Full wwPDB X-ray Structure Validation Report (i)

Oct 17, 2023 – 03:56 PM EDT

PDB ID	:	2AGV
Title	:	Crystal structure of the SR CA2+-ATPASE with BHQ and TG
Authors	:	Toyoshima, C.; Obara, K.; Norimatsu, Y.
Deposited on	:	2005-07-27
Resolution	:	2.40 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 (i) 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 (1)) were used in the production of this report:

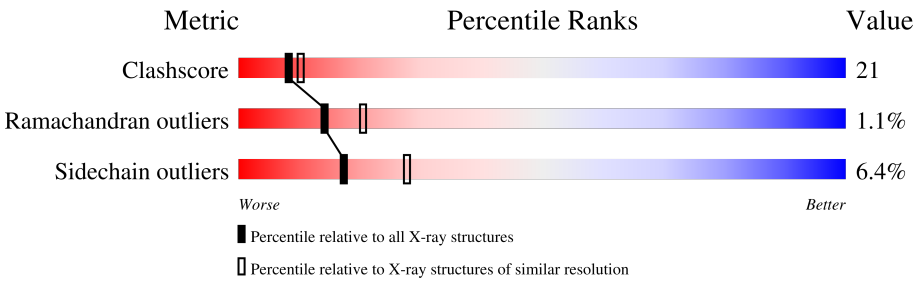
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	994	60% 36% .
1	B	994	61% 35% .

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 15830 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
			Total	C	N	O	S			
1	A	994	7671	4876	1287	1451	57	0	0	0
1	B	994	7671	4876	1287	1451	57	0	0	0

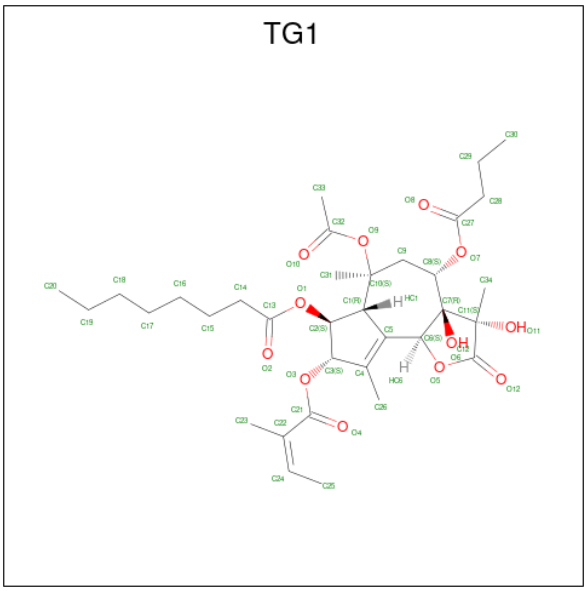
There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

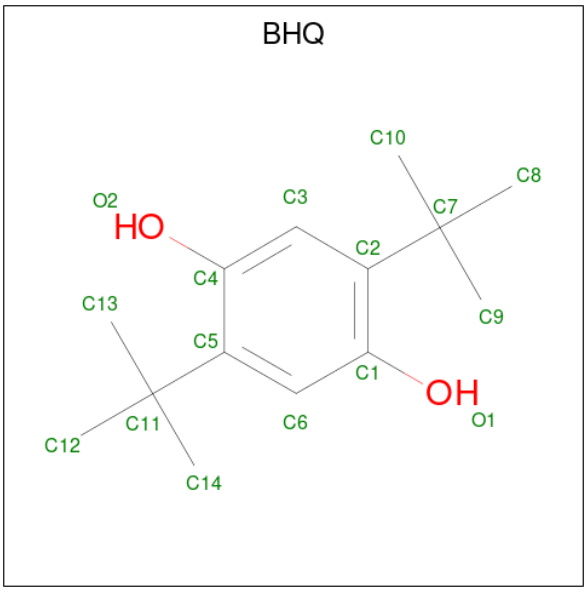
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
2	A	1	1	1	0	0
2	B	1	1	1	0	0

- Molecule 3 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)OX Y]-2-OXO-4-(1-OXOBUTOXY)-AZULENO[4,5-B]FURAN-7-YL ESTER (three-letter code: TG1) (formula: $C_{34}H_{50}O_{12}$).



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

- Molecule 4 is 2,5-DITERT-BUTYLBENZENE-1,4-DIOL (three-letter code: BHQ) (formula: $C_{14}H_{22}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	16	14	2	0	0

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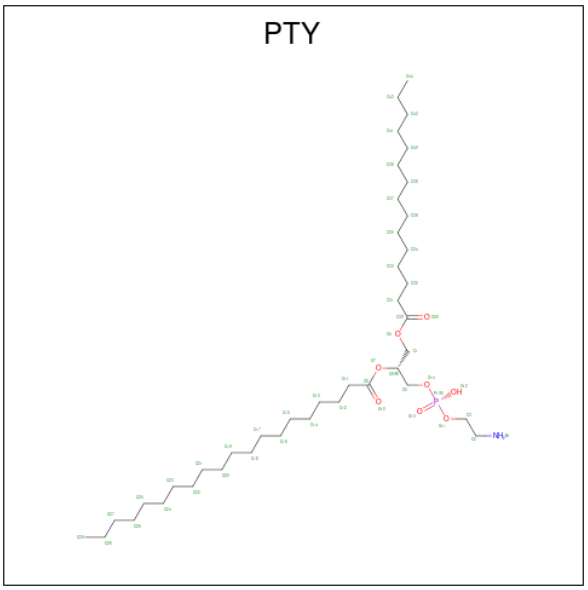
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	B	1	16	14	2	0	0

- Molecule 5 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	19	9	1	8	1	0	0
			Total	C	N	O	P		
5	A	1	19	9	1	8	1	0	0
			Total	C	N	O	P		
5	A	1	19	9	1	8	1	0	0
			Total	C	N	O	P		
5	B	1	19	9	1	8	1	0	0
			Total	C	N	O	P		
5	B	1	19	9	1	8	1	0	0
			Total	C	N	O	P		
5	B	1	19	9	1	8	1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	124	124	124	0	0
			Total	O		
6	B	124	124	124	0	0

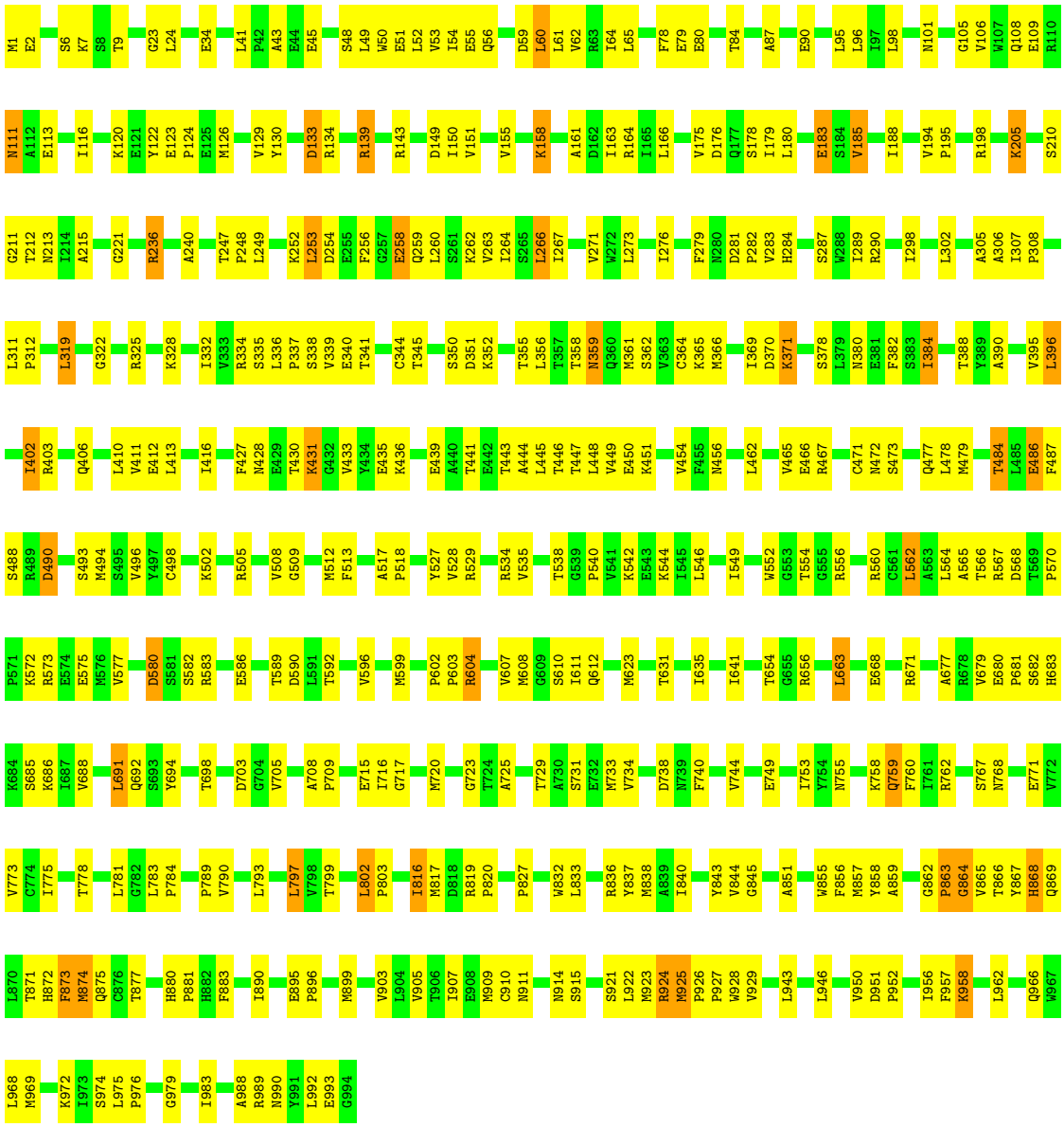
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

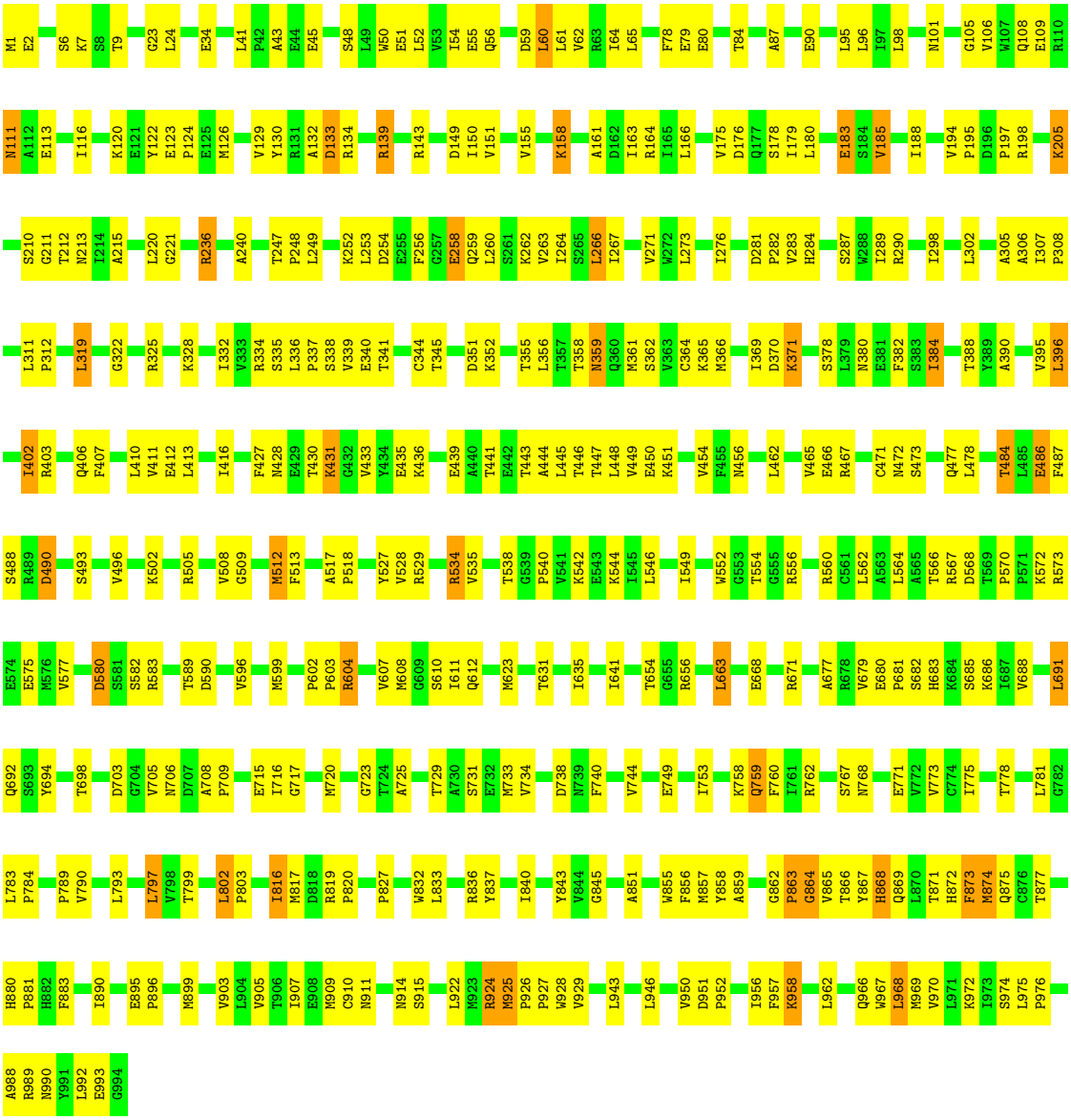
- Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1

Chain A: 60% 36% •



• Molecule 1: Sarcoplasmic/endoplasmic reticulum calcium ATPase 1

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	71.39Å 71.39Å 591.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.98 – 2.40	Depositor
% Data completeness (in resolution range)	99.8 (14.98-2.40)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.239 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15830	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PTY, BHQ, TG1, NA

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	0.42	0/7812	0.64	1/10592 (0.0%)
1	B	0.41	0/7812	0.64	2/10592 (0.0%)
All	All	0.42	0/15624	0.64	3/21184 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	505	ARG	NE-CZ-NH2	7.30	123.95	120.30
1	B	505	ARG	NE-CZ-NH2	7.30	123.95	120.30
1	B	512	MET	CG-SD-CE	5.91	109.65	100.20

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	331	0
1	B	7671	0	7764	330	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	46	0	50	3	0
3	B	46	0	50	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	16	0	22	1	0
4	B	16	0	22	1	0
5	A	57	0	33	2	0
5	B	57	0	33	2	0
6	A	124	0	0	7	0
6	B	124	0	0	7	0
All	All	15830	0	15738	660	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 21.

All (660) 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:B:567:ARG:HD3	1:B:570:PRO:HA	1.42	1.01
1:A:865:VAL:HB	1:A:868:HIS:HB2	1.42	1.01
1:B:865:VAL:HB	1:B:868:HIS:HB2	1.41	0.99
1:A:567:ARG:HD3	1:A:570:PRO:HA	1.42	0.98
1:B:126:MET:HE2	1:B:139:ARG:HD3	1.49	0.94
1:B:260:LEU:HD11	1:B:306:ALA:HB1	1.49	0.94
1:A:538:THR:HG22	1:A:540:PRO:HD2	1.48	0.93
1:B:538:THR:HG22	1:B:540:PRO:HD2	1.49	0.92
1:A:260:LEU:HD11	1:A:306:ALA:HB1	1.49	0.92
1:A:328:LYS:HE2	1:A:328:LYS:HA	1.52	0.92
1:B:328:LYS:HE2	1:B:328:LYS:HA	1.50	0.90
1:A:126:MET:HE2	1:A:139:ARG:HD3	1.54	0.87
1:A:679:VAL:HG13	1:A:683:HIS:HB2	1.57	0.86
1:B:312:PRO:HG2	6:B:3114:HOH:O	1.77	0.85
1:B:679:VAL:HG13	1:B:683:HIS:HB2	1.57	0.84
1:B:56:GLN:OE1	1:B:105:GLY:HA3	1.78	0.84
1:B:663:LEU:HD12	1:B:663:LEU:H	1.43	0.84
1:A:663:LEU:HD12	1:A:663:LEU:H	1.42	0.83
1:A:188:ILE:HD12	1:A:188:ILE:H	1.42	0.83
1:A:312:PRO:HG2	6:A:2114:HOH:O	1.79	0.83
1:B:188:ILE:HD12	1:B:188:ILE:H	1.42	0.83
1:B:865:VAL:HB	1:B:868:HIS:CB	2.10	0.81
1:A:56:GLN:OE1	1:A:105:GLY:HA3	1.80	0.79
1:B:924:ARG:HE	1:B:924:ARG:HA	1.47	0.79
1:A:855:TRP:HA	1:A:859:ALA:HB2	1.64	0.79
1:B:151:VAL:HG21	1:B:163:ILE:HD13	1.64	0.79
1:B:855:TRP:HA	1:B:859:ALA:HB2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:865:VAL:HB	1:A:868:HIS:CB	2.11	0.78
1:A:611:ILE:HD12	1:A:641:ILE:HD11	1.66	0.78
1:B:366:MET:CE	1:B:448:LEU:HD11	2.14	0.78
1:A:924:ARG:HA	1:A:924:ARG:HE	1.47	0.78
1:B:369:ILE:HG13	1:B:528:VAL:CG1	2.14	0.78
1:A:369:ILE:HG13	1:A:528:VAL:CG1	2.14	0.77
1:A:411:VAL:HG22	1:A:454:VAL:HB	1.66	0.77
1:B:668:GLU:O	1:B:671:ARG:HG2	1.85	0.77
1:A:604:ARG:O	1:A:607:VAL:HG22	1.84	0.77
1:A:151:VAL:HG21	1:A:163:ILE:HD13	1.66	0.77
1:B:604:ARG:O	1:B:607:VAL:HG22	1.84	0.77
1:B:411:VAL:HG22	1:B:454:VAL:HB	1.67	0.76
1:A:668:GLU:O	1:A:671:ARG:HG2	1.85	0.76
1:B:183:GLU:HB2	1:B:185:VAL:HG23	1.68	0.76
1:B:48:SER:OG	1:B:51:GLU:HG3	1.86	0.76
1:B:611:ILE:HD12	1:B:641:ILE:HD11	1.68	0.76
1:A:79:GLU:HG2	1:A:80:GLU:H	1.51	0.76
1:B:863:PRO:O	1:B:865:VAL:HG13	1.87	0.75
1:A:366:MET:CE	1:A:448:LEU:HD11	2.17	0.74
1:B:79:GLU:HG2	1:B:80:GLU:H	1.52	0.74
1:A:48:SER:OG	1:A:51:GLU:HG3	1.86	0.74
1:A:863:PRO:O	1:A:865:VAL:HG13	1.86	0.74
1:A:23:GLY:HA3	1:A:130:TYR:O	1.88	0.74
1:B:654:THR:HA	1:B:677:ALA:O	1.87	0.73
1:A:183:GLU:HB2	1:A:185:VAL:HG23	1.69	0.73
1:B:205:LYS:NZ	1:B:205:LYS:HB3	2.04	0.73
1:A:654:THR:HA	1:A:677:ALA:O	1.89	0.72
1:B:366:MET:HE1	1:B:448:LEU:HD11	1.72	0.72
1:A:205:LYS:NZ	1:A:205:LYS:HB3	2.04	0.72
1:B:843:TYR:OH	1:B:976:PRO:HG2	1.90	0.71
1:A:126:MET:CE	1:A:139:ARG:HD3	2.21	0.71
1:A:388:THR:CG2	1:A:390:ALA:HB3	2.21	0.71
1:B:23:GLY:HA3	1:B:130:TYR:O	1.90	0.71
1:A:843:TYR:OH	1:A:976:PRO:HG2	1.91	0.70
1:B:126:MET:CE	1:B:139:ARG:HD3	2.20	0.70
1:B:366:MET:HE1	1:B:448:LEU:HD21	1.73	0.70
1:B:388:THR:CG2	1:B:390:ALA:HB3	2.21	0.70
1:B:129:VAL:HG12	1:B:151:VAL:HG12	1.73	0.70
1:B:880:HIS:N	1:B:881:PRO:HD2	2.07	0.70
1:A:880:HIS:N	1:A:881:PRO:HD2	2.07	0.70
1:B:283:VAL:HG13	1:B:284:HIS:ND1	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:VAL:HG13	1:A:284:HIS:ND1	2.07	0.69
1:A:366:MET:HE1	1:A:448:LEU:HD21	1.75	0.69
1:A:607:VAL:O	1:A:611:ILE:HG12	1.93	0.69
1:B:573:ARG:HG3	6:B:3008:HOH:O	1.92	0.68
1:A:573:ARG:HG3	6:A:2008:HOH:O	1.90	0.68
1:A:129:VAL:HG12	1:A:151:VAL:HG12	1.76	0.68
1:B:607:VAL:O	1:B:611:ILE:HG12	1.93	0.68
1:B:679:VAL:CG1	1:B:683:HIS:HB2	2.23	0.68
1:A:679:VAL:CG1	1:A:683:HIS:HB2	2.23	0.68
1:B:988:ALA:HA	1:B:992:LEU:HD12	1.77	0.67
1:A:311:LEU:N	1:A:312:PRO:HD2	2.10	0.67
1:B:336:LEU:HB2	1:B:337:PRO:HD3	1.77	0.67
1:B:802:LEU:HB2	1:B:803:PRO:HD3	1.77	0.67
1:A:427:PHE:HB3	1:A:465:VAL:HG22	1.77	0.67
1:A:802:LEU:HB2	1:A:803:PRO:HD3	1.76	0.67
1:A:969:MET:HE3	1:A:972:LYS:HB2	1.77	0.66
1:A:988:ALA:HA	1:A:992:LEU:HD12	1.77	0.66
1:B:758:LYS:O	1:B:762:ARG:HG3	1.94	0.66
1:B:311:LEU:N	1:B:312:PRO:HD2	2.11	0.66
1:B:427:PHE:HB3	1:B:465:VAL:HG22	1.78	0.66
1:B:873:PHE:HB2	1:B:875:GLN:HE21	1.61	0.66
1:B:671:ARG:HD2	1:B:694:TYR:CZ	2.31	0.66
1:B:176:ASP:O	1:B:212:THR:HG23	1.96	0.66
1:A:176:ASP:O	1:A:212:THR:HG23	1.96	0.65
1:A:336:LEU:HB2	1:A:337:PRO:HD3	1.78	0.65
1:A:758:LYS:O	1:A:762:ARG:HG3	1.96	0.65
1:B:446:THR:O	1:B:449:VAL:HG22	1.97	0.65
1:A:446:THR:O	1:A:449:VAL:HG22	1.96	0.65
1:B:90:GLU:OE1	1:B:789:PRO:HG2	1.96	0.64
1:B:180:LEU:HA	1:B:705:VAL:HG22	1.79	0.64
1:A:671:ARG:HD2	1:A:694:TYR:CZ	2.32	0.64
1:A:943:LEU:O	1:A:946:LEU:HB3	1.97	0.64
1:B:402:ILE:HD13	1:B:402:ILE:H	1.60	0.64
1:A:366:MET:HE1	1:A:448:LEU:HD11	1.77	0.64
1:A:402:ILE:HD13	1:A:402:ILE:H	1.61	0.64
1:B:899:MET:O	1:B:903:VAL:HG23	1.98	0.64
1:B:969:MET:HE3	1:B:972:LYS:HB2	1.79	0.64
1:A:188:ILE:HD12	1:A:188:ILE:N	2.11	0.64
1:B:943:LEU:O	1:B:946:LEU:HB3	1.98	0.64
1:A:899:MET:O	1:A:903:VAL:HG23	1.98	0.64
1:A:90:GLU:OE1	1:A:789:PRO:HG2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:873:PHE:HB2	1:A:875:GLN:HE21	1.62	0.64
1:B:395:VAL:C	1:B:396:LEU:HD23	2.19	0.64
1:A:395:VAL:C	1:A:396:LEU:HD23	2.19	0.63
1:A:922:LEU:HD22	1:A:927:PRO:HG3	1.79	0.63
1:B:513:PHE:HD1	1:B:566:THR:HG22	1.62	0.63
1:A:484:THR:HB	1:A:496:VAL:HG12	1.80	0.63
1:B:922:LEU:HD22	1:B:927:PRO:HG3	1.79	0.63
1:A:50:TRP:O	1:A:54:ILE:HG12	1.99	0.63
1:A:513:PHE:HD1	1:A:566:THR:HG22	1.65	0.62
1:A:716:ILE:HD12	1:A:716:ILE:N	2.13	0.62
1:B:335:SER:HB3	1:B:338:SER:OG	1.98	0.62
1:A:335:SER:HB3	1:A:338:SER:OG	1.99	0.62
1:B:857:MET:HA	1:B:865:VAL:H	1.64	0.62
1:A:260:LEU:O	1:A:264:ILE:HG13	2.00	0.62
1:B:924:ARG:HA	1:B:924:ARG:NE	2.14	0.62
1:B:260:LEU:O	1:B:264:ILE:HG13	2.00	0.62
1:B:188:ILE:HD12	1:B:188:ILE:N	2.11	0.62
1:A:679:VAL:HG13	1:A:683:HIS:CB	2.29	0.61
1:B:370:ASP:HB3	1:B:378:SER:OG	2.00	0.61
1:A:924:ARG:HA	1:A:924:ARG:NE	2.15	0.61
1:B:484:THR:HB	1:B:496:VAL:HG12	1.81	0.61
1:A:111:ASN:HD22	1:A:111:ASN:H	1.49	0.61
1:A:857:MET:HA	1:A:865:VAL:H	1.66	0.61
1:B:679:VAL:HG13	1:B:683:HIS:CB	2.30	0.61
1:A:180:LEU:HA	1:A:705:VAL:HG22	1.81	0.61
1:A:205:LYS:HB3	1:A:205:LYS:HZ3	1.65	0.61
1:A:151:VAL:HG21	1:A:163:ILE:CD1	2.30	0.61
1:B:832:TRP:CD1	1:B:988:ALA:HB2	2.36	0.61
1:B:50:TRP:O	1:B:54:ILE:HG12	2.00	0.61
1:B:205:LYS:HB3	1:B:205:LYS:HZ3	1.65	0.61
1:A:370:ASP:HB3	1:A:378:SER:OG	2.01	0.61
1:A:631:THR:O	1:A:635:ILE:HG13	2.01	0.61
1:A:962:LEU:HB3	1:A:966:GLN:HB2	1.83	0.61
1:B:24:LEU:HD12	1:B:149:ASP:HB3	1.81	0.60
1:B:111:ASN:HD22	1:B:111:ASN:H	1.49	0.60
1:A:534:ARG:HG2	1:A:535:VAL:N	2.16	0.60
1:B:161:ALA:HA	1:B:210:SER:HB2	1.83	0.60
1:B:449:VAL:HG21	1:B:472:ASN:OD1	2.02	0.60
1:B:680:GLU:HB3	1:B:681:PRO:HD2	1.84	0.60
1:B:962:LEU:HB3	1:B:966:GLN:HB2	1.83	0.60
1:A:24:LEU:HD12	1:A:149:ASP:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:716:ILE:N	1:B:716:ILE:HD12	2.16	0.60
1:B:534:ARG:HG2	1:B:535:VAL:N	2.16	0.60
1:A:441:THR:HG23	1:A:599:MET:SD	2.41	0.59
1:A:161:ALA:HA	1:A:210:SER:HB2	1.84	0.59
1:A:428:ASN:HB2	1:A:435:GLU:HG3	1.84	0.59
1:A:212:THR:HG22	1:A:213:ASN:N	2.18	0.59
1:B:428:ASN:HB2	1:B:435:GLU:HG3	1.84	0.59
1:A:680:GLU:HB3	1:A:681:PRO:HD2	1.84	0.59
1:A:518:PRO:HB3	1:A:549:ILE:HD13	1.84	0.59
1:A:759:GLN:HG3	1:A:915:SER:O	2.03	0.59
1:A:260:LEU:HD21	1:A:307:ILE:HD13	1.84	0.59
1:B:212:THR:HG22	1:B:213:ASN:N	2.16	0.59
1:B:441:THR:HG23	1:B:599:MET:SD	2.43	0.59
1:A:262:LYS:HE3	1:A:266:LEU:HD23	1.84	0.59
1:A:832:TRP:CD1	1:A:988:ALA:HB2	2.37	0.59
1:B:260:LEU:HD21	1:B:307:ILE:HD13	1.84	0.59
1:B:259:GLN:O	1:B:263:VAL:HG23	2.03	0.59
1:B:395:VAL:HG12	1:B:402:ILE:HD11	1.85	0.59
1:B:816:ILE:HG22	1:B:817:MET:N	2.17	0.59
1:A:254:ASP:O	1:A:258:GLU:HG2	2.04	0.58
1:A:395:VAL:HG12	1:A:402:ILE:HD11	1.85	0.58
1:A:890:ILE:C	1:A:890:ILE:HD12	2.24	0.58
1:B:151:VAL:HG21	1:B:163:ILE:CD1	2.32	0.58
1:B:793:LEU:O	1:B:797:LEU:HB2	2.03	0.58
1:A:793:LEU:O	1:A:797:LEU:HB2	2.03	0.58
1:A:816:ILE:HG22	1:A:817:MET:N	2.18	0.58
1:B:267:ILE:O	1:B:271:VAL:HG23	2.03	0.58
1:B:518:PRO:HB3	1:B:549:ILE:HD13	1.85	0.58
1:A:725:ALA:O	1:A:729:THR:HG23	2.03	0.58
1:A:869:GLN:HB3	1:A:872:HIS:HB2	1.86	0.58
1:A:604:ARG:HG3	1:A:604:ARG:HH11	1.69	0.58
1:B:260:LEU:HD13	3:B:1103:TG1:H252	1.86	0.58
1:B:925:MET:HE2	1:B:929:VAL:HG21	1.86	0.58
1:A:259:GLN:O	1:A:263:VAL:HG23	2.03	0.58
1:B:725:ALA:O	1:B:729:THR:HG23	2.04	0.58
1:B:51:GLU:O	1:B:55:GLU:HG3	2.04	0.57
1:B:388:THR:HG21	1:B:390:ALA:HB3	1.85	0.57
1:B:589:THR:HG22	1:B:590:ASP:N	2.18	0.57
1:A:388:THR:HG21	1:A:390:ALA:HB3	1.86	0.57
1:B:631:THR:O	1:B:635:ILE:HG13	2.03	0.57
1:B:668:GLU:OE1	1:B:671:ARG:HD3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ILE:O	1:A:271:VAL:HG23	2.05	0.57
1:A:51:GLU:O	1:A:55:GLU:HG3	2.04	0.57
1:B:890:ILE:HD12	1:B:890:ILE:C	2.25	0.57
1:B:262:LYS:HE3	1:B:266:LEU:HD23	1.86	0.57
1:B:388:THR:HG23	1:B:390:ALA:HB3	1.87	0.57
1:B:663:LEU:H	1:B:663:LEU:CD1	2.17	0.57
1:B:869:GLN:HB3	1:B:872:HIS:HB2	1.86	0.57
1:B:254:ASP:O	1:B:258:GLU:HG2	2.05	0.57
1:A:412:GLU:OE1	1:A:529:ARG:HD2	2.04	0.57
1:B:332:ILE:HB	1:B:734:VAL:HB	1.87	0.57
1:B:720:MET:HE1	1:B:738:ASP:O	2.05	0.57
1:B:836:ARG:O	1:B:840:ILE:HG12	2.05	0.57
1:A:388:THR:HG23	1:A:390:ALA:HB3	1.86	0.56
1:A:720:MET:HE3	1:A:738:ASP:CB	2.35	0.56
1:B:527:TYR:CD1	1:B:534:ARG:HD3	2.39	0.56
1:A:352:LYS:HG3	1:A:623:MET:HE2	1.87	0.56
1:B:759:GLN:HG3	1:B:915:SER:O	2.04	0.56
1:A:449:VAL:HG21	1:A:472:ASN:OD1	2.05	0.56
1:A:816:ILE:HG22	1:A:817:MET:HG2	1.88	0.56
1:A:836:ARG:O	1:A:840:ILE:HG12	2.04	0.56
1:B:924:ARG:O	1:B:926:PRO:HD3	2.05	0.56
1:A:863:PRO:HG2	1:A:890:ILE:HD13	1.88	0.56
1:B:122:TYR:O	1:B:211:GLY:HA2	2.06	0.56
1:A:290:ARG:HH22	1:A:875:GLN:HA	1.70	0.56
1:A:668:GLU:OE1	1:A:671:ARG:HD3	2.05	0.56
1:A:905:VAL:O	1:A:909:MET:HG2	2.06	0.56
1:B:412:GLU:OE1	1:B:529:ARG:HD2	2.06	0.56
1:A:308:PRO:HB3	1:A:768:ASN:OD1	2.06	0.56
1:A:527:TYR:CD1	1:A:534:ARG:HD3	2.41	0.56
1:B:749:GLU:O	1:B:753:ILE:HG12	2.05	0.56
1:B:290:ARG:HH22	1:B:875:GLN:HA	1.70	0.56
1:B:863:PRO:HG2	1:B:890:ILE:HD13	1.88	0.56
1:A:260:LEU:HD13	3:A:1003:TG1:H252	1.88	0.55
1:A:287:SER:HB2	1:A:290:ARG:HE	1.71	0.55
1:A:332:ILE:HB	1:A:734:VAL:HB	1.88	0.55
1:B:416:ILE:HD11	1:B:566:THR:HG23	1.88	0.55
1:B:688:VAL:O	1:B:692:GLN:HG3	2.06	0.55
1:A:305:ALA:HB1	1:A:771:GLU:HB3	1.89	0.55
1:B:703:ASP:HB3	6:B:3086:HOH:O	2.07	0.55
1:A:175:VAL:CG1	1:A:212:THR:HG21	2.36	0.55
1:A:589:THR:HG22	1:A:590:ASP:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:720:MET:HE1	1:A:738:ASP:O	2.06	0.55
1:B:572:LYS:HB2	1:B:575:GLU:HG2	1.88	0.55
1:A:869:GLN:HB3	1:A:872:HIS:CB	2.37	0.55
1:A:133:ASP:O	1:A:134:ARG:HG3	2.07	0.55
1:A:188:ILE:H	1:A:188:ILE:CD1	2.18	0.55
1:A:198:ARG:HG2	1:A:198:ARG:HH11	1.72	0.55
1:A:688:VAL:O	1:A:692:GLN:HG3	2.07	0.55
1:B:198:ARG:HG2	1:B:198:ARG:HH11	1.72	0.55
1:A:990:ASN:HD21	5:A:1012:PTY:HC22	1.72	0.55
1:B:869:GLN:HB3	1:B:872:HIS:CB	2.37	0.55
1:A:975:LEU:N	1:A:976:PRO:HD2	2.23	0.54
1:B:175:VAL:CG1	1:B:212:THR:HG21	2.37	0.54
1:B:975:LEU:N	1:B:976:PRO:HD2	2.22	0.54
1:A:256:PHE:HB2	3:A:1003:TG1:H291	1.88	0.54
1:A:703:ASP:HB3	6:A:2086:HOH:O	2.07	0.54
1:A:925:MET:HE2	1:A:929:VAL:HG21	1.89	0.54
1:B:287:SER:HB2	1:B:290:ARG:HE	1.72	0.54
1:B:990:ASN:HD21	5:B:1112:PTY:HC22	1.72	0.54
1:A:338:SER:O	1:A:341:THR:HG22	2.07	0.54
1:A:924:ARG:O	1:A:926:PRO:HD3	2.06	0.54
1:B:542:LYS:O	1:B:546:LEU:HG	2.08	0.54
1:B:554:THR:HG22	1:B:554:THR:O	2.07	0.54
1:A:122:TYR:O	1:A:211:GLY:HA2	2.07	0.54
1:A:161:ALA:CA	1:A:210:SER:HB2	2.38	0.54
1:A:974:SER:C	1:A:976:PRO:HD2	2.28	0.54
1:B:41:LEU:HD23	1:B:236:ARG:HG3	1.89	0.54
1:B:133:ASP:O	1:B:134:ARG:HG3	2.07	0.54
1:B:161:ALA:CA	1:B:210:SER:HB2	2.37	0.54
1:B:816:ILE:HG22	1:B:817:MET:HG2	1.90	0.54
1:A:60:LEU:O	1:A:64:ILE:HG12	2.08	0.54
1:A:749:GLU:O	1:A:753:ILE:HG12	2.08	0.54
1:B:338:SER:O	1:B:341:THR:HG22	2.07	0.54
1:B:720:MET:HE3	1:B:738:ASP:CB	2.38	0.54
1:B:773:VAL:HG12	1:B:845:GLY:HA3	1.90	0.54
1:B:60:LEU:O	1:B:64:ILE:HG12	2.08	0.53
1:A:325:ARG:HH12	1:A:753:ILE:CD1	2.21	0.53
1:A:663:LEU:H	1:A:663:LEU:CD1	2.17	0.53
1:A:799:THR:HG21	1:A:905:VAL:HG22	1.89	0.53
1:B:256:PHE:HB2	3:B:1103:TG1:H291	1.89	0.53
1:B:335:SER:O	1:B:338:SER:HB2	2.09	0.53
1:B:762:ARG:HD2	1:B:833:LEU:HD21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:905:VAL:O	1:B:909:MET:HG2	2.08	0.53
1:B:799:THR:HG21	1:B:905:VAL:HG22	1.91	0.53
1:A:335:SER:O	1:A:338:SER:HB2	2.09	0.53
1:A:441:THR:HG21	1:A:560:ARG:NH1	2.24	0.53
1:B:604:ARG:HG3	1:B:604:ARG:HH11	1.73	0.53
1:A:416:ILE:HD11	1:A:566:THR:HG23	1.91	0.53
1:A:542:LYS:O	1:A:546:LEU:HG	2.09	0.53
1:B:974:SER:C	1:B:976:PRO:HD2	2.29	0.53
1:A:41:LEU:HD23	1:A:236:ARG:HG3	1.90	0.52
1:B:247:THR:HG21	1:B:337:PRO:O	2.08	0.52
1:B:249:LEU:O	1:B:253:LEU:HB2	2.09	0.52
1:A:108:GLN:HA	1:A:111:ASN:HD21	1.75	0.52
1:A:247:THR:HG21	1:A:337:PRO:O	2.09	0.52
1:B:108:GLN:HA	1:B:111:ASN:HD21	1.74	0.52
1:B:416:ILE:HD11	1:B:566:THR:CG2	2.39	0.52
1:A:43:ALA:HA	1:A:120:LYS:NZ	2.25	0.52
1:B:325:ARG:HH12	1:B:753:ILE:CD1	2.22	0.52
1:B:911:ASN:HA	1:B:914:ASN:HD22	1.74	0.52
1:A:369:ILE:HG13	1:A:528:VAL:HG13	1.91	0.52
1:B:305:ALA:HB1	1:B:771:GLU:HB3	1.91	0.52
1:B:308:PRO:HB3	1:B:768:ASN:OD1	2.10	0.52
1:B:355:THR:HG22	1:B:740:PHE:HB2	1.91	0.52
1:A:61:LEU:HD22	1:A:307:ILE:CD1	2.40	0.52
1:A:249:LEU:O	1:A:253:LEU:HB2	2.09	0.52
1:A:762:ARG:HD2	1:A:833:LEU:HD21	1.92	0.52
1:B:895:GLU:N	1:B:896:PRO:HD2	2.25	0.52
1:A:554:THR:O	1:A:554:THR:HG22	2.09	0.52
1:A:851:ALA:CB	1:A:903:VAL:HG21	2.40	0.52
1:B:827:PRO:HB3	6:B:3104:HOH:O	2.10	0.52
1:A:236:ARG:HD3	1:A:236:ARG:C	2.30	0.51
1:B:1:MET:CE	1:B:7:LYS:HG3	2.40	0.51
1:B:441:THR:HG21	1:B:560:ARG:NH1	2.25	0.51
1:A:604:ARG:HB2	1:A:607:VAL:HG13	1.92	0.51
1:B:784:PRO:HG3	1:B:874:MET:SD	2.50	0.51
1:B:851:ALA:CB	1:B:903:VAL:HG21	2.41	0.51
1:B:336:LEU:O	1:B:339:VAL:HG22	2.10	0.51
1:A:895:GLU:N	1:A:896:PRO:HD2	2.26	0.51
1:B:449:VAL:HG21	1:B:472:ASN:CG	2.31	0.51
1:A:365:LYS:HB3	1:A:552:TRP:CH2	2.45	0.51
1:A:416:ILE:HD11	1:A:566:THR:CG2	2.40	0.51
1:A:819:ARG:HB2	1:A:820:PRO:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:O	1:B:1:MET:HG2	2.11	0.51
1:A:166:LEU:H	1:A:221:GLY:HA2	1.76	0.51
1:A:911:ASN:HA	1:A:914:ASN:HD22	1.76	0.51
1:B:166:LEU:H	1:B:221:GLY:HA2	1.76	0.51
1:A:395:VAL:O	1:A:396:LEU:HD23	2.11	0.51
1:B:43:ALA:HA	1:B:120:LYS:NZ	2.26	0.51
1:B:328:LYS:HA	1:B:328:LYS:CE	2.33	0.51
1:A:572:LYS:HB2	1:A:575:GLU:HG2	1.92	0.51
1:B:365:LYS:HB3	1:B:552:TRP:CH2	2.46	0.51
1:B:708:ALA:HB3	1:B:709:PRO:HD3	1.93	0.51
1:A:370:ASP:O	1:A:371:LYS:HB3	2.11	0.50
1:B:61:LEU:HD22	1:B:307:ILE:CD1	2.40	0.50
1:A:827:PRO:HB3	6:A:2104:HOH:O	2.10	0.50
1:B:271:VAL:HG11	1:B:298:ILE:HD11	1.92	0.50
1:B:604:ARG:HB2	1:B:607:VAL:HG13	1.94	0.50
1:A:1:MET:CE	1:A:7:LYS:HG3	2.41	0.50
1:B:403:ARG:HD3	1:B:456:ASN:HD21	1.75	0.50
1:A:449:VAL:HG21	1:A:472:ASN:CG	2.31	0.50
1:B:236:ARG:C	1:B:236:ARG:HD3	2.32	0.50
1:A:1:MET:HG2	1:A:1:MET:O	2.11	0.50
1:A:271:VAL:HG11	1:A:298:ILE:HD11	1.94	0.50
1:A:473:SER:O	1:A:477:GLN:HG2	2.12	0.50
1:A:773:VAL:HG12	1:A:845:GLY:HA3	1.94	0.50
1:B:402:ILE:HD13	1:B:402:ILE:N	2.27	0.50
1:A:279:PHE:HB3	1:B:50:TRP:HB2	1.94	0.50
1:A:403:ARG:HD3	1:A:456:ASN:HD21	1.76	0.50
1:B:52:LEU:HD21	1:B:106:VAL:HA	1.94	0.50
1:B:395:VAL:O	1:B:396:LEU:HD23	2.12	0.49
1:B:819:ARG:HB2	1:B:820:PRO:HD2	1.93	0.49
1:A:52:LEU:HD11	1:A:109:GLU:HG3	1.94	0.49
1:A:59:ASP:HB3	1:A:62:VAL:HG22	1.94	0.49
1:A:188:ILE:HG12	1:A:486:GLU:HG2	1.94	0.49
1:A:355:THR:HG22	1:A:740:PHE:HB2	1.93	0.49
1:A:862:GLY:O	1:A:864:GLY:N	2.44	0.49
1:B:790:VAL:HG12	1:B:957:PHE:CD1	2.48	0.49
1:A:790:VAL:HG12	1:A:957:PHE:CD1	2.48	0.49
1:B:358:THR:OG1	1:B:602:PRO:HG2	2.12	0.49
1:A:98:LEU:O	1:A:101:ASN:HB3	2.13	0.49
1:A:336:LEU:O	1:A:339:VAL:HG22	2.12	0.49
1:A:867:TYR:C	1:A:869:GLN:H	2.15	0.49
1:B:370:ASP:O	1:B:371:LYS:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:784:PRO:HG3	1:A:874:MET:SD	2.53	0.49
1:B:334:ARG:HD3	1:B:731:SER:O	2.12	0.49
1:B:682:SER:O	1:B:686:LYS:HG3	2.13	0.49
1:A:338:SER:HA	1:A:341:THR:HG22	1.95	0.48
1:B:6:SER:HA	1:B:194:VAL:O	2.12	0.48
1:A:366:MET:HE3	1:A:384:ILE:CD1	2.43	0.48
1:A:723:GLY:HA3	6:A:2086:HOH:O	2.12	0.48
1:B:611:ILE:HD12	1:B:641:ILE:CD1	2.42	0.48
1:B:52:LEU:HD11	1:B:109:GLU:HG3	1.95	0.48
1:A:52:LEU:HD21	1:A:106:VAL:HA	1.94	0.48
1:A:351:ASP:O	1:A:356:LEU:HD13	2.14	0.48
1:A:682:SER:O	1:A:686:LYS:HG3	2.13	0.48
1:B:41:LEU:N	1:B:41:LEU:HD12	2.28	0.48
1:B:188:ILE:HG12	1:B:486:GLU:HG2	1.94	0.48
1:A:366:MET:CE	1:A:448:LEU:HD21	2.43	0.48
1:A:567:ARG:CD	1:A:570:PRO:HA	2.30	0.48
1:B:98:LEU:O	1:B:101:ASN:HB3	2.14	0.48
1:B:322:GLY:O	1:B:325:ARG:HB3	2.13	0.48
1:B:380:ASN:O	1:B:382:PHE:CD1	2.66	0.48
1:A:952:PRO:O	1:A:956:ILE:HG13	2.13	0.48
1:B:880:HIS:N	1:B:881:PRO:CD	2.76	0.48
1:A:325:ARG:NH1	1:A:753:ILE:CD1	2.77	0.48
1:A:358:THR:OG1	1:A:602:PRO:HG2	2.13	0.48
1:B:473:SER:O	1:B:477:GLN:HG2	2.13	0.48
1:A:366:MET:HA	1:A:596:VAL:O	2.14	0.48
1:A:175:VAL:CG1	1:A:212:THR:CG2	2.91	0.48
1:A:867:TYR:O	1:A:869:GLN:N	2.46	0.48
1:B:78:PHE:HE2	1:B:289:ILE:HD11	1.79	0.48
1:B:325:ARG:NH1	1:B:753:ILE:CD1	2.77	0.48
1:B:867:TYR:C	1:B:869:GLN:H	2.15	0.48
1:A:388:THR:HG23	1:A:390:ALA:N	2.29	0.48
1:A:708:ALA:HB3	1:A:709:PRO:HD3	1.96	0.48
1:B:388:THR:HG23	1:B:390:ALA:N	2.29	0.48
1:B:512:MET:O	1:B:566:THR:HA	2.14	0.48
1:A:79:GLU:HG2	1:A:80:GLU:N	2.24	0.47
1:A:858:TYR:CD1	1:A:858:TYR:N	2.82	0.47
1:B:338:SER:HA	1:B:341:THR:HG22	1.96	0.47
1:B:858:TYR:CD1	1:B:858:TYR:N	2.82	0.47
1:B:79:GLU:HG2	1:B:80:GLU:N	2.24	0.47
1:A:447:THR:HG22	1:A:451:LYS:HE3	1.96	0.47
1:A:691:LEU:HD23	1:A:698:THR:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:ASN:HD22	1:B:111:ASN:N	2.10	0.47
1:B:447:THR:HG22	1:B:451:LYS:HE3	1.96	0.47
1:A:198:ARG:HG2	1:A:198:ARG:NH1	2.29	0.47
1:A:252:LYS:HE3	6:A:2104:HOH:O	2.15	0.47
1:A:325:ARG:NH1	1:A:753:ILE:HD11	2.29	0.47
1:A:334:ARG:HD3	1:A:731:SER:O	2.14	0.47
1:A:402:ILE:HD13	1:A:402:ILE:N	2.28	0.47
1:A:529:ARG:HH22	1:A:568:ASP:CG	2.18	0.47
1:A:604:ARG:HH11	1:A:604:ARG:CG	2.27	0.47
1:A:880:HIS:N	1:A:881:PRO:CD	2.76	0.47
1:B:352:LYS:HG3	1:B:623:MET:HE2	1.96	0.47
1:A:380:ASN:O	1:A:382:PHE:CD1	2.68	0.47
1:B:361:MET:HB3	1:B:444:ALA:HB2	1.97	0.47
1:A:720:MET:HE3	1:A:738:ASP:HB3	1.97	0.47
1:B:41:LEU:HD13	1:B:123:GLU:OE1	2.15	0.47
1:B:773:VAL:CG1	1:B:845:GLY:HA3	2.45	0.47
1:B:867:TYR:O	1:B:869:GLN:N	2.46	0.47
1:A:111:ASN:HD22	1:A:111:ASN:N	2.09	0.47
1:A:322:GLY:O	1:A:325:ARG:HB3	2.14	0.47
1:A:512:MET:O	1:A:566:THR:HA	2.14	0.47
1:A:855:TRP:O	1:A:859:ALA:HB3	2.15	0.47
1:B:837:TYR:HB2	3:B:1103:TG1:H333	1.97	0.47
1:A:61:LEU:HD22	1:A:307:ILE:HD11	1.96	0.46
1:B:188:ILE:CG1	1:B:486:GLU:HG2	2.45	0.46
1:B:325:ARG:NH1	1:B:753:ILE:HD11	2.31	0.46
1:B:328:LYS:HE2	1:B:328:LYS:CA	2.35	0.46
1:A:188:ILE:HD13	1:A:486:GLU:HG2	1.96	0.46
1:A:188:ILE:CG1	1:A:486:GLU:HG2	2.44	0.46
1:A:403:ARG:HB3	1:A:406:GLN:OE1	2.15	0.46
1:B:59:ASP:HB3	1:B:62:VAL:HG22	1.97	0.46
1:A:41:LEU:HD12	1:A:41:LEU:N	2.30	0.46
1:A:311:LEU:N	1:A:312:PRO:CD	2.78	0.46
1:B:61:LEU:HD22	1:B:307:ILE:HD11	1.97	0.46
1:B:175:VAL:CG1	1:B:212:THR:CG2	2.93	0.46
1:B:188:ILE:H	1:B:188:ILE:CD1	2.18	0.46
1:B:403:ARG:HD3	1:B:456:ASN:OD1	2.15	0.46
1:B:723:GLY:HA3	6:B:3086:HOH:O	2.14	0.46
1:A:78:PHE:HE2	1:A:289:ILE:HD11	1.79	0.46
1:A:403:ARG:HD3	1:A:456:ASN:OD1	2.15	0.46
1:A:611:ILE:HD12	1:A:641:ILE:CD1	2.41	0.46
1:A:837:TYR:HB2	3:A:1003:TG1:H333	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:VAL:HG23	1:B:215:ALA:O	2.16	0.46
1:B:198:ARG:HG2	1:B:198:ARG:NH1	2.29	0.46
1:B:403:ARG:HB3	1:B:406:GLN:OE1	2.15	0.46
1:B:952:PRO:O	1:B:956:ILE:HG13	2.16	0.46
1:A:577:VAL:HG23	1:A:583:ARG:NH1	2.30	0.46
1:B:351:ASP:O	1:B:356:LEU:HD13	2.15	0.46
1:B:462:LEU:HB3	1:B:466:GLU:HB2	1.98	0.46
1:B:691:LEU:HD23	1:B:698:THR:HG21	1.97	0.46
1:B:65:LEU:HD12	4:B:1104:BHQ:H91	1.98	0.46
1:A:344:CYS:O	1:A:345:THR:C	2.54	0.46
1:B:366:MET:HA	1:B:596:VAL:O	2.16	0.46
1:A:155:VAL:HG23	1:A:215:ALA:O	2.16	0.46
1:A:462:LEU:HB3	1:A:466:GLU:HB2	1.98	0.46
1:B:527:TYR:HB3	1:B:534:ARG:CG	2.47	0.46
1:B:862:GLY:O	1:B:864:GLY:N	2.45	0.46
1:A:41:LEU:HD13	1:A:123:GLU:OE1	2.16	0.45
1:A:958:LYS:HE3	1:A:958:LYS:N	2.31	0.45
1:B:369:ILE:HG13	1:B:528:VAL:HG13	1.93	0.45
1:A:212:THR:CG2	1:A:213:ASN:N	2.80	0.45
1:B:344:CYS:O	1:B:345:THR:C	2.55	0.45
1:B:975:LEU:CD2	1:B:975:LEU:H	2.29	0.45
1:A:6:SER:HA	1:A:194:VAL:O	2.15	0.45
1:A:439:GLU:OE1	1:A:439:GLU:HA	2.16	0.45
1:A:975:LEU:H	1:A:975:LEU:CD2	2.29	0.45
1:B:663:LEU:HD12	1:B:663:LEU:N	2.23	0.45
1:A:663:LEU:HD12	1:A:663:LEU:N	2.23	0.45
1:A:950:VAL:HG12	1:A:952:PRO:HD2	1.98	0.45
1:A:388:THR:HG23	1:A:390:ALA:H	1.82	0.45
1:A:715:GLU:CB	1:A:716:ILE:HD12	2.47	0.45
1:B:358:THR:O	1:B:359:ASN:HB3	2.17	0.45
1:B:589:THR:CG2	1:B:590:ASP:N	2.80	0.45
1:B:212:THR:CG2	1:B:213:ASN:N	2.78	0.45
1:B:950:VAL:O	1:B:952:PRO:HD2	2.16	0.45
1:B:439:GLU:HA	1:B:439:GLU:OE1	2.17	0.45
1:B:855:TRP:O	1:B:859:ALA:HB3	2.15	0.45
1:A:366:MET:HE3	1:A:384:ILE:HD11	1.98	0.45
1:B:413:LEU:HD22	1:B:564:LEU:HD12	1.98	0.45
1:B:450:GLU:OE2	1:B:471:CYS:HB2	2.17	0.45
1:B:262:LYS:CE	1:B:266:LEU:HD23	2.47	0.45
1:B:366:MET:CE	1:B:448:LEU:HD21	2.45	0.45
1:B:388:THR:HG23	1:B:390:ALA:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:857:MET:HB2	1:B:858:TYR:CD1	2.52	0.45
1:A:361:MET:HB3	1:A:444:ALA:HB2	1.99	0.45
1:B:252:LYS:HE3	6:B:3104:HOH:O	2.16	0.45
1:B:436:LYS:HB2	1:B:443:THR:HG21	1.99	0.45
1:A:273:LEU:HA	1:A:276:ILE:HD11	1.99	0.44
1:A:816:ILE:CG2	1:A:817:MET:N	2.80	0.44
1:B:577:VAL:HG23	1:B:583:ARG:NH1	2.31	0.44
1:B:720:MET:HE3	1:B:738:ASP:HB3	1.99	0.44
1:A:194:VAL:HA	1:A:195:PRO:HD2	1.75	0.44
1:A:950:VAL:O	1:A:952:PRO:HD2	2.16	0.44
1:B:950:VAL:HG12	1:B:952:PRO:HD2	1.99	0.44
1:A:413:LEU:HD22	1:A:564:LEU:HD12	1.99	0.44
1:A:450:GLU:OE2	1:A:471:CYS:HB2	2.16	0.44
1:A:926:PRO:HA	1:A:927:PRO:HD3	1.88	0.44
1:B:188:ILE:HD13	1:B:486:GLU:HG2	1.99	0.44
1:A:176:ASP:OD1	1:A:178:SER:HB2	2.18	0.44
1:A:527:TYR:HB3	1:A:534:ARG:CG	2.47	0.44
1:A:865:VAL:HB	1:A:868:HIS:CG	2.52	0.44
1:B:126:MET:HB3	1:B:126:MET:HE3	1.87	0.44
1:B:273:LEU:HA	1:B:276:ILE:HD11	2.00	0.44
1:A:65:LEU:HD12	4:A:1004:BHQ:H91	1.99	0.44
1:A:462:LEU:HD22	1:A:466:GLU:HB3	2.00	0.44
1:B:248:PRO:HB2	1:B:340:GLU:OE2	2.18	0.44
1:B:311:LEU:N	1:B:312:PRO:CD	2.79	0.44
1:B:529:ARG:HH22	1:B:568:ASP:CG	2.20	0.44
1:B:958:LYS:N	1:B:958:LYS:HE3	2.33	0.44
1:A:179:ILE:HD13	1:A:211:GLY:O	2.18	0.44
1:A:487:PHE:HA	1:A:493:SER:O	2.17	0.44
1:B:180:LEU:O	1:B:706:ASN:ND2	2.50	0.44
1:A:262:LYS:CE	1:A:266:LEU:HD23	2.46	0.44
1:A:857:MET:HB2	1:A:858:TYR:CD1	2.53	0.44
1:A:875:GLN:C	1:A:877:THR:H	2.21	0.44
1:A:188:ILE:CD1	1:A:486:GLU:HG2	2.48	0.44
1:A:371:LYS:HE3	1:A:371:LYS:HB2	1.87	0.44
1:A:556:ARG:HH11	1:A:556:ARG:HG2	1.82	0.44
1:B:166:LEU:HG	1:B:221:GLY:HA2	2.00	0.44
1:B:411:VAL:HA	1:B:454:VAL:HG11	2.00	0.44
1:B:556:ARG:HG2	1:B:556:ARG:HH11	1.82	0.44
1:B:580:ASP:C	1:B:582:SER:N	2.71	0.44
1:B:604:ARG:HH11	1:B:604:ARG:CG	2.30	0.44
1:B:610:SER:HB3	1:B:744:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:MET:HE3	1:B:384:ILE:CD1	2.48	0.43
1:B:857:MET:HB2	1:B:858:TYR:HD1	1.83	0.43
1:A:411:VAL:HA	1:A:454:VAL:HG11	1.99	0.43
1:B:527:TYR:HB3	1:B:534:ARG:HG3	2.00	0.43
1:A:508:VAL:HG12	1:A:509:GLY:N	2.34	0.43
1:B:431:LYS:HB3	1:B:433:VAL:HG22	2.01	0.43
1:B:781:LEU:HB2	1:B:783:LEU:HG	2.01	0.43
1:B:865:VAL:HB	1:B:868:HIS:CG	2.52	0.43
1:B:875:GLN:C	1:B:877:THR:H	2.21	0.43
1:A:150:ILE:N	1:A:150:ILE:CD1	2.81	0.43
1:A:166:LEU:HG	1:A:221:GLY:HA2	2.01	0.43
1:A:366:MET:O	1:A:366:MET:HG3	2.19	0.43
1:A:565:ALA:HB1	1:A:592:THR:O	2.18	0.43
1:A:990:ASN:HD21	5:A:1012:PTY:HC31	1.83	0.43
1:B:195:PRO:O	1:B:197:PRO:HD3	2.19	0.43
1:B:41:LEU:N	1:B:41:LEU:CD1	2.82	0.43
1:B:84:THR:HA	1:B:87:ALA:HB2	2.00	0.43
1:A:124:PRO:HD3	1:A:158:LYS:HG2	2.00	0.43
1:A:328:LYS:HA	1:A:328:LYS:CE	2.35	0.43
1:A:436:LYS:HB2	1:A:443:THR:HG21	2.00	0.43
1:B:45:GLU:OE1	1:B:45:GLU:HA	2.19	0.43
1:B:150:ILE:N	1:B:150:ILE:CD1	2.82	0.43
1:B:602:PRO:HA	1:B:603:PRO:HD3	1.82	0.43
1:A:358:THR:O	1:A:359:ASN:HB3	2.19	0.43
1:A:781:LEU:O	1:A:871:THR:HG23	2.19	0.43
1:A:975:LEU:N	1:A:975:LEU:HD22	2.34	0.43
1:B:508:VAL:HG12	1:B:509:GLY:N	2.33	0.43
1:A:431:LYS:HB3	1:A:433:VAL:HG22	2.00	0.43
1:A:832:TRP:O	1:A:836:ARG:HG3	2.18	0.43
1:B:989:ARG:O	1:B:993:GLU:HG2	2.19	0.43
1:A:281:ASP:HB3	1:A:282:PRO:HD2	2.01	0.42
1:B:150:ILE:CG2	1:B:220:LEU:HD11	2.49	0.42
1:B:926:PRO:HA	1:B:927:PRO:HD3	1.88	0.42
1:B:990:ASN:HD21	5:B:1112:PTY:HC31	1.84	0.42
1:A:773:VAL:CG1	1:A:845:GLY:HA3	2.48	0.42
1:A:781:LEU:HB2	1:A:783:LEU:HG	2.00	0.42
1:B:205:LYS:NZ	1:B:205:LYS:CB	2.80	0.42
1:A:258:GLU:HG2	1:A:258:GLU:H	1.62	0.42
1:A:720:MET:HE3	1:A:738:ASP:CA	2.49	0.42
1:A:857:MET:HB2	1:A:858:TYR:HD1	1.83	0.42
1:B:767:SER:HA	6:B:3120:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:TYR:HB3	1:A:534:ARG:HG3	2.02	0.42
1:A:562:LEU:HD12	1:A:562:LEU:HA	1.90	0.42
1:B:855:TRP:HZ3	1:B:856:PHE:CE1	2.37	0.42
1:A:248:PRO:HB2	1:A:340:GLU:OE2	2.19	0.42
1:B:124:PRO:HD3	1:B:158:LYS:HG2	2.02	0.42
1:B:188:ILE:CD1	1:B:486:GLU:HG2	2.49	0.42
1:B:262:LYS:NZ	1:B:266:LEU:HD23	2.35	0.42
1:A:84:THR:HA	1:A:87:ALA:HB2	2.01	0.42
1:A:95:LEU:HD23	1:A:95:LEU:O	2.19	0.42
1:A:610:SER:HB3	1:A:744:VAL:HG21	2.02	0.42
1:B:95:LEU:O	1:B:95:LEU:HD23	2.20	0.42
1:B:139:ARG:O	1:B:139:ARG:HG3	2.20	0.42
1:B:287:SER:HB2	1:B:290:ARG:HB2	2.01	0.42
1:B:623:MET:HE1	1:B:635:ILE:HG22	2.01	0.42
1:B:671:ARG:HD2	1:B:694:TYR:OH	2.20	0.42
1:A:863:PRO:O	1:A:864:GLY:C	2.58	0.42
1:B:462:LEU:HD22	1:B:466:GLU:HB3	2.01	0.42
1:A:488:SER:C	1:A:490:ASP:N	2.72	0.42
1:A:517:ALA:HA	1:A:518:PRO:HD3	1.75	0.42
1:A:589:THR:CG2	1:A:590:ASP:N	2.81	0.42
1:B:281:ASP:HB3	1:B:282:PRO:HD2	2.01	0.42
1:B:488:SER:C	1:B:490:ASP:N	2.72	0.42
1:B:781:LEU:O	1:B:871:THR:HG23	2.20	0.42
1:A:45:GLU:OE1	1:A:45:GLU:HA	2.18	0.42
1:A:478:LEU:N	1:A:478:LEU:HD12	2.35	0.42
1:A:979:GLY:O	1:A:983:ILE:HG13	2.20	0.42
1:B:358:THR:O	1:B:359:ASN:CB	2.68	0.42
1:B:671:ARG:HB3	1:B:694:TYR:CE2	2.54	0.42
1:B:907:ILE:O	1:B:910:CYS:HB2	2.19	0.42
1:A:260:LEU:CD2	1:A:307:ILE:HD13	2.50	0.41
1:B:554:THR:O	1:B:554:THR:CG2	2.68	0.41
1:B:816:ILE:CG2	1:B:817:MET:N	2.80	0.41
1:B:832:TRP:O	1:B:836:ARG:HG3	2.20	0.41
1:A:41:LEU:N	1:A:41:LEU:CD1	2.83	0.41
1:A:126:MET:HB3	1:A:126:MET:HE3	1.85	0.41
1:A:350:SER:OG	1:A:356:LEU:HD11	2.20	0.41
1:A:602:PRO:HA	1:A:603:PRO:HD3	1.82	0.41
1:A:205:LYS:NZ	1:A:205:LYS:CB	2.80	0.41
1:A:771:GLU:O	1:A:775:ILE:HG12	2.20	0.41
1:A:775:ILE:O	1:A:778:THR:HG22	2.20	0.41
1:B:715:GLU:CB	1:B:716:ILE:HD12	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:873:PHE:CB	1:B:875:GLN:HE21	2.32	0.41
1:A:319:LEU:CD1	1:A:339:VAL:HG21	2.50	0.41
1:A:580:ASP:C	1:A:582:SER:N	2.72	0.41
1:A:926:PRO:HB3	1:A:928:TRP:CE2	2.55	0.41
1:A:989:ARG:O	1:A:993:GLU:HG2	2.20	0.41
1:B:179:ILE:HD13	1:B:211:GLY:O	2.20	0.41
1:B:260:LEU:CD2	1:B:307:ILE:HD13	2.49	0.41
1:B:926:PRO:HB3	1:B:928:TRP:CE2	2.56	0.41
1:A:319:LEU:HA	1:A:319:LEU:HD12	1.85	0.41
1:A:921:SER:C	1:A:923:MET:H	2.23	0.41
1:B:487:PHE:HA	1:B:493:SER:O	2.20	0.41
1:B:517:ALA:HA	1:B:518:PRO:HD3	1.74	0.41
1:B:771:GLU:O	1:B:775:ILE:HG12	2.21	0.41
1:A:48:SER:HG	1:A:51:GLU:HG3	1.83	0.41
1:A:755:ASN:ND2	1:A:816:ILE:HD11	2.35	0.41
1:B:366:MET:HE3	1:B:448:LEU:HD11	2.00	0.41
1:B:380:ASN:O	1:B:382:PHE:CE1	2.73	0.41
1:B:478:LEU:HD12	1:B:478:LEU:N	2.35	0.41
1:A:671:ARG:HD2	1:A:694:TYR:OH	2.21	0.41
1:A:767:SER:HA	6:A:2120:HOH:O	2.20	0.41
1:B:717:GLY:O	1:B:731:SER:HB2	2.20	0.41
1:A:49:LEU:O	1:A:53:VAL:HG23	2.20	0.41
1:A:715:GLU:C	1:A:716:ILE:HD12	2.40	0.41
1:A:717:GLY:O	1:A:731:SER:HB2	2.21	0.41
1:A:865:VAL:CB	1:A:868:HIS:HB2	2.32	0.41
1:B:176:ASP:OD1	1:B:178:SER:HB2	2.20	0.41
1:B:403:ARG:HD3	1:B:456:ASN:ND2	2.36	0.41
1:B:975:LEU:N	1:B:975:LEU:HD22	2.34	0.41
1:A:253:LEU:HD12	1:A:253:LEU:HA	1.92	0.41
1:A:382:PHE:CZ	1:A:410:LEU:HD11	2.56	0.41
1:A:671:ARG:HB3	1:A:694:TYR:CE2	2.56	0.41
1:A:855:TRP:HZ3	1:A:856:PHE:CE1	2.38	0.41
1:B:194:VAL:HA	1:B:195:PRO:HD2	1.74	0.41
1:B:319:LEU:CD1	1:B:339:VAL:HG21	2.50	0.41
1:B:802:LEU:CB	1:B:803:PRO:HD3	2.48	0.41
1:B:967:TRP:O	1:B:970:VAL:HB	2.21	0.41
1:A:262:LYS:NZ	1:A:266:LEU:HD23	2.36	0.41
1:A:844:VAL:HG22	1:A:907:ILE:HG21	2.03	0.41
1:B:116:ILE:HD11	1:B:240:ALA:HA	2.03	0.41
1:B:380:ASN:ND2	1:B:407:PHE:CE2	2.89	0.41
1:B:880:HIS:H	1:B:881:PRO:HD2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:968:LEU:HD12	1:B:968:LEU:HA	1.87	0.41
1:B:132:ALA:C	1:B:134:ARG:H	2.25	0.40
1:B:567:ARG:HG3	1:B:589:THR:O	2.21	0.40
1:A:720:MET:HE3	1:A:738:ASP:HA	2.03	0.40
1:A:975:LEU:H	1:A:975:LEU:HD22	1.85	0.40
1:B:775:ILE:O	1:B:778:THR:HG22	2.22	0.40
1:A:287:SER:HB2	1:A:290:ARG:HB2	2.02	0.40
1:A:479:MET:HB3	1:A:498:CYS:HB3	2.03	0.40
1:A:502:LYS:HG3	1:A:502:LYS:O	2.21	0.40
1:A:567:ARG:HG3	1:A:589:THR:O	2.21	0.40
1:B:502:LYS:O	1:B:502:LYS:HG3	2.21	0.40
1:B:863:PRO:O	1:B:864:GLY:C	2.58	0.40
1:B:183:GLU:C	1:B:185:VAL:H	2.23	0.40
1:B:382:PHE:CZ	1:B:410:LEU:HD11	2.57	0.40
1:A:116:ILE:HD11	1:A:240:ALA:HA	2.04	0.40
1:A:907:ILE:O	1:A:910:CYS:HB2	2.22	0.40
1:B:43:ALA:HA	1:B:120:LYS:HZ3	1.86	0.40
1:B:975:LEU:H	1:B:975:LEU:HD22	1.87	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%)	920 (93%)	61 (6%)	11 (1%)	14 20
1	B	992/994 (100%)	921 (93%)	60 (6%)	11 (1%)	14 20
All	All	1984/1988 (100%)	1841 (93%)	121 (6%)	22 (1%)	14 20

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	883	PHE
1	B	883	PHE
1	A	185	VAL
1	A	663	LEU
1	A	866	THR
1	A	868	HIS
1	A	951	ASP
1	B	185	VAL
1	B	663	LEU
1	B	866	THR
1	B	868	HIS
1	B	874	MET
1	B	951	ASP
1	A	430	THR
1	A	874	MET
1	B	430	THR
1	A	133	ASP
1	A	864	GLY
1	B	133	ASP
1	B	864	GLY
1	A	863	PRO
1	B	863	PRO

5.3.2 Protein sidechains (i)

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%)	785 (94%)	55 (6%)	17	27
1	B	840/840 (100%)	788 (94%)	52 (6%)	18	29
All	All	1680/1680 (100%)	1573 (94%)	107 (6%)	17	28

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	9	THR

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Mol	Chain	Res	Type
1	A	34	GLU
1	A	60	LEU
1	A	96	LEU
1	A	111	ASN
1	A	113	GLU
1	A	139	ARG
1	A	143	ARG
1	A	158	LYS
1	A	164	ARG
1	A	183	GLU
1	A	205	LYS
1	A	236	ARG
1	A	253	LEU
1	A	258	GLU
1	A	266	LEU
1	A	302	LEU
1	A	319	LEU
1	A	359	ASN
1	A	362	SER
1	A	364	CYS
1	A	371	LYS
1	A	384	ILE
1	A	396	LEU
1	A	402	ILE
1	A	431	LYS
1	A	445	LEU
1	A	467	ARG
1	A	484	THR
1	A	486	GLU
1	A	490	ASP
1	A	494	MET
1	A	544	LYS
1	A	562	LEU
1	A	580	ASP
1	A	586	GLU
1	A	604	ARG
1	A	608	MET
1	A	612	GLN
1	A	656	ARG
1	A	685	SER
1	A	691	LEU
1	A	733	MET

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Mol	Chain	Res	Type
1	A	759	GLN
1	A	760	PHE
1	A	797	LEU
1	A	802	LEU
1	A	816	ILE
1	A	838	MET
1	A	873	PHE
1	A	924	ARG
1	A	925	MET
1	A	958	LYS
1	A	968	LEU
1	B	2	GLU
1	B	9	THR
1	B	34	GLU
1	B	60	LEU
1	B	96	LEU
1	B	111	ASN
1	B	113	GLU
1	B	139	ARG
1	B	143	ARG
1	B	158	LYS
1	B	164	ARG
1	B	183	GLU
1	B	205	LYS
1	B	236	ARG
1	B	258	GLU
1	B	266	LEU
1	B	302	LEU
1	B	319	LEU
1	B	359	ASN
1	B	362	SER
1	B	364	CYS
1	B	371	LYS
1	B	384	ILE
1	B	396	LEU
1	B	402	ILE
1	B	431	LYS
1	B	445	LEU
1	B	467	ARG
1	B	484	THR
1	B	486	GLU
1	B	490	ASP

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Mol	Chain	Res	Type
1	B	534	ARG
1	B	544	LYS
1	B	562	LEU
1	B	580	ASP
1	B	604	ARG
1	B	608	MET
1	B	612	GLN
1	B	656	ARG
1	B	685	SER
1	B	691	LEU
1	B	733	MET
1	B	759	GLN
1	B	760	PHE
1	B	797	LEU
1	B	802	LEU
1	B	816	ILE
1	B	873	PHE
1	B	924	ARG
1	B	925	MET
1	B	958	LYS
1	B	968	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	111	ASN
1	A	244	GLN
1	A	275	ASN
1	A	359	ASN
1	A	461	ASN
1	A	875	GLN
1	A	880	HIS
1	A	914	ASN
1	A	919	ASN
1	B	108	GLN
1	B	111	ASN
1	B	244	GLN
1	B	275	ASN
1	B	359	ASN
1	B	461	ASN
1	B	875	GLN

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Mol	Chain	Res	Type
1	B	880	HIS
1	B	914	ASN
1	B	919	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
4	BHQ	B	1104	-	16,16,16	1.89	6 (37%)	26,26,26	1.33	4 (15%)
5	PTY	A	1011	-	18,18,49	1.09	1 (5%)	21,23,54	1.47	3 (14%)
5	PTY	B	1112	-	18,18,49	1.46	3 (16%)	21,23,54	1.53	2 (9%)
5	PTY	B	1113	-	18,18,49	1.21	3 (16%)	21,23,54	1.29	3 (14%)
5	PTY	A	1012	-	18,18,49	1.46	3 (16%)	21,23,54	1.54	3 (14%)
3	TG1	B	1103	-	43,48,48	1.49	10 (23%)	44,72,72	1.66	9 (20%)
5	PTY	B	1111	-	18,18,49	1.12	2 (11%)	21,23,54	1.46	3 (14%)
4	BHQ	A	1004	-	16,16,16	1.87	5 (31%)	26,26,26	1.32	4 (15%)
3	TG1	A	1003	-	43,48,48	1.45	8 (18%)	44,72,72	1.65	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	PTY	A	1013	-	18,18,49	1.20	3 (16%)	21,23,54	1.29	3 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BHQ	B	1104	-	-	0/12/12/12	0/1/1/1
5	PTY	A	1011	-	-	13/20/20/53	-
5	PTY	B	1112	-	-	10/20/20/53	-
5	PTY	B	1113	-	-	7/20/20/53	-
5	PTY	A	1012	-	-	10/20/20/53	-
3	TG1	B	1103	-	-	8/33/99/99	0/3/3/3
5	PTY	B	1111	-	-	13/20/20/53	-
4	BHQ	A	1004	-	-	0/12/12/12	0/1/1/1
3	TG1	A	1003	-	-	8/33/99/99	0/3/3/3
5	PTY	A	1013	-	-	7/20/20/53	-

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1104	BHQ	C1-C2	4.17	1.45	1.40
4	A	1004	BHQ	C1-C2	4.10	1.45	1.40
3	A	1003	TG1	O4-C21	3.96	1.29	1.21
3	B	1103	TG1	O4-C21	3.47	1.28	1.21
4	B	1104	BHQ	C6-C5	3.34	1.44	1.39
4	A	1004	BHQ	C6-C5	3.17	1.44	1.39
4	A	1004	BHQ	C4-C5	3.15	1.44	1.40
4	B	1104	BHQ	C4-C5	3.12	1.44	1.40
5	B	1112	PTY	C1-C6	3.11	1.60	1.50
5	A	1012	PTY	C1-C6	3.08	1.60	1.50
3	A	1003	TG1	C1-C5	2.92	1.56	1.51
3	B	1103	TG1	C1-C5	2.78	1.55	1.51
3	B	1103	TG1	O3-C3	2.76	1.50	1.44
3	B	1103	TG1	C21-C22	2.65	1.59	1.50
3	B	1103	TG1	O6-C7	2.65	1.47	1.43
3	A	1003	TG1	C11-C7	2.57	1.58	1.55
3	B	1103	TG1	C9-C10	2.57	1.58	1.54
3	A	1003	TG1	C21-C22	2.56	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1103	TG1	C11-C7	2.55	1.58	1.55
5	A	1012	PTY	P1-O13	2.55	1.59	1.50
3	B	1103	TG1	C9-C8	2.54	1.55	1.52
5	A	1012	PTY	C5-C6	2.51	1.58	1.50
5	B	1112	PTY	P1-O13	2.50	1.59	1.50
5	B	1112	PTY	C5-C6	2.48	1.58	1.50
3	A	1003	TG1	O3-C3	2.47	1.49	1.44
3	A	1003	TG1	C9-C10	2.47	1.58	1.54
4	A	1004	BHQ	C3-C2	2.44	1.43	1.39
5	B	1111	PTY	P1-O13	2.39	1.59	1.50
5	A	1011	PTY	P1-O13	2.32	1.59	1.50
4	B	1104	BHQ	C3-C2	2.30	1.42	1.39
5	A	1013	PTY	C5-C6	2.24	1.57	1.50
5	B	1113	PTY	C5-C6	2.24	1.57	1.50
5	A	1013	PTY	P1-O13	2.19	1.58	1.50
5	B	1113	PTY	C1-C6	2.19	1.57	1.50
3	B	1103	TG1	C33-C32	-2.19	1.42	1.49
4	B	1104	BHQ	C7-C2	2.18	1.58	1.54
5	A	1013	PTY	C1-C6	2.17	1.57	1.50
5	B	1113	PTY	P1-O13	2.16	1.58	1.50
4	B	1104	BHQ	C3-C4	2.15	1.42	1.38
3	A	1003	TG1	O6-C7	2.14	1.46	1.43
3	B	1103	TG1	C4-C5	2.08	1.36	1.34
4	A	1004	BHQ	C3-C4	2.05	1.41	1.38
5	B	1111	PTY	C2-C3	2.03	1.58	1.50
3	A	1003	TG1	C33-C32	-2.01	1.42	1.49

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1103	TG1	C10-O9-C32	5.86	135.44	121.53
3	A	1003	TG1	C10-O9-C32	5.70	135.07	121.53
5	A	1011	PTY	O7-C8-C11	4.50	119.36	111.09
5	B	1111	PTY	O7-C8-C11	4.43	119.24	111.09
5	A	1012	PTY	O4-C1-C6	4.35	121.11	108.43
5	B	1112	PTY	O4-C1-C6	4.26	120.83	108.43
4	B	1104	BHQ	C7-C2-C1	3.85	124.61	122.26
4	A	1004	BHQ	C7-C2-C1	3.84	124.60	122.26
5	A	1013	PTY	O7-C8-C11	3.22	117.02	111.09
5	B	1113	PTY	O7-C8-C11	3.21	117.00	111.09
3	A	1003	TG1	O12-C12-C11	-3.10	125.16	128.28
3	B	1103	TG1	C7-C6-C5	3.09	123.32	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1003	TG1	C7-C6-C5	2.98	123.05	115.41
3	B	1103	TG1	C24-C22-C21	2.91	132.28	120.78
3	A	1003	TG1	C24-C22-C21	2.90	132.25	120.78
3	B	1103	TG1	O12-C12-C11	-2.76	125.51	128.28
4	A	1004	BHQ	C4-C3-C2	2.66	124.01	120.21
4	B	1104	BHQ	C4-C3-C2	2.66	124.01	120.21
3	A	1003	TG1	C11-C7-C6	-2.61	98.01	103.03
3	B	1103	TG1	C11-C7-C6	-2.58	98.05	103.03
3	A	1003	TG1	O5-C12-O12	2.58	125.03	121.62
3	B	1103	TG1	O5-C12-O12	2.39	124.79	121.62
5	A	1011	PTY	C5-C6-C1	-2.35	106.23	111.79
5	A	1013	PTY	P1-O11-C3	2.29	132.84	121.59
5	B	1113	PTY	P1-O11-C3	2.28	132.82	121.59
4	B	1104	BHQ	C1-C6-C5	2.27	123.44	120.21
4	A	1004	BHQ	C1-C6-C5	2.26	123.43	120.21
3	B	1103	TG1	O7-C8-C9	2.25	110.65	106.63
5	B	1111	PTY	C5-C6-C1	-2.23	106.52	111.79
3	A	1003	TG1	O1-C13-C14	-2.21	106.73	111.50
3	A	1003	TG1	O7-C8-C9	2.19	110.54	106.63
5	A	1013	PTY	O4-C1-C6	2.13	114.64	108.43
5	B	1112	PTY	O14-P1-O13	2.13	117.39	109.07
3	B	1103	TG1	C10-C1-C5	2.12	117.80	115.26
3	B	1103	TG1	O1-C13-C14	-2.12	106.94	111.50
5	A	1011	PTY	O11-P1-O13	-2.11	100.84	109.07
5	B	1111	PTY	O11-P1-O13	-2.09	100.88	109.07
5	A	1012	PTY	O14-P1-O13	2.09	117.22	109.07
4	B	1104	BHQ	C3-C2-C1	-2.07	113.89	116.59
4	A	1004	BHQ	C3-C2-C1	-2.06	113.89	116.59
5	B	1113	PTY	O4-C1-C6	2.05	114.41	108.43
3	A	1003	TG1	C10-C1-C5	2.04	117.70	115.26
5	A	1012	PTY	O7-C8-C11	2.02	114.80	111.09

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1012	PTY	O4-C1-C6-O7
5	A	1012	PTY	N1-C2-C3-O11
5	B	1112	PTY	O4-C1-C6-O7
5	B	1112	PTY	N1-C2-C3-O11
5	A	1011	PTY	C11-C8-O7-C6
5	A	1013	PTY	C11-C8-O7-C6

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Mol	Chain	Res	Type	Atoms
5	B	1111	PTY	C11-C8-O7-C6
5	B	1113	PTY	C11-C8-O7-C6
5	A	1011	PTY	O10-C8-O7-C6
5	B	1111	PTY	O10-C8-O7-C6
5	A	1012	PTY	C11-C8-O7-C6
5	B	1112	PTY	C11-C8-O7-C6
5	A	1011	PTY	C31-C30-O4-C1
5	B	1111	PTY	C31-C30-O4-C1
5	A	1013	PTY	O10-C8-O7-C6
5	B	1113	PTY	O10-C8-O7-C6
5	B	1113	PTY	C31-C30-O4-C1
5	A	1013	PTY	C31-C30-O4-C1
5	A	1011	PTY	O30-C30-O4-C1
5	B	1111	PTY	O30-C30-O4-C1
5	A	1012	PTY	C31-C30-O4-C1
5	B	1112	PTY	C31-C30-O4-C1
5	A	1013	PTY	O30-C30-O4-C1
5	B	1113	PTY	O30-C30-O4-C1
5	A	1012	PTY	O10-C8-O7-C6
5	B	1112	PTY	O10-C8-O7-C6
5	A	1012	PTY	O30-C30-O4-C1
5	B	1112	PTY	O30-C30-O4-C1
3	A	1003	TG1	C15-C16-C17-C18
3	B	1103	TG1	C15-C16-C17-C18
3	A	1003	TG1	C14-C15-C16-C17
3	B	1103	TG1	C14-C15-C16-C17
5	A	1011	PTY	C5-O14-P1-O11
5	B	1111	PTY	C5-O14-P1-O11
3	A	1003	TG1	C27-C28-C29-C30
5	A	1011	PTY	O14-C5-C6-O7
5	B	1111	PTY	O14-C5-C6-O7
3	A	1003	TG1	C16-C17-C18-C19
3	B	1103	TG1	C16-C17-C18-C19
5	A	1012	PTY	O4-C1-C6-C5
5	B	1112	PTY	O4-C1-C6-C5
3	B	1103	TG1	C27-C28-C29-C30
5	A	1011	PTY	O4-C1-C6-O7
5	B	1111	PTY	O4-C1-C6-O7
5	A	1012	PTY	C3-O11-P1-O14
5	B	1112	PTY	C3-O11-P1-O14
5	A	1011	PTY	C5-O14-P1-O12
5	B	1111	PTY	C5-O14-P1-O12

Continued on next page...

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Mol	Chain	Res	Type	Atoms
5	A	1011	PTY	O14-C5-C6-C1
5	B	1111	PTY	O14-C5-C6-C1
5	B	1113	PTY	O14-C5-C6-C1
5	A	1011	PTY	C3-O11-P1-O14
5	A	1013	PTY	C5-O14-P1-O11
5	B	1111	PTY	C3-O11-P1-O14
5	B	1113	PTY	C5-O14-P1-O11
5	A	1013	PTY	O14-C5-C6-C1
5	A	1013	PTY	O4-C1-C6-O7
5	B	1113	PTY	O4-C1-C6-O7
3	A	1003	TG1	O3-C21-C22-C23
3	B	1103	TG1	O3-C21-C22-C23
3	B	1103	TG1	C17-C18-C19-C20
3	A	1003	TG1	C17-C18-C19-C20
5	A	1011	PTY	O4-C1-C6-C5
5	B	1111	PTY	O4-C1-C6-C5
5	A	1011	PTY	C3-O11-P1-O13
5	A	1011	PTY	C5-O14-P1-O13
5	A	1012	PTY	C3-O11-P1-O13
5	B	1111	PTY	C3-O11-P1-O13
5	B	1111	PTY	C5-O14-P1-O13
5	B	1112	PTY	C3-O11-P1-O13
3	B	1103	TG1	O7-C27-C28-C29
5	A	1012	PTY	C2-C3-O11-P1
5	B	1112	PTY	C2-C3-O11-P1
3	A	1003	TG1	O7-C27-C28-C29
3	A	1003	TG1	O1-C13-C14-C15
3	B	1103	TG1	O1-C13-C14-C15

There are no ring outliers.

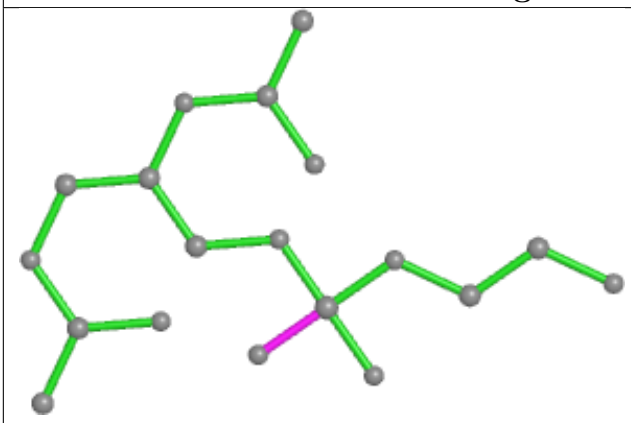
6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1104	BHQ	1	0
5	B	1112	PTY	2	0
5	A	1012	PTY	2	0
3	B	1103	TG1	3	0
4	A	1004	BHQ	1	0
3	A	1003	TG1	3	0

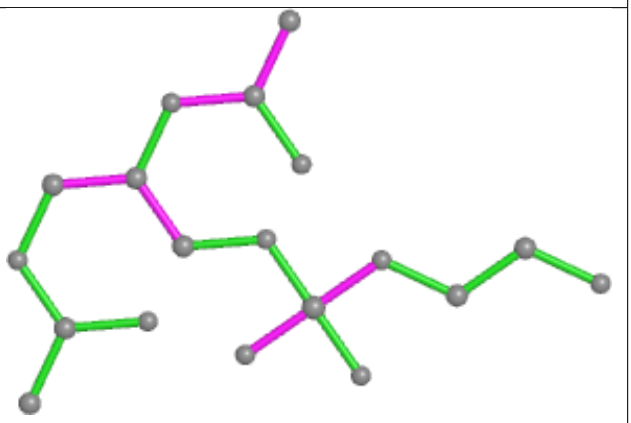
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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

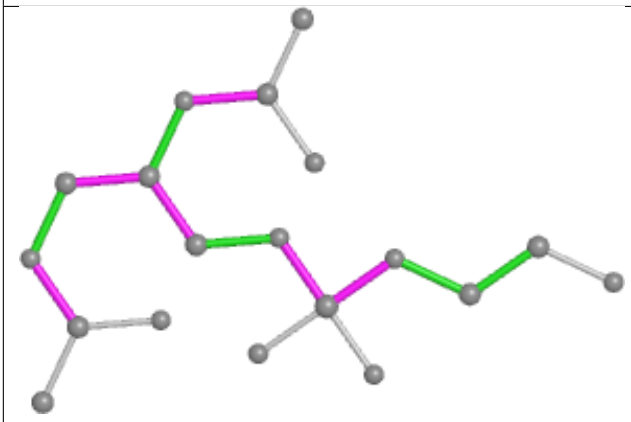
Ligand PTY A 1011



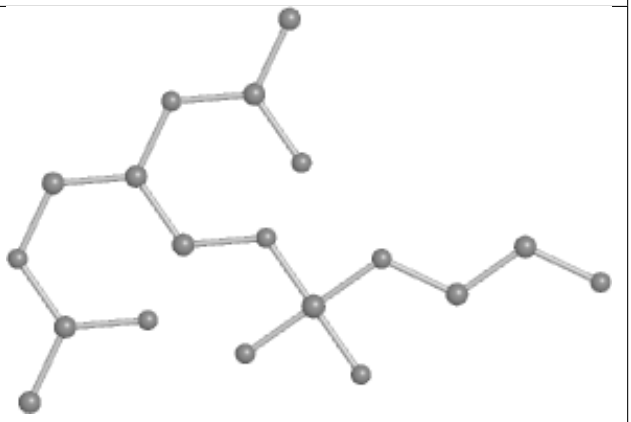
Bond lengths



Bond angles

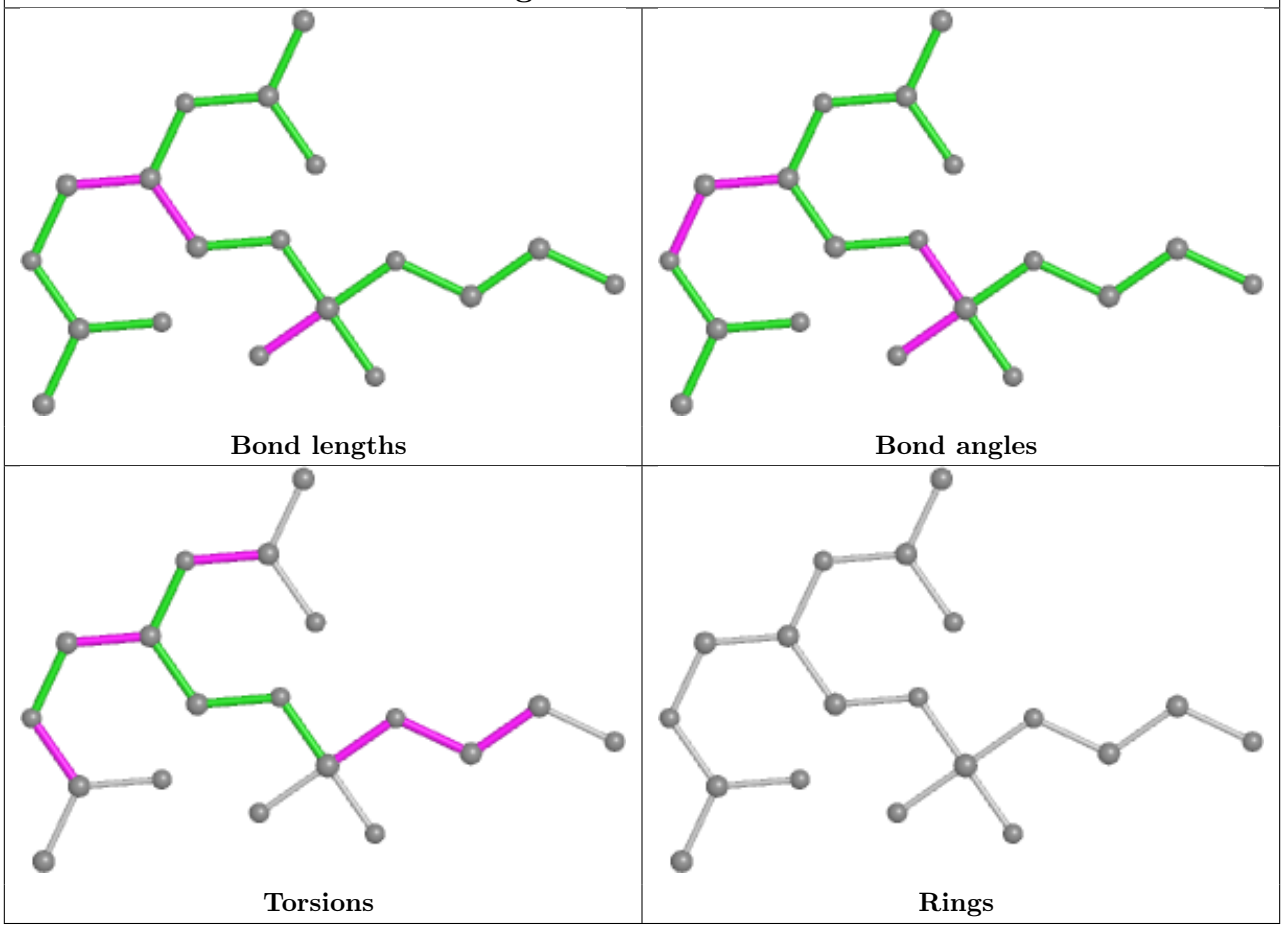


Torsions

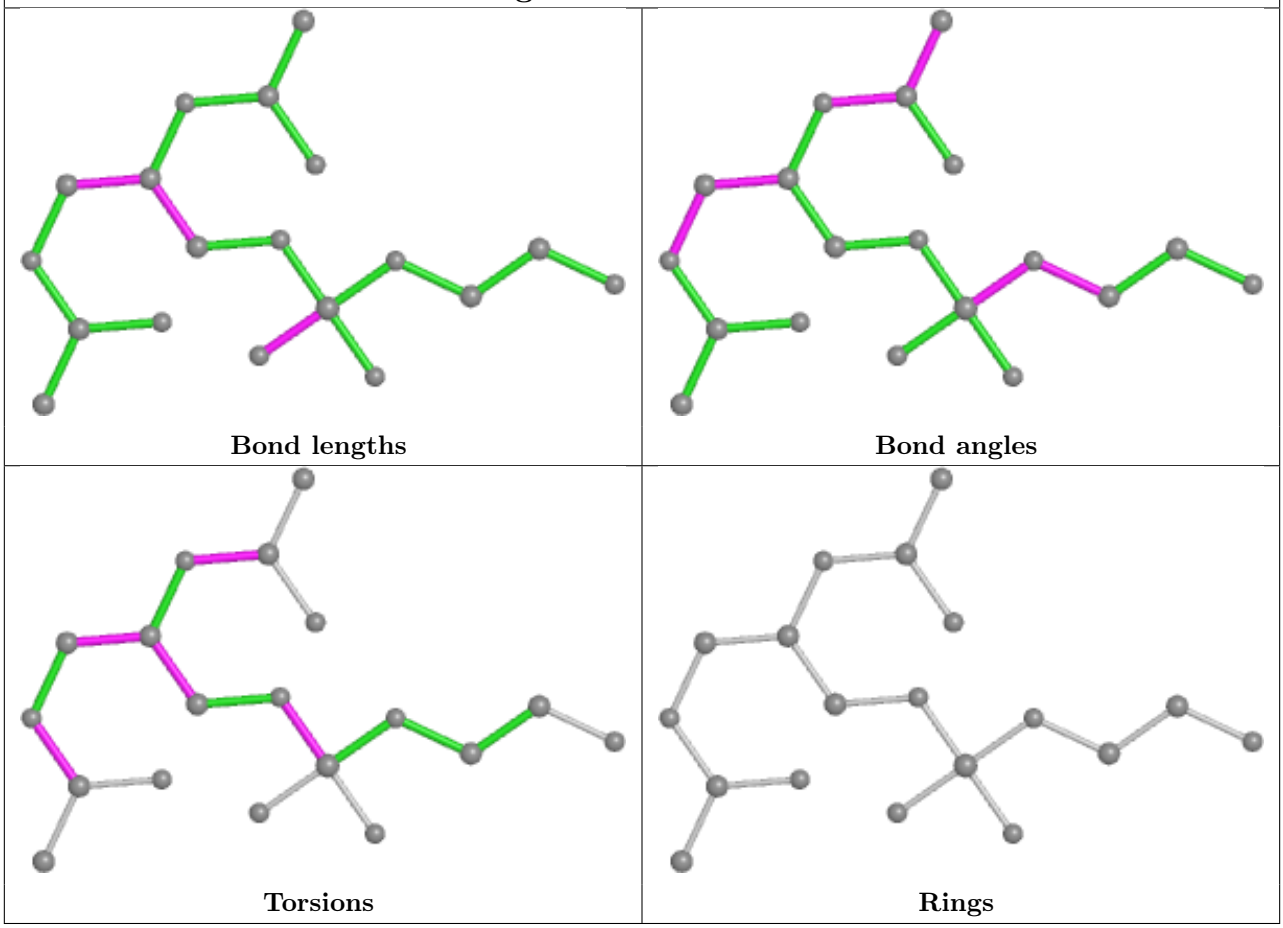


Rings

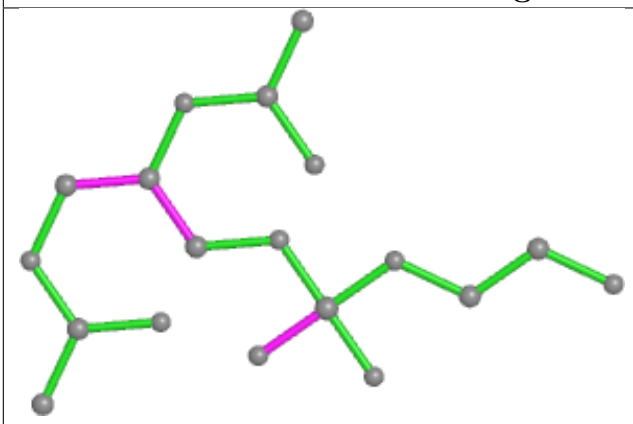
Ligand PTY B 1112



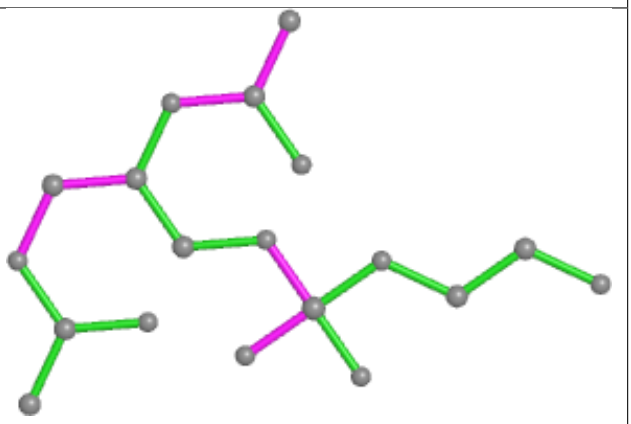
Ligand PTY B 1113



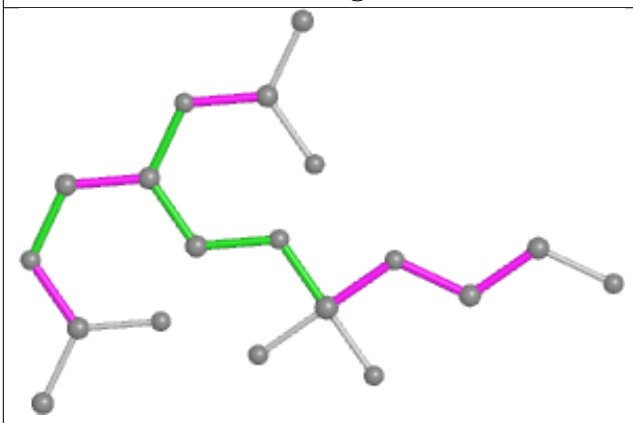
Ligand PTY A 1012



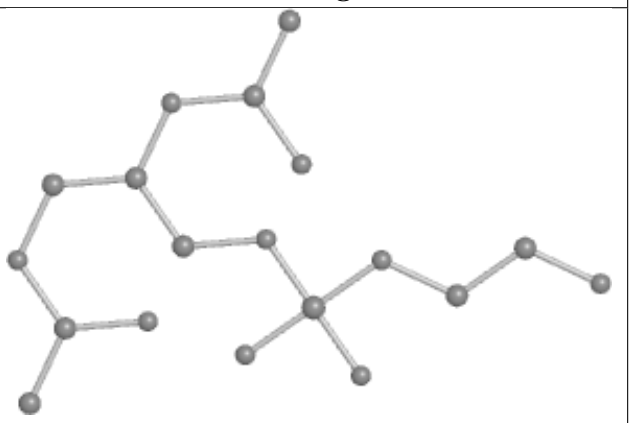
Bond lengths



Bond angles

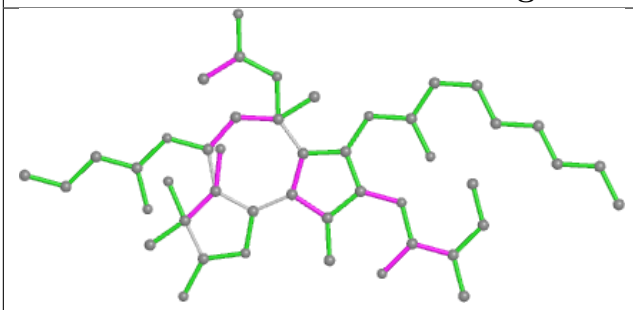


Torsions

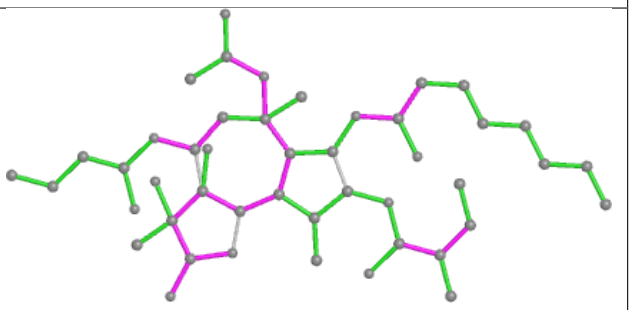


Rings

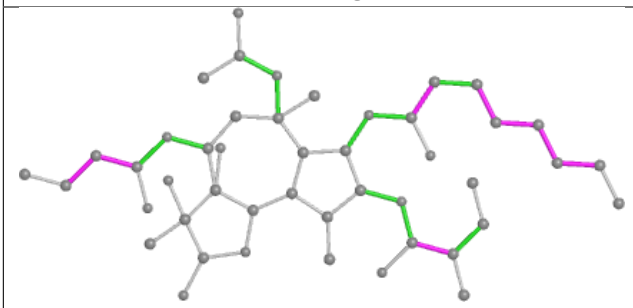
Ligand TG1 B 1103



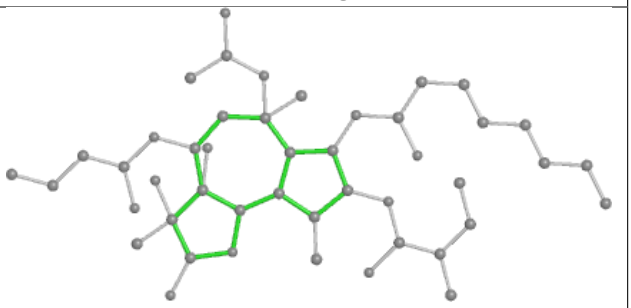
Bond lengths



Bond angles

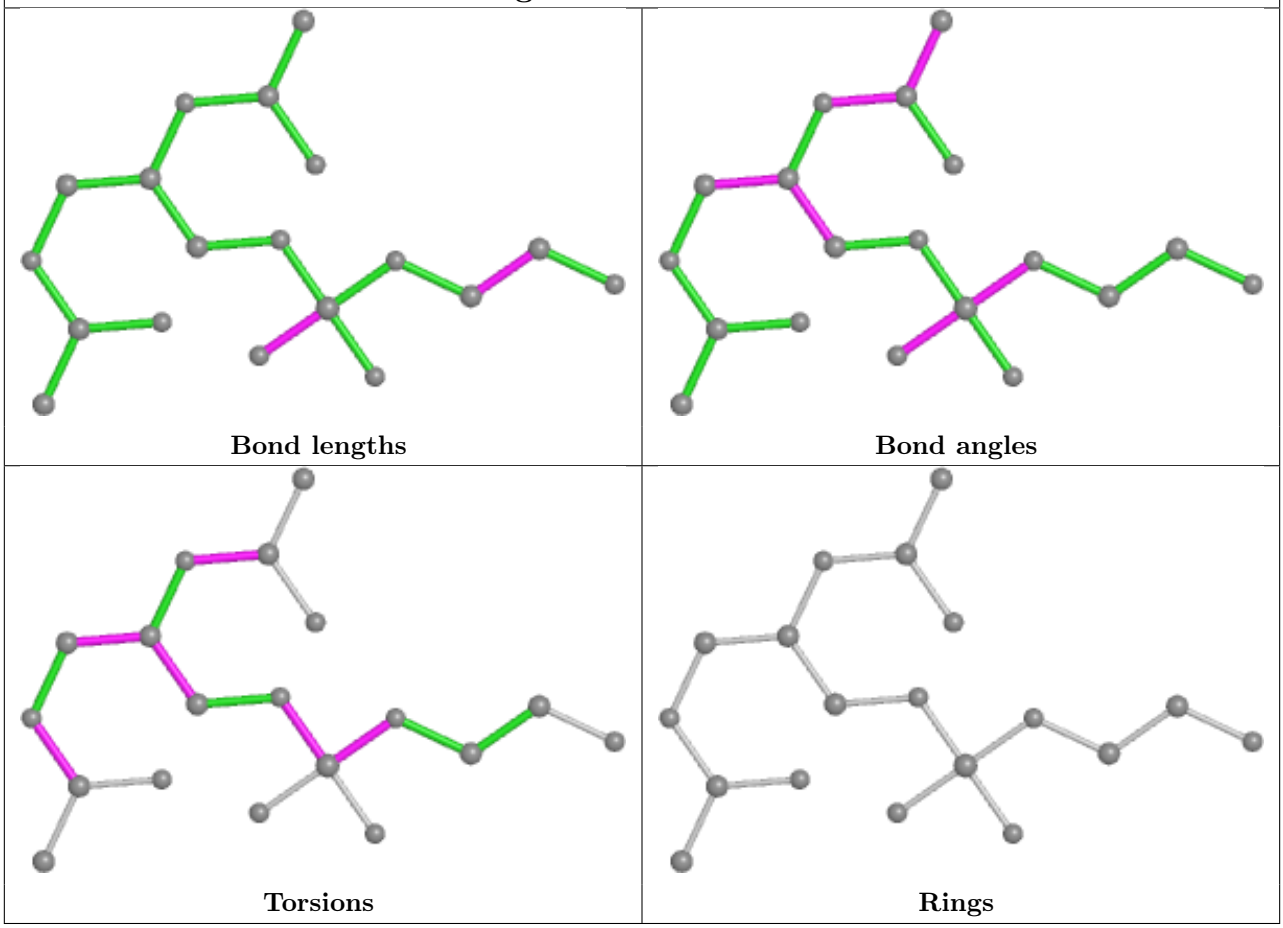


Torsions

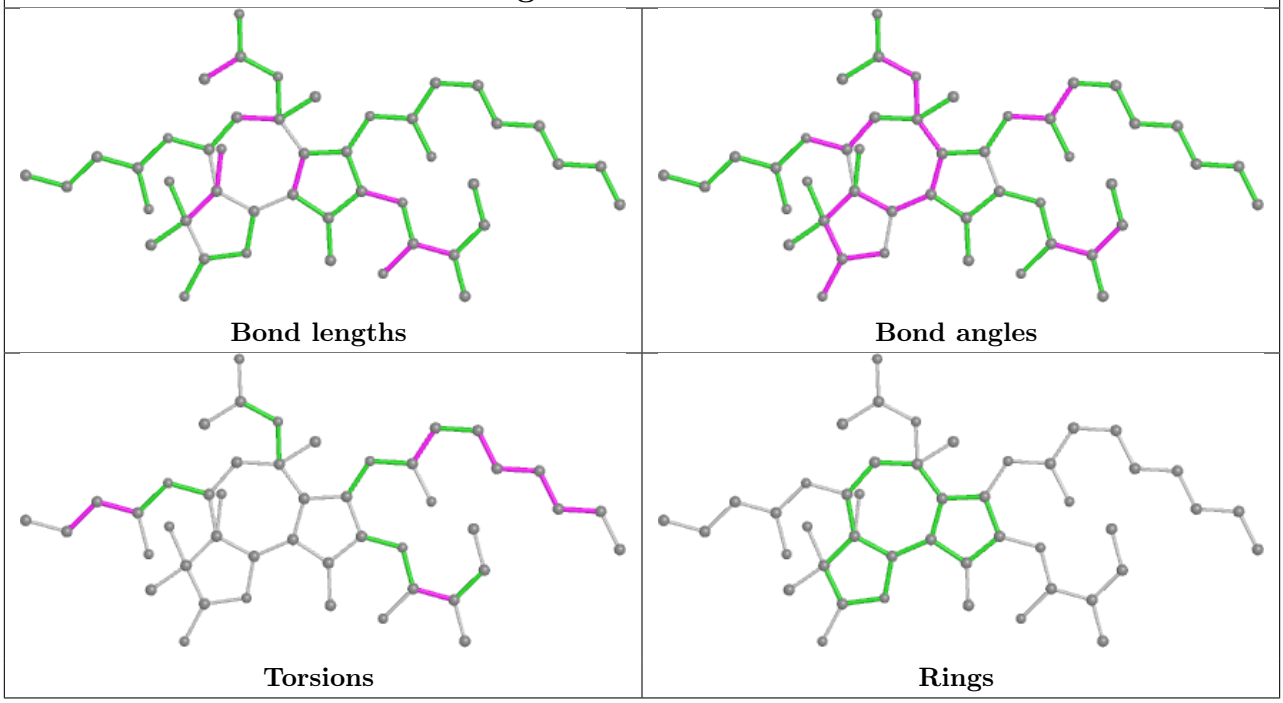


Rings

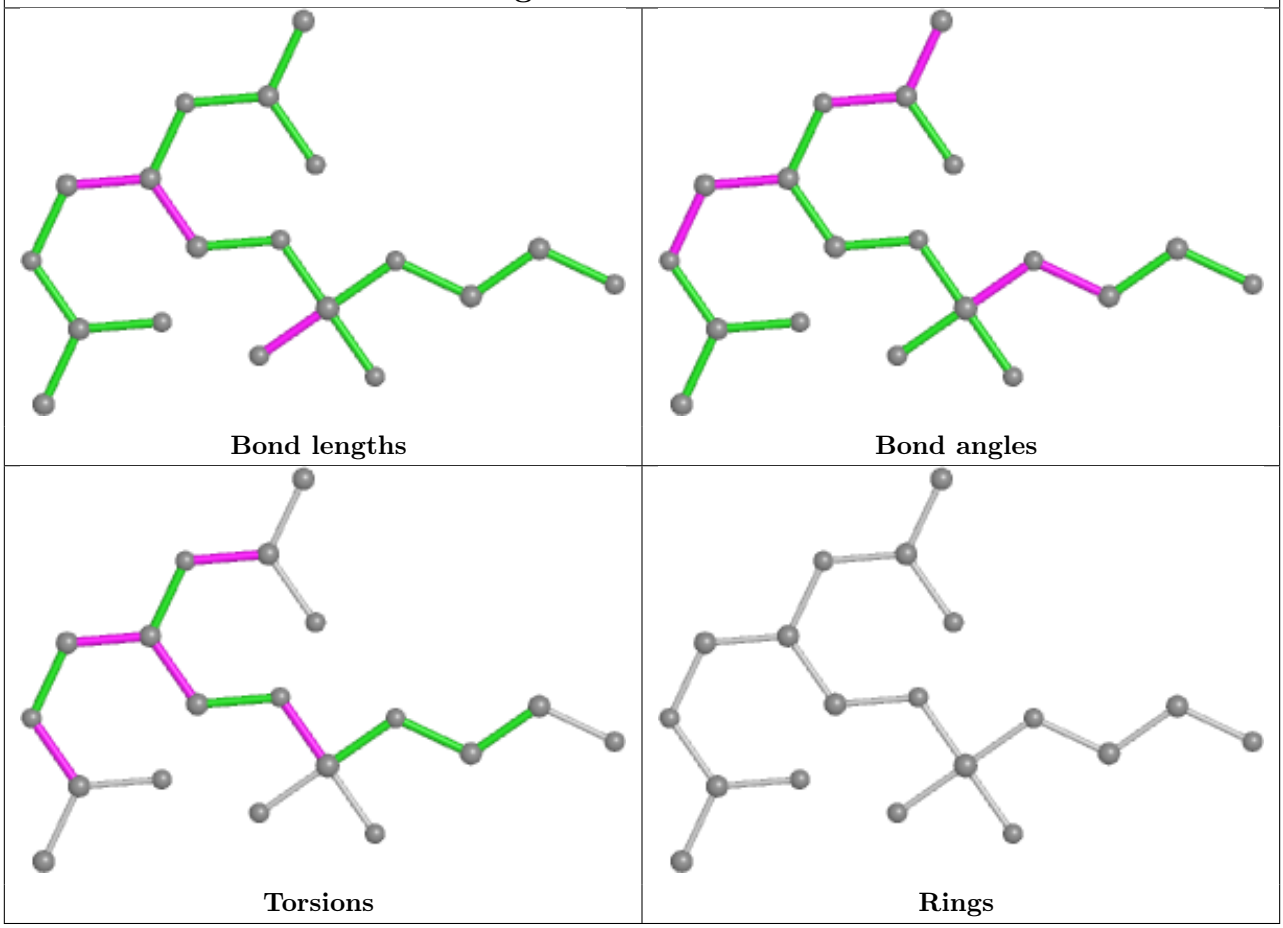
Ligand PTY B 1111



Ligand TG1 A 1003



Ligand PTY A 1013



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.