



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 12:40 pm BST

PDB ID : 1BYE
Title : GLUTATHIONE S-TRANSFERASE I FROM MAIS IN COMPLEX WITH
ATRAZINE GLUTATHIONE CONJUGATE
Authors : Prade, L.; Huber, R.; Bieseler, B.
Deposited on : 1998-10-14
Resolution : 2.80 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 following versions of software and data (see [references ⓘ](#)) 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) : 2.11

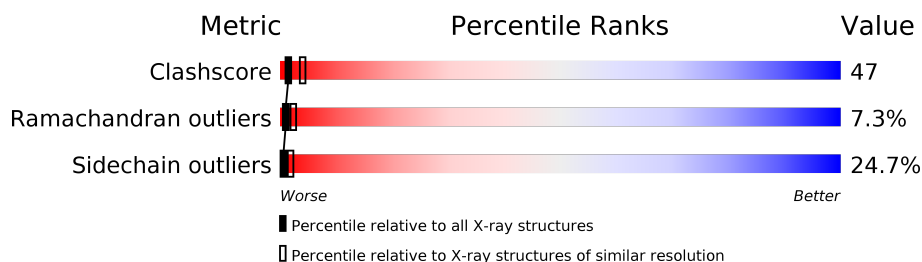
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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 on 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	213	
1	B	213	
1	C	213	
1	D	213	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ATA	A	1001	-	-	X	-

2 Entry composition [i](#)

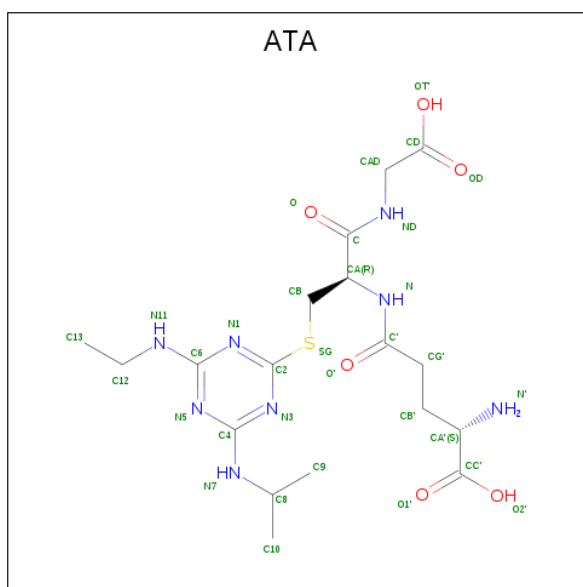
There are 3 unique types of molecules in this entry. The entry contains 6844 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called PROTEIN (GLUTATHIONE S-TRANSFERASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1666	1071	275	310	10			
1	B	213	Total	C	N	O	S	0	0	0
			1666	1071	275	310	10			
1	C	213	Total	C	N	O	S	0	0	0
			1666	1071	275	310	10			
1	D	213	Total	C	N	O	S	0	0	0
			1666	1071	275	310	10			

- Molecule 2 is ATRAZINE GLUTATHIONE CONJUGATE (three-letter code: ATA) (formula: $C_{18}H_{30}N_8O_6S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			33	18	8	6	1		
2	B	1	Total	C	N	O	S	0	0
			33	18	8	6	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			33	18	8	6	1		
2	D	1	Total	C	N	O	S	0	0
			33	18	8	6	1		

- Molecule 3 is water.

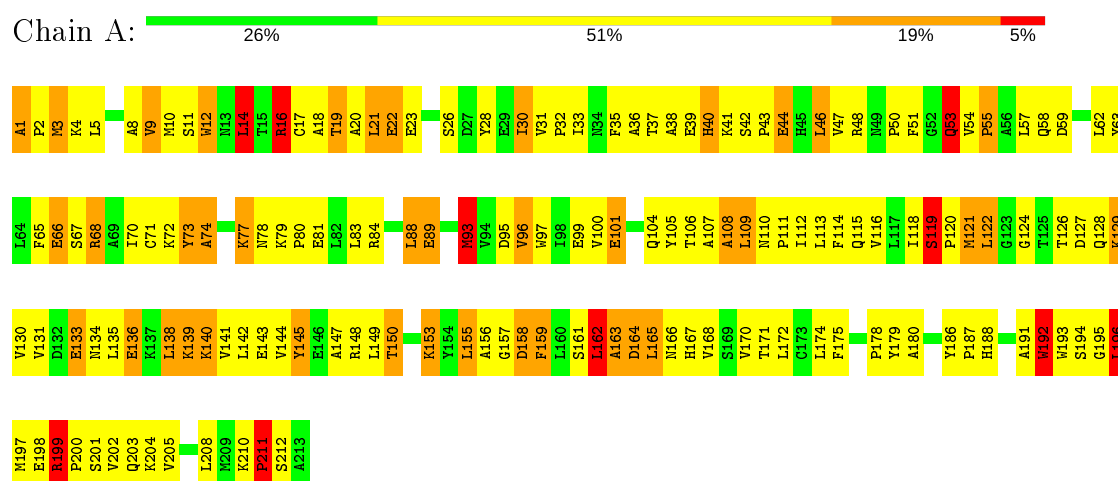
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		
3	B	12	Total	O	0	0
			12	12		
3	C	16	Total	O	0	0
			16	16		
3	D	9	Total	O	0	0
			9	9		

3 Residue-property plots

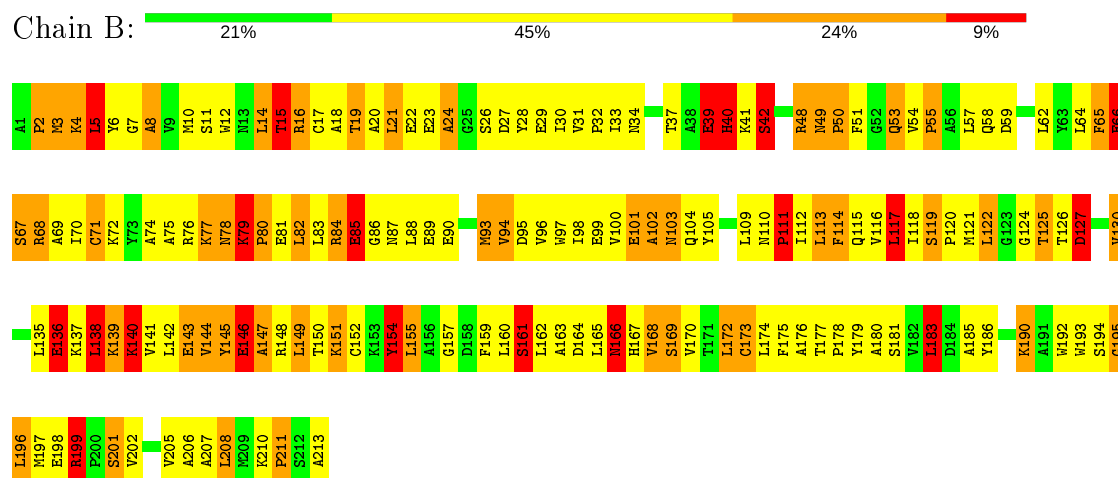
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: PROTEIN (GLUTATHIONE S-TRANSFERASE)

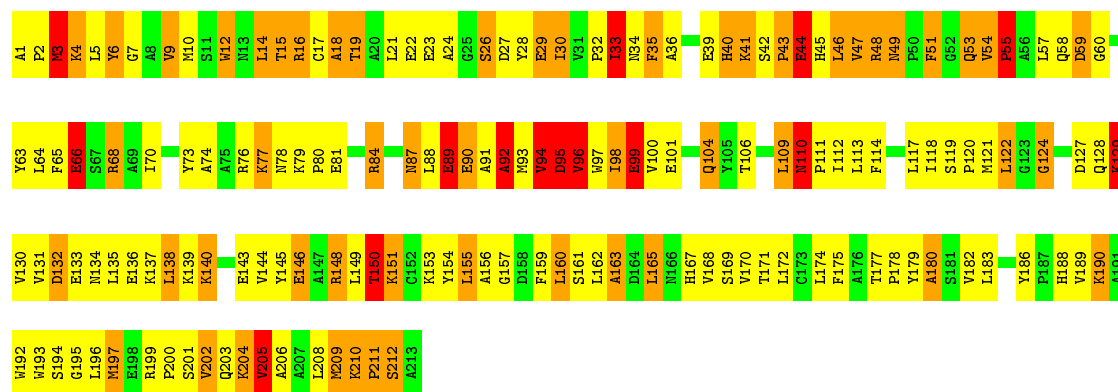


• Molecule 1: PROTEIN (GLUTATHIONE S-TRANSFERASE)



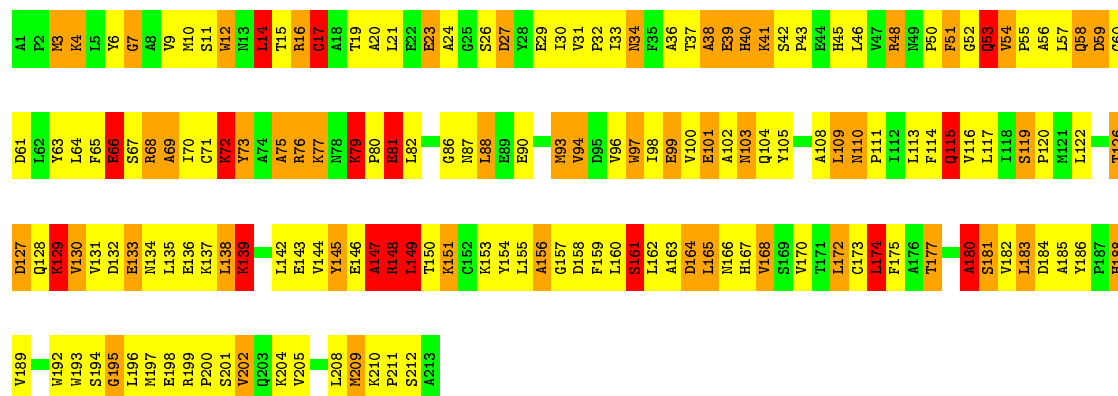
• Molecule 1: PROTEIN (GLUTATHIONE S-TRANSFERASE)





● Molecule 1: PROTEIN (GLUTATHIONE S-TRANSFERASE)

Chain D: 22% 46% 24% 8%



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	169.61Å 60.28Å 121.43Å 90.00° 126.22° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80	Depositor
% Data completeness (in resolution range)	89.6 (10.00-2.80)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.221 , 0.305	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6844	wwPDB-VP
Average B, all atoms (Å ²)	47.0	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: ATA

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	0.60	0/1704	2.02	37/2317 (1.6%)
1	B	0.55	0/1704	1.78	35/2317 (1.5%)
1	C	0.55	0/1704	1.72	21/2317 (0.9%)
1	D	0.62	0/1704	1.96	48/2317 (2.1%)
All	All	0.58	0/6816	1.87	141/9268 (1.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	15
1	B	0	21
1	C	0	27
1	D	0	24
All	All	0	87

There are no bond length outliers.

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	ARG	NE-CZ-NH2	-27.24	106.68	120.30
1	A	68	ARG	NE-CZ-NH2	-16.42	112.09	120.30
1	A	68	ARG	NE-CZ-NH1	15.24	127.92	120.30
1	B	48	ARG	NE-CZ-NH2	-15.17	112.72	120.30
1	A	199	ARG	NE-CZ-NH2	-13.64	113.48	120.30
1	D	16	ARG	NE-CZ-NH1	13.30	126.95	120.30
1	A	199	ARG	CD-NE-CZ	13.02	141.82	123.60
1	D	132	ASP	CB-CG-OD1	12.15	129.24	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	16	ARG	NE-CZ-NH2	-11.82	114.39	120.30
1	D	16	ARG	CD-NE-CZ	11.51	139.72	123.60
1	A	16	ARG	NH1-CZ-NH2	10.11	130.52	119.40
1	B	48	ARG	NE-CZ-NH1	9.93	125.27	120.30
1	C	68	ARG	NE-CZ-NH2	-9.90	115.35	120.30
1	C	92	ALA	N-CA-CB	9.64	123.60	110.10
1	B	127	ASP	CB-CG-OD2	9.59	126.93	118.30
1	B	199	ARG	CD-NE-CZ	9.57	136.99	123.60
1	A	105	TYR	CB-CG-CD2	8.74	126.25	121.00
1	C	16	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	A	12	TRP	N-CA-CB	8.63	126.13	110.60
1	C	29	GLU	CA-CB-CG	8.60	132.32	113.40
1	A	36	ALA	CB-CA-C	-8.37	97.55	110.10
1	A	199	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	B	16	ARG	NE-CZ-NH1	8.33	124.47	120.30
1	C	95	ASP	CB-CG-OD1	8.30	125.77	118.30
1	B	138	LEU	CA-CB-CG	8.26	134.29	115.30
1	B	79	LYS	CB-CA-C	8.04	126.48	110.40
1	D	164	ASP	CB-CG-OD2	7.99	125.49	118.30
1	C	84	ARG	NE-CZ-NH1	-7.94	116.33	120.30
1	A	101	GLU	CA-CB-CG	7.79	130.53	113.40
1	B	127	ASP	CB-CG-OD1	-7.75	111.32	118.30
1	A	53	GLN	CB-CG-CD	7.74	131.72	111.60
1	B	154	TYR	CB-CG-CD1	7.65	125.59	121.00
1	D	133	GLU	CA-CB-CG	7.65	130.23	113.40
1	A	148	ARG	NE-CZ-NH2	7.52	124.06	120.30
1	A	36	ALA	N-CA-CB	7.49	120.58	110.10
1	D	66	GLU	CG-CD-OE1	7.46	133.23	118.30
1	C	94	VAL	CA-CB-CG1	7.42	122.03	110.90
1	D	129	LYS	CA-CB-CG	7.34	129.55	113.40
1	C	89	GLU	OE1-CD-OE2	7.31	132.07	123.30
1	A	9	VAL	CA-CB-CG2	7.28	121.83	110.90
1	A	179	TYR	CB-CG-CD2	-7.27	116.64	121.00
1	D	68	ARG	NE-CZ-NH2	7.27	123.93	120.30
1	A	119	SER	N-CA-CB	7.12	121.18	110.50
1	B	117	LEU	CA-CB-CG	7.08	131.58	115.30
1	C	148	ARG	CD-NE-CZ	7.01	133.41	123.60
1	B	154	TYR	CB-CG-CD2	-6.84	116.90	121.00
1	A	31	VAL	CB-CA-C	-6.83	98.41	111.40
1	A	196	LEU	CA-CB-CG	6.82	130.98	115.30
1	D	69	ALA	N-CA-CB	6.79	119.61	110.10
1	D	66	GLU	O-C-N	-6.78	111.85	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	40	HIS	CA-C-N	6.77	132.09	117.20
1	C	96	VAL	CA-C-N	6.66	131.84	117.20
1	B	48	ARG	CD-NE-CZ	6.48	132.67	123.60
1	D	168	VAL	CA-CB-CG1	6.47	120.60	110.90
1	B	8	ALA	O-C-N	-6.46	112.37	122.70
1	D	3	MET	CA-CB-CG	6.45	124.26	113.30
1	B	145	TYR	CB-CG-CD2	6.41	124.85	121.00
1	B	211	PRO	CA-N-CD	-6.36	102.60	111.50
1	A	108	ALA	CB-CA-C	-6.33	100.61	110.10
1	D	104	GLN	CB-CA-C	6.31	123.02	110.40
1	D	132	ASP	CB-CA-C	6.23	122.86	110.40
1	B	103	ASN	CB-CG-ND2	6.22	131.63	116.70
1	D	14	LEU	CA-CB-CG	-6.22	100.99	115.30
1	C	90	GLU	CA-CB-CG	6.21	127.06	113.40
1	D	66	GLU	C-N-CA	6.20	137.19	121.70
1	A	22	GLU	OE1-CD-OE2	6.19	130.73	123.30
1	B	101	GLU	OE1-CD-OE2	-6.19	115.87	123.30
1	D	115	GLN	CA-C-N	6.17	130.79	117.20
1	C	59	ASP	CB-CG-OD1	-6.17	112.75	118.30
1	A	136	GLU	N-CA-CB	6.16	121.68	110.60
1	D	17	CYS	O-C-N	-6.16	112.85	122.70
1	A	14	LEU	CA-CB-CG	-6.14	101.17	115.30
1	C	4	LYS	CA-CB-CG	6.09	126.80	113.40
1	C	9	VAL	CB-CA-C	-6.08	99.85	111.40
1	D	39	GLU	OE1-CD-OE2	-6.03	116.07	123.30
1	A	9	VAL	CG1-CB-CG2	-5.92	101.44	110.90
1	A	108	ALA	N-CA-C	5.92	126.97	111.00
1	D	126	THR	CA-C-N	5.92	130.21	117.20
1	C	16	ARG	NH1-CZ-NH2	5.91	125.90	119.40
1	C	68	ARG	NH1-CZ-NH2	5.89	125.88	119.40
1	D	24	ALA	CA-C-N	5.88	127.96	116.20
1	B	183	LEU	CA-CB-CG	5.86	128.78	115.30
1	D	27	ASP	CA-C-O	5.78	132.24	120.10
1	C	68	ARG	O-C-N	-5.76	113.48	122.70
1	B	96	VAL	CA-CB-CG2	-5.75	102.27	110.90
1	D	10	MET	CA-CB-CG	5.75	123.08	113.30
1	B	199	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	A	48	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	B	66	GLU	OE1-CD-OE2	5.67	130.11	123.30
1	B	71	CYS	N-CA-CB	-5.67	100.40	110.60
1	D	129	LYS	CB-CG-CD	5.65	126.29	111.60
1	A	145	TYR	CB-CG-CD1	5.65	124.39	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	143	GLU	CA-CB-CG	5.64	125.81	113.40
1	D	148	ARG	CA-C-O	-5.58	108.38	120.10
1	B	66	GLU	N-CA-C	5.56	126.01	111.00
1	D	177	THR	CA-CB-OG1	-5.55	97.34	109.00
1	D	126	THR	O-C-N	-5.53	113.85	122.70
1	B	111	PRO	CA-C-N	5.53	129.36	117.20
1	B	39	GLU	O-C-N	-5.52	113.87	122.70
1	D	180	ALA	CA-C-N	5.50	129.31	117.20
1	A	63	TYR	O-C-N	-5.49	113.91	122.70
1	D	79	LYS	CB-CG-CD	5.49	125.88	111.60
1	D	73	TYR	O-C-N	-5.49	113.92	122.70
1	A	211	PRO	O-C-N	-5.47	113.95	122.70
1	C	129	LYS	CA-CB-CG	5.44	125.37	113.40
1	A	129	LYS	O-C-N	5.44	131.40	122.70
1	B	71	CYS	CB-CA-C	5.42	121.24	110.40
1	D	17	CYS	CA-C-N	5.42	129.11	117.20
1	B	166	ASN	CA-C-N	5.41	129.11	117.20
1	A	138	LEU	CB-CA-C	5.40	120.46	110.20
1	A	191	ALA	CB-CA-C	-5.40	102.00	110.10
1	C	81	GLU	OE1-CD-OE2	-5.39	116.83	123.30
1	A	143	GLU	CA-CB-CG	5.38	125.25	113.40
1	B	127	ASP	O-C-N	-5.38	114.09	122.70
1	D	59	ASP	N-CA-CB	5.38	120.28	110.60
1	D	149	LEU	N-CA-CB	5.36	121.12	110.40
1	D	148	ARG	CA-C-N	5.35	128.96	117.20
1	C	35	PHE	N-CA-CB	-5.33	101.01	110.60
1	D	129	LYS	CB-CA-C	5.32	121.05	110.40
1	A	21	LEU	CA-C-N	5.32	128.91	117.20
1	D	174	LEU	CA-CB-CG	5.31	127.52	115.30
1	D	94	VAL	CA-C-N	5.31	128.88	117.20
1	D	105	TYR	CA-CB-CG	5.31	123.48	113.40
1	D	66	GLU	OE1-CD-OE2	-5.30	116.94	123.30
1	D	130	VAL	CG1-CB-CG2	-5.29	102.43	110.90
1	D	81	GLU	OE1-CD-OE2	-5.29	116.96	123.30
1	D	139	LYS	CA-CB-CG	5.24	124.94	113.40
1	A	192	TRP	CA-CB-CG	5.24	123.65	113.70
1	D	159	PHE	N-CA-CB	-5.24	101.18	110.60
1	B	102	ALA	CA-C-N	5.17	128.58	117.20
1	A	57	LEU	CA-CB-CG	5.15	127.15	115.30
1	D	115	GLN	O-C-N	-5.13	114.49	122.70
1	D	103	ASN	N-CA-CB	5.12	119.82	110.60
1	B	99	GLU	CB-CA-C	5.11	120.62	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	50	PRO	CA-N-CD	-5.10	104.36	111.50
1	B	173	CYS	CA-C-N	5.09	128.41	117.20
1	A	74	ALA	N-CA-CB	5.06	117.19	110.10
1	D	161	SER	O-C-N	-5.04	114.63	122.70
1	B	65	PHE	O-C-N	-5.03	114.65	122.70
1	B	122	LEU	CA-CB-CG	5.01	126.83	115.30
1	C	33	ILE	CB-CG1-CD1	5.01	127.93	113.90

There are no chirality outliers.

All (87) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	ALA	Peptide
1	A	107	ALA	Peptide
1	A	11	SER	Mainchain
1	A	119	SER	Mainchain
1	A	124	GLY	Peptide
1	A	162	LEU	Peptide
1	A	178	PRO	Mainchain
1	A	186	TYR	Mainchain
1	A	20	ALA	Peptide
1	A	211	PRO	Peptide
1	A	35	PHE	Mainchain
1	A	37	THR	Mainchain
1	A	55	PRO	Peptide
1	A	80	PRO	Mainchain
1	A	93	MET	Peptide
1	B	119	SER	Mainchain
1	B	127	ASP	Mainchain
1	B	135	LEU	Peptide
1	B	144	VAL	Mainchain
1	B	146	GLU	Peptide
1	B	15	THR	Peptide
1	B	161	SER	Peptide
1	B	175	PHE	Mainchain,Peptide
1	B	185	ALA	Peptide
1	B	201	SER	Peptide
1	B	24	ALA	Peptide
1	B	39	GLU	Peptide
1	B	42	SER	Peptide
1	B	55	PRO	Peptide
1	B	77	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	B	78	ASN	Peptide
1	B	8	ALA	Mainchain
1	B	80	PRO	Mainchain
1	B	85	GLU	Peptide
1	B	93	MET	Peptide
1	C	12	TRP	Mainchain
1	C	124	GLY	Peptide
1	C	127	ASP	Mainchain
1	C	129	LYS	Peptide
1	C	150	THR	Mainchain
1	C	157	GLY	Mainchain
1	C	160	LEU	Mainchain
1	C	165	LEU	Mainchain
1	C	17	CYS	Peptide
1	C	180	ALA	Peptide
1	C	19	THR	Mainchain
1	C	194	SER	Peptide
1	C	205	VAL	Mainchain
1	C	3	MET	Mainchain
1	C	30	ILE	Peptide
1	C	35	PHE	Peptide
1	C	43	PRO	Peptide
1	C	49	ASN	Mainchain
1	C	54	VAL	Peptide
1	C	55	PRO	Peptide
1	C	6	TYR	Peptide
1	C	66	GLU	Mainchain
1	C	68	ARG	Sidechain
1	C	91	ALA	Peptide
1	C	92	ALA	Mainchain
1	C	94	VAL	Mainchain
1	C	99	GLU	Mainchain
1	D	102	ALA	Mainchain
1	D	114	PHE	Peptide
1	D	12	TRP	Peptide
1	D	147	ALA	Mainchain
1	D	149	LEU	Peptide
1	D	156	ALA	Peptide
1	D	16	ARG	Mainchain
1	D	17	CYS	Mainchain
1	D	173	CYS	Mainchain
1	D	177	THR	Mainchain

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Mol	Chain	Res	Type	Group
1	D	188	HIS	Mainchain
1	D	195	GLY	Mainchain
1	D	23	GLU	Peptide
1	D	38	ALA	Mainchain
1	D	43	PRO	Peptide
1	D	51	PHE	Peptide
1	D	53	GLN	Mainchain
1	D	58	GLN	Mainchain
1	D	7	GLY	Mainchain
1	D	72	LYS	Mainchain
1	D	75	ALA	Mainchain
1	D	77	LYS	Mainchain
1	D	93	MET	Peptide
1	D	97	TRP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1666	0	1676	149	0
1	B	1666	0	1676	181	0
1	C	1666	0	1676	156	0
1	D	1666	0	1676	164	0
2	A	33	0	28	21	0
2	B	33	0	28	4	0
2	C	33	0	28	4	0
2	D	33	0	28	7	0
3	A	11	0	0	1	0
3	B	12	0	0	2	0
3	C	16	0	0	0	0
3	D	9	0	0	2	0
All	All	6844	0	6816	639	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 47.

All (639) 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)
2:A:1001:ATA:N3	2:A:1001:ATA:O	1.89	1.04
2:D:1004:ATA:OT'	2:D:1004:ATA:O	1.77	1.02
2:A:1001:ATA:N5	2:A:1001:ATA:C9	2.22	1.01
1:C:66:GLU:HG3	1:D:99:GLU:HB3	1.41	1.00
1:D:153:LYS:HE3	1:D:158:ASP:HB3	1.42	0.98
2:A:1001:ATA:SG	2:A:1001:ATA:O	2.25	0.94
1:C:43:PRO:HA	1:C:46:LEU:HB2	1.53	0.91
1:B:18:ALA:HA	1:B:21:LEU:HD12	1.53	0.90
1:A:16:ARG:HD3	1:A:166:ASN:HD22	1.37	0.89
2:A:1001:ATA:N5	2:A:1001:ATA:H93	1.87	0.88
1:C:33:ILE:HG23	1:C:39:GLU:HG3	1.54	0.88
1:B:94:VAL:HG22	1:B:161:SER:HB3	1.56	0.88
1:B:98:ILE:HD11	1:B:162:LEU:HB3	1.57	0.87
1:D:53:GLN:NE2	2:D:1004:ATA:HG'1	1.89	0.87
1:A:99:GLU:HB3	1:B:66:GLU:HG2	1.57	0.86
1:C:33:ILE:HD12	1:C:45:HIS:HD2	1.39	0.86
1:C:172:LEU:HB3	1:C:209:MET:HE1	1.58	0.85
1:D:94:VAL:HG22	1:D:161:SER:HB3	1.58	0.83
1:A:21:LEU:HD23	1:A:74:ALA:HB2	1.61	0.83
1:B:97:TRP:HA	1:B:100:VAL:HG12	1.60	0.83
1:C:149:LEU:HD21	1:C:155:LEU:HD13	1.60	0.83
1:D:57:LEU:HD12	1:D:58:GLN:H	1.44	0.83
1:B:53:GLN:NE2	2:B:1002:ATA:HG'1	1.93	0.82
1:C:119:SER:HB3	1:C:120:PRO:HD3	1.61	0.82
1:D:34:ASN:HD21	1:D:36:ALA:HB3	1.42	0.82
1:B:15:THR:HG22	1:B:205:VAL:HG13	1.61	0.81
1:C:19:THR:HG21	1:C:168:VAL:HG21	1.62	0.81
1:C:106:THR:HG22	1:C:170:VAL:HG21	1.61	0.81
1:D:75:ALA:HB1	1:D:82:LEU:HB2	1.61	0.81
1:A:149:LEU:HD21	1:A:155:LEU:HD12	1.63	0.81
1:D:54:VAL:HB	1:D:55:PRO:HA	1.62	0.79
1:A:83:LEU:HD21	1:A:162:LEU:HD12	1.64	0.79
1:D:66:GLU:HG3	2:D:1004:ATA:HN'2	1.48	0.79
1:D:11:SER:HB3	1:D:14:LEU:HB2	1.66	0.78
1:D:136:GLU:HA	1:D:139:LYS:HG2	1.64	0.78
1:A:168:VAL:HG11	1:A:202:VAL:HG22	1.66	0.78
1:C:1:ALA:H2	1:C:2:PRO:HD2	1.49	0.78
1:B:20:ALA:HB2	1:B:71:CYS:SG	2.24	0.78
1:D:7:GLY:HA3	1:D:14:LEU:HD11	1.66	0.77
1:A:153:LYS:HG3	1:A:158:ASP:HB3	1.66	0.77
1:B:50:PRO:HD2	1:B:65:PHE:CE1	2.19	0.77
1:C:33:ILE:HD12	1:C:45:HIS:CD2	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:GLU:HB2	1:B:167:HIS:CE1	2.20	0.77
1:B:79:LYS:HG2	1:B:82:LEU:HD22	1.67	0.77
1:D:155:LEU:HB2	1:D:164:ASP:OD1	1.85	0.77
1:B:23:GLU:HG2	1:B:165:LEU:HD11	1.67	0.76
1:C:144:VAL:HG13	1:D:50:PRO:HB2	1.68	0.75
1:C:98:ILE:HD11	1:C:162:LEU:HB3	1.69	0.75
1:D:3:MET:HB3	1:D:57:LEU:HD11	1.68	0.75
1:D:109:LEU:HD11	1:D:174:LEU:HG	1.68	0.75
2:A:1001:ATA:C2	2:A:1001:ATA:O	2.35	0.75
2:A:1001:ATA:N5	2:A:1001:ATA:H92	2.01	0.74
1:B:14:LEU:HA	1:B:55:PRO:HG3	1.69	0.74
1:D:197:MET:HA	1:D:202:VAL:HG21	1.68	0.74
1:B:6:TYR:O	1:B:14:LEU:HD11	1.87	0.74
1:D:115:GLN:HG3	1:D:130:VAL:CG2	2.16	0.74
1:A:150:THR:HG23	1:A:188:HIS:CE1	2.23	0.74
1:C:1:ALA:N	1:C:2:PRO:HD2	2.03	0.73
1:B:183:LEU:HD12	1:B:190:LYS:HA	1.70	0.73
1:C:118:ILE:O	1:C:122:LEU:HB2	1.88	0.73
1:B:168:VAL:HG21	1:B:202:VAL:HG22	1.69	0.73
1:C:149:LEU:HD12	1:C:189:VAL:HA	1.69	0.73
1:B:83:LEU:O	1:B:84:ARG:HB2	1.89	0.73
1:A:118:ILE:HG13	2:A:1001:ATA:H121	1.69	0.73
1:D:55:PRO:HD2	2:D:1004:ATA:O1'	1.88	0.73
1:D:109:LEU:O	1:D:113:LEU:HG	1.90	0.72
1:C:118:ILE:HG12	2:C:1003:ATA:H133	1.71	0.72
1:C:79:LYS:N	1:C:80:PRO:HD3	2.05	0.71
1:B:101:GLU:HB2	1:B:167:HIS:HE1	1.56	0.71
1:D:87:ASN:HB3	1:D:90:GLU:HB2	1.73	0.71
1:D:146:GLU:OE1	1:D:146:GLU:HA	1.89	0.70
1:A:16:ARG:HG2	1:A:67:SER:OG	1.90	0.70
1:B:84:ARG:HG3	1:B:159:PHE:CE2	2.25	0.70
1:D:66:GLU:O	1:D:68:ARG:N	2.24	0.70
1:C:14:LEU:CD2	1:C:55:PRO:HB3	2.22	0.70
1:C:1:ALA:N	1:C:2:PRO:CD	2.55	0.70
1:D:58:GLN:HE21	1:D:63:TYR:HE1	1.40	0.69
1:B:4:LYS:HD3	1:B:58:GLN:OE1	1.93	0.69
1:A:19:THR:HB	1:A:205:VAL:HG21	1.74	0.69
1:B:210:LYS:HB3	1:B:211:PRO:HD2	1.74	0.68
1:B:161:SER:HB2	1:B:163:ALA:H	1.59	0.68
1:A:62:LEU:HD23	1:A:73:TYR:OH	1.93	0.68
1:B:87:ASN:HB3	1:B:90:GLU:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:TRP:HA	1:C:15:THR:HG23	1.76	0.68
1:C:24:ALA:O	1:C:78:ASN:HB3	1.95	0.67
1:C:77:LYS:HB3	1:C:78:ASN:HD22	1.60	0.66
1:D:115:GLN:HG3	1:D:130:VAL:HG21	1.76	0.66
1:D:34:ASN:ND2	1:D:36:ALA:HB3	2.11	0.66
1:D:21:LEU:O	1:D:26:SER:HB3	1.95	0.66
1:A:9:VAL:HA	1:A:14:LEU:HD22	1.76	0.66
1:B:177:THR:HB	1:B:178:PRO:HD2	1.78	0.65
1:A:16:ARG:HD3	1:A:166:ASN:ND2	2.09	0.65
1:A:106:THR:HG23	1:A:170:VAL:HG11	1.78	0.65
1:C:5:LEU:HD23	1:C:30:ILE:HG12	1.79	0.65
1:D:98:ILE:HG13	1:D:163:ALA:HB2	1.79	0.65
1:D:146:GLU:OE1	1:D:189:VAL:HG23	1.96	0.65
1:A:119:SER:N	1:A:120:PRO:HD2	2.12	0.65
1:A:164:ASP:OD2	1:A:192:TRP:NE1	2.29	0.65
1:B:148:ARG:HA	1:B:151:LYS:HE2	1.78	0.65
1:A:149:LEU:HD21	1:A:155:LEU:CD1	2.27	0.64
1:C:100:VAL:HG12	1:C:145:TYR:OH	1.97	0.64
1:D:65:PHE:HA	1:D:70:ILE:HD11	1.79	0.64
1:B:19:THR:HG21	1:B:168:VAL:HG22	1.79	0.64
1:B:54:VAL:HB	1:B:55:PRO:HA	1.78	0.64
1:A:68:ARG:HH21	1:A:101:GLU:CD	2.01	0.64
1:A:128:GLN:O	1:A:128:GLN:HG3	1.97	0.64
1:B:199:ARG:HH11	1:B:199:ARG:HB3	1.63	0.63
1:C:174:LEU:O	1:C:180:ALA:HB2	1.97	0.63
1:B:97:TRP:CE3	1:B:100:VAL:HG11	2.33	0.63
1:B:75:ALA:HB1	1:B:83:LEU:HG	1.80	0.63
1:C:23:GLU:OE2	1:C:199:ARG:NH1	2.31	0.63
1:A:65:PHE:O	1:A:66:GLU:HB2	1.99	0.63
1:B:34:ASN:HB3	1:B:37:THR:HG1	1.63	0.63
1:D:197:MET:HA	1:D:202:VAL:CG2	2.28	0.63
1:D:210:LYS:N	1:D:211:PRO:HD2	2.13	0.63
1:C:53:GLN:HE21	2:C:1003:ATA:HN	1.45	0.63
1:D:172:LEU:HB3	1:D:209:MET:HE1	1.82	0.62
1:A:101:GLU:HB2	1:A:167:HIS:NE2	2.14	0.62
1:A:88:LEU:HD11	1:B:76:ARG:O	1.99	0.62
1:A:168:VAL:HA	1:A:193:TRP:HZ3	1.63	0.62
1:C:136:GLU:O	1:C:140:LYS:HG2	2.00	0.62
2:D:1004:ATA:OT'	2:D:1004:ATA:C	2.36	0.62
1:C:51:PHE:O	1:C:53:GLN:HG2	1.99	0.62
1:C:149:LEU:O	1:C:188:HIS:HB3	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:LEU:HD12	1:D:58:GLN:N	2.15	0.61
1:C:45:HIS:NE2	1:C:54:VAL:HG12	2.16	0.61
2:A:1001:ATA:H122	2:A:1001:ATA:C9	2.30	0.61
1:B:48:ARG:O	1:B:49:ASN:HB2	1.99	0.61
1:D:54:VAL:CB	1:D:55:PRO:HA	2.31	0.61
1:A:10:MET:HB2	2:A:1001:ATA:H132	1.82	0.61
1:C:7:GLY:HA3	1:C:14:LEU:HD21	1.80	0.61
1:C:51:PHE:HE2	1:D:100:VAL:HG22	1.66	0.61
1:D:45:HIS:HA	1:D:48:ARG:HE	1.64	0.61
1:A:119:SER:H	1:A:120:PRO:HD2	1.65	0.61
1:A:89:GLU:HG3	1:B:62:LEU:HD13	1.81	0.61
1:B:93:MET:HE3	1:B:148:ARG:HH22	1.66	0.61
1:C:109:LEU:O	1:C:113:LEU:HG	2.00	0.61
1:C:65:PHE:O	1:D:96:VAL:HG23	2.01	0.61
1:D:194:SER:O	1:D:198:GLU:HG3	2.01	0.60
1:D:64:LEU:HD11	1:D:73:TYR:CD2	2.36	0.60
1:A:171:THR:HG22	1:A:175:PHE:HE1	1.66	0.60
1:A:5:LEU:CD2	1:A:18:ALA:HB2	2.31	0.60
1:A:33:ILE:HD12	1:A:39:GLU:HG2	1.83	0.60
1:A:55:PRO:HD2	2:A:1001:ATA:O1'	2.02	0.60
1:B:109:LEU:HA	1:B:112:ILE:HD12	1.83	0.60
1:A:30:ILE:HD11	1:A:208:LEU:HD21	1.84	0.60
1:B:2:PRO:HG3	1:B:27:ASP:HB3	1.84	0.60
1:B:93:MET:CE	1:B:148:ARG:HH22	2.16	0.59
1:B:53:GLN:HE21	2:B:1002:ATA:HG'1	1.61	0.59
1:D:101:GLU:HB2	1:D:167:HIS:NE2	2.17	0.59
1:D:12:TRP:HA	1:D:15:THR:HG22	1.83	0.59
1:D:111:PRO:HG2	1:D:134:ASN:ND2	2.17	0.59
1:C:26:SER:HA	1:C:78:ASN:OD1	2.02	0.59
1:A:72:LYS:HG2	1:B:95:ASP:OD2	2.03	0.59
1:B:207:ALA:O	1:B:211:PRO:HD2	2.02	0.59
1:B:4:LYS:HA	1:B:29:GLU:O	2.03	0.59
1:D:182:VAL:HG22	1:D:186:TYR:HE1	1.68	0.59
1:A:22:GLU:HB2	1:A:201:SER:HB2	1.83	0.59
1:D:50:PRO:HD2	1:D:65:PHE:CE2	2.38	0.59
1:C:145:TYR:HE2	1:C:167:HIS:HE2	1.49	0.59
1:B:16:ARG:NH1	1:B:67:SER:OG	2.34	0.58
1:B:144:VAL:O	1:B:146:GLU:N	2.36	0.58
1:B:116:VAL:O	1:B:117:LEU:HD23	2.03	0.58
1:D:116:VAL:O	1:D:117:LEU:HG	2.03	0.58
1:D:116:VAL:HG12	1:D:116:VAL:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:VAL:HG12	1:A:145:TYR:OH	2.04	0.58
1:D:66:GLU:HG3	2:D:1004:ATA:N'	2.16	0.58
1:B:149:LEU:HA	1:B:152:CYS:O	2.03	0.58
1:D:150:THR:HG23	1:D:188:HIS:CE1	2.39	0.58
1:D:136:GLU:HA	1:D:139:LYS:CG	2.33	0.57
1:B:64:LEU:O	1:B:70:ILE:HD11	2.04	0.57
1:A:119:SER:N	1:A:120:PRO:CD	2.65	0.57
1:C:94:VAL:O	1:C:98:ILE:HB	2.03	0.57
1:B:168:VAL:HG11	1:B:196:LEU:HG	1.87	0.57
1:B:74:ALA:O	1:B:78:ASN:HB2	2.04	0.57
1:A:51:PHE:CZ	1:B:144:VAL:HG11	2.39	0.57
1:B:149:LEU:HD21	1:B:155:LEU:HD13	1.87	0.57
1:B:34:ASN:HB3	1:B:37:THR:OG1	2.04	0.57
1:C:76:ARG:HG2	1:D:88:LEU:HD23	1.87	0.57
1:D:115:GLN:HG3	1:D:130:VAL:HG23	1.86	0.57
1:D:196:LEU:O	1:D:196:LEU:HD13	2.04	0.57
1:C:78:ASN:O	1:C:79:LYS:HB2	2.04	0.57
1:C:96:VAL:O	1:C:98:ILE:N	2.38	0.57
1:B:195:GLY:O	1:B:199:ARG:HG2	2.05	0.57
1:A:21:LEU:CD2	1:A:74:ALA:HB2	2.35	0.56
1:C:53:GLN:NE2	2:C:1003:ATA:HN	2.03	0.56
1:C:15:THR:O	1:C:18:ALA:HB3	2.05	0.56
1:A:144:VAL:O	1:A:147:ALA:N	2.38	0.56
1:D:33:ILE:HG23	1:D:39:GLU:HB3	1.86	0.56
1:D:168:VAL:HG22	1:D:196:LEU:HD11	1.87	0.56
1:D:33:ILE:HG21	1:D:40:HIS:HB3	1.87	0.56
1:C:79:LYS:H	1:C:80:PRO:HD3	1.69	0.56
1:B:4:LYS:HB2	1:B:6:TYR:CE2	2.41	0.56
1:C:99:GLU:OE1	1:D:68:ARG:HB3	2.06	0.56
1:D:79:LYS:HG2	1:D:82:LEU:HG	1.87	0.56
1:C:110:ASN:O	1:C:113:LEU:N	2.39	0.56
1:B:84:ARG:HD2	1:B:90:GLU:OE1	2.06	0.56
1:B:164:ASP:HB2	3:B:1013:HOH:O	2.05	0.56
1:C:106:THR:HA	1:C:109:LEU:HB3	1.87	0.56
1:B:68:ARG:NH1	1:B:101:GLU:OE1	2.38	0.56
1:A:157:GLY:HA3	1:A:159:PHE:CE1	2.40	0.56
1:B:164:ASP:OD1	1:B:192:TRP:NE1	2.36	0.56
1:D:135:LEU:O	1:D:135:LEU:HG	2.06	0.55
1:D:175:PHE:HA	1:D:180:ALA:HB2	1.88	0.55
1:C:99:GLU:HB3	1:D:66:GLU:HG2	1.89	0.55
1:C:21:LEU:HD23	1:C:74:ALA:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:VAL:O	1:D:205:VAL:HG12	2.07	0.55
1:B:210:LYS:HB3	1:B:211:PRO:CD	2.36	0.55
1:B:87:ASN:ND2	1:B:90:GLU:HG3	2.22	0.55
1:A:33:ILE:HG23	1:A:39:GLU:HB3	1.88	0.54
1:A:88:LEU:HD11	1:B:76:ARG:HG3	1.87	0.54
1:C:15:THR:HG21	1:C:209:MET:SD	2.47	0.54
1:D:149:LEU:CD2	1:D:155:LEU:HD23	2.36	0.54
1:A:23:GLU:HG2	1:A:201:SER:OG	2.07	0.54
1:A:99:GLU:HB3	1:B:66:GLU:CG	2.34	0.54
1:B:2:PRO:HB3	1:B:27:ASP:HB3	1.88	0.54
1:B:142:LEU:HB3	1:B:186:TYR:CE2	2.43	0.54
1:D:145:TYR:H	1:D:145:TYR:HD1	1.54	0.54
1:D:38:ALA:HA	1:D:40:HIS:CD2	2.42	0.54
1:A:65:PHE:HD1	1:A:66:GLU:HG2	1.73	0.54
1:C:202:VAL:O	1:C:205:VAL:HG12	2.07	0.54
1:B:7:GLY:HA3	1:B:54:VAL:HG21	1.88	0.54
1:A:118:ILE:CG1	2:A:1001:ATA:H93	2.38	0.54
1:A:168:VAL:HA	1:A:193:TRP:CZ3	2.43	0.54
1:A:140:LYS:HE2	1:A:140:LYS:HA	1.90	0.54
1:A:93:MET:HB3	1:A:156:ALA:HB1	1.90	0.54
1:A:112:ILE:HD13	1:A:135:LEU:HD13	1.89	0.54
1:B:15:THR:CG2	1:B:205:VAL:HG13	2.34	0.54
1:D:101:GLU:HB2	1:D:167:HIS:CD2	2.43	0.54
1:D:135:LEU:O	1:D:139:LYS:HG2	2.08	0.54
1:D:185:ALA:HB3	1:D:186:TYR:CE1	2.42	0.54
1:B:97:TRP:HA	1:B:100:VAL:CG1	2.35	0.54
1:C:65:PHE:HA	1:C:70:ILE:HD11	1.90	0.54
1:C:63:TYR:O	1:C:64:LEU:HD23	2.07	0.53
1:D:185:ALA:HB3	1:D:186:TYR:CD1	2.43	0.53
1:D:3:MET:HG2	1:D:59:ASP:HA	1.89	0.53
1:C:88:LEU:HD11	1:D:76:ARG:O	2.07	0.53
1:D:100:VAL:HG12	1:D:145:TYR:OH	2.08	0.53
1:B:183:LEU:CD1	1:B:190:LYS:HA	2.37	0.53
1:B:19:THR:HG21	1:B:168:VAL:CG2	2.37	0.53
1:D:174:LEU:O	1:D:180:ALA:HB2	2.08	0.53
1:B:71:CYS:O	1:B:162:LEU:HD11	2.08	0.53
1:C:3:MET:HG2	1:C:27:ASP:O	2.08	0.53
1:A:73:TYR:O	1:A:77:LYS:HB2	2.08	0.53
1:B:147:ALA:O	1:B:148:ARG:C	2.46	0.53
1:B:2:PRO:CB	1:B:27:ASP:HB3	2.39	0.53
1:B:75:ALA:HB2	1:B:162:LEU:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:THR:O	1:C:175:PHE:HD1	1.91	0.53
1:D:142:LEU:CD2	1:D:189:VAL:HG11	2.39	0.53
1:D:42:SER:O	1:D:46:LEU:HG	2.08	0.53
1:B:67:SER:HB3	2:B:1002:ATA:O2'	2.09	0.53
1:B:12:TRP:CD1	1:B:170:VAL:HG22	2.43	0.53
1:B:68:ARG:HG2	1:B:68:ARG:HH11	1.74	0.53
1:C:149:LEU:HD13	1:C:192:TRP:CB	2.38	0.53
1:B:146:GLU:O	1:B:150:THR:N	2.41	0.53
1:C:6:TYR:CE2	1:C:48:ARG:HG2	2.43	0.53
1:D:79:LYS:NZ	1:D:79:LYS:HB2	2.23	0.53
1:A:131:VAL:O	1:A:135:LEU:HB2	2.09	0.52
1:C:179:TYR:O	1:C:182:VAL:HG12	2.09	0.52
1:C:149:LEU:HD13	1:C:192:TRP:HB3	1.91	0.52
1:A:9:VAL:HA	1:A:14:LEU:CD2	2.39	0.52
1:A:12:TRP:CH2	1:A:118:ILE:HD11	2.44	0.52
1:D:17:CYS:O	1:D:20:ALA:HB3	2.08	0.52
1:B:115:GLN:HG3	1:B:130:VAL:HG22	1.90	0.52
1:B:177:THR:OG1	1:B:179:TYR:HB2	2.09	0.52
1:A:89:GLU:OE2	1:B:62:LEU:HD22	2.09	0.52
1:D:93:MET:O	1:D:96:VAL:HG12	2.10	0.52
1:C:4:LYS:HB2	1:C:58:GLN:HB3	1.92	0.52
1:B:79:LYS:CG	1:B:82:LEU:HD22	2.38	0.52
1:A:84:ARG:NH2	1:A:159:PHE:HB3	2.25	0.52
1:C:49:ASN:ND2	1:C:53:GLN:O	2.42	0.52
1:D:127:ASP:HB3	1:D:130:VAL:HG22	1.91	0.52
1:B:72:LYS:O	1:B:75:ALA:HB3	2.09	0.52
1:A:22:GLU:OE2	1:A:28:TYR:HE1	1.93	0.51
1:A:78:ASN:O	1:A:79:LYS:HB2	2.10	0.51
1:B:3:MET:HE3	1:B:57:LEU:HD21	1.92	0.51
2:A:1001:ATA:HG'2	2:A:1001:ATA:O1'	1.96	0.51
1:A:12:TRP:CD1	1:A:170:VAL:HG12	2.45	0.51
1:C:109:LEU:HD23	1:C:138:LEU:HD13	1.91	0.51
1:C:146:GLU:HB2	1:C:189:VAL:HG23	1.91	0.51
1:B:82:LEU:O	1:B:161:SER:HA	2.11	0.51
1:A:144:VAL:O	1:A:145:TYR:C	2.47	0.51
1:B:2:PRO:CG	1:B:27:ASP:HB3	2.41	0.51
1:C:110:ASN:HB3	1:C:111:PRO:CD	2.40	0.51
1:C:205:VAL:O	1:C:206:ALA:C	2.49	0.51
1:B:125:THR:O	1:B:126:THR:C	2.48	0.51
1:B:205:VAL:HA	1:B:208:LEU:HD12	1.93	0.51
1:A:162:LEU:O	1:A:163:ALA:C	2.49	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:TRP:O	1:C:197:MET:HB2	2.11	0.51
1:C:199:ARG:O	1:C:203:GLN:HG2	2.11	0.51
1:C:145:TYR:HE2	1:C:167:HIS:NE2	2.07	0.51
1:A:12:TRP:HH2	1:A:118:ILE:HD11	1.76	0.51
1:A:79:LYS:HG3	1:A:81:GLU:OE1	2.11	0.51
1:B:4:LYS:CD	1:B:4:LYS:H	2.24	0.51
1:C:16:ARG:HB2	1:C:169:SER:HB3	1.92	0.51
1:B:17:CYS:HB3	1:B:70:ILE:HG22	1.92	0.51
1:C:94:VAL:HG22	1:C:161:SER:OG	2.11	0.51
1:D:130:VAL:HG23	1:D:131:VAL:N	2.26	0.51
1:C:14:LEU:HD13	1:C:14:LEU:O	2.10	0.50
1:C:19:THR:HG21	1:C:168:VAL:CG2	2.37	0.50
1:C:44:GLU:O	1:C:47:VAL:HG23	2.11	0.50
1:A:65:PHE:HA	1:A:70:ILE:HD11	1.92	0.50
1:C:34:ASN:H	1:C:39:GLU:CD	2.14	0.50
1:D:134:ASN:HA	1:D:137:LYS:HB2	1.93	0.50
1:D:72:LYS:O	1:D:75:ALA:N	2.43	0.50
1:B:205:VAL:HA	1:B:208:LEU:HB2	1.94	0.50
1:D:23:GLU:HG2	1:D:165:LEU:HD21	1.93	0.50
1:A:1:ALA:N	1:A:2:PRO:HD3	2.26	0.50
1:B:193:TRP:O	1:B:196:LEU:N	2.42	0.50
1:D:127:ASP:HB3	1:D:130:VAL:CG2	2.40	0.50
1:D:153:LYS:CE	1:D:158:ASP:HB3	2.30	0.50
1:D:59:ASP:O	1:D:61:ASP:N	2.44	0.50
1:A:8:ALA:O	1:A:14:LEU:HD22	2.12	0.50
1:B:164:ASP:O	1:B:167:HIS:HB2	2.12	0.50
1:B:69:ALA:O	1:B:72:LYS:HB2	2.12	0.50
1:B:146:GLU:CG	1:B:186:TYR:HB3	2.41	0.50
1:A:130:VAL:HA	1:A:133:GLU:HG2	1.94	0.50
1:B:174:LEU:HB3	1:B:180:ALA:HB2	1.92	0.50
1:C:22:GLU:HB2	1:C:201:SER:HB2	1.94	0.50
1:C:96:VAL:N	1:D:69:ALA:HB2	2.27	0.50
1:D:115:GLN:CG	1:D:130:VAL:HG21	2.42	0.50
1:D:195:GLY:HA2	1:D:198:GLU:CD	2.31	0.50
1:D:199:ARG:HB2	1:D:202:VAL:HG13	1.93	0.50
1:A:115:GLN:HB3	1:A:126:THR:HG23	1.94	0.50
1:A:171:THR:HB	1:A:193:TRP:CH2	2.46	0.50
1:A:23:GLU:CD	1:A:199:ARG:HE	2.13	0.49
1:A:23:GLU:OE2	1:A:199:ARG:NE	2.45	0.49
1:C:128:GLN:NE2	1:C:132:ASP:OD1	2.41	0.49
1:C:165:LEU:O	1:C:168:VAL:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:TYR:HB2	1:D:157:GLY:O	2.12	0.49
1:B:137:LYS:O	1:B:141:VAL:HG23	2.13	0.49
1:B:168:VAL:CG1	1:B:196:LEU:HG	2.41	0.49
1:B:24:ALA:HB1	1:B:78:ASN:CB	2.41	0.49
1:D:154:TYR:CE2	1:D:160:LEU:HD23	2.47	0.49
1:A:104:GLN:O	1:A:141:VAL:HG21	2.13	0.49
1:A:153:LYS:HB2	1:A:158:ASP:HA	1.94	0.49
1:A:106:THR:CG2	1:A:170:VAL:HG11	2.42	0.49
1:A:144:VAL:HG21	1:B:51:PHE:CD1	2.48	0.49
1:C:65:PHE:O	1:C:66:GLU:HB2	2.12	0.49
1:A:194:SER:O	1:A:195:GLY:C	2.50	0.49
1:A:4:LYS:HD2	1:A:58:GLN:OE1	2.12	0.49
1:A:51:PHE:CD1	1:B:144:VAL:HG21	2.47	0.49
1:C:143:GLU:HG2	1:C:186:TYR:CE1	2.48	0.49
1:B:109:LEU:CD1	1:B:170:VAL:HG12	2.43	0.49
1:B:119:SER:N	1:B:120:PRO:CD	2.76	0.49
1:D:101:GLU:HG3	1:D:167:HIS:CD2	2.48	0.49
1:D:65:PHE:HA	1:D:70:ILE:CD1	2.43	0.49
1:B:144:VAL:O	1:B:145:TYR:C	2.51	0.49
1:D:33:ILE:CG2	1:D:40:HIS:HB3	2.43	0.49
1:B:146:GLU:HG3	1:B:186:TYR:HB3	1.93	0.49
1:C:78:ASN:HD22	1:C:78:ASN:N	2.10	0.49
1:B:83:LEU:O	1:B:84:ARG:CB	2.61	0.48
1:C:14:LEU:HD23	1:C:55:PRO:HB3	1.94	0.48
1:A:116:VAL:O	1:A:116:VAL:HG12	2.14	0.48
1:B:97:TRP:CA	1:B:100:VAL:HG12	2.38	0.48
1:B:14:LEU:CA	1:B:55:PRO:HG3	2.41	0.48
1:B:68:ARG:HH12	1:B:101:GLU:CD	2.16	0.48
1:D:181:SER:O	1:D:184:ASP:OD1	2.32	0.48
1:D:58:GLN:NE2	1:D:63:TYR:HE1	2.11	0.48
1:A:122:LEU:H	1:A:122:LEU:HD12	1.78	0.48
1:A:1:ALA:N	1:A:2:PRO:CD	2.76	0.48
1:A:51:PHE:CE1	1:B:144:VAL:HG21	2.48	0.48
1:B:22:GLU:HB3	1:B:201:SER:OG	2.12	0.48
1:A:118:ILE:HD12	1:A:118:ILE:H	1.79	0.48
1:B:94:VAL:CG2	1:B:161:SER:HB3	2.36	0.48
1:B:172:LEU:HD21	1:B:202:VAL:HG13	1.94	0.48
1:D:148:ARG:O	1:D:148:ARG:HG3	2.12	0.48
1:D:40:HIS:CE1	1:D:41:LYS:HZ3	2.31	0.48
1:D:53:GLN:HB3	2:D:1004:ATA:N	2.28	0.48
1:A:3:MET:O	1:A:28:TYR:HA	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:TRP:CG	1:B:170:VAL:HG22	2.49	0.48
1:C:114:PHE:HD1	1:C:118:ILE:HB	1.77	0.48
1:C:84:ARG:HB3	1:C:87:ASN:HD21	1.77	0.48
1:D:162:LEU:HG	1:D:162:LEU:O	2.12	0.48
1:B:152:CYS:SG	1:B:157:GLY:HA2	2.54	0.48
1:B:34:ASN:OD1	1:B:37:THR:N	2.46	0.48
1:C:129:LYS:O	1:C:133:GLU:HB2	2.13	0.48
1:B:113:LEU:CD1	1:B:173:CYS:HB2	2.42	0.48
1:B:62:LEU:HA	1:B:62:LEU:HD12	1.79	0.48
1:D:101:GLU:HG3	1:D:167:HIS:HD2	1.78	0.48
1:A:59:ASP:OD2	1:A:77:LYS:NZ	2.47	0.48
1:A:53:GLN:HB3	2:A:1001:ATA:CD	2.44	0.48
1:A:108:ALA:HB1	1:A:138:LEU:HB2	1.96	0.48
1:A:14:LEU:O	1:A:14:LEU:HG	2.12	0.47
1:A:83:LEU:CD2	1:A:162:LEU:HD12	2.40	0.47
1:C:12:TRP:O	1:C:169:SER:HB2	2.14	0.47
1:C:34:ASN:H	1:C:39:GLU:CG	2.26	0.47
1:C:45:HIS:O	1:C:45:HIS:ND1	2.46	0.47
1:D:97:TRP:CZ3	1:D:100:VAL:HG11	2.49	0.47
1:D:79:LYS:HZ3	1:D:79:LYS:HB2	1.78	0.47
1:A:162:LEU:O	1:A:165:LEU:N	2.47	0.47
1:A:38:ALA:HA	1:A:40:HIS:CE1	2.49	0.47
1:A:78:ASN:O	1:A:79:LYS:CB	2.62	0.47
1:A:96:VAL:HG12	1:A:97:TRP:CD1	2.50	0.47
1:B:4:LYS:HD2	1:B:58:GLN:HB3	1.96	0.47
1:A:10:MET:CG	2:A:1001:ATA:H132	2.45	0.47
1:A:43:PRO:HA	1:A:46:LEU:HD12	1.96	0.47
1:C:23:GLU:O	1:C:23:GLU:HG3	2.14	0.47
1:C:84:ARG:HH21	1:C:159:PHE:HB3	1.79	0.47
1:C:51:PHE:CD1	1:D:144:VAL:HG21	2.50	0.47
1:D:149:LEU:HD21	1:D:155:LEU:HD23	1.95	0.47
1:C:22:GLU:CB	1:C:201:SER:HB2	2.45	0.47
1:D:23:GLU:OE2	1:D:199:ARG:NE	2.47	0.47
1:B:147:ALA:O	1:B:151:LYS:HG3	2.15	0.47
1:B:197:MET:HA	1:B:202:VAL:HG11	1.96	0.47
1:C:210:LYS:HD2	1:C:210:LYS:N	2.29	0.47
1:C:88:LEU:O	1:C:89:GLU:C	2.49	0.47
1:D:75:ALA:CB	1:D:82:LEU:HB2	2.39	0.47
1:B:39:GLU:O	1:B:42:SER:OG	2.33	0.47
1:A:118:ILE:HG12	2:A:1001:ATA:H93	1.97	0.46
1:A:4:LYS:HB2	1:A:58:GLN:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:VAL:HB	1:D:55:PRO:CA	2.36	0.46
1:A:171:THR:O	1:A:175:PHE:HD1	1.98	0.46
1:B:159:PHE:N	1:B:159:PHE:CD1	2.83	0.46
1:B:62:LEU:HG	1:B:64:LEU:HD21	1.96	0.46
1:C:90:GLU:HB3	1:C:159:PHE:CZ	2.51	0.46
1:C:172:LEU:CB	1:C:209:MET:HE1	2.36	0.46
1:C:48:ARG:CD	1:C:48:ARG:H	2.29	0.46
1:A:108:ALA:O	1:A:112:ILE:HG13	2.16	0.46
1:B:202:VAL:O	1:B:206:ALA:N	2.48	0.46
1:D:156:ALA:HB3	1:D:161:SER:OG	2.15	0.46
1:B:29:GLU:HG3	1:B:29:GLU:O	2.16	0.46
1:C:204:LYS:HG2	1:C:204:LYS:O	2.15	0.46
1:D:139:LYS:HE2	1:D:139:LYS:HB3	1.71	0.46
1:B:139:LYS:O	1:B:142:LEU:N	2.46	0.46
1:C:15:THR:HG21	1:C:209:MET:CG	2.45	0.46
1:C:39:GLU:HA	1:C:42:SER:CB	2.45	0.46
1:C:88:LEU:HD23	1:C:88:LEU:C	2.35	0.46
1:A:171:THR:HB	1:A:193:TRP:CZ3	2.50	0.46
1:D:71:CYS:HB3	1:D:162:LEU:HD11	1.98	0.46
1:A:118:ILE:HG21	2:A:1001:ATA:H8	1.97	0.46
1:A:153:LYS:CG	1:A:158:ASP:HB3	2.42	0.46
1:B:3:MET:SD	1:B:59:ASP:OD2	2.74	0.46
1:C:148:ARG:HD2	1:C:148:ARG:HA	1.78	0.46
1:D:168:VAL:HG11	1:D:202:VAL:HB	1.96	0.46
1:B:173:CYS:O	1:B:176:ALA:HB3	2.15	0.46
1:B:31:VAL:HA	1:B:32:PRO:HD3	1.85	0.46
1:B:82:LEU:HD12	1:B:160:LEU:O	2.15	0.46
1:C:28:TYR:HE1	1:C:30:ILE:HG13	1.81	0.46
1:A:95:ASP:OD1	1:B:72:LYS:NZ	2.46	0.46
1:B:161:SER:N	3:B:1013:HOH:O	2.44	0.46
1:C:66:GLU:HA	2:C:1003:ATA:O1'	2.15	0.46
1:D:172:LEU:CB	1:D:209:MET:HE1	2.44	0.46
1:B:142:LEU:HB3	1:B:186:TYR:CD2	2.51	0.46
1:B:210:LYS:CB	1:B:211:PRO:CD	2.94	0.46
1:B:67:SER:O	1:B:71:CYS:HB2	2.16	0.46
2:A:1001:ATA:H122	2:A:1001:ATA:H92	1.95	0.45
1:A:1:ALA:H3	1:A:2:PRO:HD3	1.81	0.45
1:C:175:PHE:HZ	1:C:183:LEU:HD22	1.81	0.45
1:C:94:VAL:HG23	1:C:156:ALA:HB1	1.97	0.45
1:A:68:ARG:NH2	1:A:101:GLU:OE2	2.48	0.45
1:A:21:LEU:HD23	1:A:74:ALA:CB	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ASP:OD1	1:B:127:ASP:C	2.53	0.45
1:A:16:ARG:CD	1:A:166:ASN:HD22	2.19	0.45
1:A:200:PRO:HG2	1:A:201:SER:H	1.82	0.45
1:A:95:ASP:O	1:A:96:VAL:C	2.54	0.45
1:B:33:ILE:CG2	1:B:40:HIS:H	2.30	0.45
1:C:197:MET:HA	1:C:202:VAL:HG11	1.97	0.45
1:A:71:CYS:O	1:A:162:LEU:HD11	2.16	0.45
1:A:16:ARG:NE	1:A:166:ASN:O	2.42	0.45
1:D:57:LEU:N	1:D:64:LEU:O	2.48	0.45
1:A:118:ILE:HG22	1:A:122:LEU:HD11	1.97	0.45
1:A:138:LEU:O	1:A:142:LEU:HG	2.17	0.45
1:A:101:GLU:HG3	1:A:167:HIS:CD2	2.52	0.45
1:C:24:ALA:HA	1:C:79:LYS:HD3	1.99	0.45
1:A:145:TYR:CE2	1:A:167:HIS:HE1	2.35	0.45
1:C:45:HIS:HA	1:C:48:ARG:CD	2.46	0.45
1:A:157:GLY:HA3	1:A:159:PHE:CD1	2.52	0.45
1:A:50:PRO:HD2	1:A:65:PHE:CE2	2.52	0.45
1:B:3:MET:O	1:B:28:TYR:HA	2.17	0.45
1:B:62:LEU:CD2	1:B:64:LEU:HD21	2.47	0.45
1:C:175:PHE:CZ	1:C:183:LEU:HD22	2.52	0.45
1:A:16:ARG:HD3	1:A:166:ASN:HA	1.98	0.45
1:C:79:LYS:N	1:C:80:PRO:CD	2.77	0.45
1:A:200:PRO:HA	1:A:203:GLN:NE2	2.31	0.44
1:A:10:MET:CB	2:A:1001:ATA:H132	2.48	0.44
1:A:22:GLU:OE2	1:A:28:TYR:CE1	2.70	0.44
1:B:114:PHE:HB2	1:B:118:ILE:HB	1.98	0.44
1:C:106:THR:CG2	1:C:170:VAL:HG21	2.40	0.44
1:A:109:LEU:O	1:A:110:ASN:C	2.55	0.44
1:A:44:GLU:O	1:A:47:VAL:HG13	2.17	0.44
1:C:162:LEU:O	1:C:163:ALA:C	2.55	0.44
1:C:190:LYS:HZ3	1:C:193:TRP:HD1	1.66	0.44
1:D:196:LEU:O	1:D:202:VAL:HG21	2.17	0.44
1:D:75:ALA:HB2	1:D:82:LEU:HD12	2.00	0.44
1:C:95:ASP:O	1:C:96:VAL:C	2.56	0.44
1:D:147:ALA:O	1:D:148:ARG:C	2.56	0.44
1:D:12:TRP:CD1	1:D:170:VAL:HG12	2.52	0.44
1:A:118:ILE:O	1:A:118:ILE:HG22	2.17	0.44
1:B:190:LYS:O	1:B:193:TRP:HB3	2.18	0.44
1:B:76:ARG:HA	1:B:80:PRO:HG3	2.00	0.44
1:C:12:TRP:CZ2	1:C:110:ASN:ND2	2.85	0.44
1:D:210:LYS:N	1:D:211:PRO:CD	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:LEU:O	1:C:139:LYS:HB2	2.17	0.44
1:C:1:ALA:H2	1:C:2:PRO:CD	2.20	0.44
1:C:30:ILE:O	1:C:32:PRO:HD3	2.18	0.44
1:B:54:VAL:HA	1:B:55:PRO:C	2.38	0.44
1:D:193:TRP:NE1	1:D:197:MET:HE2	2.33	0.44
1:B:120:PRO:HA	1:B:124:GLY:O	2.18	0.44
1:B:34:ASN:CB	1:B:37:THR:HG1	2.29	0.44
1:D:68:ARG:NH2	1:D:101:GLU:OE1	2.49	0.44
1:D:81:GLU:CD	1:D:81:GLU:H	2.21	0.44
1:A:149:LEU:O	1:A:188:HIS:HB3	2.18	0.43
1:A:26:SER:OG	1:A:78:ASN:ND2	2.46	0.43
1:B:136:GLU:O	1:B:139:LYS:HB2	2.18	0.43
1:C:3:MET:HE1	1:C:73:TYR:HE2	1.82	0.43
1:D:119:SER:CB	1:D:120:PRO:HD3	2.48	0.43
1:A:17:CYS:O	1:A:19:THR:N	2.43	0.43
1:B:119:SER:N	1:B:120:PRO:HD2	2.33	0.43
1:D:128:GLN:O	1:D:129:LYS:C	2.54	0.43
1:D:182:VAL:O	1:D:183:LEU:C	2.54	0.43
1:D:31:VAL:HA	1:D:32:PRO:HD3	1.88	0.43
1:B:114:PHE:CB	1:B:118:ILE:HB	2.48	0.43
1:B:168:VAL:O	1:B:169:SER:C	2.57	0.43
1:B:65:PHE:HB2	1:B:66:GLU:H	1.63	0.43
1:C:168:VAL:HG12	1:C:193:TRP:CZ3	2.53	0.43
1:D:23:GLU:HB2	1:D:201:SER:CB	2.47	0.43
1:A:65:PHE:O	1:A:66:GLU:CB	2.60	0.43
1:B:17:CYS:O	1:B:20:ALA:HB3	2.18	0.43
1:B:62:LEU:HG	1:B:64:LEU:CD2	2.49	0.43
1:C:104:GLN:HE21	1:C:104:GLN:HB2	1.68	0.43
1:D:167:HIS:HD1	1:D:192:TRP:HH2	1.64	0.43
1:A:114:PHE:O	1:A:115:GLN:C	2.56	0.43
1:A:118:ILE:HG13	2:A:1001:ATA:H93	2.01	0.43
1:B:138:LEU:O	1:B:142:LEU:HG	2.18	0.43
1:C:143:GLU:HG2	1:C:186:TYR:HE1	1.83	0.43
1:D:145:TYR:O	1:D:149:LEU:HG	2.18	0.43
1:B:140:LYS:HD3	1:B:140:LYS:H	1.83	0.43
1:B:3:MET:HA	1:B:4:LYS:HE3	2.00	0.43
1:C:40:HIS:CD2	1:C:41:LYS:H	2.37	0.43
1:D:189:VAL:HG23	1:D:189:VAL:H	1.59	0.43
1:C:95:ASP:OD2	1:D:72:LYS:HD2	2.19	0.43
1:A:59:ASP:O	1:A:62:LEU:HB3	2.19	0.43
1:C:154:TYR:HD1	1:C:192:TRP:CD1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:GLU:HA	1:C:42:SER:OG	2.18	0.43
1:D:4:LYS:HD2	1:D:6:TYR:OH	2.18	0.43
1:A:81:GLU:CD	1:A:81:GLU:H	2.21	0.43
1:A:99:GLU:OE1	1:A:99:GLU:HA	2.19	0.43
1:B:165:LEU:O	1:B:166:ASN:C	2.56	0.43
1:D:115:GLN:CD	1:D:130:VAL:HG21	2.39	0.43
1:D:69:ALA:O	1:D:70:ILE:C	2.57	0.43
1:B:109:LEU:HD23	1:B:109:LEU:HA	1.73	0.43
1:C:110:ASN:HD22	1:C:110:ASN:HA	1.71	0.43
1:A:192:TRP:O	1:A:196:LEU:HB3	2.18	0.43
2:A:1001:ATA:O1'	2:A:1001:ATA:CG'	2.64	0.42
1:A:174:LEU:O	1:A:180:ALA:HB2	2.19	0.42
1:B:81:GLU:CD	1:B:81:GLU:H	2.23	0.42
1:D:73:TYR:N	3:D:1007:HOH:O	2.47	0.42
1:B:3:MET:CE	1:B:57:LEU:HD21	2.48	0.42
1:D:165:LEU:O	1:D:168:VAL:HG23	2.19	0.42
1:D:79:LYS:N	1:D:80:PRO:HD3	2.34	0.42
1:A:194:SER:O	1:A:197:MET:HB2	2.18	0.42
1:B:4:LYS:HD2	1:B:4:LYS:H	1.84	0.42
1:C:22:GLU:OE2	1:C:204:LYS:HE2	2.19	0.42
1:C:4:LYS:N	1:C:58:GLN:O	2.48	0.42
1:D:68:ARG:HB2	3:D:1005:HOH:O	2.18	0.42
1:B:152:CYS:HB3	1:B:157:GLY:O	2.19	0.42
1:C:109:LEU:HD12	1:C:170:VAL:HB	2.01	0.42
1:C:3:MET:HE3	1:C:59:ASP:OD1	2.19	0.42
3:A:1005:HOH:O	2:B:1002:ATA:HA'	2.20	0.42
1:B:101:GLU:O	1:B:103:ASN:N	2.52	0.42
1:C:190:LYS:NZ	1:C:193:TRP:HD1	2.17	0.42
1:C:144:VAL:CG1	1:D:50:PRO:HB2	2.43	0.42
1:C:7:GLY:HA3	1:C:14:LEU:CD2	2.49	0.42
1:D:115:GLN:HA	1:D:115:GLN:HE21	1.84	0.42
1:B:198:GLU:O	1:B:199:ARG:C	2.57	0.42
1:D:48:ARG:HG3	1:D:48:ARG:H	1.70	0.42
1:A:118:ILE:O	1:A:121:MET:HB2	2.20	0.42
1:B:143:GLU:O	1:B:144:VAL:O	2.37	0.42
1:C:175:PHE:CE2	1:C:180:ALA:HB1	2.55	0.42
1:D:77:LYS:O	1:D:77:LYS:HG2	2.20	0.42
1:D:99:GLU:O	1:D:103:ASN:ND2	2.52	0.42
1:C:150:THR:HG22	1:C:151:LYS:HG2	2.02	0.41
1:D:119:SER:HB3	1:D:120:PRO:HD3	2.02	0.41
1:A:119:SER:O	1:A:122:LEU:N	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:LYS:HE3	1:A:139:LYS:HB3	1.86	0.41
1:C:209:MET:O	1:C:210:LYS:HB2	2.20	0.41
1:D:174:LEU:HD13	1:D:180:ALA:HA	2.02	0.41
1:A:33:ILE:HA	1:A:33:ILE:HD13	1.94	0.41
1:B:21:LEU:HA	1:B:24:ALA:HB3	2.02	0.41
1:D:64:LEU:CD1	1:D:73:TYR:CD2	3.02	0.41
1:D:96:VAL:HG13	1:D:97:TRP:N	2.36	0.41
1:A:30:ILE:CD1	1:A:208:LEU:HD21	2.49	0.41
1:B:116:VAL:O	1:B:116:VAL:HG12	2.20	0.41
1:C:112:ILE:HD11	1:C:135:LEU:N	2.35	0.41
1:D:147:ALA:O	1:D:149:LEU:N	2.53	0.41
1:D:154:TYR:HD2	1:D:164:ASP:OD2	2.03	0.41
1:D:145:TYR:CE2	1:D:167:HIS:HE1	2.37	0.41
1:D:34:ASN:HD21	1:D:36:ALA:CB	2.23	0.41
1:D:50:PRO:CD	1:D:65:PHE:CE2	3.03	0.41
1:A:134:ASN:O	1:A:135:LEU:C	2.56	0.41
1:B:165:LEU:O	1:B:167:HIS:N	2.53	0.41
1:C:150:THR:OG1	1:C:188:HIS:CD2	2.73	0.41
1:D:48:ARG:O	1:D:56:ALA:HB1	2.21	0.41
1:C:150:THR:HG22	1:C:151:LYS:HD3	2.03	0.41
1:C:196:LEU:O	1:C:202:VAL:HG21	2.20	0.41
1:C:14:LEU:HD22	1:C:55:PRO:HB3	1.99	0.41
1:C:95:ASP:O	1:C:96:VAL:O	2.38	0.41
1:D:154:TYR:HB3	1:D:164:ASP:OD2	2.20	0.41
1:C:144:VAL:HG21	1:D:51:PHE:CD1	2.55	0.41
1:B:4:LYS:CD	1:B:58:GLN:HB3	2.51	0.41
1:C:211:PRO:HG2	1:C:212:SER:H	1.84	0.41
1:D:109:LEU:HD22	1:D:138:LEU:CD1	2.51	0.41
2:A:1001:ATA:H122	2:A:1001:ATA:H93	2.02	0.41
1:A:198:GLU:O	1:A:199:ARG:C	2.59	0.41
1:B:205:VAL:HA	1:B:208:LEU:CD1	2.51	0.41
1:C:162:LEU:HD23	1:C:162:LEU:HA	1.72	0.41
1:B:154:TYR:HB3	1:B:155:LEU:H	1.69	0.41
1:B:33:ILE:HA	1:B:39:GLU:OE2	2.20	0.41
1:B:77:LYS:HG2	1:B:78:ASN:OD1	2.21	0.41
1:A:127:ASP:O	1:A:131:VAL:HG23	2.21	0.41
1:A:168:VAL:O	1:A:172:LEU:HG	2.20	0.41
1:B:207:ALA:HA	1:B:210:LYS:HB3	2.03	0.41
1:C:134:ASN:HA	1:C:137:LYS:HB2	2.03	0.41
1:C:18:ALA:HB1	1:C:205:VAL:HG23	2.02	0.41
1:D:142:LEU:HD22	1:D:189:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:VAL:O	1:D:209:MET:HB3	2.21	0.41
1:C:201:SER:O	1:C:202:VAL:C	2.59	0.41
1:C:39:GLU:HA	1:C:42:SER:HB2	2.03	0.41
1:D:145:TYR:HE2	1:D:167:HIS:HE1	1.67	0.41
1:A:149:LEU:CD2	1:A:155:LEU:HD12	2.41	0.40
1:B:109:LEU:HD12	1:B:170:VAL:HG12	2.01	0.40
1:B:83:LEU:HB3	1:B:85:GLU:HG2	2.04	0.40
1:D:130:VAL:HG23	1:D:131:VAL:H	1.86	0.40
1:D:108:ALA:O	1:D:138:LEU:HB2	2.21	0.40
1:A:114:PHE:HA	1:A:118:ILE:HD13	2.02	0.40
1:B:110:ASN:N	1:B:111:PRO:CD	2.85	0.40
1:B:119:SER:H	1:B:120:PRO:HD2	1.85	0.40
1:C:43:PRO:O	1:C:47:VAL:HG22	2.21	0.40
1:A:110:ASN:O	1:A:113:LEU:HB2	2.21	0.40
1:B:23:GLU:HG2	1:B:165:LEU:CD1	2.44	0.40
1:C:128:GLN:HG3	1:C:128:GLN:O	2.21	0.40
1:A:111:PRO:O	1:A:112:ILE:C	2.60	0.40
1:B:84:ARG:NH1	1:B:84:ARG:HG2	2.36	0.40
1:D:9:VAL:HG11	1:D:208:LEU:HD22	2.02	0.40
1:B:10:MET:HB3	1:B:213:ALA:HB3	2.03	0.40
1:B:5:LEU:O	1:B:30:ILE:HG23	2.22	0.40
1:C:16:ARG:HB2	1:C:169:SER:CB	2.52	0.40
1:D:110:ASN:HD22	1:D:110:ASN:HA	1.60	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	211/213 (99%)	163 (77%)	40 (19%)	8 (4%)	3 10
1	B	211/213 (99%)	142 (67%)	52 (25%)	17 (8%)	1 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	211/213 (99%)	154 (73%)	35 (17%)	22 (10%)	0	1
1	D	211/213 (99%)	159 (75%)	37 (18%)	15 (7%)	1	2
All	All	844/852 (99%)	618 (73%)	164 (19%)	62 (7%)	1	2

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	VAL
1	A	163	ALA
1	A	211	PRO
1	B	40	HIS
1	B	66	GLU
1	B	166	ASN
1	C	36	ALA
1	C	96	VAL
1	C	131	VAL
1	D	60	GLY
1	D	67	SER
1	D	126	THR
1	D	145	TYR
1	D	180	ALA
1	A	44	GLU
1	B	5	LEU
1	B	102	ALA
1	B	136	GLU
1	B	147	ALA
1	C	60	GLY
1	C	95	ASP
1	C	163	ALA
1	C	195	GLY
1	C	202	VAL
1	C	211	PRO
1	D	86	GLY
1	A	162	LEU
1	B	117	LEU
1	B	139	LYS
1	B	169	SER
1	C	18	ALA
1	C	44	GLU
1	C	55	PRO
1	C	66	GLU

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Mol	Chain	Res	Type
1	C	89	GLU
1	C	92	ALA
1	C	124	GLY
1	D	17	CYS
1	D	166	ASN
1	A	46	LEU
1	A	66	GLU
1	B	105	TYR
1	B	140	LYS
1	C	138	LEU
1	D	52	GLY
1	D	127	ASP
1	D	151	LYS
1	C	51	PHE
1	C	109	LEU
1	C	110	ASN
1	C	178	PRO
1	D	115	GLN
1	D	148	ARG
1	D	174	LEU
1	C	97	TRP
1	D	147	ALA
1	B	86	GLY
1	A	42	SER
1	B	49	ASN
1	B	111	PRO
1	B	94	VAL
1	B	195	GLY

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	178/178 (100%)	140 (79%)	38 (21%)	1	3
1	B	178/178 (100%)	130 (73%)	48 (27%)	0	1
1	C	178/178 (100%)	130 (73%)	48 (27%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	178/178 (100%)	136 (76%)	42 (24%)	1	2
All	All	712/712 (100%)	536 (75%)	176 (25%)	0	2

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	MET
1	A	14	LEU
1	A	16	ARG
1	A	19	THR
1	A	30	ILE
1	A	32	PRO
1	A	40	HIS
1	A	41	LYS
1	A	53	GLN
1	A	54	VAL
1	A	73	TYR
1	A	77	LYS
1	A	88	LEU
1	A	89	GLU
1	A	93	MET
1	A	109	LEU
1	A	121	MET
1	A	122	LEU
1	A	129	LYS
1	A	133	GLU
1	A	136	GLU
1	A	139	LYS
1	A	140	LYS
1	A	150	THR
1	A	153	LYS
1	A	155	LEU
1	A	158	ASP
1	A	159	PHE
1	A	161	SER
1	A	164	ASP
1	A	165	LEU
1	A	187	PRO
1	A	192	TRP
1	A	196	LEU
1	A	199	ARG
1	A	204	LYS

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Mol	Chain	Res	Type
1	A	210	LYS
1	A	212	SER
1	B	2	PRO
1	B	3	MET
1	B	4	LYS
1	B	5	LEU
1	B	11	SER
1	B	14	LEU
1	B	15	THR
1	B	19	THR
1	B	21	LEU
1	B	26	SER
1	B	41	LYS
1	B	42	SER
1	B	53	GLN
1	B	66	GLU
1	B	67	SER
1	B	68	ARG
1	B	79	LYS
1	B	82	LEU
1	B	84	ARG
1	B	85	GLU
1	B	88	LEU
1	B	89	GLU
1	B	104	GLN
1	B	113	LEU
1	B	114	PHE
1	B	121	MET
1	B	122	LEU
1	B	125	THR
1	B	130	VAL
1	B	136	GLU
1	B	138	LEU
1	B	140	LYS
1	B	143	GLU
1	B	146	GLU
1	B	149	LEU
1	B	151	LYS
1	B	154	TYR
1	B	155	LEU
1	B	161	SER
1	B	168	VAL

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Mol	Chain	Res	Type
1	B	172	LEU
1	B	181	SER
1	B	183	LEU
1	B	190	LYS
1	B	194	SER
1	B	196	LEU
1	B	199	ARG
1	B	208	LEU
1	C	3	MET
1	C	9	VAL
1	C	10	MET
1	C	14	LEU
1	C	15	THR
1	C	26	SER
1	C	29	GLU
1	C	33	ILE
1	C	40	HIS
1	C	41	LYS
1	C	44	GLU
1	C	46	LEU
1	C	47	VAL
1	C	48	ARG
1	C	53	GLN
1	C	57	LEU
1	C	77	LYS
1	C	87	ASN
1	C	93	MET
1	C	94	VAL
1	C	98	ILE
1	C	99	GLU
1	C	101	GLU
1	C	104	GLN
1	C	110	ASN
1	C	117	LEU
1	C	121	MET
1	C	122	LEU
1	C	129	LYS
1	C	130	VAL
1	C	132	ASP
1	C	140	LYS
1	C	146	GLU
1	C	150	THR

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Mol	Chain	Res	Type
1	C	151	LYS
1	C	153	LYS
1	C	155	LEU
1	C	160	LEU
1	C	177	THR
1	C	190	LYS
1	C	197	MET
1	C	200	PRO
1	C	204	LYS
1	C	205	VAL
1	C	208	LEU
1	C	209	MET
1	C	210	LYS
1	C	212	SER
1	D	4	LYS
1	D	14	LEU
1	D	19	THR
1	D	27	ASP
1	D	29	GLU
1	D	30	ILE
1	D	34	ASN
1	D	37	THR
1	D	40	HIS
1	D	41	LYS
1	D	48	ARG
1	D	53	GLN
1	D	54	VAL
1	D	66	GLU
1	D	72	LYS
1	D	76	ARG
1	D	79	LYS
1	D	81	GLU
1	D	88	LEU
1	D	99	GLU
1	D	101	GLU
1	D	109	LEU
1	D	110	ASN
1	D	119	SER
1	D	122	LEU
1	D	129	LYS
1	D	133	GLU
1	D	138	LEU

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Mol	Chain	Res	Type
1	D	139	LYS
1	D	149	LEU
1	D	151	LYS
1	D	161	SER
1	D	165	LEU
1	D	172	LEU
1	D	174	LEU
1	D	181	SER
1	D	183	LEU
1	D	200	PRO
1	D	202	VAL
1	D	204	LYS
1	D	209	MET
1	D	212	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	78	ASN
1	A	128	GLN
1	A	134	ASN
1	A	166	ASN
1	A	167	HIS
1	A	188	HIS
1	A	203	GLN
1	B	40	HIS
1	B	53	GLN
1	B	104	GLN
1	B	203	GLN
1	C	40	HIS
1	C	53	GLN
1	C	78	ASN
1	C	87	ASN
1	C	104	GLN
1	C	110	ASN
1	C	166	ASN
1	C	188	HIS
1	D	34	ASN
1	D	40	HIS
1	D	45	HIS
1	D	53	GLN

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Mol	Chain	Res	Type
1	D	58	GLN
1	D	110	ASN
1	D	115	GLN
1	D	134	ASN
1	D	167	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ATA	A	1001	-	26,33,33	3.16	2 (7%)	33,43,43	3.35	9 (27%)
2	ATA	B	1002	-	26,33,33	3.05	2 (7%)	33,43,43	3.31	14 (42%)
2	ATA	C	1003	-	26,33,33	3.24	2 (7%)	33,43,43	2.72	8 (24%)
2	ATA	D	1004	-	26,33,33	3.29	3 (11%)	33,43,43	3.70	14 (42%)

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATA	A	1001	-	-	14/28/34/34	0/1/1/1
2	ATA	B	1002	-	-	10/28/34/34	0/1/1/1
2	ATA	C	1003	-	-	16/28/34/34	0/1/1/1
2	ATA	D	1004	-	-	15/28/34/34	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1003	ATA	C4-N7	13.08	1.51	1.34
2	D	1004	ATA	C4-N7	12.66	1.51	1.34
2	A	1001	ATA	C4-N7	12.22	1.50	1.34
2	B	1002	ATA	C4-N7	11.98	1.50	1.34
2	D	1004	ATA	C6-N11	10.22	1.50	1.34
2	A	1001	ATA	C6-N11	9.66	1.49	1.34
2	C	1003	ATA	C6-N11	9.32	1.48	1.34
2	B	1002	ATA	C6-N11	9.16	1.48	1.34
2	D	1004	ATA	C8-N7	2.44	1.51	1.46

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1004	ATA	C12-N11-C6	-13.33	107.41	123.85
2	A	1001	ATA	C12-N11-C6	-12.59	108.32	123.85
2	D	1004	ATA	C4-N7-C8	-12.25	114.47	124.53
2	C	1003	ATA	C12-N11-C6	-11.23	110.00	123.85
2	B	1002	ATA	C12-N11-C6	-10.88	110.43	123.85
2	A	1001	ATA	C4-N7-C8	-10.68	115.76	124.53
2	B	1002	ATA	CAD-ND-C	-6.48	113.02	122.34
2	C	1003	ATA	C4-N7-C8	-6.44	119.24	124.53
2	B	1002	ATA	O-C-ND	-6.41	109.23	122.99
2	B	1002	ATA	C10-C8-N7	5.16	121.17	109.94
2	B	1002	ATA	O-C-CA	4.69	130.32	120.45
2	B	1002	ATA	O'-C'-CG'	-4.55	113.69	122.02
2	A	1001	ATA	N7-C4-N3	4.35	123.72	117.18
2	D	1004	ATA	N1-C6-N5	-4.25	119.52	126.23
2	B	1002	ATA	C-CA-N	3.86	121.65	111.16
2	C	1003	ATA	CA-N-C'	3.76	131.31	121.65
2	A	1001	ATA	C10-C8-N7	3.75	118.11	109.94
2	B	1002	ATA	CA-N-C'	3.72	131.22	121.65
2	B	1002	ATA	N7-C4-N3	3.70	122.73	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1003	ATA	C10-C8-N7	3.67	117.93	109.94
2	C	1003	ATA	O'-C'-CG'	-3.60	115.43	122.02
2	A	1001	ATA	O'-C'-N	-3.40	117.22	122.95
2	D	1004	ATA	N3-C2-N1	-3.31	120.88	126.95
2	D	1004	ATA	CAD-ND-C	3.20	126.94	122.34
2	B	1002	ATA	O'-C'-N	3.14	128.26	122.95
2	A	1001	ATA	C2-N3-C4	-3.13	112.09	113.85
2	A	1001	ATA	O'-C'-CG'	-3.07	116.39	122.02
2	D	1004	ATA	CA-N-C'	3.02	129.42	121.65
2	B	1002	ATA	C9-C8-N7	2.96	116.39	109.94
2	D	1004	ATA	CB'-CG'-C'	2.94	119.60	113.04
2	D	1004	ATA	C4-N5-C6	-2.89	108.98	113.89
2	C	1003	ATA	N7-C4-N3	2.83	121.43	117.18
2	D	1004	ATA	O'-C'-CG'	-2.80	116.90	122.02
2	C	1003	ATA	N7-C4-N5	-2.80	112.98	117.18
2	D	1004	ATA	C2-N3-C4	-2.74	112.31	113.85
2	D	1004	ATA	CB-CA-N	2.56	117.91	111.00
2	C	1003	ATA	N3-C4-N5	-2.45	122.35	126.23
2	A	1001	ATA	N7-C4-N5	-2.42	113.54	117.18
2	B	1002	ATA	C10-C8-C9	2.31	116.73	111.58
2	B	1002	ATA	CB-CA-C	2.29	114.70	109.73
2	D	1004	ATA	N3-C4-N5	-2.28	122.62	126.23
2	B	1002	ATA	N7-C4-N5	-2.28	113.76	117.18
2	A	1001	ATA	N3-C4-N5	-2.21	122.73	126.23
2	D	1004	ATA	N7-C4-N3	2.20	120.48	117.18
2	D	1004	ATA	N11-C6-N5	-2.19	113.39	117.19

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	ATA	N'-CA'-CB'-CG'
2	A	1001	ATA	CC'-CA'-CB'-CG'
2	A	1001	ATA	N1-C2-SG-CB
2	A	1001	ATA	N3-C2-SG-CB
2	A	1001	ATA	N5-C4-N7-C8
2	A	1001	ATA	N3-C4-N7-C8
2	A	1001	ATA	N-CA-CB-SG
2	A	1001	ATA	C-CA-CB-SG
2	A	1001	ATA	C9-C8-N7-C4
2	B	1002	ATA	N5-C6-N11-C12
2	B	1002	ATA	N1-C6-N11-C12

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Mol	Chain	Res	Type	Atoms
2	B	1002	ATA	C10-C8-N7-C4
2	C	1003	ATA	O'-C'-N-CA
2	C	1003	ATA	N5-C6-N11-C12
2	C	1003	ATA	N3-C2-SG-CB
2	C	1003	ATA	N5-C4-N7-C8
2	C	1003	ATA	N3-C4-N7-C8
2	C	1003	ATA	C-CA-CB-SG
2	C	1003	ATA	CA-C-ND-CAD
2	C	1003	ATA	O-C-ND-CAD
2	D	1004	ATA	O'-C'-N-CA
2	D	1004	ATA	N1-C6-N11-C12
2	D	1004	ATA	N5-C4-N7-C8
2	D	1004	ATA	N3-C4-N7-C8
2	D	1004	ATA	C-CA-CB-SG
2	D	1004	ATA	C10-C8-N7-C4
2	D	1004	ATA	CD-CAD-ND-C
2	A	1001	ATA	O-C-ND-CAD
2	B	1002	ATA	O-C-ND-CAD
2	A	1001	ATA	CA-C-ND-CAD
2	B	1002	ATA	O'-C'-N-CA
2	B	1002	ATA	CA-C-ND-CAD
2	C	1003	ATA	N1-C6-N11-C12
2	A	1001	ATA	CA'-CB'-CG'-C'
2	A	1001	ATA	O'-C'-N-CA
2	D	1004	ATA	O-C-ND-CAD
2	C	1003	ATA	CB-CA-N-C'
2	D	1004	ATA	CB-CA-N-C'
2	B	1002	ATA	CG'-C'-N-CA
2	D	1004	ATA	C-CA-N-C'
2	C	1003	ATA	N1-C2-SG-CB
2	B	1002	ATA	CA'-CB'-CG'-C'
2	C	1003	ATA	CG'-C'-N-CA
2	C	1003	ATA	CA-CB-SG-C2
2	D	1004	ATA	CA-CB-SG-C2
2	D	1004	ATA	ND-C-CA-N
2	C	1003	ATA	N-CA-CB-SG
2	C	1003	ATA	O-C-CA-N
2	B	1002	ATA	N'-CA'-CB'-CG'
2	D	1004	ATA	CA'-CB'-CG'-C'
2	A	1001	ATA	CD-CAD-ND-C
2	D	1004	ATA	N5-C6-N11-C12
2	C	1003	ATA	C-CA-N-C'

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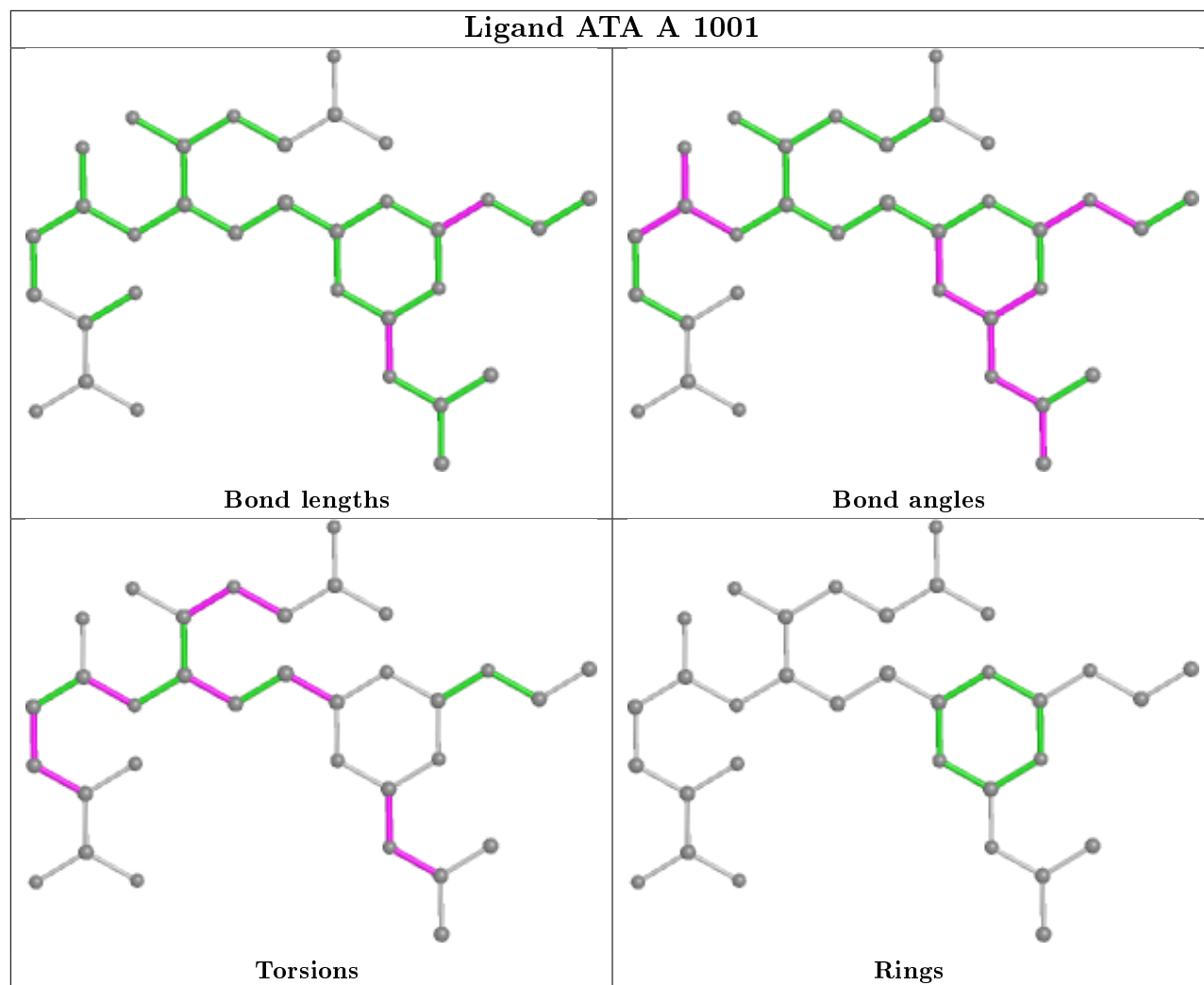
Mol	Chain	Res	Type	Atoms
2	B	1002	ATA	C-CA-CB-SG
2	D	1004	ATA	CA-C-ND-CAD

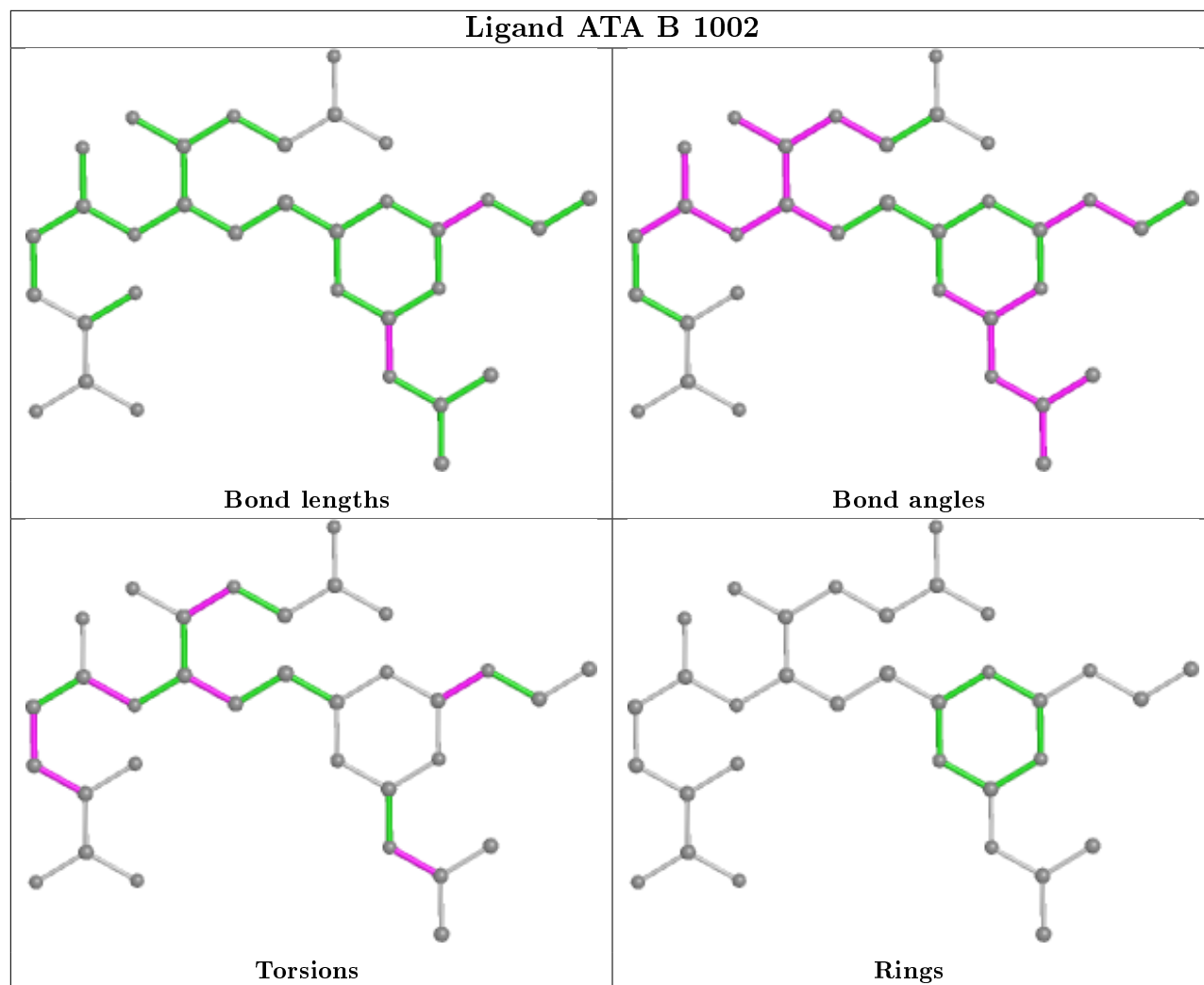
There are no ring outliers.

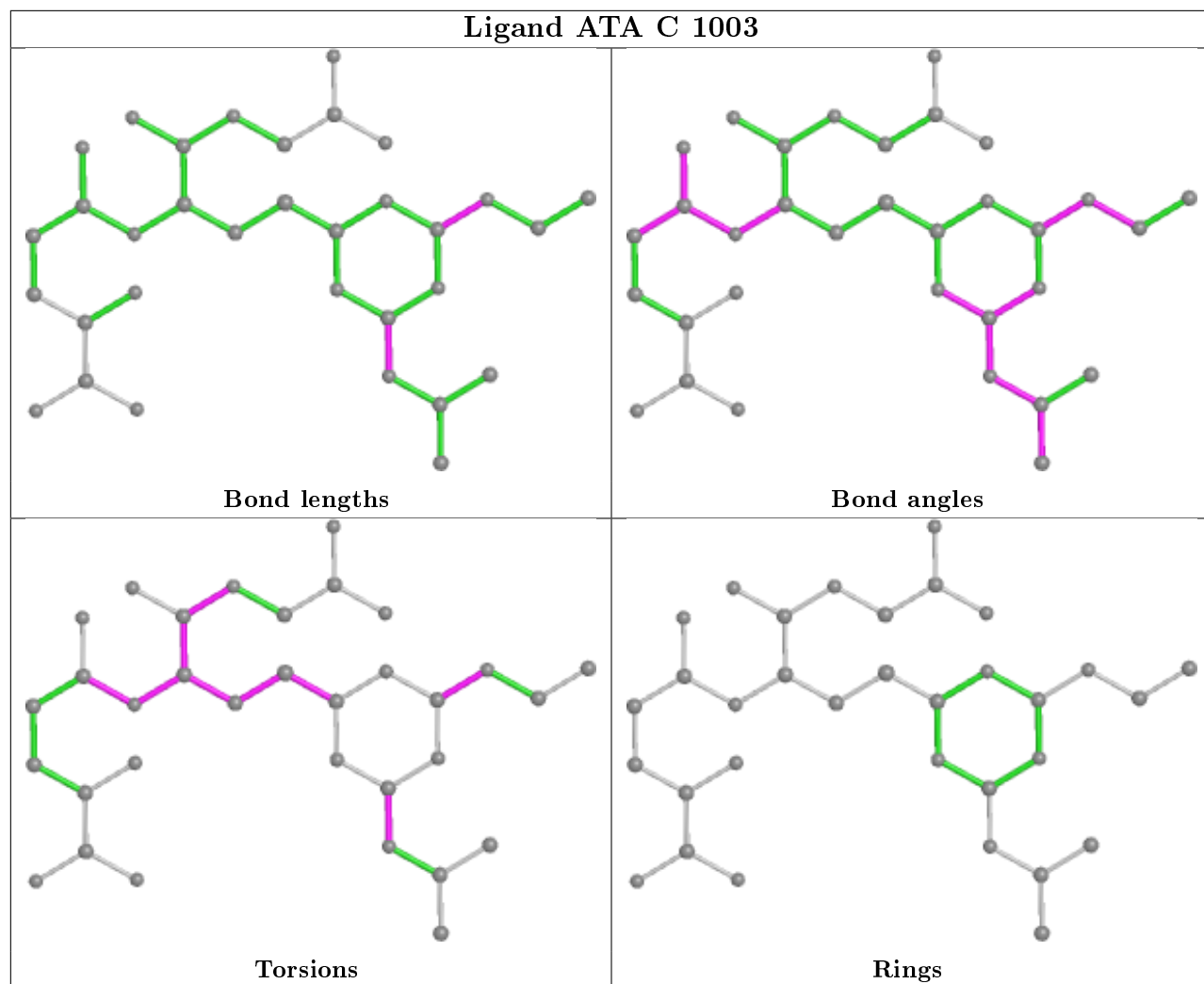
4 monomers are involved in 36 short contacts:

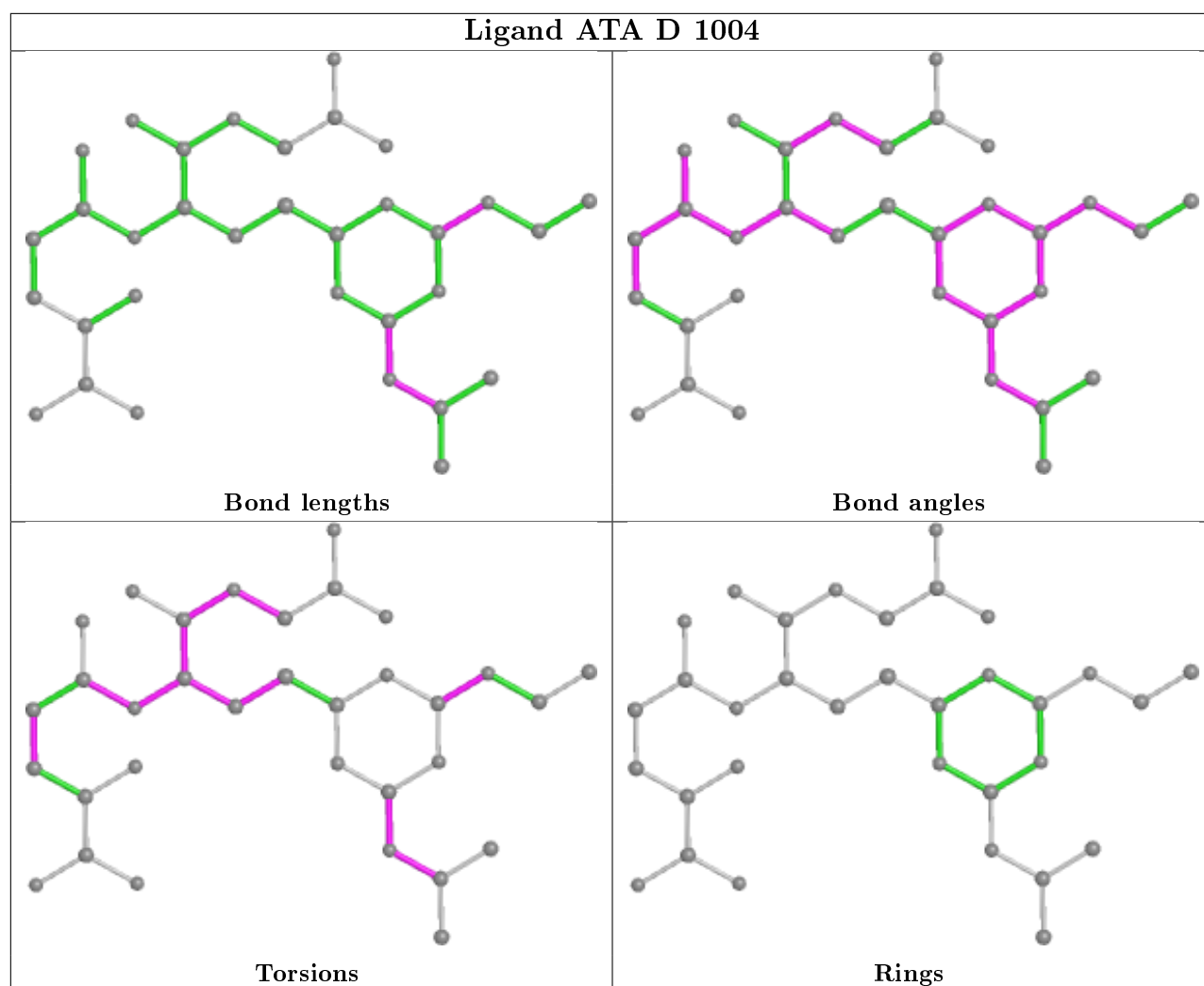
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	ATA	21	0
2	B	1002	ATA	4	0
2	C	1003	ATA	4	0
2	D	1004	ATA	7	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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.