.29	0.46
1:B:893:ALA:HB1	1:B:895:GLU:OE1	2.16	0.46
1:C:574:GLU:CD	1:C:574:GLU:H	2.24	0.46
1:C:810:ASN:HA	1:C:930:ASN:ND2	2.29	0.46
1:A:289:ILE:O	1:A:290:ARG:HD2	2.16	0.46
1:B:574:GLU:CD	1:B:574:GLU:H	2.23	0.46
1:C:332:ILE:CD1	1:C:736:ALA:HB2	2.45	0.46
1:C:865:VAL:CG1	1:C:869:GLN:HB2	2.42	0.46
1:C:337:PRO:O	1:C:340:GLU:HG3	2.16	0.46
1:D:950:VAL:HB	1:D:953:LEU:HD12	1.97	0.46
1:D:971:LEU:O	1:D:975:LEU:HB2	2.17	0.46
1:A:950:VAL:C	1:A:952:PRO:HD2	2.41	0.45
1:B:541:VAL:O	1:B:545:ILE:HG12	2.16	0.45
1:C:50:TRP:O	1:C:54:ILE:HG13	2.17	0.45
1:C:600:LEU:O	1:C:602:PRO:HD3	2.16	0.45
1:C:757:MET:O	1:C:761:ILE:HG13	2.16	0.45
1:C:967:TRP:O	1:C:971:LEU:HG	2.17	0.45
1:D:289:ILE:O	1:D:290:ARG:HD2	2.16	0.45
1:D:518:PRO:HB3	1:D:549:ILE:HD13	1.98	0.45
1:D:862:GLY:N	1:D:863:PRO:HD3	2.30	0.45
1:D:919:ASN:O	1:D:989:ARG:HD3	2.16	0.45
1:D:950:VAL:C	1:D:952:PRO:HD2	2.41	0.45
1:A:200:VAL:HG13	1:A:680:GLU:CG	2.45	0.45
1:A:919:ASN:O	1:A:989:ARG:HD3	2.15	0.45
1:B:965:THR:HA	1:B:968:LEU:HD12	1.97	0.45
1:C:443:THR:O	1:C:447:THR:HG23	2.16	0.45
1:D:83:GLU:C	1:D:85:ILE:H	2.24	0.45
1:D:495:SER:HB3	1:D:514:VAL:HG22	1.97	0.45
1:A:200:VAL:HG12	1:A:202:GLN:HE21	1.81	0.45
1:A:971:LEU:O	1:A:975:LEU:HB2	2.17	0.45
1:B:851:ALA:HB1	1:B:899:MET:HE3	1.97	0.45
1:C:97:ILE:CD1	1:C:797:LEU:HD11	2.46	0.45
1:D:59:ASP:HB3	1:D:62:VAL:HG22	1.98	0.45
1:D:913:LEU:HD22	1:D:927:PRO:HB3	1.97	0.45
1:A:352:LYS:HA	1:A:356:LEU:HB2	1.98	0.45
1:B:768:ASN:O	1:B:772:VAL:HG23	2.16	0.45
1:C:96:LEU:O	1:C:96:LEU:HD23	2.16	0.45
1:C:116:ILE:HD12	1:C:236:ARG:HG2	1.99	0.45
1:C:836:ARG:NH2	1:C:985:LYS:HE2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:326:MET:HE1	1:D:339:VAL:HG12	1.99	0.45
1:D:342:LEU:HD12	1:D:733:MET:HE1	1.98	0.45
1:D:926:PRO:O	1:D:929:VAL:HG23	2.17	0.45
1:A:326:MET:HE1	1:A:339:VAL:HG12	1.99	0.45
1:A:796:ASN:HA	7:A:2131:HOH:O	2.15	0.45
1:A:899:MET:O	1:A:903:VAL:HG23	2.16	0.45
1:B:683:HIS:O	1:B:687:ILE:HG13	2.16	0.45
1:B:886:LEU:N	1:B:886:LEU:HD23	2.31	0.45
1:C:320:ALA:O	1:C:324:ARG:HG3	2.15	0.45
1:C:811:PRO:HG3	1:C:929:VAL:HG12	1.99	0.45
1:C:851:ALA:HB1	1:C:899:MET:HE3	1.97	0.45
1:D:77:TRP:C	1:D:79:GLU:H	2.25	0.45
1:D:701:THR:HA	1:D:718:ILE:O	2.15	0.45
1:D:893:ALA:O	1:D:896:PRO:HD2	2.17	0.45
1:A:269:VAL:O	1:A:273:LEU:HG	2.17	0.45
1:A:862:GLY:N	1:A:863:PRO:HD3	2.31	0.45
1:B:116:ILE:HD12	1:B:236:ARG:HG2	1.99	0.45
1:B:781:LEU:HD23	1:B:783:LEU:HD11	1.97	0.45
1:B:811:PRO:HG3	1:B:929:VAL:HG12	1.99	0.45
1:B:967:TRP:O	1:B:971:LEU:HG	2.17	0.45
1:C:893:ALA:HB1	1:C:895:GLU:OE1	2.17	0.45
1:D:829:ILE:HD12	1:D:837:TYR:CD1	2.51	0.45
1:A:83:GLU:C	1:A:85:ILE:H	2.25	0.45
1:A:367:PHE:C	1:A:367:PHE:CD2	2.95	0.45
1:B:329:LYS:O	1:B:330:ASN:HB2	2.16	0.45
1:B:449:VAL:CG2	1:B:472:ASN:CG	2.89	0.45
1:C:305:ALA:HB2	1:C:792:LEU:HD13	1.98	0.45
1:C:971:LEU:HA	1:C:975:LEU:HD23	1.99	0.45
1:D:914:ASN:HB3	1:D:981:ASP:OD2	2.17	0.45
1:C:423:SER:HB3	1:C:437:VAL:O	2.17	0.45
1:D:228:VAL:O	1:D:228:VAL:HG12	2.16	0.45
1:D:768:ASN:O	1:D:772:VAL:HG23	2.16	0.45
1:D:950:VAL:HG12	1:D:952:PRO:HG2	1.99	0.45
1:A:77:TRP:C	1:A:79:GLU:H	2.25	0.45
1:A:360:GLN:HG2	1:A:389:TYR:CE2	2.52	0.45
1:A:893:ALA:O	1:A:896:PRO:HD2	2.17	0.45
1:A:950:VAL:HG12	1:A:952:PRO:HG2	1.99	0.45
1:B:838:MET:HE3	1:B:838:MET:HA	1.99	0.45
1:B:971:LEU:HA	1:B:975:LEU:HD23	1.99	0.45
1:C:190:HIS:O	1:C:206:ASN:HA	2.17	0.45
1:C:768:ASN:O	1:C:772:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:VAL:HG22	1:D:217:GLY:H	1.81	0.45
1:D:367:PHE:C	1:D:367:PHE:CD2	2.95	0.45
1:D:899:MET:O	1:D:903:VAL:HG23	2.17	0.45
1:D:943:LEU:O	1:D:947:ILE:HG13	2.16	0.45
1:D:954:PRO:HB3	1:D:959:LEU:O	2.17	0.45
1:A:518:PRO:HB3	1:A:549:ILE:HD13	1.99	0.45
1:A:950:VAL:HB	1:A:953:LEU:HD12	1.98	0.45
1:B:256:PHE:CE1	1:B:765:ILE:HD11	2.52	0.45
1:B:767:SER:O	1:B:771:GLU:HG3	2.16	0.45
1:C:59:ASP:OD2	1:C:62:VAL:HG23	2.16	0.45
1:C:352:LYS:HE2	7:C:4068:HOH:O	2.16	0.45
1:C:760:PHE:CD1	1:C:760:PHE:C	2.95	0.45
1:C:835:PHE:O	1:C:838:MET:HB3	2.17	0.45
1:D:65:LEU:HD11	1:D:307:ILE:HG21	1.99	0.45
1:A:59:ASP:HB3	1:A:62:VAL:HG22	1.99	0.44
1:A:913:LEU:HD22	1:A:927:PRO:HB3	1.98	0.44
1:A:914:ASN:HB3	1:A:981:ASP:OD2	2.17	0.44
1:B:97:ILE:CD1	1:B:797:LEU:HD11	2.47	0.44
1:C:177:GLN:NE2	1:C:189:LYS:NZ	2.65	0.44
1:C:701:THR:HA	1:C:718:ILE:O	2.17	0.44
1:D:236:ARG:HD3	1:D:236:ARG:C	2.42	0.44
1:D:814:LEU:N	1:D:814:LEU:HD12	2.32	0.44
1:A:303:ALA:O	1:A:307:ILE:HG12	2.17	0.44
1:C:758:LYS:HZ1	1:C:828:LEU:HD23	1.83	0.44
1:D:186:SER:HB3	7:D:5524:HOH:O	2.17	0.44
1:A:954:PRO:HB3	1:A:959:LEU:O	2.17	0.44
1:C:947:ILE:HD11	1:C:957:PHE:CG	2.52	0.44
1:A:236:ARG:HD3	1:A:236:ARG:C	2.42	0.44
1:A:481:LYS:HG3	1:A:496:VAL:HB	1.99	0.44
1:B:116:ILE:O	1:B:120:LYS:HG3	2.18	0.44
1:B:701:THR:HA	1:B:718:ILE:O	2.17	0.44
1:C:329:LYS:O	1:C:330:ASN:HB2	2.17	0.44
1:C:838:MET:HE3	1:C:838:MET:HA	1.99	0.44
1:C:886:LEU:HD23	1:C:886:LEU:N	2.33	0.44
1:D:360:GLN:HG2	1:D:389:TYR:CE2	2.52	0.44
1:A:206:ASN:C	1:A:206:ASN:HD22	2.24	0.44
1:A:228:VAL:O	1:A:228:VAL:HG12	2.17	0.44
1:A:679:VAL:HG13	1:A:683:HIS:CB	2.35	0.44
1:A:783:LEU:HB3	1:A:784:PRO:HD2	1.99	0.44
1:B:332:ILE:CD1	1:B:736:ALA:HB2	2.47	0.44
1:B:367:PHE:C	1:B:367:PHE:CD2	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:947:ILE:HD11	1:B:957:PHE:CG	2.53	0.44
1:C:116:ILE:O	1:C:120:LYS:HG3	2.18	0.44
1:C:187:VAL:CG2	1:C:189:LYS:HE2	2.47	0.44
1:C:788:ILE:HG12	1:C:791:GLN:OE1	2.17	0.44
1:C:856:PHE:CZ	1:C:891:PHE:HA	2.53	0.44
1:C:914:ASN:HD22	1:C:914:ASN:HA	1.56	0.44
1:D:783:LEU:HB3	1:D:784:PRO:HD2	1.98	0.44
1:D:984:LEU:HD23	1:D:987:ILE:HD12	1.99	0.44
1:A:12:CYS:SG	1:A:164:ARG:HG3	2.57	0.44
1:A:65:LEU:HD11	1:A:307:ILE:HG21	1.99	0.44
1:A:69:ALA:HB2	1:A:94:ILE:HG21	2.00	0.44
1:A:336:LEU:N	1:A:337:PRO:HD2	2.33	0.44
1:B:59:ASP:OD2	1:B:62:VAL:HG23	2.17	0.44
1:B:856:PHE:CZ	1:B:891:PHE:HA	2.53	0.44
1:C:89:VAL:O	1:C:93:VAL:HG23	2.18	0.44
1:D:269:VAL:O	1:D:273:LEU:HG	2.18	0.44
1:D:855:TRP:HA	1:D:859:ALA:HB2	1.99	0.44
1:A:943:LEU:O	1:A:947:ILE:HG13	2.17	0.44
1:B:835:PHE:O	1:B:838:MET:HB3	2.18	0.44
1:C:344:CYS:SG	1:C:697:ILE:HG13	2.58	0.44
1:C:450:GLU:OE1	1:C:467:ARG:NH2	2.49	0.44
1:C:646:GLU:OE2	1:C:651:ARG:NH1	2.51	0.44
1:D:353:THR:HA	1:D:357:THR:HG1	1.83	0.44
1:A:984:LEU:HD23	1:A:987:ILE:HD12	1.99	0.44
1:B:896:PRO:O	1:B:899:MET:HB2	2.18	0.44
1:C:758:LYS:NZ	1:C:828:LEU:HD23	2.33	0.44
1:C:767:SER:O	1:C:771:GLU:HG3	2.17	0.44
1:C:921:SER:HB2	1:C:989:ARG:NH2	2.14	0.44
1:D:370:ASP:HB3	1:D:378:SER:OG	2.18	0.44
1:D:573:ARG:HH21	1:D:573:ARG:HG3	1.83	0.44
1:D:678:ARG:HB3	7:D:5069:HOH:O	2.17	0.44
1:A:814:LEU:HD12	1:A:814:LEU:N	2.33	0.44
1:A:922:LEU:N	1:A:922:LEU:HD12	2.33	0.44
1:C:978:ILE:O	1:C:982:GLU:HB2	2.18	0.44
1:D:69:ALA:HB2	1:D:94:ILE:HG21	2.00	0.44
1:A:491:ARG:HG2	1:A:493:SER:OG	2.17	0.43
1:A:926:PRO:HA	1:A:927:PRO:HD3	1.83	0.43
1:B:320:ALA:O	1:B:324:ARG:HG3	2.17	0.43
1:D:796:ASN:HA	7:D:5131:HOH:O	2.16	0.43
1:A:768:ASN:O	1:A:772:VAL:HG23	2.18	0.43
1:B:454:VAL:HG22	7:B:3034:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:760:PHE:CD1	1:B:760:PHE:C	2.96	0.43
1:C:328:LYS:HB3	1:C:328:LYS:HZ2	1.82	0.43
1:D:200:VAL:HG13	1:D:680:GLU:CG	2.48	0.43
1:D:214:ILE:HD12	1:D:214:ILE:N	2.33	0.43
1:A:687:ILE:O	1:A:691:LEU:HD22	2.18	0.43
1:A:855:TRP:HA	1:A:859:ALA:HB2	2.00	0.43
1:B:149:ASP:HB2	7:B:3093:HOH:O	2.19	0.43
1:B:389:TYR:HB3	1:B:425:LEU:HD11	2.00	0.43
1:D:303:ALA:O	1:D:307:ILE:HG12	2.18	0.43
1:D:862:GLY:H	1:D:863:PRO:HD3	1.83	0.43
1:A:862:GLY:H	1:A:863:PRO:HD3	1.83	0.43
1:B:80:GLU:CG	1:B:82:GLU:HG2	2.45	0.43
1:B:443:THR:O	1:B:447:THR:HG23	2.18	0.43
1:B:921:SER:HB2	1:B:989:ARG:NH2	2.14	0.43
1:C:1:MET:HE3	1:C:15:TYR:HB3	2.00	0.43
1:C:129:VAL:HG12	1:C:151:VAL:HG22	1.98	0.43
1:C:256:PHE:CE1	1:C:765:ILE:HD11	2.53	0.43
1:C:953:LEU:N	1:C:954:PRO:HD2	2.33	0.43
1:D:336:LEU:N	1:D:337:PRO:HD2	2.34	0.43
1:B:423:SER:HB3	1:B:437:VAL:O	2.19	0.43
1:B:465:VAL:HG23	1:B:466:GLU:N	2.33	0.43
1:C:80:GLU:CG	1:C:82:GLU:HG2	2.45	0.43
1:C:449:VAL:CG2	1:C:472:ASN:CG	2.91	0.43
1:B:549:ILE:HD11	1:B:596:VAL:HG21	2.00	0.43
1:B:914:ASN:HD22	1:B:914:ASN:HA	1.57	0.43
1:B:919:ASN:HD22	1:B:988:ALA:HB3	1.83	0.43
1:C:367:PHE:C	1:C:367:PHE:CD2	2.96	0.43
1:C:454:VAL:HG22	7:C:4034:HOH:O	2.18	0.43
1:D:481:LYS:HG3	1:D:496:VAL:HB	2.01	0.43
1:A:20:GLU:HB3	7:A:2516:HOH:O	2.18	0.43
1:A:930:ASN:OD1	1:A:932:TRP:HB2	2.19	0.43
1:B:352:LYS:HE2	7:B:3068:HOH:O	2.17	0.43
1:C:149:ASP:HB2	7:C:4093:HOH:O	2.19	0.43
1:D:49:LEU:C	1:D:51:GLU:H	2.26	0.43
1:A:49:LEU:C	1:A:51:GLU:H	2.26	0.43
1:A:283:VAL:HG22	1:A:286:GLY:H	1.84	0.43
1:B:458:GLU:H	1:B:458:GLU:CD	2.26	0.43
1:B:555:GLY:C	1:B:557:ASP:N	2.74	0.43
1:B:903:VAL:HG22	1:B:970:VAL:HG13	2.01	0.43
1:C:458:GLU:H	1:C:458:GLU:CD	2.26	0.43
1:D:12:CYS:SG	1:D:164:ARG:HG3	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:926:PRO:HA	1:D:927:PRO:HD3	1.83	0.43
1:A:280:ASN:N	1:A:280:ASN:HD22	2.16	0.43
1:A:459:VAL:HB	1:A:467:ARG:HD3	2.00	0.43
1:A:831:GLY:O	1:A:834:PHE:HB3	2.19	0.43
1:B:953:LEU:N	1:B:954:PRO:HD2	2.33	0.43
1:D:200:VAL:CG1	1:D:201:ASN:N	2.82	0.43
1:D:352:LYS:HA	1:D:356:LEU:HB2	2.00	0.43
1:D:930:ASN:OD1	1:D:932:TRP:HB2	2.19	0.43
1:A:295:TYR:C	1:A:297:LYS:H	2.27	0.43
1:A:600:LEU:O	1:A:602:PRO:HD3	2.19	0.43
1:B:332:ILE:N	1:B:332:ILE:CD1	2.82	0.43
1:B:978:ILE:O	1:B:982:GLU:HB2	2.19	0.43
1:C:788:ILE:HB	1:C:789:PRO:HD2	2.01	0.43
1:C:919:ASN:HD22	1:C:988:ALA:HB3	1.83	0.43
1:D:21:THR:HG22	1:D:21:THR:O	2.17	0.43
1:D:831:GLY:O	1:D:834:PHE:HB3	2.19	0.43
1:B:104:VAL:O	1:B:108:GLN:HG3	2.19	0.42
1:B:449:VAL:HG21	1:B:472:ASN:OD1	2.19	0.42
1:B:788:ILE:HB	1:B:789:PRO:HD2	2.01	0.42
1:B:788:ILE:HG12	1:B:791:GLN:OE1	2.19	0.42
1:C:389:TYR:HB3	1:C:425:LEU:HD11	2.00	0.42
1:C:758:LYS:HE3	1:C:762:ARG:NH2	2.34	0.42
1:D:46:GLY:C	1:D:48:SER:H	2.27	0.42
1:D:295:TYR:C	1:D:297:LYS:H	2.27	0.42
1:D:654:THR:HA	1:D:677:ALA:O	2.18	0.42
1:A:336:LEU:O	1:A:339:VAL:HG22	2.19	0.42
1:A:459:VAL:HB	1:A:467:ARG:CD	2.49	0.42
1:A:558:THR:HG22	1:A:558:THR:O	2.18	0.42
1:C:555:GLY:C	1:C:557:ASP:N	2.74	0.42
1:C:896:PRO:O	1:C:899:MET:HB2	2.19	0.42
1:C:903:VAL:HG22	1:C:970:VAL:HG13	2.01	0.42
1:D:922:LEU:HD12	1:D:922:LEU:N	2.34	0.42
1:A:18:VAL:HG12	1:A:24:LEU:HD23	2.02	0.42
1:B:89:VAL:O	1:B:93:VAL:HG23	2.19	0.42
1:B:473:SER:HA	1:B:476:ARG:NH1	2.34	0.42
1:B:757:MET:O	1:B:761:ILE:HG13	2.19	0.42
1:C:104:VAL:O	1:C:108:GLN:HG3	2.19	0.42
1:C:765:ILE:O	1:C:769:VAL:HG23	2.19	0.42
1:D:280:ASN:N	1:D:280:ASN:HD22	2.16	0.42
1:D:558:THR:O	1:D:558:THR:HG22	2.18	0.42
1:A:179:ILE:O	1:A:705:VAL:HG22	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:840:ILE:O	1:A:844:VAL:HG23	2.19	0.42
1:B:266:LEU:HD13	1:B:266:LEU:O	2.20	0.42
1:B:372:VAL:HG22	1:B:377:CYS:HB2	2.01	0.42
1:B:413:LEU:C	1:B:413:LEU:HD23	2.44	0.42
1:B:765:ILE:O	1:B:769:VAL:HG23	2.19	0.42
1:D:209:PHE:O	1:D:212:THR:HB	2.20	0.42
1:A:185:VAL:HG13	1:A:185:VAL:O	2.19	0.42
1:A:893:ALA:HA	1:A:894:PRO:HD3	1.86	0.42
1:A:951:ASP:O	1:A:954:PRO:HD2	2.18	0.42
1:B:646:GLU:OE2	1:B:651:ARG:NH1	2.52	0.42
1:D:283:VAL:HG22	1:D:286:GLY:H	1.85	0.42
1:D:717:GLY:O	1:D:731:SER:HB3	2.19	0.42
1:B:542:LYS:HD2	7:B:3003:HOH:O	2.19	0.42
1:D:459:VAL:HB	1:D:467:ARG:CD	2.49	0.42
1:B:862:GLY:N	1:B:863:PRO:HD3	2.35	0.42
1:C:325:ARG:NH1	1:C:753:ILE:HD11	2.35	0.42
1:D:336:LEU:O	1:D:339:VAL:HG22	2.20	0.42
1:D:765:ILE:O	1:D:769:VAL:HG23	2.20	0.42
1:A:446:THR:HG23	1:A:472:ASN:ND2	2.34	0.42
1:A:604:ARG:HB2	1:A:607:VAL:HG23	2.02	0.42
1:B:187:VAL:CG2	1:B:189:LYS:HE2	2.50	0.42
1:B:758:LYS:NZ	1:B:828:LEU:HD23	2.35	0.42
1:C:654:THR:HA	1:C:677:ALA:O	2.20	0.42
1:C:862:GLY:N	1:C:863:PRO:HD3	2.35	0.42
1:D:459:VAL:HB	1:D:467:ARG:HD3	2.01	0.42
1:A:46:GLY:C	1:A:48:SER:H	2.28	0.42
1:A:200:VAL:HG12	1:A:202:GLN:NE2	2.34	0.42
1:A:209:PHE:O	1:A:212:THR:HB	2.20	0.42
1:A:214:ILE:N	1:A:214:ILE:HD12	2.35	0.42
1:A:606:GLU:HG3	1:A:739:ASN:OD1	2.20	0.42
1:A:765:ILE:O	1:A:769:VAL:HG23	2.20	0.42
1:C:473:SER:HA	1:C:476:ARG:HH11	1.85	0.42
1:C:876:CYS:SG	1:C:884:GLU:OE1	2.78	0.42
1:D:239:MET:SD	1:D:708:ALA:HB1	2.60	0.42
1:A:175:VAL:CG1	1:A:212:THR:CG2	2.97	0.41
1:B:473:SER:HA	1:B:476:ARG:HH11	1.85	0.41
1:C:75:LEU:HD23	1:C:297:LYS:HD2	2.01	0.41
1:C:465:VAL:HG23	1:C:466:GLU:N	2.35	0.41
1:D:18:VAL:HG12	1:D:24:LEU:HD23	2.02	0.41
1:D:179:ILE:O	1:D:705:VAL:HG22	2.19	0.41
1:B:325:ARG:NH1	1:B:753:ILE:HD11	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:905:VAL:O	1:C:909:MET:HG2	2.19	0.41
1:D:185:VAL:HG13	1:D:185:VAL:O	2.20	0.41
1:D:212:THR:CG2	1:D:213:ASN:N	2.82	0.41
1:D:491:ARG:HG2	1:D:493:SER:OG	2.19	0.41
1:A:206:ASN:HD22	1:A:206:ASN:H	1.68	0.41
1:A:239:MET:SD	1:A:708:ALA:HB1	2.60	0.41
1:C:413:LEU:HD23	1:C:413:LEU:C	2.45	0.41
1:D:412:GLU:OE2	1:D:566:THR:CG2	2.66	0.41
1:D:604:ARG:HB2	1:D:607:VAL:HG23	2.03	0.41
1:D:893:ALA:HA	1:D:894:PRO:HD3	1.86	0.41
1:A:624:ILE:HD13	1:A:687:ILE:CD1	2.51	0.41
1:B:758:LYS:HE3	1:B:762:ARG:NH2	2.35	0.41
1:C:1:MET:HE2	1:C:7:LYS:HE2	2.02	0.41
1:C:983:ILE:O	1:C:987:ILE:HG13	2.19	0.41
1:C:100:ALA:O	1:C:104:VAL:HG23	2.20	0.41
1:C:473:SER:HA	1:C:476:ARG:NH1	2.35	0.41
1:D:840:ILE:O	1:D:844:VAL:HG23	2.20	0.41
1:A:567:ARG:HD2	1:A:570:PRO:CA	2.48	0.41
1:A:924:ARG:HA	1:A:924:ARG:HE	1.86	0.41
1:C:975:LEU:N	1:C:976:PRO:CD	2.82	0.41
1:D:795:VAL:HA	1:D:799:THR:CB	2.49	0.41
1:D:843:TYR:OH	1:D:976:PRO:HG2	2.20	0.41
1:A:941:MET:O	1:A:944:HIS:HB3	2.20	0.41
1:B:65:LEU:HG	1:B:94:ILE:HD11	2.03	0.41
1:B:90:GLU:O	1:B:94:ILE:HG22	2.21	0.41
1:B:501:ALA:C	1:B:503:SER:N	2.79	0.41
1:B:922:LEU:HD12	1:B:922:LEU:N	2.36	0.41
1:C:23:GLY:HA3	1:C:130:TYR:O	2.20	0.41
1:C:656:ARG:HA	1:C:656:ARG:HD3	1.92	0.41
1:D:198:ARG:HE	1:D:656:ARG:HH22	1.69	0.41
1:B:491:ARG:NH1	1:B:588:GLU:OE1	2.54	0.41
1:B:975:LEU:N	1:B:976:PRO:CD	2.82	0.41
1:D:198:ARG:HE	1:D:656:ARG:NH2	2.18	0.41
1:D:255:GLU:O	1:D:258:GLU:HB2	2.20	0.41
1:D:366:MET:HA	1:D:596:VAL:O	2.21	0.41
1:B:1:MET:HE3	1:B:15:TYR:HB3	2.00	0.41
1:B:88:PHE:C	1:B:91:PRO:HD2	2.46	0.41
1:B:102:ALA:O	1:B:106:VAL:HG23	2.21	0.41
1:B:166:LEU:HD11	1:B:222:ILE:HB	2.02	0.41
1:B:322:GLY:O	1:B:326:MET:HG3	2.20	0.41
1:B:654:THR:HA	1:B:677:ALA:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:656:ARG:HD3	1:B:656:ARG:HA	1.92	0.41
1:B:876:CYS:SG	1:B:884:GLU:OE1	2.79	0.41
1:B:983:ILE:O	1:B:987:ILE:HG13	2.20	0.41
1:C:491:ARG:NH1	1:C:588:GLU:OE1	2.54	0.41
1:C:491:ARG:HH11	1:C:588:GLU:CD	2.29	0.41
1:D:446:THR:HG23	1:D:472:ASN:ND2	2.35	0.41
1:D:491:ARG:NH1	1:D:588:GLU:OE1	2.54	0.41
1:D:567:ARG:HD2	1:D:570:PRO:CA	2.48	0.41
1:D:807:LEU:C	1:D:809:PHE:H	2.27	0.41
1:D:924:ARG:HE	1:D:924:ARG:HA	1.86	0.41
1:D:941:MET:O	1:D:944:HIS:HB3	2.20	0.41
1:D:951:ASP:O	1:D:954:PRO:HD2	2.20	0.41
1:A:198:ARG:HE	1:A:656:ARG:NH2	2.19	0.41
1:A:325:ARG:O	1:A:328:LYS:HB3	2.21	0.41
1:A:795:VAL:HA	1:A:799:THR:CB	2.50	0.41
1:B:90:GLU:HB2	1:B:790:VAL:HG22	2.03	0.41
1:C:962:LEU:HB2	1:C:966:GLN:HB2	2.02	0.41
1:D:868:HIS:C	1:D:870:LEU:H	2.28	0.41
1:A:654:THR:HA	1:A:677:ALA:O	2.21	0.40
1:A:843:TYR:OH	1:A:976:PRO:HG2	2.20	0.40
1:C:88:PHE:C	1:C:91:PRO:HD2	2.46	0.40
1:C:922:LEU:N	1:C:922:LEU:HD12	2.36	0.40
1:A:255:GLU:O	1:A:258:GLU:HB2	2.21	0.40
1:A:366:MET:HA	1:A:596:VAL:O	2.21	0.40
1:B:1:MET:HE2	1:B:7:LYS:HE2	2.03	0.40
1:B:8:SER:OG	1:B:11:GLU:HG3	2.22	0.40
1:B:179:ILE:O	1:B:705:VAL:HG22	2.21	0.40
1:B:905:VAL:O	1:B:909:MET:HG2	2.20	0.40
1:B:910:CYS:HB3	1:B:978:ILE:CG1	2.51	0.40
1:B:962:LEU:HB2	1:B:966:GLN:HB2	2.02	0.40
1:C:100:ALA:O	1:C:103:ILE:HG22	2.21	0.40
1:C:102:ALA:O	1:C:106:VAL:HG23	2.22	0.40
1:C:266:LEU:HD13	1:C:266:LEU:O	2.21	0.40
1:C:777:LEU:HD12	1:C:845:GLY:O	2.21	0.40
1:C:962:LEU:HG	1:C:967:TRP:NE1	2.36	0.40
1:A:916:LEU:CD1	1:A:927:PRO:HA	2.52	0.40
1:B:100:ALA:O	1:B:104:VAL:HG23	2.21	0.40
1:B:777:LEU:HD12	1:B:845:GLY:O	2.21	0.40
1:B:962:LEU:HG	1:B:967:TRP:NE1	2.36	0.40
1:C:90:GLU:O	1:C:94:ILE:HG22	2.22	0.40
1:C:389:TYR:HA	1:C:447:THR:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:501:ALA:C	1:C:503:SER:N	2.80	0.40
1:D:20:GLU:HB3	7:D:5516:HOH:O	2.20	0.40
1:D:485:LEU:HD22	1:D:584:PHE:CE2	2.56	0.40
1:D:600:LEU:O	1:D:602:PRO:HD3	2.22	0.40
1:D:971:LEU:HA	1:D:975:LEU:HD23	2.02	0.40
1:A:858:TYR:CD1	1:A:858:TYR:N	2.89	0.40
1:A:971:LEU:HA	1:A:975:LEU:HD23	2.02	0.40
1:C:39:ASN:OD1	1:C:226:THR:HB	2.21	0.40
1:D:263:VAL:O	1:D:267:ILE:HG13	2.21	0.40
1:D:771:GLU:O	1:D:775:ILE:HG12	2.22	0.40
1:D:670:CYS:HB3	1:D:691:LEU:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	992/994 (100%)	932 (94%)	51 (5%)	9 (1%)	14	17
1	B	992/994 (100%)	934 (94%)	52 (5%)	6 (1%)	21	27
1	C	992/994 (100%)	933 (94%)	53 (5%)	6 (1%)	21	27
1	D	992/994 (100%)	931 (94%)	52 (5%)	9 (1%)	14	17
All	All	3968/3976 (100%)	3730 (94%)	208 (5%)	30 (1%)	16	20

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	882	HIS
1	B	882	HIS
1	C	882	HIS
1	D	882	HIS

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Mol	Chain	Res	Type
1	A	961	ALA
1	D	961	ALA
1	A	992	LEU
1	B	663	LEU
1	C	663	LEU
1	D	992	LEU
1	A	243	GLU
1	A	282	PRO
1	B	241	ALA
1	D	243	GLU
1	D	282	PRO
1	A	862	GLY
1	A	953	LEU
1	C	241	ALA
1	C	950	VAL
1	D	862	GLY
1	B	950	VAL
1	B	953	LEU
1	C	953	LEU
1	D	953	LEU
1	A	291	GLY
1	A	950	VAL
1	D	291	GLY
1	B	862	GLY
1	C	862	GLY
1	D	950	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	840/840 (100%)	808 (96%)	32 (4%)	29	44
1	B	840/840 (100%)	804 (96%)	36 (4%)	26	39
1	C	840/840 (100%)	803 (96%)	37 (4%)	25	38
1	D	840/840 (100%)	807 (96%)	33 (4%)	28	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3360/3360 (100%)	3222 (96%)	138 (4%)	27	41

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LEU
1	A	44	GLU
1	A	45	GLU
1	A	121	GLU
1	A	187	VAL
1	A	202	GLN
1	A	206	ASN
1	A	255	GLU
1	A	266	LEU
1	A	342	LEU
1	A	356	LEU
1	A	413	LEU
1	A	486	GLU
1	A	534	ARG
1	A	544	LYS
1	A	562	LEU
1	A	566	THR
1	A	567	ARG
1	A	574	GLU
1	A	602	PRO
1	A	620	ARG
1	A	631	THR
1	A	656	ARG
1	A	660	ASP
1	A	678	ARG
1	A	687	ILE
1	A	691	LEU
1	A	705	VAL
1	A	829	ILE
1	A	882	HIS
1	A	964	LEU
1	A	972	LYS
1	B	9	THR
1	B	22	THR
1	B	41	LEU
1	B	134	ARG
1	B	202	GLN

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Mol	Chain	Res	Type
1	B	212	THR
1	B	242	THR
1	B	319	LEU
1	B	328	LYS
1	B	340	GLU
1	B	342	LEU
1	B	356	LEU
1	B	361	MET
1	B	394	GLU
1	B	406	GLN
1	B	445	LEU
1	B	449	VAL
1	B	460	ARG
1	B	467	ARG
1	B	484	THR
1	B	534	ARG
1	B	544	LYS
1	B	562	LEU
1	B	566	THR
1	B	572	LYS
1	B	589	THR
1	B	620	ARG
1	B	631	THR
1	B	679	VAL
1	B	691	LEU
1	B	705	VAL
1	B	713	LYS
1	B	765	ILE
1	B	882	HIS
1	B	914	ASN
1	B	962	LEU
1	C	9	THR
1	C	22	THR
1	C	41	LEU
1	C	134	ARG
1	C	202	GLN
1	C	212	THR
1	C	242	THR
1	C	319	LEU
1	C	328	LYS
1	C	340	GLU
1	C	342	LEU

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Mol	Chain	Res	Type
1	C	356	LEU
1	C	361	MET
1	C	394	GLU
1	C	406	GLN
1	C	445	LEU
1	C	449	VAL
1	C	460	ARG
1	C	467	ARG
1	C	484	THR
1	C	534	ARG
1	C	544	LYS
1	C	562	LEU
1	C	566	THR
1	C	572	LYS
1	C	589	THR
1	C	620	ARG
1	C	631	THR
1	C	679	VAL
1	C	691	LEU
1	C	701	THR
1	C	705	VAL
1	C	713	LYS
1	C	765	ILE
1	C	882	HIS
1	C	914	ASN
1	C	962	LEU
1	D	41	LEU
1	D	44	GLU
1	D	45	GLU
1	D	121	GLU
1	D	187	VAL
1	D	202	GLN
1	D	255	GLU
1	D	266	LEU
1	D	342	LEU
1	D	356	LEU
1	D	413	LEU
1	D	486	GLU
1	D	534	ARG
1	D	544	LYS
1	D	554	THR
1	D	562	LEU

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Mol	Chain	Res	Type
1	D	566	THR
1	D	567	ARG
1	D	574	GLU
1	D	602	PRO
1	D	620	ARG
1	D	631	THR
1	D	656	ARG
1	D	660	ASP
1	D	671	ARG
1	D	678	ARG
1	D	687	ILE
1	D	691	LEU
1	D	705	VAL
1	D	829	ILE
1	D	882	HIS
1	D	964	LEU
1	D	972	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	202	GLN
1	A	206	ASN
1	A	280	ASN
1	A	359	ASN
1	A	472	ASN
1	A	869	GLN
1	A	872	HIS
1	A	911	ASN
1	A	914	ASN
1	A	920	GLN
1	A	966	GLN
1	B	38	HIS
1	B	108	GLN
1	B	138	GLN
1	B	275	ASN
1	B	278	HIS
1	B	359	ASN
1	B	406	GLN
1	B	472	ASN
1	B	510	ASN

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Mol	Chain	Res	Type
1	B	768	ASN
1	B	869	GLN
1	B	914	ASN
1	B	919	ASN
1	C	38	HIS
1	C	108	GLN
1	C	138	GLN
1	C	177	GLN
1	C	244	GLN
1	C	275	ASN
1	C	278	HIS
1	C	359	ASN
1	C	406	GLN
1	C	472	ASN
1	C	510	ASN
1	C	914	ASN
1	C	919	ASN
1	D	114	ASN
1	D	238	GLN
1	D	280	ASN
1	D	359	ASN
1	D	472	ASN
1	D	911	ASN
1	D	914	ASN
1	D	920	GLN
1	D	966	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

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	TG1	A	1003	-	44,48,48	1.75	11 (25%)	47,72,72	1.70	10 (21%)
4	MF4	B	1098	2,1	0,4,4	-	-	-	-	-
5	ADP	C	1202	2	28,29,29	1.57	8 (28%)	43,45,45	2.15	13 (30%)
6	TG1	C	1203	-	44,48,48	1.77	11 (25%)	47,72,72	1.74	9 (19%)
4	MF4	D	1298	2,1	0,4,4	-	-	-	-	-
5	ADP	A	1002	2	28,29,29	1.58	7 (25%)	43,45,45	2.20	14 (32%)
6	TG1	B	1103	-	44,48,48	1.76	11 (25%)	47,72,72	1.75	9 (19%)
5	ADP	D	1302	2	28,29,29	1.58	7 (25%)	43,45,45	2.21	14 (32%)
4	MF4	C	1198	2,1	0,4,4	-	-	-	-	-
6	TG1	D	1303	-	44,48,48	1.74	11 (25%)	47,72,72	1.71	11 (23%)
5	ADP	B	1102	2	28,29,29	1.61	8 (28%)	43,45,45	2.17	13 (30%)
4	MF4	A	998	2,1	0,4,4	-	-	-	-	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	TG1	A	1003	-	-	9/33/99/99	0/3/3/3
5	ADP	C	1202	2	-	6/16/32/32	0/3/3/3
6	TG1	C	1203	-	-	12/33/99/99	0/3/3/3
5	ADP	A	1002	2	-	4/16/32/32	0/3/3/3
6	TG1	B	1103	-	-	11/33/99/99	0/3/3/3
5	ADP	D	1302	2	-	4/16/32/32	0/3/3/3
6	TG1	D	1303	-	-	9/33/99/99	0/3/3/3
5	ADP	B	1102	2	-	6/16/32/32	0/3/3/3

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1203	TG1	O4-C21	6.12	1.33	1.21
6	B	1103	TG1	O4-C21	5.98	1.33	1.21
6	A	1003	TG1	O4-C21	5.70	1.33	1.21
6	D	1303	TG1	O4-C21	5.56	1.32	1.21
5	B	1102	ADP	C5-N7	-3.66	1.32	1.39
6	C	1203	TG1	C3-C4	3.63	1.55	1.50
6	B	1103	TG1	C3-C4	3.59	1.54	1.50
5	C	1202	ADP	C5-N7	-3.53	1.32	1.39
6	D	1303	TG1	C3-C4	3.46	1.54	1.50
5	D	1302	ADP	C5-N7	-3.45	1.32	1.39
6	B	1103	TG1	O6-C7	3.42	1.48	1.43
5	A	1002	ADP	C5-N7	-3.42	1.32	1.39
6	A	1003	TG1	C3-C4	3.38	1.54	1.50
6	B	1103	TG1	C9-C10	3.30	1.59	1.54
6	C	1203	TG1	C9-C10	3.27	1.59	1.54
6	C	1203	TG1	O6-C7	3.26	1.48	1.43
6	D	1303	TG1	O6-C7	3.22	1.48	1.43
6	A	1003	TG1	O6-C7	3.18	1.48	1.43
5	D	1302	ADP	C5-C4	3.07	1.44	1.39
5	A	1002	ADP	C5-C4	3.07	1.44	1.39
6	D	1303	TG1	C1-C2	2.98	1.59	1.54
6	D	1303	TG1	C34-C11	2.95	1.57	1.53
6	A	1003	TG1	C9-C10	2.88	1.59	1.54
6	A	1003	TG1	C1-C2	2.88	1.59	1.54
6	D	1303	TG1	C9-C10	2.85	1.59	1.54
6	C	1203	TG1	C11-C7	2.80	1.59	1.55
6	A	1003	TG1	C34-C11	2.79	1.57	1.53
5	B	1102	ADP	C5-C4	2.79	1.44	1.39
6	B	1103	TG1	C34-C11	2.78	1.57	1.53
5	C	1202	ADP	C5-C4	2.75	1.44	1.39
6	B	1103	TG1	C11-C7	2.67	1.58	1.55
6	B	1103	TG1	C9-C8	2.66	1.55	1.52
6	C	1203	TG1	C34-C11	2.65	1.56	1.53
6	C	1203	TG1	C9-C8	2.65	1.55	1.52
6	D	1303	TG1	C11-C7	2.64	1.58	1.55
5	A	1002	ADP	C4-N3	2.61	1.39	1.34
5	B	1102	ADP	C4-N3	2.57	1.39	1.34
5	C	1202	ADP	C4-N3	2.53	1.39	1.34
5	D	1302	ADP	C4-N9	-2.46	1.32	1.37
5	D	1302	ADP	PB-O2B	2.45	1.63	1.54
5	A	1002	ADP	PB-O2B	2.45	1.63	1.54
5	D	1302	ADP	C4-N3	2.45	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1003	TG1	C11-C7	2.40	1.58	1.55
6	C	1203	TG1	C1-C2	2.39	1.58	1.54
5	B	1102	ADP	PB-O2B	2.36	1.63	1.54
5	C	1202	ADP	PB-O2B	2.35	1.63	1.54
6	B	1103	TG1	C1-C2	2.34	1.58	1.54
6	A	1003	TG1	O3-C3	2.34	1.49	1.44
5	A	1002	ADP	C4-N9	-2.29	1.32	1.37
5	B	1102	ADP	C2-N1	2.27	1.38	1.33
6	C	1203	TG1	C1-C5	2.27	1.55	1.51
6	A	1003	TG1	C9-C8	2.24	1.55	1.52
5	B	1102	ADP	C4-N9	-2.22	1.33	1.37
6	D	1303	TG1	C9-C8	2.20	1.55	1.52
6	A	1003	TG1	C1-C5	2.19	1.54	1.51
6	D	1303	TG1	C1-C5	2.19	1.54	1.51
5	D	1302	ADP	C8-N7	2.18	1.35	1.31
6	A	1003	TG1	O7-C27	2.15	1.40	1.34
5	C	1202	ADP	C4-N9	-2.14	1.33	1.37
6	C	1203	TG1	C31-C10	2.14	1.56	1.52
6	B	1103	TG1	C31-C10	2.14	1.56	1.52
6	D	1303	TG1	O7-C27	2.13	1.40	1.34
5	C	1202	ADP	C2-N1	2.12	1.37	1.33
5	B	1102	ADP	C2'-C1'	-2.12	1.46	1.53
5	A	1002	ADP	C2-N1	2.11	1.37	1.33
6	B	1103	TG1	C1-C5	2.11	1.54	1.51
5	A	1002	ADP	C8-N7	2.08	1.35	1.31
5	B	1102	ADP	C2-N3	2.07	1.37	1.33
6	B	1103	TG1	O1-C13	2.06	1.40	1.34
5	C	1202	ADP	C2'-C1'	-2.04	1.47	1.53
5	C	1202	ADP	C8-N7	2.03	1.35	1.31
6	D	1303	TG1	O3-C3	2.03	1.48	1.44
6	C	1203	TG1	O1-C13	2.02	1.40	1.34
5	D	1302	ADP	C2-N1	2.00	1.37	1.33

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1302	ADP	N3-C2-N1	-7.01	117.97	128.58
5	B	1102	ADP	N3-C2-N1	-6.99	118.01	128.58
5	A	1002	ADP	N3-C2-N1	-6.97	118.02	128.58
5	C	1202	ADP	N3-C2-N1	-6.95	118.06	128.58
6	D	1303	TG1	C10-O9-C32	5.65	134.59	121.36
6	A	1003	TG1	C10-O9-C32	5.64	134.58	121.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1103	TG1	C10-O9-C32	5.63	134.56	121.36
6	C	1203	TG1	C10-O9-C32	5.57	134.42	121.36
5	A	1002	ADP	C5-C4-N3	-5.14	119.64	126.72
5	D	1302	ADP	C5-C4-N3	-5.11	119.68	126.72
5	B	1102	ADP	C5-C4-N3	-5.00	119.83	126.72
5	C	1202	ADP	C5-C4-N3	-4.99	119.85	126.72
5	D	1302	ADP	C2-N3-C4	4.78	123.50	111.83
5	A	1002	ADP	C2-N3-C4	4.76	123.46	111.83
5	C	1202	ADP	C2-N3-C4	4.67	123.23	111.83
5	B	1102	ADP	C2-N3-C4	4.62	123.12	111.83
6	B	1103	TG1	C2-O1-C13	4.15	124.33	117.59
6	C	1203	TG1	C2-O1-C13	4.06	124.19	117.59
6	D	1303	TG1	O12-C12-C11	-4.01	124.22	128.28
6	A	1003	TG1	O12-C12-C11	-3.96	124.27	128.28
6	C	1203	TG1	O12-C12-C11	-3.82	124.42	128.28
6	B	1103	TG1	O12-C12-C11	-3.81	124.42	128.28
5	A	1002	ADP	C4-C5-N7	-3.65	106.41	110.58
6	D	1303	TG1	O1-C2-C3	-3.61	103.37	110.18
5	D	1302	ADP	C4-C5-N7	-3.59	106.47	110.58
6	A	1003	TG1	O1-C2-C3	-3.47	103.63	110.18
5	B	1102	ADP	C4-C5-N7	-3.46	106.62	110.58
5	B	1102	ADP	C5-N7-C8	3.42	108.83	103.45
5	A	1002	ADP	C5-N7-C8	3.41	108.81	103.45
6	B	1103	TG1	O3-C21-O4	3.34	129.64	123.40
6	C	1203	TG1	O3-C21-O4	3.34	129.63	123.40
5	D	1302	ADP	C5-N7-C8	3.31	108.66	103.45
5	C	1202	ADP	C5-N7-C8	3.25	108.55	103.45
5	C	1202	ADP	C4-C5-N7	-3.23	106.89	110.58
5	B	1102	ADP	N9-C8-N7	-3.10	109.53	113.94
5	D	1302	ADP	N9-C8-N7	-3.07	109.57	113.94
5	C	1202	ADP	O4'-C1'-N9	3.07	113.98	108.09
5	C	1202	ADP	N3-C4-N9	3.07	132.38	127.17
5	B	1102	ADP	O4'-C1'-N9	3.07	113.98	108.09
6	B	1103	TG1	C7-C6-C5	3.06	123.44	115.41
6	C	1203	TG1	C7-C6-C5	3.04	123.41	115.41
5	A	1002	ADP	N9-C8-N7	-3.03	109.63	113.94
5	C	1202	ADP	N9-C8-N7	-3.02	109.66	113.94
5	D	1302	ADP	N3-C4-N9	2.98	132.24	127.17
5	B	1102	ADP	N3-C4-N9	2.96	132.21	127.17
6	D	1303	TG1	C7-C6-C5	2.96	123.19	115.41
6	A	1003	TG1	C7-C6-C5	2.96	123.18	115.41
5	A	1002	ADP	N3-C4-N9	2.94	132.16	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1302	ADP	O4'-C1'-C2'	2.84	112.69	106.62
5	A	1002	ADP	C6-C5-N7	2.81	137.50	132.09
5	A	1002	ADP	O4'-C1'-C2'	2.80	112.60	106.62
6	D	1303	TG1	O3-C21-O4	2.79	128.60	123.40
6	A	1003	TG1	O3-C21-O4	2.78	128.59	123.40
5	D	1302	ADP	C6-C5-N7	2.77	137.44	132.09
5	D	1302	ADP	O2'-C2'-C1'	2.73	119.52	110.10
6	B	1103	TG1	C24-C22-C21	2.72	130.99	120.79
6	D	1303	TG1	O5-C12-O12	2.70	125.10	121.60
6	C	1203	TG1	C24-C22-C21	2.70	130.93	120.79
5	D	1302	ADP	O4'-C1'-N9	2.70	113.28	108.09
5	A	1002	ADP	O2'-C2'-C1'	2.70	119.39	110.10
5	C	1202	ADP	O4'-C1'-C2'	2.69	112.37	106.62
5	B	1102	ADP	O4'-C1'-C2'	2.69	112.36	106.62
6	A	1003	TG1	C24-C22-C21	2.66	130.79	120.79
6	A	1003	TG1	O5-C12-O12	2.65	125.04	121.60
6	D	1303	TG1	C24-C22-C21	2.65	130.76	120.79
5	C	1202	ADP	O2'-C2'-C1'	2.59	119.03	110.10
5	B	1102	ADP	O2'-C2'-C1'	2.59	119.01	110.10
5	B	1102	ADP	C6-C5-N7	2.56	137.03	132.09
5	A	1002	ADP	O4'-C1'-N9	2.54	112.97	108.09
6	B	1103	TG1	O5-C12-O12	2.52	124.86	121.60
6	B	1103	TG1	O7-C8-C9	2.45	111.01	106.63
6	C	1203	TG1	O5-C12-O12	2.44	124.76	121.60
5	C	1202	ADP	C6-C5-N7	2.41	136.73	132.09
6	C	1203	TG1	O7-C8-C9	2.37	110.87	106.63
5	D	1302	ADP	C2'-C3'-C4'	2.36	107.17	102.61
6	B	1103	TG1	C23-C22-C21	-2.36	110.07	116.12
5	D	1302	ADP	C2-N1-C6	2.35	122.59	118.73
6	C	1203	TG1	C23-C22-C21	-2.34	110.10	116.12
5	A	1002	ADP	C2'-C3'-C4'	2.33	107.11	102.61
6	A	1003	TG1	O4-C21-C22	-2.32	117.91	125.28
6	D	1303	TG1	O4-C21-C22	-2.31	117.95	125.28
5	A	1002	ADP	C2-N1-C6	2.24	122.40	118.73
5	C	1202	ADP	C2-N1-C6	2.20	122.34	118.73
5	A	1002	ADP	C5-C4-N9	2.18	108.18	105.81
6	D	1303	TG1	C2-O1-C13	2.10	121.00	117.59
5	C	1202	ADP	C2'-C3'-C4'	2.09	106.66	102.61
5	B	1102	ADP	C2-N1-C6	2.08	122.16	118.73
5	D	1302	ADP	C5-C4-N9	2.08	108.08	105.81
6	D	1303	TG1	C8-O7-C27	2.06	121.79	118.03
6	D	1303	TG1	C23-C22-C21	-2.06	110.84	116.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1003	TG1	C8-O7-C27	2.06	121.78	118.03
5	B	1102	ADP	C2'-C3'-C4'	2.05	106.57	102.61
6	A	1003	TG1	C23-C22-C21	-2.05	110.86	116.12

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1102	ADP	O4'-C4'-C5'-O5'
5	C	1202	ADP	O4'-C4'-C5'-O5'
6	A	1003	TG1	O3-C21-C22-C23
6	A	1003	TG1	O3-C21-C22-C24
6	B	1103	TG1	O3-C21-C22-C23
6	C	1203	TG1	O3-C21-C22-C23
6	D	1303	TG1	O3-C21-C22-C23
6	D	1303	TG1	O3-C21-C22-C24
5	A	1002	ADP	C3'-C4'-C5'-O5'
5	B	1102	ADP	C3'-C4'-C5'-O5'
5	C	1202	ADP	C3'-C4'-C5'-O5'
5	D	1302	ADP	C3'-C4'-C5'-O5'
6	A	1003	TG1	O4-C21-C22-C23
6	B	1103	TG1	O4-C21-C22-C23
6	C	1203	TG1	O4-C21-C22-C23
6	D	1303	TG1	O4-C21-C22-C23
6	A	1003	TG1	O4-C21-C22-C24
6	C	1203	TG1	O4-C21-C22-C24
6	D	1303	TG1	O4-C21-C22-C24
6	B	1103	TG1	O3-C21-C22-C24
6	C	1203	TG1	O3-C21-C22-C24
6	A	1003	TG1	C22-C21-O3-C3
6	D	1303	TG1	C22-C21-O3-C3
5	A	1002	ADP	O4'-C4'-C5'-O5'
5	D	1302	ADP	O4'-C4'-C5'-O5'
6	B	1103	TG1	O4-C21-C22-C24
6	B	1103	TG1	C22-C21-O3-C3
6	C	1203	TG1	C22-C21-O3-C3
6	B	1103	TG1	C14-C15-C16-C17
6	C	1203	TG1	C14-C15-C16-C17
6	D	1303	TG1	C17-C18-C19-C20
6	A	1003	TG1	C17-C18-C19-C20
6	A	1003	TG1	C15-C16-C17-C18
6	D	1303	TG1	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
6	B	1103	TG1	C17-C18-C19-C20
6	C	1203	TG1	C17-C18-C19-C20
5	A	1002	ADP	PB-O3A-PA-O5'
5	B	1102	ADP	PB-O3A-PA-O5'
5	C	1202	ADP	PB-O3A-PA-O5'
5	D	1302	ADP	PB-O3A-PA-O5'
5	C	1202	ADP	PA-O3A-PB-O1B
6	B	1103	TG1	C15-C16-C17-C18
6	C	1203	TG1	C15-C16-C17-C18
5	B	1102	ADP	PA-O3A-PB-O1B
6	A	1003	TG1	C14-C15-C16-C17
6	B	1103	TG1	C16-C17-C18-C19
6	C	1203	TG1	C16-C17-C18-C19
6	D	1303	TG1	C14-C15-C16-C17
5	A	1002	ADP	PA-O3A-PB-O2B
5	B	1102	ADP	PA-O3A-PB-O2B
5	B	1102	ADP	PA-O3A-PB-O3B
5	C	1202	ADP	PA-O3A-PB-O2B
5	C	1202	ADP	PA-O3A-PB-O3B
5	D	1302	ADP	PA-O3A-PB-O2B
6	B	1103	TG1	O1-C13-C14-C15
6	C	1203	TG1	O1-C13-C14-C15
6	A	1003	TG1	O1-C13-C14-C15
6	D	1303	TG1	O1-C13-C14-C15
6	C	1203	TG1	O2-C13-C14-C15
6	C	1203	TG1	O7-C27-C28-C29
6	B	1103	TG1	O2-C13-C14-C15

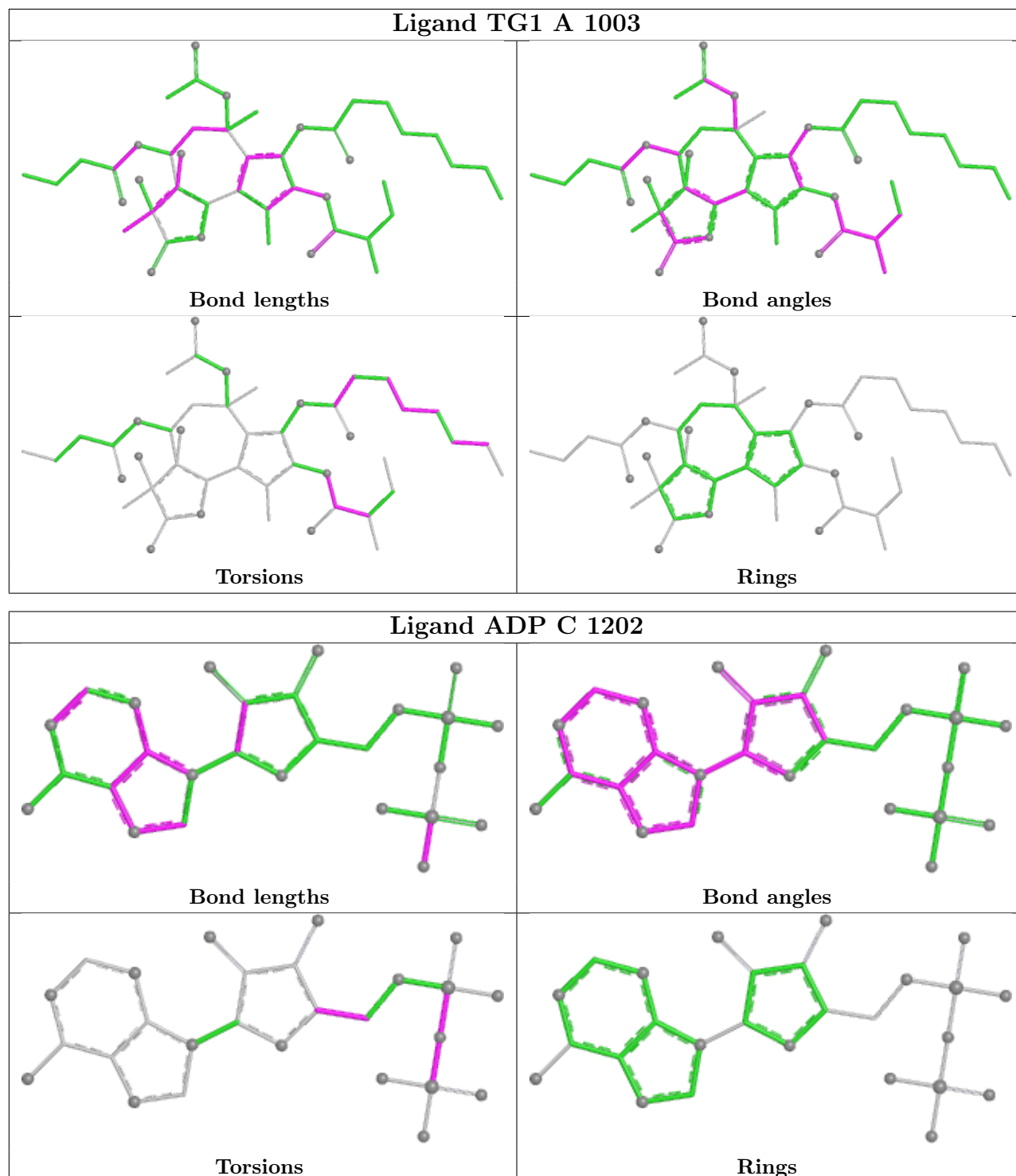
There are no ring outliers.

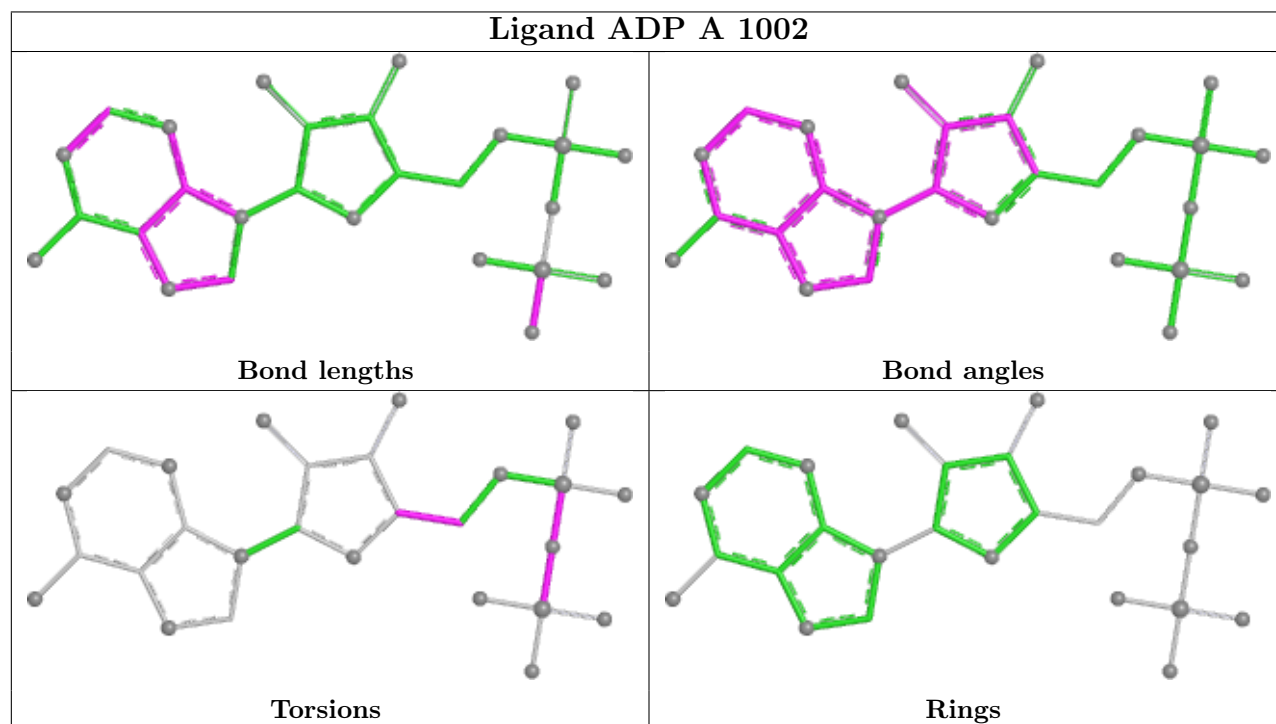
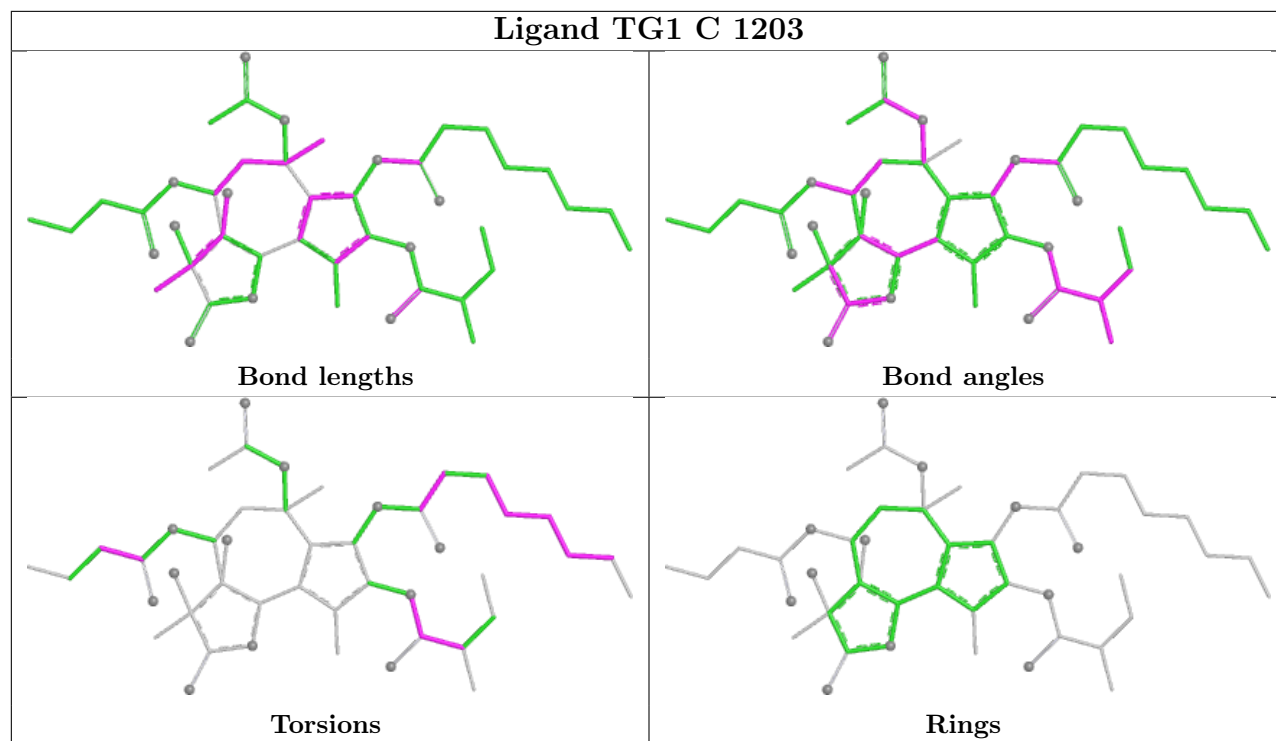
4 monomers are involved in 8 short contacts:

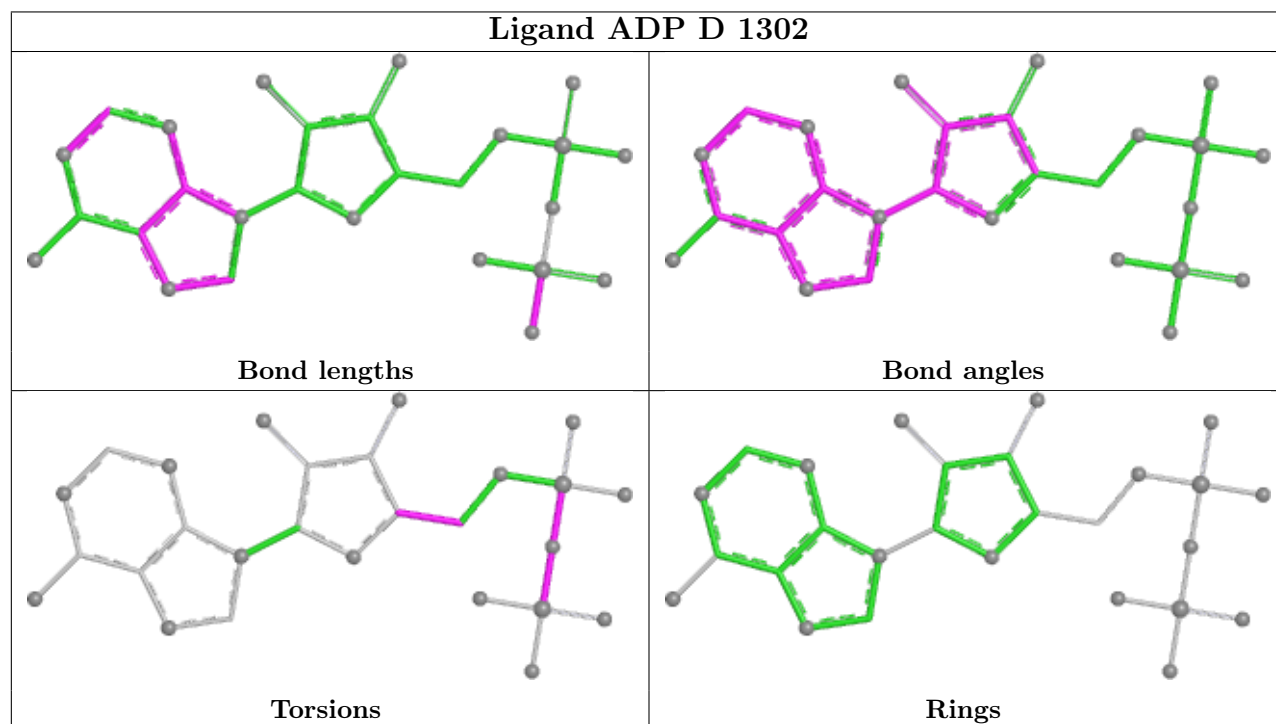
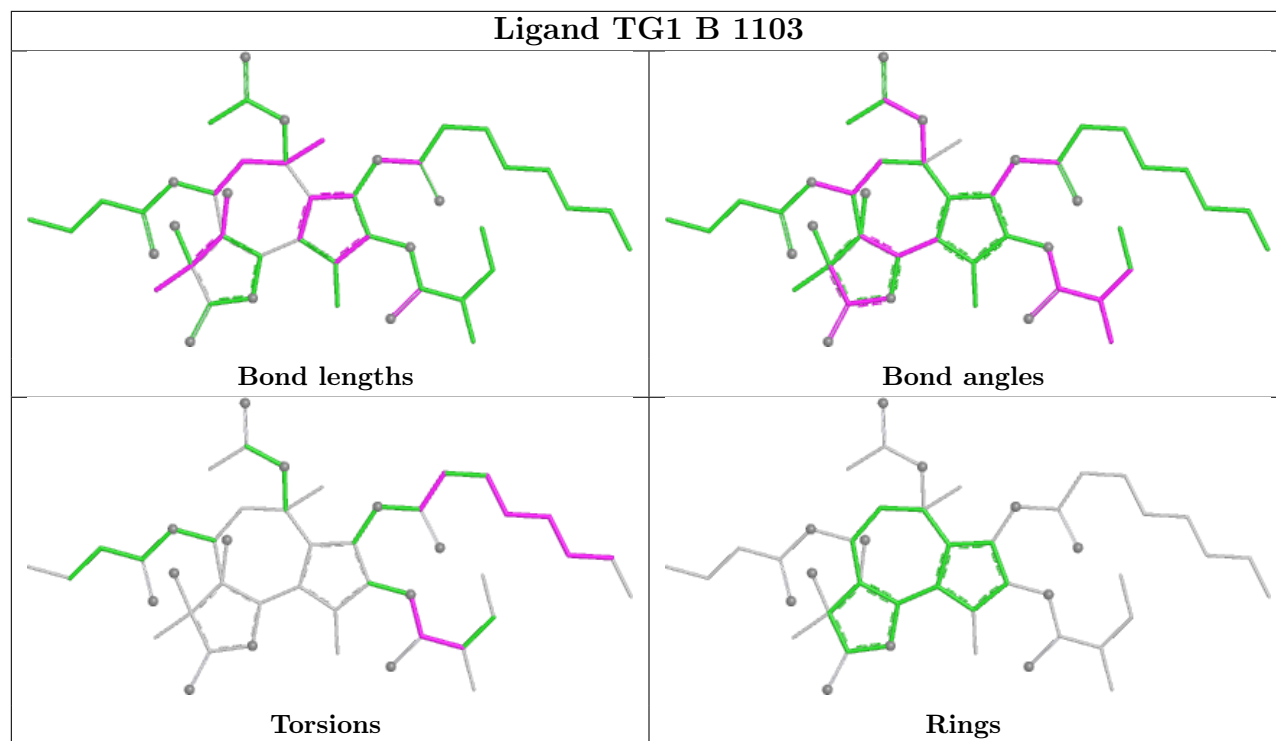
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1202	ADP	2	0
6	C	1203	TG1	2	0
6	B	1103	TG1	2	0
5	B	1102	ADP	2	0

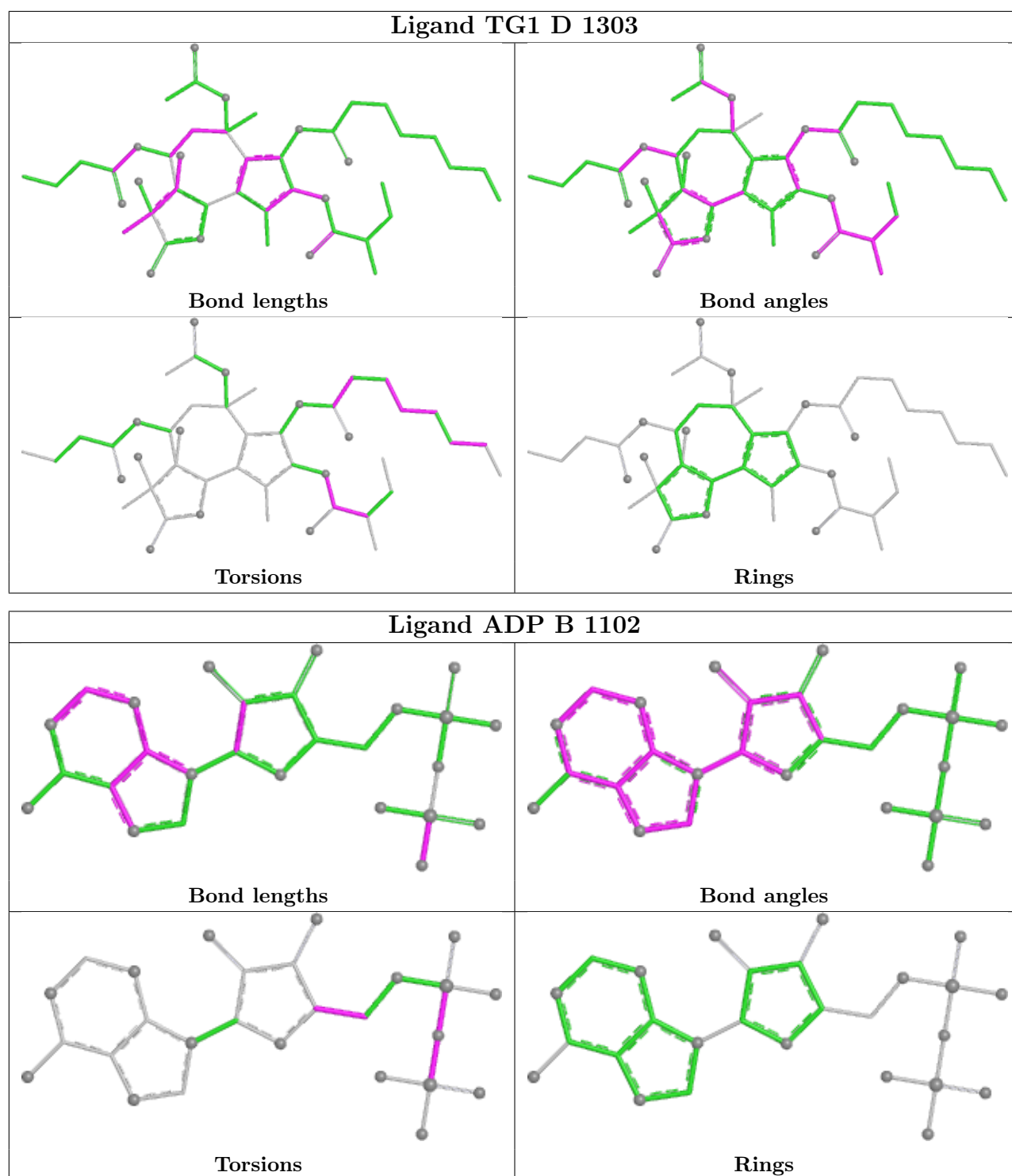
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.