



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:26 AM UTC

PDB ID : 2WPO / pdb_00002wpo
Title : HCMV protease inhibitor complex
Authors : Tong, L.; Qian, C.; Massariol, M.-J.; Deziel, R.; Yoakim, C.; Lagace, L.
Deposited on : 1998-08-04
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

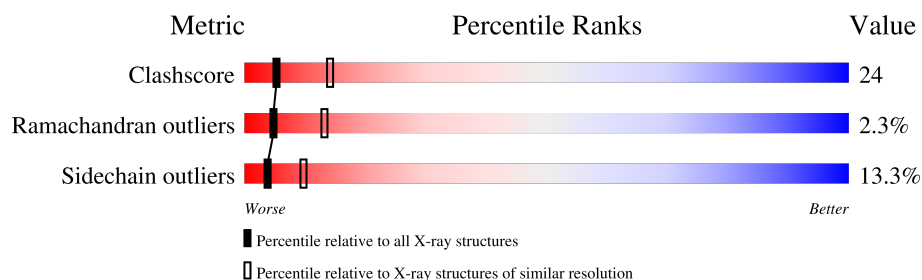
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	256	
1	B	256	
1	C	256	
1	D	256	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9072 atoms, of which 1680 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.

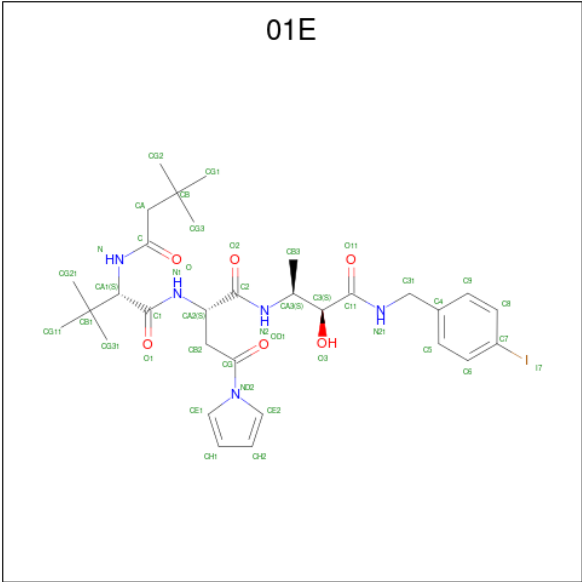
- Molecule 1 is a protein called HUMAN CYTOMEGALOVIRUS PROTEASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	230	Total	C	H	N	O	S	0	0	0
			2221	1128	416	327	343	7			
1	B	230	Total	C	H	N	O	S	0	0	0
			2221	1128	416	327	343	7			
1	C	230	Total	C	H	N	O	S	0	0	0
			2221	1128	416	327	343	7			
1	D	230	Total	C	H	N	O	S	0	0	0
			2221	1128	416	327	343	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	GLN	ALA	engineered mutation	UNP P16753
A	181	MET	THR	engineered mutation	UNP P16753
A	229	MET	LEU	engineered mutation	UNP P16753
B	143	GLN	ALA	engineered mutation	UNP P16753
B	181	MET	THR	engineered mutation	UNP P16753
B	229	MET	LEU	engineered mutation	UNP P16753
C	143	GLN	ALA	engineered mutation	UNP P16753
C	181	MET	THR	engineered mutation	UNP P16753
C	229	MET	LEU	engineered mutation	UNP P16753
D	143	GLN	ALA	engineered mutation	UNP P16753
D	181	MET	THR	engineered mutation	UNP P16753
D	229	MET	LEU	engineered mutation	UNP P16753

- Molecule 2 is (2S)-2-(3,3-dimethylbutanoylamino)-N-[(2S)-1-[(2S,3S)-3-hydroxy-4-[(4-iodophenyl)methylamino]-4-oxo-butan-2-yl]amino]-1,4-dioxo-4-pyrrol-1-yl-butan-2-yl]-3,3-dimethyl-butanamide (CCD ID: 01E) (formula: C₃₁H₄₄IN₅O₆).



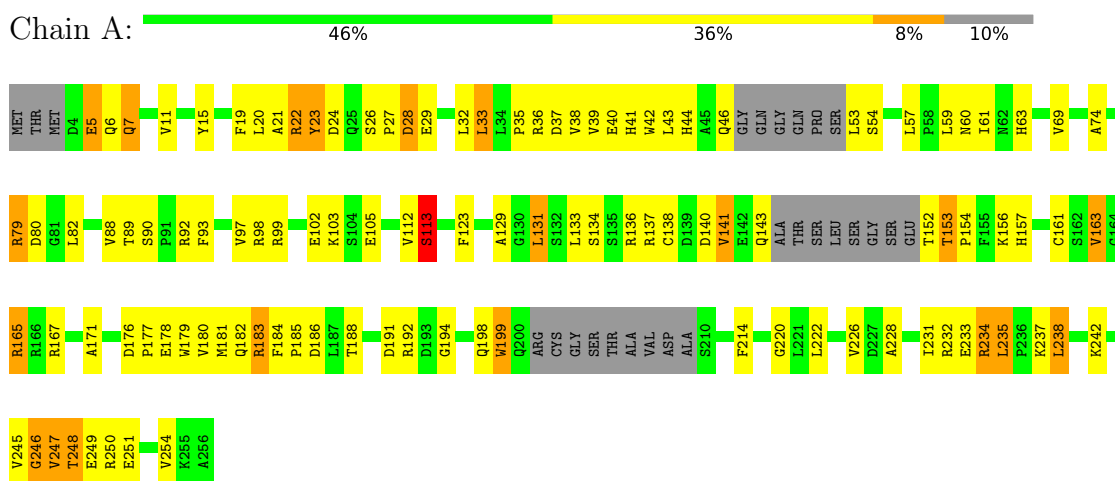
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	I	N	O	0	0
			47	31	4	1	5	6		
2	B	1	Total	C	H	I	N	O	0	0
			47	31	4	1	5	6		
2	C	1	Total	C	H	I	N	O	0	0
			47	31	4	1	5	6		
2	D	1	Total	C	H	I	N	O	0	0
			47	31	4	1	5	6		

3 Residue-property plots

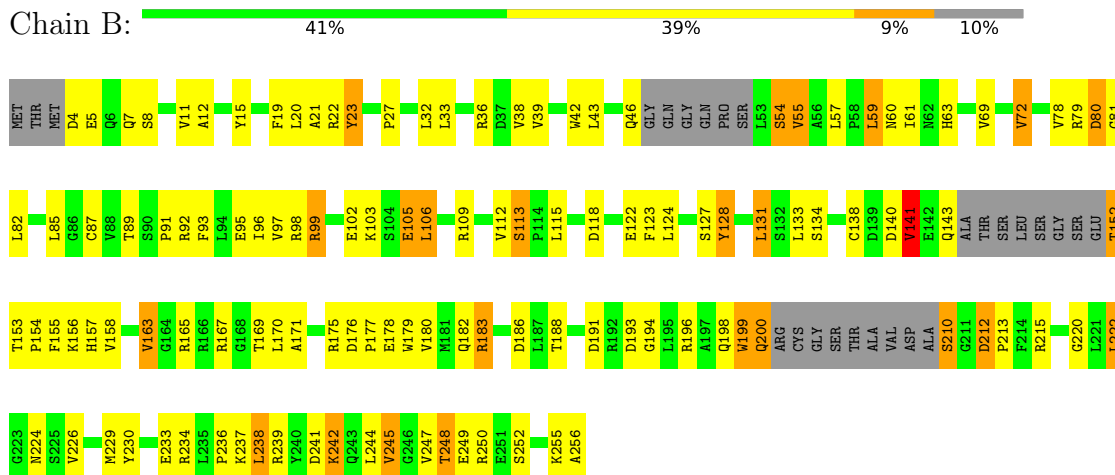
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: HUMAN CYTOMEGALOVIRUS PROTEASE

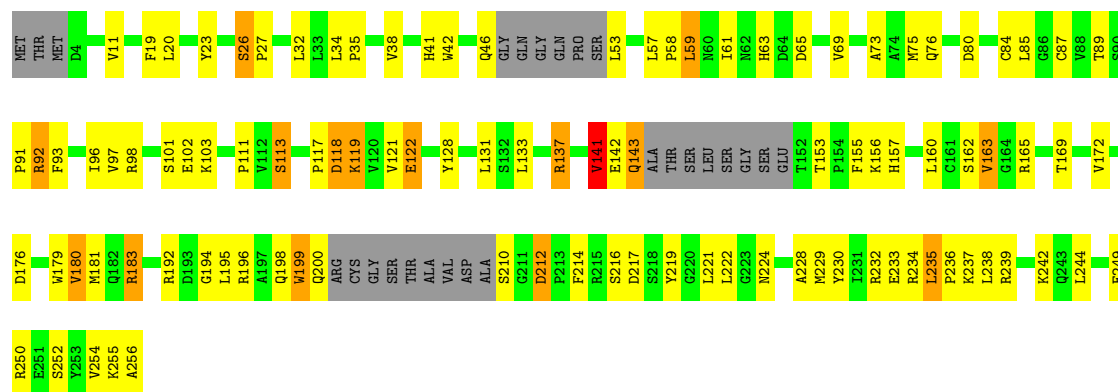


• Molecule 1: HUMAN CYTOMEGALOVIRUS PROTEASE



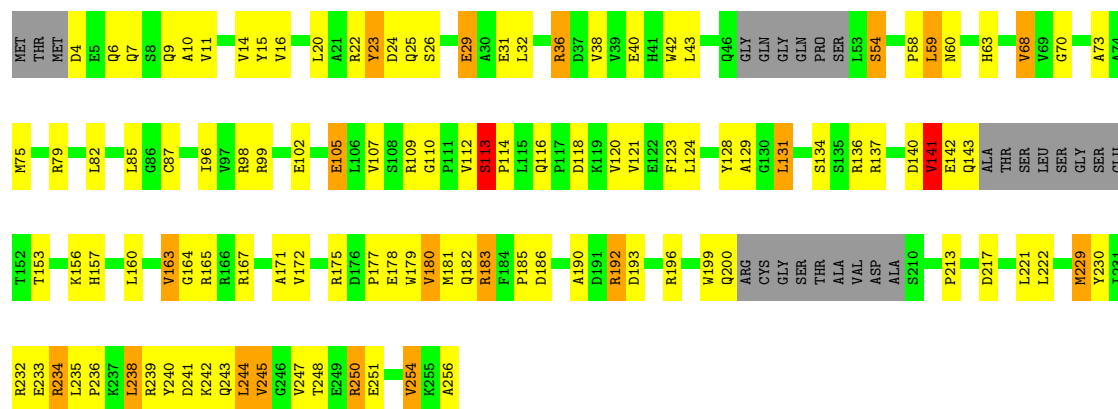
• Molecule 1: HUMAN CYTOMEGALOVIRUS PROTEASE





● Molecule 1: HUMAN CYTOMEGALOVIRUS PROTEASE

Chain D: 45% 36% 7% 10%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	107.80 Å 53.40 Å 212.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.70	Depositor
% Data completeness (in resolution range)	92.0 (6.00-2.70)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.226 , 0.332	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9072	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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: 01E

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	0.64	0/1840	1.08	10/2491 (0.4%)
1	B	0.67	1/1840 (0.1%)	1.13	9/2491 (0.4%)
1	C	0.64	0/1840	1.11	11/2491 (0.4%)
1	D	0.67	0/1840	1.14	9/2491 (0.4%)
All	All	0.66	1/7360 (0.0%)	1.11	39/9964 (0.4%)

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	B	0	1
1	C	0	1
1	D	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	55	VAL	CA-CB	6.03	1.60	1.54

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	SER	N-CA-C	7.50	126.39	109.81
1	D	20	LEU	N-CA-C	-7.47	104.19	113.38
1	B	113	SER	N-CA-C	7.04	125.38	109.81
1	A	176	ASP	CA-C-N	6.96	126.66	119.56
1	A	176	ASP	C-N-CA	6.96	126.66	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	113	SER	N-CA-C	6.83	124.89	109.81
1	B	222	LEU	N-CA-C	-6.81	103.78	111.07
1	D	250	ARG	N-CA-C	-6.61	98.87	107.73
1	C	141	VAL	N-CA-C	6.55	122.97	109.34
1	A	246	GLY	N-CA-C	6.38	122.41	114.37
1	B	212	ASP	CA-C-N	6.37	126.08	119.64
1	B	212	ASP	C-N-CA	6.37	126.08	119.64
1	A	6	GLN	N-CA-C	-6.27	104.45	111.28
1	C	34	LEU	CA-C-N	6.22	126.19	119.78
1	C	34	LEU	C-N-CA	6.22	126.19	119.78
1	C	80	ASP	N-CA-C	6.08	120.69	113.28
1	C	26	SER	CA-C-N	6.03	126.04	119.89
1	C	26	SER	C-N-CA	6.03	126.04	119.89
1	B	248	THR	N-CA-C	-5.92	104.75	111.14
1	D	113	SER	N-CA-C	5.85	122.74	109.81
1	B	59	LEU	N-CA-C	-5.71	99.11	108.41
1	A	129	ALA	N-CA-C	5.67	119.94	113.19
1	C	119	LYS	N-CA-C	5.59	117.82	111.11
1	D	110	GLY	CA-C-N	5.59	126.83	119.84
1	D	110	GLY	C-N-CA	5.59	126.83	119.84
1	D	153	THR	CA-C-N	5.58	125.19	119.56
1	D	153	THR	C-N-CA	5.58	125.19	119.56
1	B	106	LEU	N-CA-C	-5.53	104.89	111.03
1	C	212	ASP	CA-C-N	5.48	125.17	119.64
1	C	212	ASP	C-N-CA	5.48	125.17	119.64
1	D	186	ASP	N-CA-C	5.47	117.33	111.36
1	D	129	ALA	N-CA-C	5.44	119.67	113.19
1	C	198	GLN	N-CA-C	5.24	117.39	111.11
1	A	90	SER	CA-C-N	5.13	124.30	118.97
1	A	90	SER	C-N-CA	5.13	124.30	118.97
1	B	39	VAL	CB-CA-C	-5.11	105.34	111.88
1	A	153	THR	N-CA-C	5.08	118.97	108.71
1	A	165	ARG	N-CA-C	-5.03	105.99	111.82
1	B	186	ASP	N-CA-C	5.00	116.73	111.28

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	230	TYR	Sidechain
1	C	230	TYR	Sidechain
1	D	230	TYR	Sidechain

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	1805	416	1768	98	0
1	B	1805	416	1768	108	1
1	C	1805	416	1768	80	0
1	D	1805	416	1768	90	1
2	A	43	4	43	3	0
2	B	43	4	43	5	0
2	C	43	4	43	6	0
2	D	43	4	43	1	0
All	All	7392	1680	7244	355	1

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 24.

All (355) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:VAL:HG22	1:A:143:GLN:HB2	1.51	0.92
1:A:242:LYS:HD3	1:A:254:VAL:HG11	1.49	0.92
1:A:136:ARG:HD2	1:A:154:PRO:HB3	1.52	0.90
1:D:243:GLN:HG3	1:D:248:THR:HG21	1.54	0.88
1:B:46:GLN:HG3	1:B:154:PRO:HD2	1.59	0.84
1:B:72:VAL:HG21	1:B:158:VAL:HG21	1.60	0.84
1:C:165:ARG:HD3	2:C:257:O1E:HA4	1.60	0.81
1:C:235:LEU:HD23	1:D:232:ARG:HG3	1.62	0.81
1:C:163:VAL:HG13	1:C:234:ARG:HG3	1.61	0.81
1:B:36:ARG:HH12	1:B:79:ARG:HA	1.47	0.79
1:B:183:ARG:CD	1:B:252:SER:HB3	2.14	0.78
1:B:122:GLU:HB3	1:B:255:LYS:HZ1	1.49	0.77
1:A:103:LYS:HG3	1:B:220:GLY:HA2	1.68	0.76
1:A:181:MET:HE2	1:A:199:TRP:HZ2	1.51	0.76
1:D:241:ASP:O	1:D:245:VAL:HG23	1.86	0.75
1:B:131:LEU:HD13	1:B:171:ALA:HB2	1.67	0.75
1:C:234:ARG:HH12	1:D:234:ARG:HH22	1.32	0.75
1:B:242:LYS:HE2	1:B:248:THR:HG22	1.69	0.74
1:B:167:ARG:HG2	1:B:167:ARG:HH11	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:LEU:HD21	1:C:75:MET:HE2	1.70	0.74
1:B:93:PHE:O	1:B:97:VAL:HG23	1.88	0.74
1:B:194:GLY:O	1:B:198:GLN:HG3	1.88	0.74
1:B:183:ARG:HD3	1:B:252:SER:HB3	1.68	0.74
1:C:239:ARG:NH2	1:D:232:ARG:HG2	2.06	0.71
1:D:178:GLU:O	1:D:182:GLN:HG2	1.91	0.71
1:A:131:LEU:HD13	1:A:171:ALA:HB2	1.72	0.71
1:C:239:ARG:HH21	1:D:232:ARG:HG2	1.55	0.71
1:A:167:ARG:HG2	1:A:167:ARG:HH11	1.57	0.70
1:C:239:ARG:HA	1:C:242:LYS:HD3	1.74	0.70
1:D:23:TYR:CE2	1:D:36:ARG:HD3	2.27	0.69
1:B:36:ARG:NH1	1:B:79:ARG:HH11	1.91	0.68
1:B:163:VAL:HG13	1:B:238:LEU:HD21	1.76	0.68
1:A:226:VAL:HG12	1:B:106:LEU:HD22	1.76	0.68
1:B:46:GLN:CG	1:B:153:THR:HA	2.24	0.68
1:A:181:MET:HE2	1:A:199:TRP:CZ2	2.28	0.68
1:C:93:PHE:O	1:C:97:VAL:HG23	1.94	0.68
1:A:183:ARG:O	1:A:185:PRO:HD3	1.94	0.67
1:D:14:VAL:HG11	1:D:124:LEU:HD12	1.76	0.67
1:D:43:LEU:HD21	1:D:75:MET:HE2	1.77	0.66
1:B:61:ILE:HD11	1:B:69:VAL:HG11	1.76	0.66
1:B:233:GLU:O	1:B:237:LYS:HG3	1.96	0.66
1:A:19:PHE:CG	1:A:22:ARG:HD3	2.29	0.66
1:C:233:GLU:C	1:C:236:PRO:HD2	2.20	0.66
1:C:181:MET:HE3	1:C:192:ARG:HB3	1.77	0.66
1:D:25:GLN:NE2	1:D:244:LEU:HD11	2.10	0.66
1:A:112:VAL:HG21	1:A:251:GLU:CG	2.26	0.65
1:D:131:LEU:HD13	1:D:171:ALA:HB2	1.77	0.65
1:A:112:VAL:HG21	1:A:251:GLU:HG3	1.79	0.65
1:D:183:ARG:O	1:D:185:PRO:HD3	1.97	0.65
1:A:27:PRO:HG2	1:A:33:LEU:HD23	1.78	0.64
1:B:156:LYS:NZ	2:B:257:O1E:H21	2.12	0.64
1:B:183:ARG:HB2	1:B:183:ARG:NH1	2.11	0.64
1:C:234:ARG:HH22	1:D:234:ARG:HH12	1.45	0.64
1:A:42:TRP:HH2	1:A:138:CYS:HB2	1.61	0.64
1:B:163:VAL:HG13	1:B:238:LEU:CD2	2.27	0.63
1:B:241:ASP:O	1:B:245:VAL:HG23	1.98	0.63
1:B:128:TYR:N	1:B:128:TYR:CD1	2.64	0.63
1:C:101:SER:HB2	1:C:119:LYS:HB3	1.80	0.63
1:A:161:CYS:SG	1:A:163:VAL:O	2.56	0.62
1:C:61:ILE:HD11	1:C:69:VAL:HG11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:VAL:CG1	1:C:234:ARG:HG3	2.28	0.61
1:B:183:ARG:HD2	1:B:252:SER:HB3	1.82	0.61
1:D:73:ALA:HB1	1:D:199:TRP:HB3	1.81	0.61
1:C:87:CYS:SG	1:C:89:THR:HG23	2.41	0.61
1:C:96:ILE:HG21	1:C:221:LEU:HD12	1.82	0.61
1:A:61:ILE:HD11	1:A:93:PHE:CZ	2.36	0.61
1:B:15:TYR:CE2	1:B:177:PRO:HD3	2.36	0.61
1:B:196:ARG:O	1:B:200:GLN:HB2	2.01	0.61
1:C:41:HIS:HD2	1:C:42:TRP:HD1	1.49	0.60
1:B:152:THR:HG23	1:B:154:PRO:HD3	1.83	0.60
1:C:53:LEU:HD21	1:C:75:MET:CE	2.30	0.60
1:C:73:ALA:HB1	1:C:199:TRP:HB3	1.83	0.60
1:B:152:THR:CG2	1:B:154:PRO:HD3	2.31	0.60
1:C:172:VAL:HG11	1:C:183:ARG:HG2	1.82	0.60
1:A:183:ARG:N	1:A:183:ARG:HD2	2.16	0.60
1:B:38:VAL:HG22	1:B:143:GLN:HB2	1.83	0.60
1:D:134:SER:OG	1:D:156:LYS:HD3	2.01	0.60
1:B:134:SER:OG	1:B:156:LYS:HE2	2.02	0.59
1:D:38:VAL:HG22	1:D:143:GLN:HB2	1.82	0.59
1:B:93:PHE:HZ	1:B:128:TYR:HE2	1.51	0.59
1:B:156:LYS:HZ1	2:B:257:O1E:H21	1.67	0.59
1:D:36:ARG:O	1:D:40:GLU:HG3	2.03	0.58
1:D:112:VAL:HG21	1:D:251:GLU:HG3	1.83	0.58
1:D:22:ARG:NH2	1:D:245:VAL:HA	2.19	0.58
1:C:133:LEU:HD21	1:C:155:PHE:CE1	2.38	0.58
1:B:183:ARG:HB2	1:B:183:ARG:HH11	1.69	0.57
1:D:163:VAL:HG13	1:D:238:LEU:HD13	1.86	0.57
1:D:172:VAL:HG11	1:D:183:ARG:HG2	1.84	0.57
1:B:163:VAL:HG22	1:B:234:ARG:HG3	1.86	0.57
1:B:92:ARG:O	1:B:96:ILE:HG13	2.03	0.57
1:C:46:GLN:HE22	1:C:57:LEU:HD11	1.70	0.57
1:A:11:VAL:HG12	1:A:11:VAL:O	2.02	0.57
1:B:238:LEU:HB3	1:B:256:ALA:HB1	1.87	0.57
1:A:178:GLU:O	1:A:182:GLN:HG2	2.05	0.57
1:A:79:ARG:HE	1:A:79:ARG:N	2.02	0.56
1:A:23:TYR:CE2	1:A:36:ARG:HD3	2.40	0.56
1:D:16:VAL:O	1:D:85:LEU:HD22	2.06	0.56
1:B:93:PHE:CE2	1:B:124:LEU:HD21	2.40	0.56
1:B:95:GLU:OE2	1:B:98:ARG:NH2	2.38	0.56
1:B:127:SER:HB3	1:B:128:TYR:CE1	2.40	0.56
1:D:15:TYR:CD2	1:D:177:PRO:HB3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:GLN:OE1	1:A:153:THR:HA	2.06	0.55
1:A:28:ASP:HB2	1:A:29:GLU:OE1	2.06	0.55
1:C:233:GLU:O	1:C:236:PRO:HD2	2.06	0.55
1:D:60:ASN:HD21	1:D:157:HIS:CD2	2.24	0.55
1:A:232:ARG:HG2	1:B:239:ARG:NH2	2.22	0.55
1:B:79:ARG:HA	1:B:79:ARG:HH11	1.71	0.55
1:B:122:GLU:HB3	1:B:255:LYS:NZ	2.20	0.55
1:C:84:CYS:SG	1:C:131:LEU:HD21	2.47	0.55
1:A:46:GLN:NE2	1:A:153:THR:HB	2.22	0.54
1:C:27:PRO:HB3	1:C:32:LEU:HB2	1.87	0.54
1:A:163:VAL:HG22	1:A:234:ARG:HD2	1.89	0.54
1:B:19:PHE:HD1	1:B:82:LEU:O	1.89	0.54
1:A:38:VAL:HG11	1:A:138:CYS:SG	2.47	0.54
1:A:33:LEU:HD13	1:A:35:PRO:HG3	1.88	0.54
1:C:35:PRO:HB2	1:C:38:VAL:HG23	1.90	0.54
1:D:140:ASP:O	1:D:141:VAL:HB	2.08	0.54
1:D:112:VAL:HG21	1:D:251:GLU:CG	2.37	0.54
1:B:178:GLU:O	1:B:182:GLN:HG2	2.08	0.54
1:C:181:MET:CE	1:C:192:ARG:HB3	2.38	0.53
1:C:192:ARG:HA	1:C:195:LEU:HD12	1.88	0.53
1:D:15:TYR:HD2	1:D:85:LEU:HD11	1.72	0.53
1:D:42:TRP:CH2	1:D:136:ARG:HG2	2.43	0.53
1:A:92:ARG:HD2	1:A:214:PHE:HD2	1.74	0.53
1:C:122:GLU:HG2	1:C:255:LYS:NZ	2.23	0.53
1:C:165:ARG:CD	2:C:257:01E:HA4	2.37	0.53
1:A:177:PRO:HB2	1:A:199:TRP:CH2	2.44	0.53
1:C:35:PRO:HD2	1:C:38:VAL:HG21	1.90	0.53
1:A:22:ARG:HH11	1:A:22:ARG:HB3	1.73	0.52
1:A:249:GLU:O	1:A:250:ARG:HG2	2.08	0.52
1:A:165:ARG:HB2	2:A:257:01E:HB1	1.90	0.52
1:A:220:GLY:HA2	1:B:103:LYS:HG3	1.91	0.52
1:B:22:ARG:HG3	1:B:244:LEU:HD21	1.91	0.52
1:D:120:VAL:O	1:D:124:LEU:HG	2.10	0.52
1:A:42:TRP:CH2	1:A:138:CYS:HB2	2.43	0.52
1:A:152:THR:HG23	1:A:154:PRO:HD3	1.91	0.52
1:A:179:TRP:NE1	1:A:183:ARG:NH1	2.58	0.52
1:C:38:VAL:HG22	1:C:143:GLN:HG3	1.92	0.52
1:A:181:MET:SD	1:A:192:ARG:HG2	2.50	0.52
1:D:179:TRP:CE2	1:D:183:ARG:NH1	2.77	0.52
1:A:131:LEU:HD13	1:A:171:ALA:CB	2.40	0.52
1:B:27:PRO:HB3	1:B:32:LEU:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:ASP:O	1:C:180:VAL:HG12	2.10	0.52
1:B:19:PHE:HE1	1:B:78:VAL:HG21	1.74	0.52
1:C:141:VAL:O	1:C:141:VAL:HG13	2.10	0.52
1:D:196:ARG:O	1:D:200:GLN:HB2	2.09	0.52
1:D:98:ARG:O	1:D:102:GLU:HG2	2.10	0.51
1:C:133:LEU:HD21	1:C:155:PHE:CD1	2.45	0.51
1:D:190:ALA:O	1:D:193:ASP:HB3	2.10	0.51
1:B:46:GLN:HG2	1:B:153:THR:HA	1.91	0.51
1:B:196:ARG:HA	1:B:199:TRP:CE2	2.46	0.51
1:A:234:ARG:NH2	1:B:229:MET:O	2.40	0.51
1:D:163:VAL:HG22	1:D:234:ARG:HG3	1.92	0.51
1:B:36:ARG:NH1	1:B:79:ARG:HA	2.23	0.51
1:A:42:TRP:CZ2	1:A:136:ARG:HD3	2.46	0.51
1:A:60:ASN:ND2	1:A:157:HIS:CD2	2.78	0.51
1:C:11:VAL:O	1:C:11:VAL:HG12	2.11	0.50
1:B:167:ARG:HG2	1:B:167:ARG:NH1	2.24	0.50
1:C:156:LYS:HD3	2:C:257:O1E:H21	1.94	0.50
1:B:7:GLN:HG3	1:B:98:ARG:NE	2.27	0.50
1:B:42:TRP:CH2	1:B:138:CYS:HB2	2.46	0.50
1:B:72:VAL:HG21	1:B:158:VAL:CG2	2.36	0.50
1:C:76:GLN:HE22	1:C:194:GLY:HA3	1.75	0.50
1:C:98:ARG:O	1:C:102:GLU:HG2	2.11	0.50
1:B:22:ARG:NH1	1:B:80:ASP:HB3	2.27	0.50
1:A:20:LEU:HD22	1:A:133:LEU:HB2	1.93	0.50
1:B:165:ARG:HD3	2:B:257:O1E:HA4	1.92	0.50
1:A:242:LYS:HG2	1:A:248:THR:HG23	1.94	0.49
1:B:93:PHE:HE2	1:B:124:LEU:HD21	1.77	0.49
1:A:74:ALA:HA	1:A:198:GLN:OE1	2.12	0.49
1:A:167:ARG:CZ	1:A:167:ARG:HA	2.42	0.49
1:A:232:ARG:HG2	1:B:239:ARG:HH22	1.76	0.49
1:D:112:VAL:O	1:D:114:PRO:HD2	2.12	0.49
1:A:182:GLN:HA	1:A:182:GLN:OE1	2.12	0.49
1:D:70:GLY:HA3	1:D:87:CYS:O	2.12	0.49
1:D:233:GLU:O	1:D:236:PRO:HD2	2.13	0.49
1:B:42:TRP:HH2	1:B:138:CYS:HB2	1.76	0.49
1:C:41:HIS:CD2	1:C:42:TRP:HD1	2.31	0.49
1:D:163:VAL:HG12	1:D:164:GLY:H	1.78	0.49
1:A:228:ALA:HA	1:A:231:ILE:HD12	1.95	0.49
1:B:118:ASP:O	1:B:122:GLU:HG3	2.12	0.49
1:A:242:LYS:CD	1:A:254:VAL:HG11	2.33	0.49
1:B:97:VAL:HG13	1:B:123:PHE:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:ASP:OD2	1:B:178:GLU:HB2	2.12	0.48
1:D:22:ARG:O	1:D:24:ASP:N	2.46	0.48
1:B:215:ARG:HH11	1:B:215:ARG:HG3	1.78	0.48
1:B:249:GLU:O	1:B:250:ARG:HG2	2.13	0.48
1:C:232:ARG:HG2	1:D:239:ARG:NH2	2.28	0.48
1:D:233:GLU:C	1:D:236:PRO:HD2	2.38	0.48
1:D:113:SER:HB3	1:D:114:PRO:CD	2.44	0.48
1:D:217:ASP:N	1:D:217:ASP:OD1	2.47	0.48
1:B:97:VAL:HG13	1:B:123:PHE:HD2	1.78	0.48
1:D:167:ARG:HD3	1:D:240:TYR:HD2	1.78	0.48
1:D:183:ARG:O	1:D:250:ARG:HG3	2.13	0.48
1:A:226:VAL:HG12	1:B:106:LEU:CD2	2.43	0.48
1:B:38:VAL:HG22	1:B:143:GLN:CB	2.45	0.47
1:B:133:LEU:HD12	1:B:134:SER:H	1.79	0.47
1:A:140:ASP:O	1:A:141:VAL:HB	2.14	0.47
1:C:196:ARG:HG2	1:C:200:GLN:OE1	2.15	0.47
1:A:165:ARG:HD3	2:A:257:01E:HA4	1.96	0.47
1:C:92:ARG:HB2	1:C:212:ASP:OD2	2.15	0.47
1:C:249:GLU:O	1:C:250:ARG:HD3	2.14	0.47
1:D:96:ILE:HG21	1:D:221:LEU:HD12	1.95	0.47
1:A:235:LEU:HD12	1:A:235:LEU:HA	1.70	0.47
1:C:41:HIS:HD2	1:C:42:TRP:CD1	2.30	0.47
1:C:118:ASP:HB3	1:C:121:VAL:HB	1.95	0.47
1:A:46:GLN:OE1	1:A:154:PRO:HD2	2.15	0.47
1:B:127:SER:HB3	1:B:128:TYR:CD1	2.50	0.47
1:D:181:MET:SD	1:D:192:ARG:HG2	2.55	0.47
1:B:163:VAL:CG2	1:B:234:ARG:HG3	2.45	0.46
1:A:69:VAL:HB	1:A:88:VAL:HG13	1.96	0.46
1:C:19:PHE:O	1:C:169:THR:HG22	2.16	0.46
1:C:254:VAL:HG12	1:C:256:ALA:OXT	2.16	0.46
1:A:194:GLY:O	1:A:198:GLN:HG3	2.16	0.46
1:B:179:TRP:O	1:B:183:ARG:NH1	2.45	0.46
1:A:19:PHE:CB	1:A:22:ARG:HD3	2.45	0.46
1:B:170:LEU:HD13	1:B:238:LEU:HD12	1.97	0.46
1:C:162:SER:HB3	1:C:228:ALA:HB1	1.98	0.46
1:D:183:ARG:HE	1:D:183:ARG:HA	1.80	0.46
1:D:59:LEU:HD11	1:D:160:LEU:HD21	1.98	0.46
1:B:156:LYS:HZ1	2:B:257:01E:HE2	1.79	0.46
1:D:167:ARG:HD3	1:D:240:TYR:CD2	2.51	0.46
1:B:19:PHE:O	1:B:169:THR:HA	2.15	0.46
1:D:112:VAL:CG2	1:D:251:GLU:HG3	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:GLN:O	1:D:9:GLN:HB3	2.16	0.46
1:D:75:MET:HE3	1:D:82:LEU:HD11	1.98	0.46
1:B:165:ARG:HB2	2:B:257:01E:HB1	1.97	0.45
1:A:242:LYS:HG3	1:A:247:VAL:HB	1.98	0.45
1:B:21:ALA:O	1:B:81:GLY:HA3	2.16	0.45
1:B:122:GLU:CB	1:B:255:LYS:HZ1	2.22	0.45
1:D:10:ALA:HA	1:D:175:ARG:NH2	2.32	0.45
1:D:137:ARG:HG2	2:D:257:01E:HG32	1.98	0.45
1:B:112:VAL:HG23	1:B:115:LEU:HD12	1.99	0.45
1:D:242:LYS:HD2	1:D:256:ALA:O	2.16	0.45
1:D:29:GLU:HB3	1:D:31:GLU:HG2	1.98	0.45
1:A:226:VAL:HG22	1:B:127:SER:OG	2.16	0.45
1:A:233:GLU:O	1:A:237:LYS:HG3	2.16	0.45
1:C:179:TRP:O	1:C:183:ARG:NH1	2.47	0.45
1:D:60:ASN:ND2	1:D:157:HIS:CD2	2.85	0.45
1:D:247:VAL:HG11	1:D:254:VAL:HG21	1.99	0.45
1:B:23:TYR:CD2	1:B:81:GLY:HA2	2.52	0.45
1:B:36:ARG:HH12	1:B:79:ARG:HH11	1.59	0.45
1:D:22:ARG:HH21	1:D:245:VAL:HA	1.81	0.45
1:B:60:ASN:OD1	1:B:63:HIS:HA	2.17	0.45
1:A:60:ASN:HD21	1:A:157:HIS:CD2	2.35	0.45
1:C:87:CYS:SG	1:C:89:THR:CG2	3.05	0.45
1:D:58:PRO:HG2	1:D:157:HIS:HB2	1.99	0.45
1:A:5:GLU:H	1:A:5:GLU:HG2	1.70	0.44
1:A:140:ASP:O	1:A:141:VAL:CB	2.65	0.44
1:B:188:THR:O	1:B:191:ASP:HB2	2.17	0.44
1:A:97:VAL:HG12	1:A:97:VAL:O	2.17	0.44
1:B:46:GLN:OE1	1:B:155:PHE:HB2	2.17	0.44
1:D:123:PHE:CD1	1:D:123:PHE:C	2.95	0.44
1:D:182:GLN:HE22	1:D:192:ARG:HD2	1.82	0.44
1:A:238:LEU:HD12	1:A:238:LEU:HA	1.89	0.44
1:C:232:ARG:HG2	1:D:239:ARG:HH21	1.82	0.44
1:A:112:VAL:HG23	1:A:112:VAL:O	2.18	0.44
1:A:188:THR:O	1:A:191:ASP:HB2	2.18	0.44
1:A:112:VAL:HG21	1:A:251:GLU:OE2	2.16	0.44
1:C:181:MET:HE3	1:C:192:ARG:CB	2.45	0.44
1:A:246:GLY:O	1:A:248:THR:N	2.51	0.44
1:A:7:GLN:O	1:A:11:VAL:HG23	2.17	0.44
1:A:134:SER:OG	1:A:156:LYS:HD3	2.17	0.44
1:B:12:ALA:O	1:B:175:ARG:NH1	2.51	0.44
1:D:238:LEU:HD12	1:D:238:LEU:HA	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:GLN:OE1	1:A:154:PRO:CD	2.66	0.43
1:C:63:HIS:CE1	2:C:257:O1E:HB2	2.53	0.43
1:C:103:LYS:HB3	1:C:103:LYS:HE3	1.78	0.43
1:A:39:VAL:O	1:A:43:LEU:HG	2.17	0.43
1:D:11:VAL:HG12	1:D:11:VAL:O	2.18	0.43
1:C:20:LEU:HD13	1:C:133:LEU:HD13	2.00	0.43
1:B:131:LEU:HD13	1:B:171:ALA:CB	2.43	0.43
1:B:212:ASP:HA	1:B:213:PRO:HD2	1.85	0.43
1:D:180:VAL:O	1:D:183:ARG:HB2	2.18	0.43
1:C:137:ARG:HH11	1:C:137:ARG:CG	2.31	0.43
1:A:41:HIS:C	1:A:41:HIS:CD2	2.96	0.43
1:B:99:ARG:O	1:B:102:GLU:HB2	2.19	0.43
1:C:128:TYR:HB3	1:C:160:LEU:HB3	2.00	0.43
1:C:229:MET:HG2	1:D:234:ARG:NH2	2.33	0.43
1:B:87:CYS:SG	1:B:89:THR:HG22	2.58	0.43
1:A:15:TYR:CD1	1:A:177:PRO:HD3	2.54	0.43
1:A:27:PRO:HB3	1:A:32:LEU:HB2	2.00	0.43
1:B:36:ARG:HH12	1:B:79:ARG:HD3	1.83	0.43
1:C:183:ARG:O	1:C:250:ARG:HG3	2.18	0.43
1:C:233:GLU:O	1:C:237:LYS:HD2	2.18	0.43
1:D:163:VAL:CG2	1:D:234:ARG:HG3	2.49	0.43
1:A:46:GLN:CD	1:A:153:THR:HA	2.44	0.43
1:B:93:PHE:CZ	1:B:128:TYR:HE2	2.33	0.43
1:D:193:ASP:HA	1:D:196:ARG:NH1	2.34	0.43
1:B:233:GLU:C	1:B:236:PRO:HD2	2.44	0.42
1:A:42:TRP:CE2	1:A:136:ARG:HD3	2.53	0.42
1:A:57:LEU:H	1:A:57:LEU:CD1	2.32	0.42
1:A:184:PHE:HD2	1:A:245:VAL:CG1	2.33	0.42
1:B:20:LEU:HD13	1:B:133:LEU:HD22	2.01	0.42
1:B:156:LYS:HE3	1:B:157:HIS:CE1	2.54	0.42
1:C:179:TRP:HH2	1:C:252:SER:HA	1.83	0.42
1:C:216:SER:OG	1:C:217:ASP:N	2.51	0.42
1:D:254:VAL:HG12	1:D:256:ALA:OXT	2.18	0.42
1:A:179:TRP:CE2	1:A:183:ARG:NH1	2.88	0.42
1:C:219:TYR:CE2	1:D:99:ARG:HD2	2.54	0.42
1:B:19:PHE:HE1	1:B:78:VAL:CG2	2.32	0.42
1:B:89:THR:O	1:B:91:PRO:HD3	2.20	0.42
1:B:215:ARG:HG3	1:B:215:ARG:NH1	2.34	0.42
1:A:97:VAL:HG13	1:A:123:PHE:CD1	2.54	0.42
1:C:219:TYR:CD2	1:D:99:ARG:HD2	2.54	0.42
1:D:128:TYR:HB3	1:D:160:LEU:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:LEU:HD12	1:D:131:LEU:HA	1.89	0.42
1:A:63:HIS:HA	1:A:157:HIS:HE2	1.85	0.42
1:C:196:ARG:HG2	1:C:200:GLN:CD	2.45	0.42
1:A:179:TRP:CD1	1:D:114:PRO:HG3	2.55	0.42
1:B:11:VAL:O	1:B:11:VAL:CG1	2.67	0.42
1:B:27:PRO:HG2	1:B:33:LEU:HD23	2.02	0.42
1:B:247:VAL:O	1:B:247:VAL:HG12	2.19	0.42
1:D:68:VAL:HG12	1:D:213:PRO:HB2	2.02	0.42
1:A:42:TRP:O	1:A:43:LEU:C	2.62	0.41
1:A:165:ARG:HB2	2:A:257:01E:CB3	2.49	0.41
1:A:113:SER:O	1:D:116:GLN:NE2	2.53	0.41
1:B:140:ASP:O	1:B:141:VAL:HB	2.20	0.41
1:C:58:PRO:HG2	1:C:157:HIS:HB2	2.02	0.41
1:C:163:VAL:HG23	2:C:257:01E:H9	2.03	0.41
1:D:179:TRP:NE1	1:D:183:ARG:NH1	2.67	0.41
1:C:172:VAL:CG1	1:C:183:ARG:HG2	2.50	0.41
1:D:118:ASP:HB3	1:D:121:VAL:HB	2.02	0.41
1:C:53:LEU:HD11	1:C:75:MET:HE3	2.02	0.41
1:C:176:ASP:HB3	1:C:179:TRP:HB2	2.03	0.41
1:A:74:ALA:HB2	1:A:199:TRP:HD1	1.85	0.41
1:C:214:PHE:CZ	1:C:216:SER:HB3	2.55	0.41
1:C:242:LYS:HD2	1:C:256:ALA:OXT	2.20	0.41
1:D:240:TYR:O	1:D:244:LEU:HB2	2.20	0.41
1:B:103:LYS:HB3	1:B:103:LYS:HE3	1.89	0.41
1:D:23:TYR:HE2	1:D:36:ARG:HD3	1.82	0.41
1:D:63:HIS:HA	1:D:157:HIS:HE2	1.86	0.41
1:D:112:VAL:HG21	1:D:251:GLU:OE2	2.21	0.41
1:A:28:ASP:OD1	1:A:28:ASP:N	2.53	0.41
1:A:37:ASP:O	1:A:40:GLU:HB2	2.20	0.41
1:A:123:PHE:CD1	1:A:123:PHE:C	2.99	0.41
1:B:22:ARG:HD2	1:B:80:ASP:O	2.21	0.41
1:B:167:ARG:HA	1:B:167:ARG:CZ	2.51	0.41
1:C:59:LEU:CD2	1:C:160:LEU:HG	2.51	0.41
1:D:32:LEU:HD21	1:D:165:ARG:NH1	2.34	0.41
1:B:105:GLU:O	1:B:109:ARG:HG3	2.21	0.41
1:D:185:PRO:HG3	1:D:250:ARG:NE	2.36	0.41
1:A:38:VAL:HG21	1:A:138:CYS:SG	2.61	0.40
1:C:59:LEU:HD22	1:C:160:LEU:HG	2.03	0.40
1:C:59:LEU:HD21	1:C:160:LEU:CD2	2.51	0.40
1:D:105:GLU:O	1:D:109:ARG:HG3	2.21	0.40
1:A:69:VAL:HG12	1:A:93:PHE:CG	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:TRP:CE3	1:B:200:GLN:NE2	2.87	0.40
1:C:63:HIS:NE2	2:C:257:O1E:O11	2.52	0.40
1:A:167:ARG:HG2	1:A:167:ARG:NH1	2.31	0.40
1:D:38:VAL:HG22	1:D:143:GLN:CB	2.50	0.40
1:A:20:LEU:HB2	1:A:82:LEU:HD23	2.03	0.40
1:A:98:ARG:O	1:A:102:GLU:HG2	2.21	0.40
1:C:91:PRO:HD2	1:C:212:ASP:HB2	2.03	0.40
1:C:234:ARG:NH2	1:D:229:MET:O	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:SER:HG	1:D:250:ARG:HH22[3_465]	1.28	0.32

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	222/256 (87%)	196 (88%)	20 (9%)	6 (3%)	4	10
1	B	222/256 (87%)	205 (92%)	13 (6%)	4 (2%)	6	18
1	C	222/256 (87%)	194 (87%)	24 (11%)	4 (2%)	6	18
1	D	222/256 (87%)	198 (89%)	18 (8%)	6 (3%)	4	10
All	All	888/1024 (87%)	793 (89%)	75 (8%)	20 (2%)	5	13

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	SER
1	A	113	SER

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Mol	Chain	Res	Type
1	A	141	VAL
1	B	54	SER
1	B	113	SER
1	B	141	VAL
1	C	113	SER
1	C	141	VAL
1	D	113	SER
1	D	141	VAL
1	C	23	TYR
1	D	23	TYR
1	B	23	TYR
1	A	23	TYR
1	D	54	SER
1	A	21	ALA
1	D	234	ARG
1	D	254	VAL
1	C	111	PRO
1	A	247	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	196/215 (91%)	169 (86%)	27 (14%)	3	9
1	B	196/215 (91%)	166 (85%)	30 (15%)	3	7
1	C	196/215 (91%)	173 (88%)	23 (12%)	5	13
1	D	196/215 (91%)	172 (88%)	24 (12%)	5	12
All	All	784/860 (91%)	680 (87%)	104 (13%)	4	10

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	7	GLN
1	A	22	ARG

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Mol	Chain	Res	Type
1	A	24	ASP
1	A	26	SER
1	A	28	ASP
1	A	33	LEU
1	A	44	HIS
1	A	53	LEU
1	A	59	LEU
1	A	79	ARG
1	A	80	ASP
1	A	89	THR
1	A	99	ARG
1	A	105	GLU
1	A	131	LEU
1	A	137	ARG
1	A	163	VAL
1	A	180	VAL
1	A	183	ARG
1	A	186	ASP
1	A	199	TRP
1	A	222	LEU
1	A	234	ARG
1	A	235	LEU
1	A	238	LEU
1	A	248	THR
1	B	4	ASP
1	B	5	GLU
1	B	8	SER
1	B	43	LEU
1	B	54	SER
1	B	55	VAL
1	B	57	LEU
1	B	59	LEU
1	B	72	VAL
1	B	80	ASP
1	B	85	LEU
1	B	99	ARG
1	B	105	GLU
1	B	128	TYR
1	B	131	LEU
1	B	141	VAL
1	B	152	THR
1	B	163	VAL

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Mol	Chain	Res	Type
1	B	180	VAL
1	B	183	ARG
1	B	193	ASP
1	B	199	TRP
1	B	200	GLN
1	B	210	SER
1	B	222	LEU
1	B	224	ASN
1	B	226	VAL
1	B	238	LEU
1	B	242	LYS
1	B	245	VAL
1	C	26	SER
1	C	59	LEU
1	C	65	ASP
1	C	85	LEU
1	C	92	ARG
1	C	117	PRO
1	C	118	ASP
1	C	122	GLU
1	C	137	ARG
1	C	141	VAL
1	C	142	GLU
1	C	143	GLN
1	C	153	THR
1	C	163	VAL
1	C	180	VAL
1	C	183	ARG
1	C	199	TRP
1	C	210	SER
1	C	222	LEU
1	C	224	ASN
1	C	235	LEU
1	C	238	LEU
1	C	244	LEU
1	D	4	ASP
1	D	7	GLN
1	D	26	SER
1	D	29	GLU
1	D	36	ARG
1	D	54	SER
1	D	59	LEU

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Mol	Chain	Res	Type
1	D	68	VAL
1	D	79	ARG
1	D	105	GLU
1	D	107	VAL
1	D	131	LEU
1	D	141	VAL
1	D	142	GLU
1	D	163	VAL
1	D	180	VAL
1	D	183	ARG
1	D	192	ARG
1	D	222	LEU
1	D	229	MET
1	D	235	LEU
1	D	238	LEU
1	D	244	LEU
1	D	245	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	41	HIS
1	A	243	GLN
1	B	25	GLN
1	B	224	ASN
1	C	7	GLN
1	C	41	HIS
1	C	76	GLN
1	C	200	GLN
1	D	25	GLN
1	D	182	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	01E	D	257	1	44,44,44	1.71	5 (11%)	57,63,63	1.79	6 (10%)
2	01E	B	257	1	44,44,44	1.83	6 (13%)	57,63,63	1.60	4 (7%)
2	01E	C	257	1	44,44,44	1.78	6 (13%)	57,63,63	1.32	4 (7%)
2	01E	A	257	1	44,44,44	1.75	7 (15%)	57,63,63	1.73	5 (8%)

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	01E	D	257	1	-	3/52/52/52	0/2/2/2
2	01E	B	257	1	-	3/52/52/52	0/2/2/2
2	01E	C	257	1	-	2/52/52/52	0/2/2/2
2	01E	A	257	1	-	3/52/52/52	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	257	01E	CE1-CH1	7.31	1.52	1.37
2	B	257	01E	CE2-CH2	6.73	1.51	1.37
2	D	257	01E	CE2-CH2	6.71	1.51	1.37
2	A	257	01E	CE1-CH1	6.60	1.51	1.37
2	A	257	01E	CE2-CH2	6.25	1.50	1.37
2	C	257	01E	CE2-CH2	6.21	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	257	01E	CE1-CH1	6.20	1.50	1.37
2	D	257	01E	CE1-CH1	5.99	1.50	1.37
2	C	257	01E	CE1-ND2	3.87	1.45	1.38
2	C	257	01E	CE2-ND2	3.75	1.45	1.38
2	D	257	01E	CE1-ND2	3.58	1.45	1.38
2	B	257	01E	CG-ND2	-3.56	1.32	1.38
2	D	257	01E	CG-ND2	-3.20	1.33	1.38
2	A	257	01E	CE2-ND2	2.98	1.44	1.38
2	C	257	01E	CH2-CH1	2.94	1.50	1.41
2	B	257	01E	CH2-CH1	2.93	1.50	1.41
2	A	257	01E	CG-ND2	-2.88	1.34	1.38
2	A	257	01E	CH2-CH1	2.82	1.50	1.41
2	B	257	01E	CE1-ND2	2.76	1.43	1.38
2	D	257	01E	CH2-CH1	2.72	1.49	1.41
2	C	257	01E	CG-ND2	-2.72	1.34	1.38
2	A	257	01E	CE1-ND2	2.56	1.43	1.38
2	B	257	01E	CE2-ND2	2.53	1.43	1.38
2	A	257	01E	C3-CA3	2.38	1.56	1.54

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	257	01E	CE2-ND2-CE1	9.15	117.62	108.41
2	D	257	01E	CE2-ND2-CE1	8.95	117.42	108.41
2	B	257	01E	CE2-ND2-CE1	8.77	117.24	108.41
2	D	257	01E	CH2-CE2-ND2	-6.90	100.95	107.86
2	C	257	01E	CE2-ND2-CE1	6.50	114.96	108.41
2	A	257	01E	CH2-CE2-ND2	-5.48	102.37	107.86
2	B	257	01E	CH1-CE1-ND2	-5.43	102.42	107.86
2	A	257	01E	CH1-CE1-ND2	-5.34	102.51	107.86
2	D	257	01E	CH1-CE1-ND2	-5.08	102.77	107.86
2	C	257	01E	CH1-CE1-ND2	-4.17	103.68	107.86
2	B	257	01E	CH2-CE2-ND2	-3.79	104.06	107.86
2	C	257	01E	CH2-CE2-ND2	-3.45	104.41	107.86
2	C	257	01E	CB3-CA3-C3	-2.48	110.08	112.56
2	B	257	01E	CB3-CA3-C3	-2.28	110.28	112.56
2	A	257	01E	CB3-CA3-C3	-2.22	110.33	112.56
2	A	257	01E	C3-CA3-N2	2.22	113.11	110.10
2	D	257	01E	C3-CA3-N2	2.11	112.95	110.10
2	D	257	01E	CB3-CA3-C3	-2.06	110.49	112.56
2	D	257	01E	CB1-CA1-C1	-2.04	110.73	112.97

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	257	01E	O3-C3-CA3-N2
2	A	257	01E	C11-C3-CA3-CB3
2	B	257	01E	O3-C3-CA3-N2
2	B	257	01E	C11-C3-CA3-CB3
2	D	257	01E	O3-C3-CA3-N2
2	A	257	01E	C11-C3-CA3-N2
2	B	257	01E	C11-C3-CA3-N2
2	C	257	01E	O3-C3-CA3-N2
2	C	257	01E	C11-C3-CA3-N2
2	D	257	01E	C11-C3-CA3-CB3
2	D	257	01E	C11-C3-CA3-N2

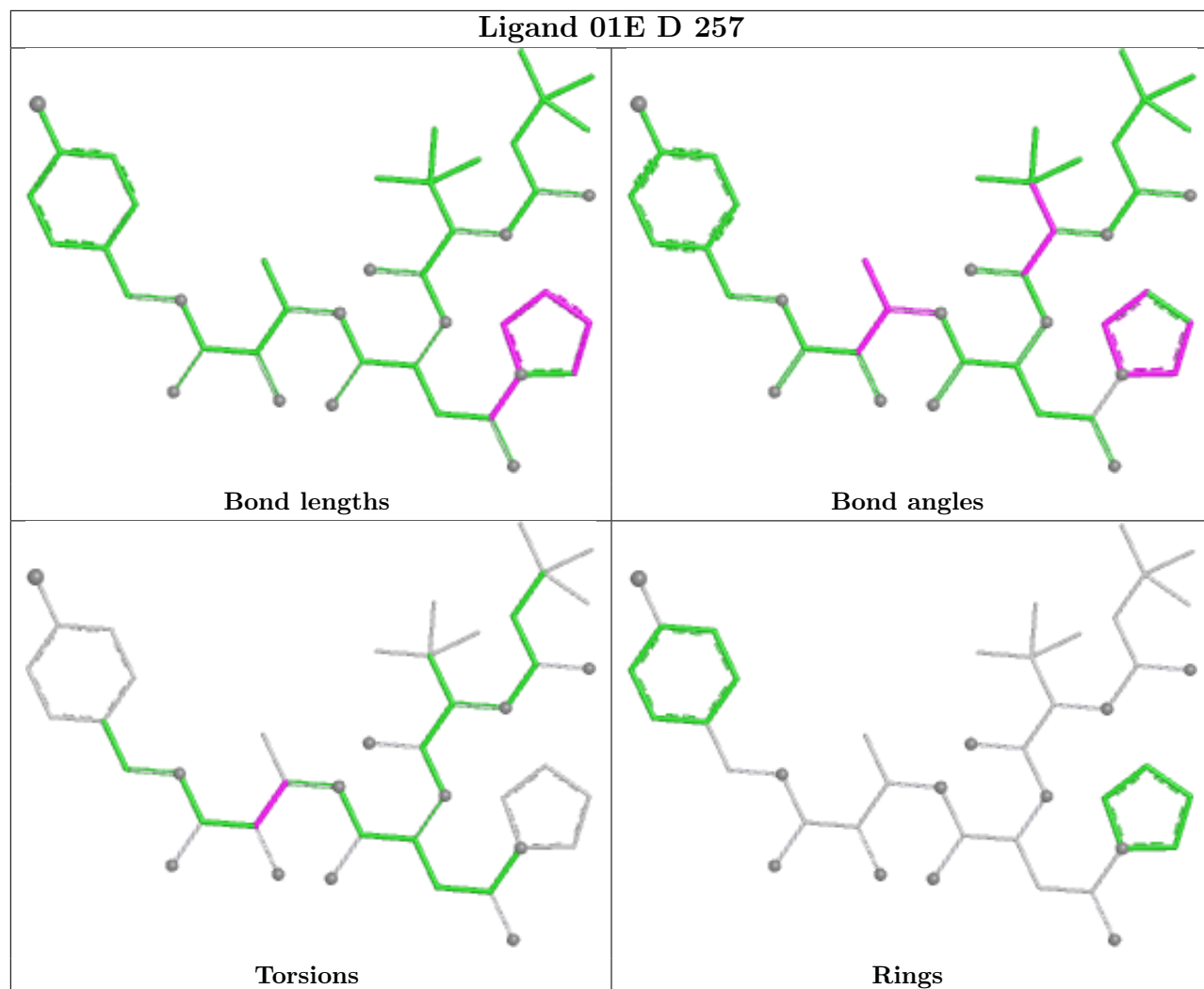
There are no ring outliers.

4 monomers are involved in 15 short contacts:

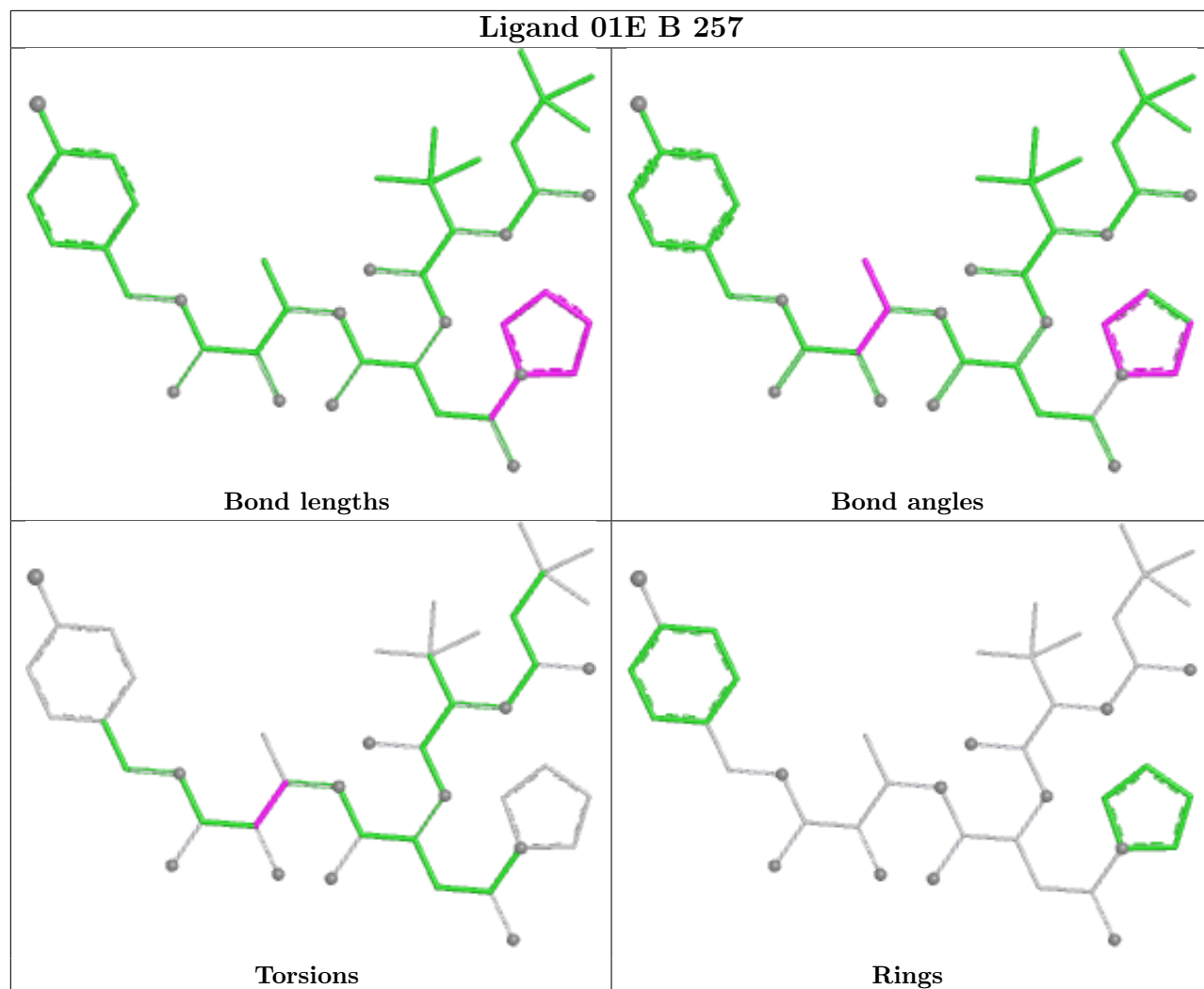
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	257	01E	1	0
2	B	257	01E	5	0
2	C	257	01E	6	0
2	A	257	01E	3	0

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

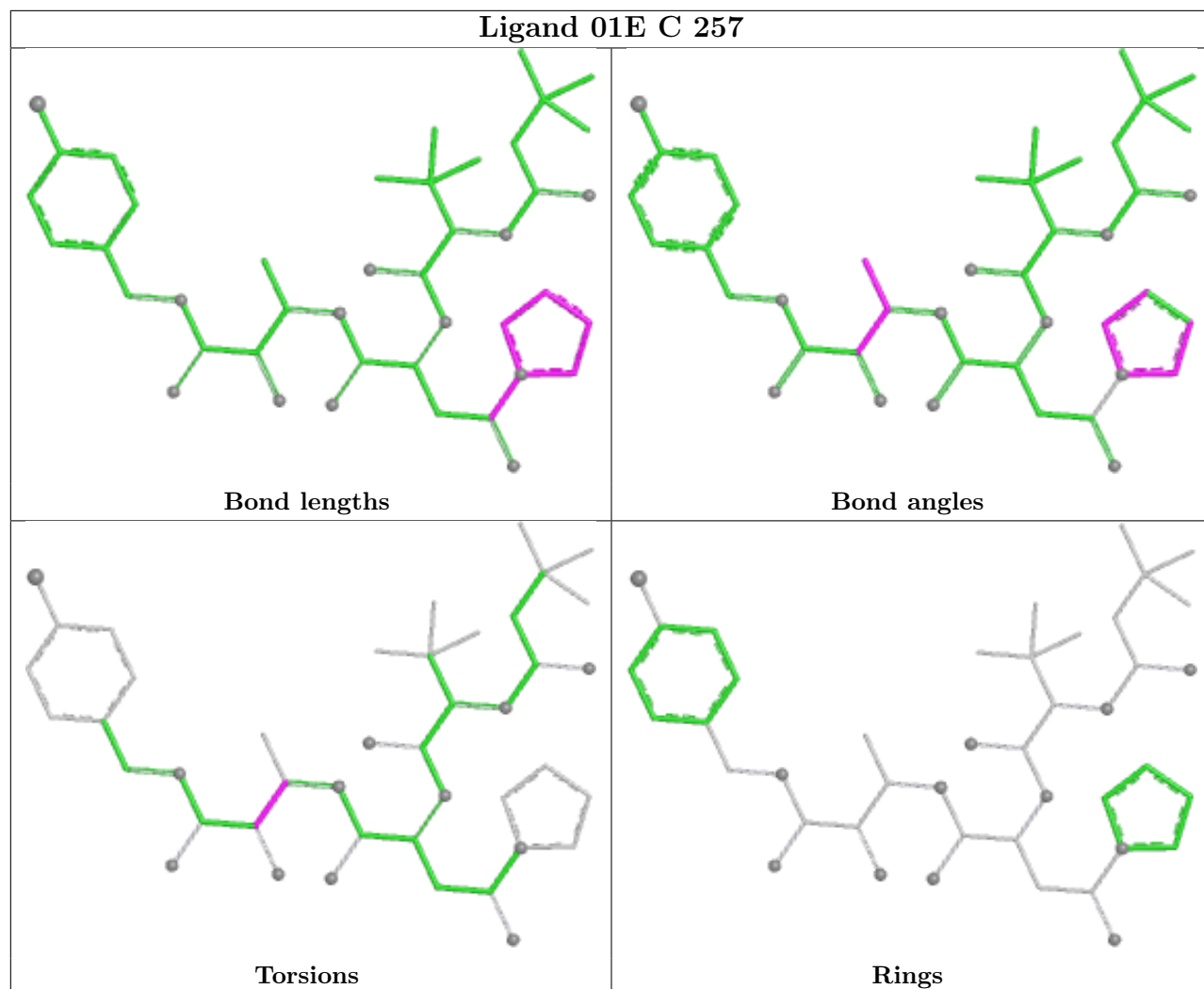
Ligand 01E D 257

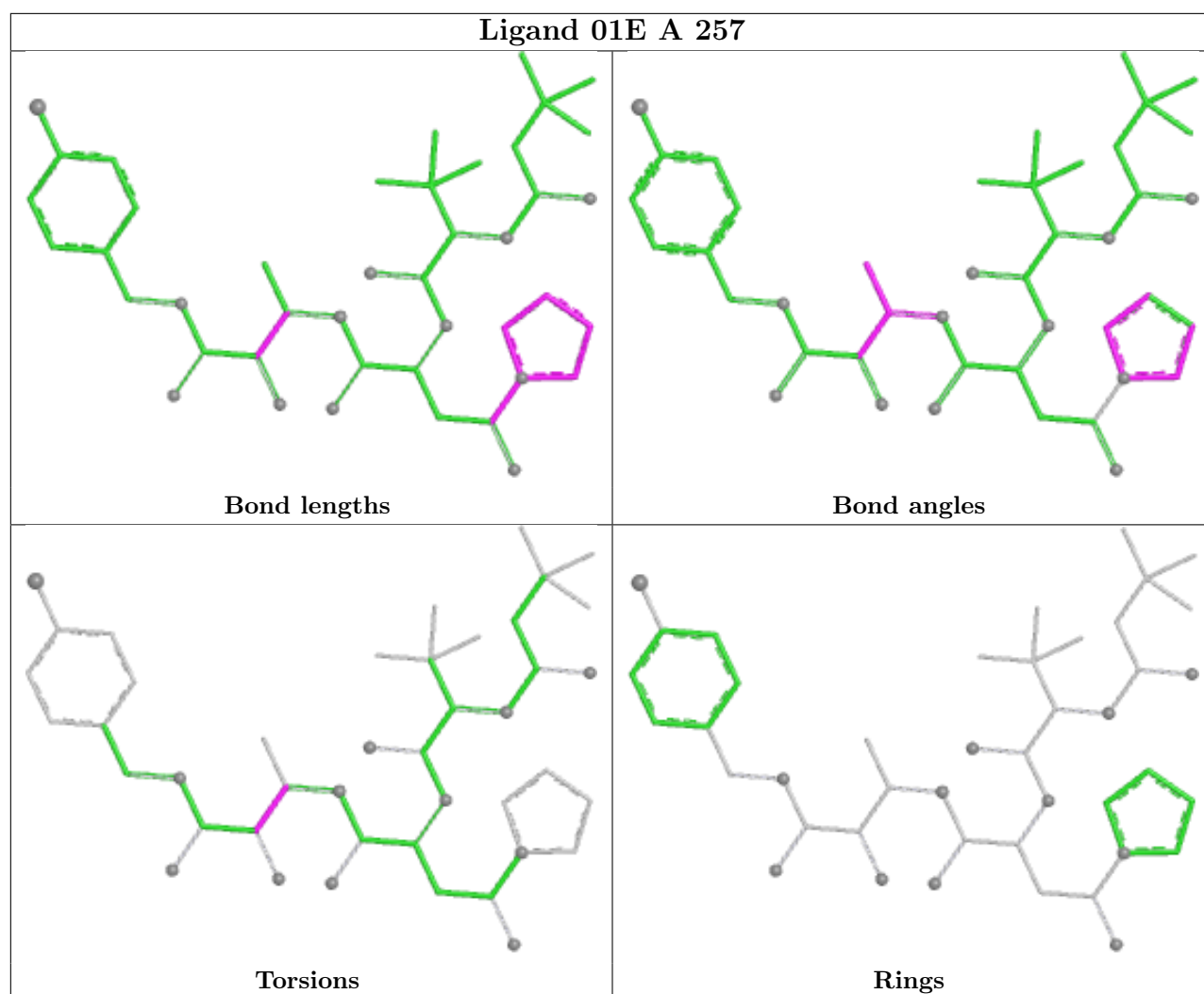


Ligand 01E B 257



Ligand 01E C 257





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.