



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:13 AM UTC

PDB ID : 4JK4 / pdb_00004jk4
Title : Crystal Structure of Bovine Serum Albumin in complex with 3,5-diiodosalicylic acid
Authors : Zielinski, K.; Bujacz, A.; Sekula, B.; Bujacz, G.
Deposited on : 2013-03-09
Resolution : 2.65 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

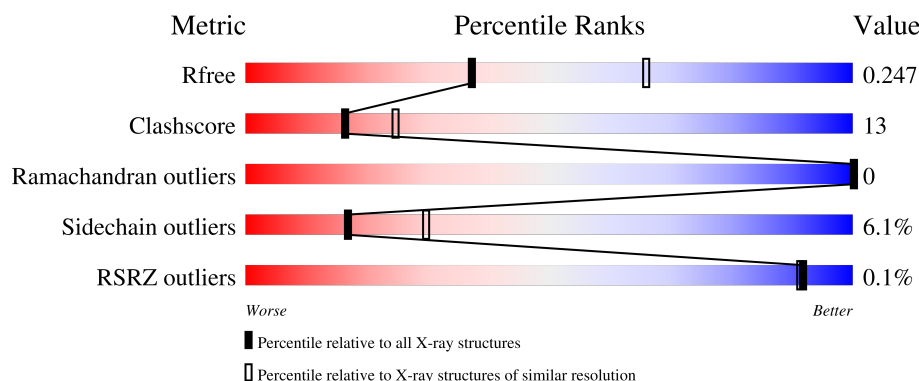
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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

Mol	Chain	Length	Quality of chain
1	A	583	 66% 31% .
1	B	583	 68% 28% .

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	DIU	B	603	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 9643 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.

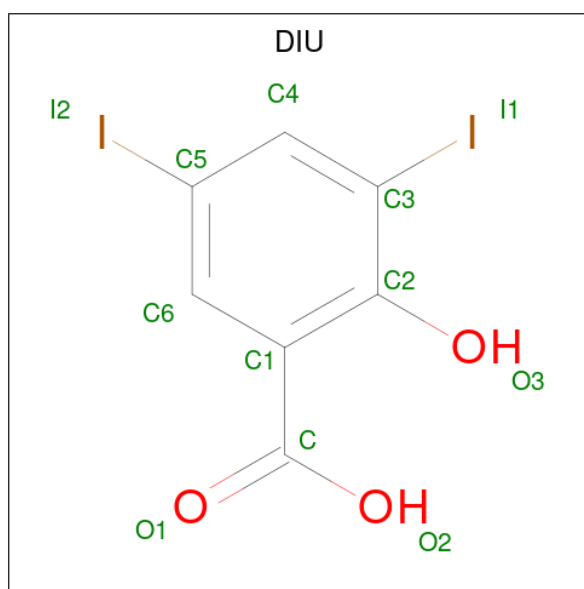
- Molecule 1 is a protein called Serum albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	0	3	0
			4668	2944	782	903	39			
1	B	582	Total	C	N	O	S	0	0	0
			4645	2931	780	895	39			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	190	THR	ALA	variant	UNP P02769
B	190	THR	ALA	variant	UNP P02769

- Molecule 2 is 2-HYDROXY-3,5-DIIDO-BENZOIC ACID (CCD ID: DIU) (formula: $C_7H_4I_2O_3$).



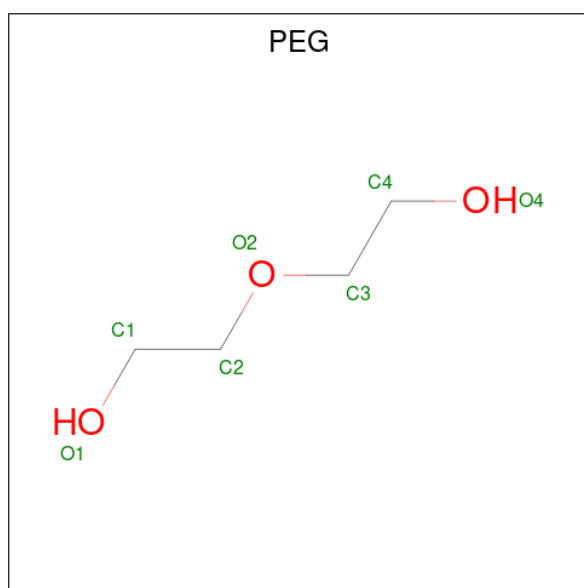
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	I	O	0	0
			12	7	2	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	I	O	0	0
			12	7	2	3		
2	A	1	Total	C	I	O	0	0
			12	7	2	3		
2	A	1	Total	C	I	O	0	0
			12	7	2	3		
2	B	1	Total	C	I	O	0	0
			12	7	2	3		
2	B	1	Total	C	I	O	0	0
			12	7	2	3		
2	B	1	Total	C	I	O	0	0
			12	7	2	3		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



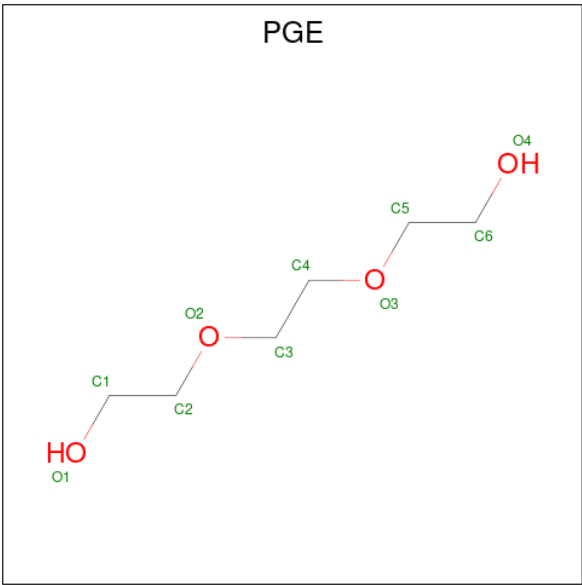
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			16	10	6		
4	A	1	Total	C	O	0	0
			16	10	6		
4	B	1	Total	C	O	0	0
			16	10	6		

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total	Ca	0	0
			4	4		
6	B	3	Total	Ca	0	0
			3	3		

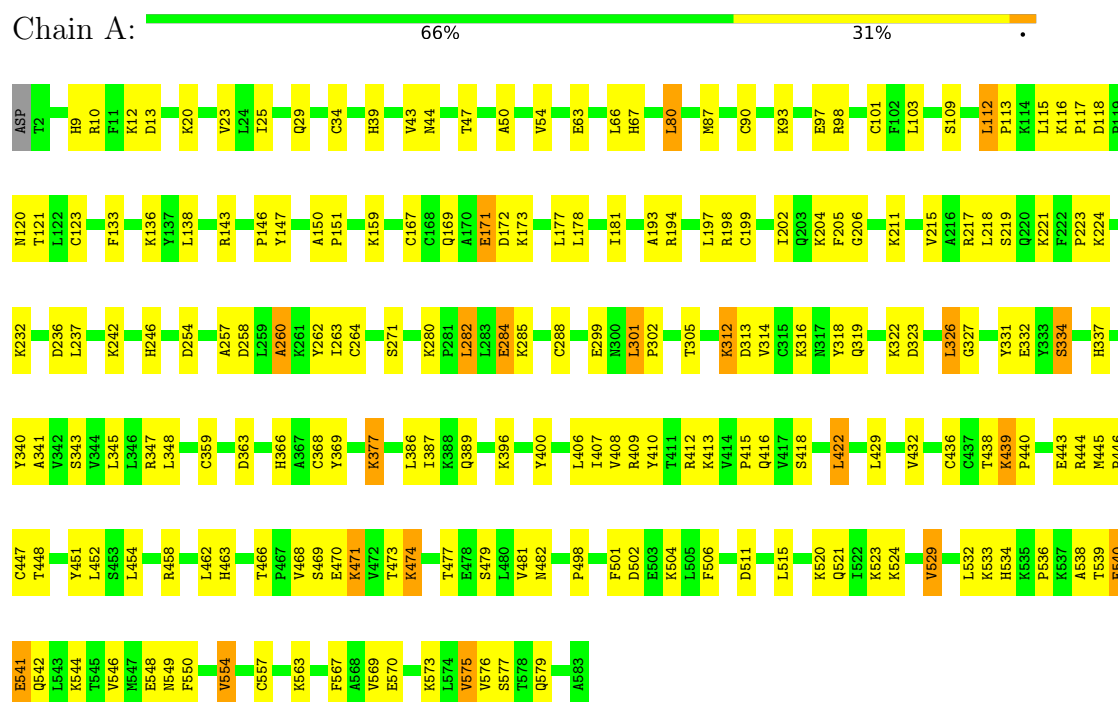
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	82	Total	O	0	0
			82	82		
7	B	63	Total	O	0	0
			63	63		

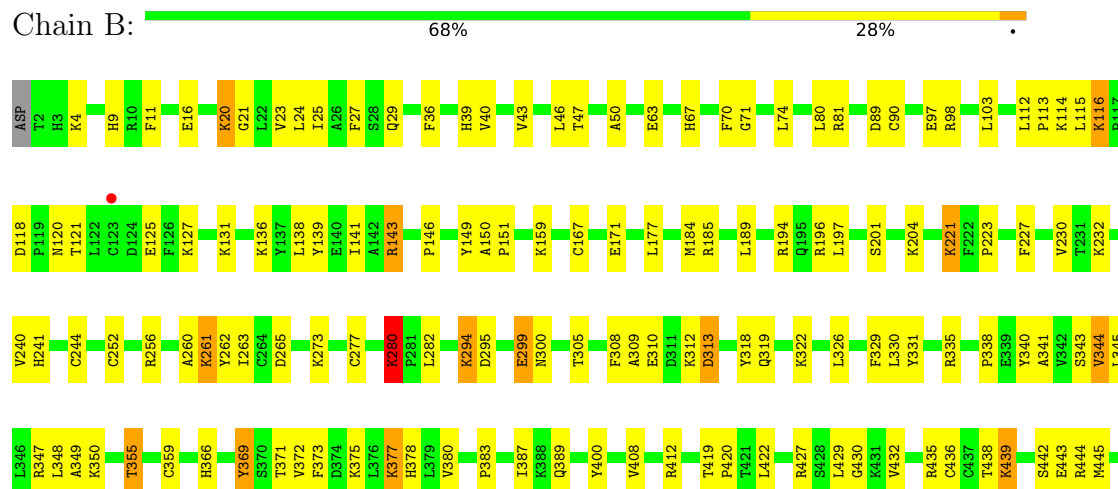
3 Residue-property plots

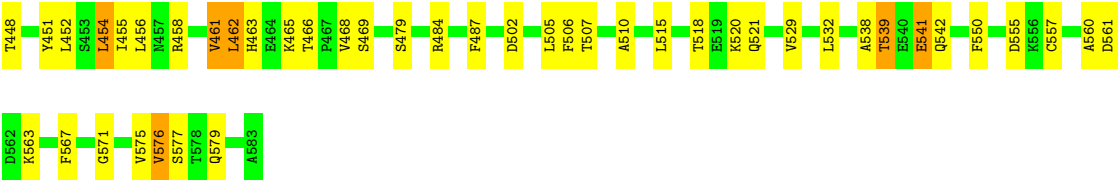
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Serum albumin



• Molecule 1: Serum albumin





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	215.41Å 44.80Å 146.90Å 90.00° 115.77° 90.00°	Depositor
Resolution (Å)	36.53 – 2.65 36.53 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.6 (36.53-2.65) 98.6 (36.53-2.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.188 , 0.246 0.192 , 0.247	Depositor DCC
R_{free} test set	1844 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	60.8	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9643	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DIU, CA, PGE, 1PE, PEG

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	1.21	11/4766 (0.2%)	1.36	31/6434 (0.5%)
1	B	1.09	6/4740 (0.1%)	1.30	22/6399 (0.3%)
All	All	1.15	17/9506 (0.2%)	1.33	53/12833 (0.4%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	240	VAL	CA-CB	6.55	1.61	1.54
1	B	263	ILE	CA-CB	6.44	1.61	1.54
1	A	257	ALA	CA-CB	-6.28	1.43	1.53
1	A	529	VAL	CA-CB	6.24	1.61	1.54
1	B	189	LEU	C-O	6.05	1.31	1.24
1	A	147	TYR	CA-CB	-5.91	1.45	1.53
1	B	461	VAL	CA-CB	5.80	1.62	1.54
1	B	50	ALA	CA-CB	-5.71	1.44	1.53
1	A	237	LEU	C-O	5.71	1.30	1.24
1	A	178	LEU	C-O	-5.56	1.19	1.24
1	A	263	ILE	CA-CB	5.52	1.61	1.54
1	A	199	CYS	C-O	-5.43	1.17	1.24
1	B	70	PHE	CA-C	5.41	1.59	1.52
1	A	202	ILE	CA-CB	5.28	1.60	1.54
1	A	150	ALA	CA-CB	5.27	1.60	1.53
1	A	50	ALA	CA-CB	-5.18	1.45	1.53
1	A	151	PRO	CA-C	5.13	1.60	1.52

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	LYS	CA-C-N	10.89	130.65	119.76
1	B	116	LYS	C-N-CA	10.89	130.65	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	280	LYS	CA-C-N	10.82	131.50	119.92
1	B	280	LYS	C-N-CA	10.82	131.50	119.92
1	A	301	LEU	CA-C-N	9.10	126.31	119.66
1	A	301	LEU	C-N-CA	9.10	126.31	119.66
1	A	337	HIS	CA-C-N	-8.55	110.63	120.12
1	A	337	HIS	C-N-CA	-8.55	110.63	120.12
1	B	571	GLY	CA-C-N	-8.22	111.25	119.56
1	B	571	GLY	C-N-CA	-8.22	111.25	119.56
1	B	282	LEU	N-CA-C	7.93	120.70	111.02
1	B	241	HIS	N-CA-C	7.68	119.65	111.28
1	A	260	ALA	N-CA-C	-7.21	103.50	111.36
1	A	299[A]	GLU	N-CA-C	7.03	118.94	111.28
1	A	299[B]	GLU	N-CA-C	7.03	118.94	111.28
1	B	21	GLY	N-CA-C	-6.96	104.07	112.49
1	B	252	CYS	N-CA-C	-6.51	104.11	111.14
1	A	282	LEU	N-CA-C	6.49	118.94	111.02
1	A	219	SER	N-CA-C	-6.37	104.44	111.82
1	A	569	VAL	N-CA-C	6.34	117.69	111.67
1	B	529	VAL	CB-CA-C	-6.01	104.28	111.97
1	A	418	SER	N-CA-C	5.97	119.12	110.28
1	A	109	SER	CA-C-N	5.91	125.67	119.76
1	A	109	SER	C-N-CA	5.91	125.67	119.76
1	A	271	SER	N-CA-C	5.84	117.98	108.76
1	B	576	VAL	N-CA-C	5.82	115.94	110.30
1	A	327	GLY	N-CA-C	-5.67	105.92	112.50
1	B	507	THR	CB-CA-C	5.66	119.57	109.38
1	B	221	LYS	CA-C-N	-5.60	116.55	123.21
1	B	221	LYS	C-N-CA	-5.60	116.55	123.21
1	B	462	LEU	N-CA-C	-5.59	105.27	111.36
1	B	439	LYS	N-CA-C	5.54	116.87	109.83
1	B	80	LEU	N-CA-C	5.47	116.93	110.97
1	A	112	LEU	CA-C-N	5.43	126.63	119.84
1	A	112	LEU	C-N-CA	5.43	126.63	119.84
1	A	302	PRO	O-C-N	5.42	123.80	121.31
1	B	444	ARG	N-CA-C	5.41	116.86	111.07
1	A	567	PHE	N-CA-C	-5.37	105.42	111.28
1	B	359	CYS	N-CA-C	5.37	117.22	111.36
1	A	334	SER	CA-C-N	-5.37	112.01	120.60
1	A	334	SER	C-N-CA	-5.37	112.01	120.60
1	A	80	LEU	N-CA-C	5.34	116.79	110.97
1	A	377	LYS	N-CA-C	5.31	117.07	111.28
1	A	554	VAL	CB-CA-C	-5.26	105.24	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	557	CYS	N-CA-C	5.23	117.89	111.82
1	A	118	ASP	CA-C-N	5.22	125.28	119.32
1	A	118	ASP	C-N-CA	5.22	125.28	119.32
1	B	312	LYS	N-CA-C	-5.20	106.89	113.18
1	A	167	CYS	N-CA-C	5.16	117.81	111.82
1	A	206	GLY	CA-C-N	5.14	127.43	120.38
1	A	206	GLY	C-N-CA	5.14	127.43	120.38
1	A	575	VAL	N-CA-C	-5.13	105.49	110.42
1	A	439	LYS	N-CA-C	5.01	116.01	109.64

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4668	0	4573	121	0
1	B	4645	0	4559	121	0
2	A	48	0	8	5	0
2	B	48	0	9	10	0
3	A	7	0	10	2	0
3	B	7	0	10	3	0
4	A	32	0	44	3	0
4	B	16	0	22	0	0
5	A	10	0	14	1	0
5	B	10	0	14	2	0
6	A	4	0	0	0	0
6	B	3	0	0	0	0
7	A	82	0	0	6	0
7	B	63	0	0	9	0
All	All	9643	0	9263	243	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 13.

All (243) 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:340:TYR:HA	1:A:445:MET:HE3	1.48	0.96
1:A:463:HIS:HE1	1:A:469:SER:H	1.15	0.93
1:B:432:VAL:HG22	1:B:451:TYR:CD2	2.16	0.80
1:B:11:PHE:HE2	1:B:47:THR:HG23	1.47	0.79
1:B:71:GLY:HA3	7:B:704:HOH:O	1.86	0.74
1:B:432:VAL:HG22	1:B:451:TYR:HD2	1.54	0.73
1:B:223:PRO:O	1:B:335:ARG:NH1	2.23	0.72
1:A:280:LYS:HD3	1:A:284:GLU:OE1	1.90	0.71
1:B:25:ILE:HD11	1:B:138:LEU:HD22	1.74	0.70
1:B:273:LYS:NZ	7:B:757:HOH:O	2.25	0.69
1:B:319:GLN:NE2	7:B:721:HOH:O	2.26	0.69
1:A:498:PRO:HG3	1:A:536:PRO:HG2	1.77	0.67
1:A:412:ARG:NH2	1:A:538:ALA:O	2.28	0.66
1:B:463:HIS:HE1	1:B:469:SER:H	1.42	0.66
1:A:23:VAL:HG12	1:A:43:VAL:HG22	1.77	0.65
1:B:451:TYR:O	1:B:455:ILE:HG12	1.97	0.64
1:A:575:VAL:O	1:A:579:GLN:HG3	1.97	0.64
1:B:185:ARG:HD2	7:B:751:HOH:O	1.96	0.64
1:A:470:GLU:OE1	1:A:470:GLU:N	2.31	0.64
1:A:93:LYS:HD3	1:A:97:GLU:HB3	1.81	0.63
1:A:515:LEU:O	1:A:520:LYS:NZ	2.31	0.63
1:A:115:LEU:HD22	3:A:605:PEG:H42	1.81	0.63
1:A:481:VAL:HG12	4:A:607:1PE:H232	1.82	0.62
1:A:570:GLU:HA	1:A:573:LYS:HD2	1.80	0.62
1:A:25:ILE:HD11	1:A:138:LEU:HD22	1.82	0.62
1:A:280:LYS:NZ	1:A:288:CYS:SG	2.74	0.60
1:A:463:HIS:CE1	1:A:469:SER:H	2.07	0.60
1:B:115:LEU:HD22	3:B:605:PEG:H31	1.84	0.60
1:B:139:TYR:CE1	1:B:143:ARG:HD2	2.36	0.60
1:B:429:LEU:O	1:B:432:VAL:HG23	2.02	0.60
1:A:171:GLU:CD	1:A:171:GLU:H	2.10	0.59
1:B:451:TYR:CZ	1:B:455:ILE:HD11	2.37	0.59
1:A:20:LYS:NZ	1:A:44:ASN:OD1	2.32	0.58
1:B:305:THR:HA	1:B:373:PHE:CE2	2.38	0.58
1:A:63:GLU:OE1	1:A:63:GLU:N	2.27	0.58
1:B:11:PHE:CE2	1:B:47:THR:HG23	2.36	0.57
1:A:466:THR:O	1:A:466:THR:OG1	2.13	0.57
1:B:456:LEU:HD13	1:B:487:PHE:CD2	2.40	0.57
1:B:313:ASP:N	1:B:313:ASP:OD1	2.38	0.57
1:A:43:VAL:O	1:A:47:THR:OG1	2.20	0.56
1:B:373:PHE:O	1:B:377:LYS:HD3	2.04	0.56
1:B:502:ASP:HB3	1:B:505:LEU:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:560:ALA:HA	7:B:763:HOH:O	2.05	0.56
1:A:501:PHE:HB2	1:A:534:HIS:CE1	2.40	0.56
1:A:217:ARG:NH1	7:A:703:HOH:O	2.36	0.56
1:A:479:SER:OG	1:A:482:ASN:HB2	2.05	0.56
1:B:463:HIS:CE1	1:B:469:SER:H	2.22	0.56
1:B:539:THR:HG23	1:B:541:GLU:CD	2.31	0.56
1:A:387:ILE:HG12	2:A:602:DIU:H4	1.87	0.55
1:A:539:THR:HG23	1:A:542:GLN:OE1	2.06	0.55
1:A:506:PHE:HB3	5:A:608:PGE:H2	1.89	0.55
1:B:151:PRO:HB2	1:B:256:ARG:NH1	2.22	0.55
1:A:221:LYS:O	1:A:223:PRO:HD3	2.06	0.55
1:B:29:GLN:HG2	1:B:146:PRO:HA	1.88	0.55
1:A:444:ARG:O	1:A:448:THR:HG23	2.07	0.54
1:B:223:PRO:HD2	1:B:295:ASP:HB3	1.88	0.54
1:B:366:HIS:HA	1:B:369:TYR:CE1	2.43	0.54
1:B:463:HIS:CE1	1:B:468:VAL:H	2.26	0.54
1:A:194:ARG:HA	1:A:454:LEU:HD21	1.88	0.54
1:B:23:VAL:HG12	1:B:43:VAL:HG22	1.89	0.54
1:A:120:ASN:OD1	1:A:121:THR:N	2.40	0.54
1:B:115:LEU:CB	2:B:603:DIU:H6	2.38	0.53
1:A:9:HIS:NE2	1:A:13:ASP:OD2	2.41	0.53
1:A:123:CYS:SG	1:A:173:LYS:HD2	2.48	0.53
1:A:406:LEU:HD13	1:A:429:LEU:CB	2.38	0.53
1:A:542:GLN:O	1:A:546:VAL:HG23	2.08	0.53
1:A:318:TYR:HE1	1:A:326:LEU:HD22	1.74	0.53
1:B:120:ASN:OD1	1:B:121:THR:N	2.42	0.53
1:B:171:GLU:N	1:B:171:GLU:OE1	2.42	0.53
1:B:299:GLU:H	1:B:299:GLU:CD	2.14	0.53
1:B:223:PRO:HB3	1:B:335:ARG:HB2	1.91	0.53
1:B:318:TYR:O	1:B:322:LYS:HG3	2.08	0.52
1:A:67:HIS:HE1	7:A:763:HOH:O	1.91	0.52
1:A:198:ARG:NH2	2:A:604:DIU:O2	2.43	0.52
1:A:443:GLU:O	1:A:446:PRO:HD2	2.10	0.52
1:A:264:CYS:SG	1:A:285:LYS:HD3	2.50	0.52
1:B:16:GLU:O	1:B:20:LYS:HG3	2.10	0.52
1:A:80:LEU:HD11	1:A:87:MET:HE3	1.92	0.51
1:A:479:SER:HA	7:A:779:HOH:O	2.10	0.51
1:B:39:HIS:O	1:B:43:VAL:HG23	2.10	0.51
1:B:341:ALA:O	1:B:344:VAL:HG12	2.10	0.51
1:A:221:LYS:C	1:A:223:PRO:HD3	2.35	0.51
1:B:261:LYS:NZ	1:B:265:ASP:OD1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:SER:O	1:A:347:ARG:HG3	2.10	0.51
1:A:406:LEU:HD13	1:A:429:LEU:HB3	1.91	0.50
1:A:258:ASP:HB3	7:A:771:HOH:O	2.11	0.50
1:B:67:HIS:HD2	7:B:759:HOH:O	1.95	0.50
1:A:331:TYR:HD2	1:A:332:GLU:HG2	1.76	0.50
1:A:463:HIS:CE1	1:A:468:VAL:H	2.29	0.50
1:A:242:LYS:HG2	1:A:246:HIS:CE1	2.47	0.50
1:B:185:ARG:HG3	2:B:603:DIU:C2	2.42	0.50
1:A:415:PRO:O	1:A:533:LYS:HE2	2.12	0.50
1:A:115:LEU:HD12	2:A:603:DIU:O2	2.12	0.49
1:A:550:PHE:O	1:A:554:VAL:HG23	2.12	0.49
1:A:313:ASP:O	1:A:314:VAL:C	2.55	0.49
1:A:34:CYS:HB2	1:A:39:HIS:CE1	2.46	0.49
1:B:412:ARG:NH2	1:B:538:ALA:O	2.46	0.49
1:B:97:GLU:OE1	1:B:97:GLU:N	2.46	0.49
1:B:227:PHE:HB2	1:B:331:TYR:CE2	2.48	0.49
1:A:541:GLU:CD	1:A:541:GLU:N	2.71	0.49
1:A:366:HIS:HA	1:A:369:TYR:CE2	2.48	0.48
1:A:474:LYS:HB2	1:A:474:LYS:HE3	1.55	0.48
1:B:432:VAL:HG22	1:B:451:TYR:CE2	2.48	0.48
1:A:323:ASP:OD1	1:A:323:ASP:N	2.40	0.48
1:B:454:LEU:CD1	2:B:604:DIU:I1	3.31	0.48
1:B:136:LYS:HB3	3:B:605:PEG:H12	1.96	0.48
1:B:260:ALA:HB2	2:B:601:DIU:I2	2.83	0.48
1:B:309:ALA:HB2	1:B:373:PHE:HE2	1.77	0.48
1:A:322:LYS:O	1:A:326:LEU:HB2	2.14	0.48
1:B:103:LEU:HD23	1:B:103:LEU:HA	1.57	0.48
1:B:541:GLU:CD	1:B:542:GLN:H	2.15	0.48
1:B:90:CYS:O	1:B:98:ARG:HG3	2.14	0.47
1:B:125:GLU:OE2	1:B:136:LYS:NZ	2.31	0.47
1:B:427:ARG:O	1:B:430:GLY:N	2.47	0.47
1:A:422:LEU:HD13	1:A:422:LEU:HA	1.76	0.47
1:B:184:MET:HB3	2:B:603:DIU:I1	2.83	0.47
1:A:436:CYS:O	1:A:439:LYS:HB2	2.15	0.47
1:B:67:HIS:CD2	7:B:759:HOH:O	2.66	0.47
1:B:131:LYS:HA	1:B:131:LYS:HD3	1.67	0.47
1:A:204:LYS:HB2	1:A:205:PHE:CD2	2.49	0.47
1:B:36:PHE:O	1:B:40:VAL:HG23	2.15	0.47
1:A:557:CYS:O	1:A:563:LYS:HB3	2.15	0.47
1:A:576:VAL:HG11	4:A:606:1PE:H131	1.97	0.47
1:A:429:LEU:O	1:A:432:VAL:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:LYS:HE3	1:B:262:TYR:CE1	2.49	0.47
1:A:169:GLN:OE1	1:A:169:GLN:HA	2.15	0.46
1:A:232:LYS:NZ	1:A:236:ASP:OD2	2.47	0.46
1:B:506:PHE:CD1	5:B:607:PGE:H12	2.50	0.46
1:B:116:LYS:HA	1:B:116:LYS:HD3	1.70	0.46
1:B:355:THR:HG21	1:B:372:VAL:HG23	1.97	0.46
1:B:458:ARG:CZ	1:B:462:LEU:HD21	2.46	0.46
1:B:326:LEU:O	1:B:329:PHE:HB3	2.16	0.46
1:B:63:GLU:OE1	1:B:63:GLU:N	2.37	0.46
1:A:451:TYR:O	1:A:454:LEU:HB2	2.15	0.46
1:B:429:LEU:HD23	1:B:429:LEU:HA	1.71	0.46
1:A:443:GLU:C	1:A:446:PRO:HD2	2.41	0.46
1:A:502:ASP:OD1	1:A:504:LYS:HG3	2.15	0.46
1:A:448:THR:O	1:A:452:LEU:HG	2.16	0.46
1:B:98:ARG:NH1	7:B:705:HOH:O	2.49	0.46
1:B:27:PHE:HE1	1:B:74:LEU:HD23	1.81	0.46
1:A:479:SER:OG	1:A:479:SER:O	2.32	0.45
1:B:115:LEU:HB3	2:B:603:DIU:H6	1.98	0.45
1:B:454:LEU:HD11	2:B:604:DIU:I1	2.87	0.45
1:B:139:TYR:CZ	1:B:143:ARG:HD2	2.51	0.45
1:B:221:LYS:C	1:B:223:PRO:HD3	2.42	0.45
1:A:301:LEU:HD23	1:A:301:LEU:HA	1.78	0.45
1:B:322:LYS:O	1:B:326:LEU:HD13	2.15	0.45
1:A:439:LYS:HD3	1:A:440:PRO:HD2	1.98	0.45
1:A:458:ARG:NE	1:A:462:LEU:HD11	2.31	0.45
1:B:294:LYS:HD2	1:B:338:PRO:HB2	1.98	0.45
1:B:310:GLU:HA	1:B:366:HIS:HE1	1.81	0.45
1:A:400:TYR:OH	1:A:524:LYS:NZ	2.36	0.45
1:A:541:GLU:CD	1:A:541:GLU:H	2.24	0.45
1:B:387:ILE:HG12	2:B:602:DIU:I2	2.86	0.45
1:A:400:TYR:CE2	1:A:521:GLN:HG2	2.51	0.44
1:A:540:GLU:H	1:A:540:GLU:HG3	1.53	0.44
1:B:422:LEU:HD23	1:B:422:LEU:HA	1.72	0.44
1:B:439:LYS:NZ	1:B:443:GLU:CD	2.75	0.44
1:B:194:ARG:O	1:B:197:LEU:HB3	2.18	0.44
1:B:204:LYS:HA	1:B:204:LYS:HD3	1.82	0.44
1:A:197:LEU:HD12	1:A:197:LEU:O	2.17	0.44
1:B:330:LEU:HD13	1:B:349:ALA:HB2	2.00	0.44
1:B:550:PHE:CD1	5:B:607:PGE:H42	2.53	0.44
1:A:408:VAL:HG22	1:A:532:LEU:HD11	1.99	0.44
1:A:9:HIS:CD2	1:A:13:ASP:OD2	2.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ALA:CB	1:A:454:LEU:HD22	2.48	0.43
1:A:359:CYS:HB3	1:A:368:CYS:HB3	1.92	0.43
1:B:81:ARG:NH2	1:B:89:ASP:OD1	2.50	0.43
1:A:366:HIS:HD2	1:A:369:TYR:CE1	2.36	0.43
1:B:510:ALA:HA	1:B:567:PHE:CE2	2.53	0.43
1:B:541:GLU:OE1	1:B:542:GLN:N	2.26	0.43
1:B:9:HIS:C	1:B:9:HIS:CD2	2.95	0.43
1:A:90:CYS:O	1:A:98:ARG:HG3	2.18	0.43
1:A:93:LYS:HE2	7:A:759:HOH:O	2.19	0.43
1:A:443:GLU:HG2	1:A:447:CYS:HB2	2.01	0.43
1:A:544:LYS:O	1:A:548:GLU:HG3	2.18	0.43
1:B:448:THR:O	1:B:452:LEU:HG	2.18	0.43
1:A:10:ARG:NH1	1:A:254:ASP:OD2	2.51	0.43
1:A:348:LEU:HA	1:A:348:LEU:HD23	1.67	0.43
1:A:473:THR:O	1:A:477:THR:HG23	2.19	0.43
1:B:308:PHE:CZ	1:B:329:PHE:HA	2.54	0.43
1:B:429:LEU:HG	1:B:455:ILE:HG21	2.00	0.43
1:B:118:ASP:HB3	1:B:121:THR:OG1	2.18	0.43
1:B:451:TYR:CE2	1:B:455:ILE:HD11	2.53	0.43
1:A:549:ASN:N	1:A:549:ASN:HD22	2.17	0.43
1:A:573:LYS:HG2	4:A:606:1PE:H222	2.01	0.43
1:B:343:SER:O	1:B:347:ARG:HG3	2.18	0.43
1:A:20:LYS:HD3	1:A:47:THR:HG21	2.00	0.43
2:B:603:DIU:I2	3:B:605:PEG:H32	2.89	0.43
1:A:407:ILE:HG23	1:A:529:VAL:HG22	2.01	0.42
1:A:570:GLU:O	1:A:573:LYS:HB2	2.18	0.42
1:B:150:ALA:HB3	1:B:151:PRO:HD3	2.00	0.42
1:A:29:GLN:HG2	1:A:146:PRO:HA	2.01	0.42
1:A:112:LEU:HA	1:A:113:PRO:HD2	1.75	0.42
1:A:116:LYS:HA	1:A:117:PRO:HD2	1.92	0.42
1:B:345:LEU:HD23	1:B:345:LEU:HA	1.86	0.42
1:B:466:THR:O	1:B:466:THR:OG1	2.29	0.42
1:B:149:TYR:HE2	2:B:601:DIU:O1	2.02	0.42
1:B:515:LEU:O	1:B:520:LYS:NZ	2.52	0.42
1:A:103:LEU:HD23	1:A:103:LEU:HA	1.48	0.42
1:B:167:CYS:HB3	1:B:177:LEU:HG	2.01	0.42
1:B:435:ARG:O	1:B:439:LYS:HD2	2.18	0.42
1:A:334:SER:OG	1:A:345:LEU:HD13	2.19	0.42
1:A:400:TYR:CD1	1:A:400:TYR:C	2.97	0.42
1:B:400:TYR:CE1	1:B:521:GLN:HG2	2.54	0.42
1:A:181:ILE:HD13	1:A:181:ILE:HG21	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ALA:HB2	1:A:446:PRO:HA	2.02	0.42
1:B:277:CYS:HA	1:B:280:LYS:HZ3	1.84	0.42
1:A:313:ASP:O	1:A:316:LYS:N	2.53	0.42
1:B:348:LEU:HD23	1:B:348:LEU:HA	1.84	0.42
1:A:410:TYR:HA	1:A:413:LYS:HB2	2.02	0.42
1:A:12:LYS:HE3	1:A:54:VAL:HG13	2.02	0.42
1:A:396:LYS:HA	7:A:718:HOH:O	2.20	0.42
1:B:112:LEU:HA	1:B:113:PRO:HD2	1.88	0.42
1:B:256:ARG:HD3	7:B:718:HOH:O	2.20	0.42
1:B:408:VAL:O	1:B:412:ARG:HG3	2.20	0.42
1:B:419:THR:HB	1:B:420:PRO:HD3	2.01	0.42
1:B:439:LYS:HZ1	1:B:443:GLU:CD	2.27	0.42
1:B:452:LEU:HD13	1:B:484:ARG:HG3	2.02	0.41
1:A:115:LEU:HD22	3:A:605:PEG:C4	2.50	0.41
1:B:24:LEU:HA	1:B:24:LEU:HD12	1.78	0.41
1:B:196:ARG:HD2	1:B:196:ARG:HA	1.76	0.41
1:B:318:TYR:CE1	1:B:322:LYS:HG2	2.54	0.41
1:B:340:TYR:HA	1:B:445:MET:HE3	2.02	0.41
1:A:204:LYS:HB2	1:A:205:PHE:CE2	2.56	0.41
1:A:312:LYS:HA	1:A:312:LYS:HD2	1.44	0.41
1:B:375:LYS:O	1:B:378:HIS:ND1	2.48	0.41
1:B:575:VAL:O	1:B:579:GLN:HG3	2.20	0.41
1:A:133:PHE:HA	1:A:136:LYS:HE2	2.02	0.41
1:A:409:ARG:NH2	2:A:602:DIU:O1	2.53	0.41
1:A:260:ALA:HB2	2:A:601:DIU:I2	2.91	0.41
1:A:211:LYS:O	1:A:215:VAL:HG23	2.20	0.41
1:A:232:LYS:HE3	1:A:262:TYR:CE1	2.56	0.41
1:A:193:ALA:HB1	1:A:454:LEU:HD22	2.02	0.41
1:A:470:GLU:CD	1:A:471:LYS:N	2.79	0.41
1:B:121:THR:O	1:B:125:GLU:HG3	2.21	0.41
1:B:380:VAL:O	1:B:383:PRO:HD2	2.21	0.41
1:B:576:VAL:O	1:B:577:SER:C	2.62	0.41
1:A:171:GLU:CD	1:A:172:ASP:H	2.28	0.41
1:B:436:CYS:HA	1:B:439:LYS:HD2	2.02	0.40
1:B:46:LEU:HD12	1:B:46:LEU:HA	1.92	0.40
1:B:408:VAL:HA	1:B:532:LEU:CD2	2.51	0.40
1:A:171:GLU:CD	1:A:171:GLU:N	2.78	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	583/583 (100%)	570 (98%)	13 (2%)	0	100	100
1	B	535/583 (92%)	521 (97%)	14 (3%)	0	100	100
All	All	1118/1166 (96%)	1091 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	523/521 (100%)	495 (95%)	28 (5%)	20	35
1	B	520/521 (100%)	485 (93%)	35 (7%)	15	25
All	All	1043/1042 (100%)	980 (94%)	63 (6%)	17	30

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	LEU
1	A	101	CYS
1	A	143	ARG
1	A	159	LYS
1	A	171	GLU
1	A	177	LEU
1	A	218	LEU
1	A	224	LYS

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Mol	Chain	Res	Type
1	A	282	LEU
1	A	284	GLU
1	A	305	THR
1	A	312	LYS
1	A	319	GLN
1	A	326	LEU
1	A	363	ASP
1	A	377	LYS
1	A	386	LEU
1	A	389	GLN
1	A	416	GLN
1	A	422	LEU
1	A	438	THR
1	A	471	LYS
1	A	474	LYS
1	A	511	ASP
1	A	523	LYS
1	A	540	GLU
1	A	541	GLU
1	A	577	SER
1	B	4	LYS
1	B	20	LYS
1	B	114	LYS
1	B	127	LYS
1	B	141	ILE
1	B	143	ARG
1	B	159	LYS
1	B	201	SER
1	B	230	VAL
1	B	244	CYS
1	B	261	LYS
1	B	280	LYS
1	B	294	LYS
1	B	299	GLU
1	B	300	ASN
1	B	313	ASP
1	B	344	VAL
1	B	350	LYS
1	B	355	THR
1	B	369	TYR
1	B	371	THR
1	B	377	LYS

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Mol	Chain	Res	Type
1	B	389	GLN
1	B	438	THR
1	B	442	SER
1	B	454	LEU
1	B	461	VAL
1	B	465	LYS
1	B	479	SER
1	B	518	THR
1	B	539	THR
1	B	541	GLU
1	B	555	ASP
1	B	561	ASP
1	B	563	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	161	ASN
1	A	246	HIS
1	A	319	GLN
1	A	366	HIS
1	A	378	HIS
1	A	384	GLN
1	A	463	HIS
1	A	549	ASN
1	B	161	ASN
1	B	241	HIS
1	B	366	HIS
1	B	384	GLN
1	B	393	GLN
1	B	463	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 7 are monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DIU	A	601	-	12,12,12	2.12	4 (33%)	17,17,17	1.30	2 (11%)
2	DIU	B	601	-	12,12,12	2.30	5 (41%)	17,17,17	1.09	1 (5%)
2	DIU	A	604	-	12,12,12	2.95	6 (50%)	17,17,17	0.90	0
2	DIU	B	604	-	12,12,12	3.06	7 (58%)	17,17,17	1.02	0
2	DIU	A	602	-	12,12,12	1.89	4 (33%)	17,17,17	0.85	0
3	PEG	B	605	-	6,6,6	0.65	0	5,5,5	0.64	0
4	1PE	A	606	-	15,15,15	0.84	0	14,14,14	1.24	2 (14%)
4	1PE	A	607	-	15,15,15	0.99	0	14,14,14	0.95	0
2	DIU	B	603	-	12,12,12	2.34	5 (41%)	17,17,17	1.14	2 (11%)
2	DIU	A	603	-	12,12,12	2.01	5 (41%)	17,17,17	0.99	1 (5%)
3	PEG	A	605	-	6,6,6	0.72	0	5,5,5	0.95	0
5	PGE	B	607	-	9,9,9	0.68	0	8,8,8	0.33	0
5	PGE	A	608	-	9,9,9	0.61	0	8,8,8	0.79	0
2	DIU	B	602	-	12,12,12	1.46	2 (16%)	17,17,17	0.84	0
4	1PE	B	606	-	15,15,15	0.82	0	14,14,14	0.68	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DIU	A	601	-	-	0/4/4/4	0/1/1/1
2	DIU	B	601	-	-	0/4/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DIU	A	604	-	-	2/4/4/4	0/1/1/1
2	DIU	B	604	-	-	0/4/4/4	0/1/1/1
2	DIU	A	602	-	-	2/4/4/4	0/1/1/1
3	PEG	B	605	-	-	2/4/4/4	-
4	1PE	A	606	-	-	6/13/13/13	-
4	1PE	A	607	-	-	5/13/13/13	-
2	DIU	B	603	-	-	2/4/4/4	0/1/1/1
2	DIU	A	603	-	-	0/4/4/4	0/1/1/1
3	PEG	A	605	-	-	0/4/4/4	-
5	PGE	B	607	-	-	2/7/7/7	-
5	PGE	A	608	-	-	3/7/7/7	-
2	DIU	B	602	-	-	0/4/4/4	0/1/1/1
4	1PE	B	606	-	-	9/13/13/13	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	604	DIU	C1-C2	5.00	1.49	1.41
2	A	604	DIU	C3-I1	4.96	2.20	2.10
2	B	604	DIU	C2-C3	4.92	1.50	1.40
2	B	601	DIU	C2-C3	4.92	1.50	1.40
2	B	604	DIU	C3-I1	4.78	2.20	2.10
2	B	604	DIU	C1-C2	4.54	1.48	1.41
2	A	604	DIU	C2-C3	4.34	1.49	1.40
2	B	604	DIU	C4-C5	4.29	1.47	1.38
2	B	603	DIU	C6-C5	4.27	1.47	1.38
2	A	603	DIU	C6-C5	3.95	1.46	1.38
2	A	601	DIU	C2-C3	3.87	1.48	1.40
2	A	604	DIU	C4-C5	3.87	1.46	1.38
2	A	601	DIU	C1-C2	3.70	1.47	1.41
2	B	603	DIU	C3-I1	-3.69	2.02	2.10
2	B	601	DIU	C1-C2	3.61	1.47	1.41
2	A	601	DIU	O1-C	3.51	1.32	1.22
2	B	602	DIU	C2-C3	3.19	1.46	1.40
2	A	602	DIU	C1-C2	3.16	1.46	1.41
2	B	604	DIU	C5-I2	3.14	2.18	2.10
2	B	603	DIU	C2-C3	3.06	1.46	1.40
2	A	602	DIU	C2-C3	3.01	1.46	1.40
2	B	601	DIU	C5-I2	-2.92	2.02	2.10
2	A	603	DIU	C2-C3	2.91	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	604	DIU	C6-C5	2.79	1.44	1.38
2	A	602	DIU	C6-C5	2.78	1.44	1.38
2	A	603	DIU	C1-C2	2.66	1.45	1.41
2	B	604	DIU	C4-C3	2.60	1.44	1.39
2	B	603	DIU	C1-C2	2.43	1.45	1.41
2	A	603	DIU	C3-I1	-2.40	2.05	2.10
2	B	603	DIU	C1-C	2.38	1.54	1.49
2	B	601	DIU	C6-C5	2.29	1.43	1.38
2	B	602	DIU	C6-C5	2.22	1.43	1.38
2	A	601	DIU	C6-C1	2.22	1.43	1.39
2	A	604	DIU	C5-I2	2.20	2.15	2.10
2	B	601	DIU	O3-C2	-2.12	1.32	1.36
2	A	603	DIU	C1-C	2.11	1.54	1.49
2	B	604	DIU	C6-C5	2.08	1.42	1.38
2	A	602	DIU	C4-C5	2.06	1.42	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	DIU	C3-C4-C5	3.74	122.90	119.42
4	A	606	1PE	OH5-C14-C24	-3.18	95.85	110.35
2	B	603	DIU	C3-C4-C5	2.63	121.87	119.42
2	B	601	DIU	C3-C4-C5	2.35	121.61	119.42
4	A	606	1PE	OH3-C22-C12	2.21	119.83	110.11
2	A	603	DIU	C3-C4-C5	2.17	121.44	119.42
2	A	601	DIU	C2-C3-I1	2.05	122.34	119.35
2	B	603	DIU	C6-C5-I2	2.04	122.26	119.38

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	606	1PE	OH4-C13-C23-OH3
4	B	606	1PE	OH7-C16-C26-OH6
5	B	607	PGE	O2-C3-C4-O3
4	A	606	1PE	OH4-C13-C23-OH3
4	A	606	1PE	OH5-C14-C24-OH4
2	B	603	DIU	O2-C-C1-C2
2	B	603	DIU	O1-C-C1-C2
4	A	606	1PE	OH6-C15-C25-OH5
4	B	606	1PE	C16-C26-OH6-C15
4	A	607	1PE	C12-C22-OH3-C23

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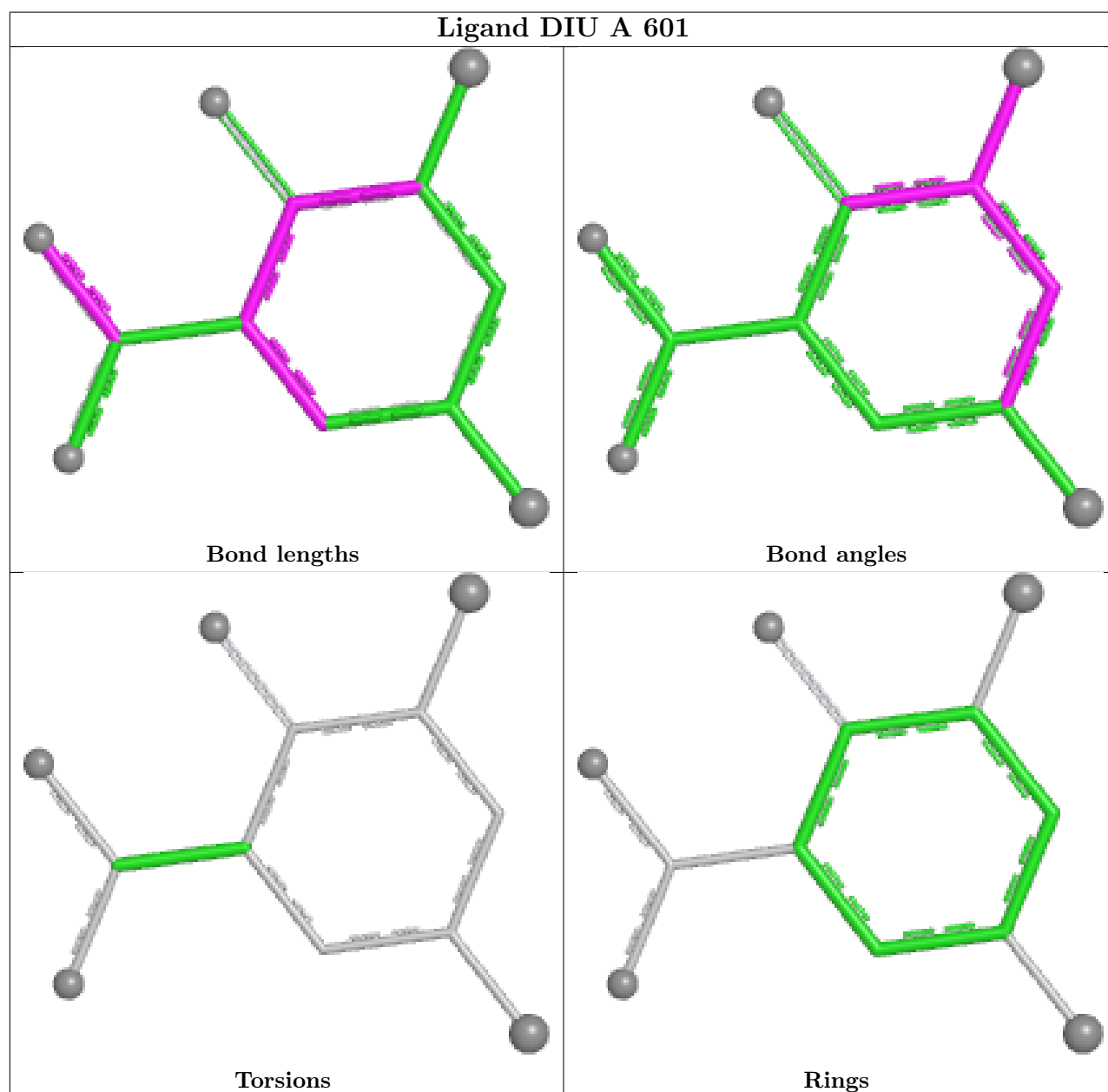
Mol	Chain	Res	Type	Atoms
4	B	606	1PE	C24-C14-OH5-C25
4	B	606	1PE	C15-C25-OH5-C14
4	A	607	1PE	C25-C15-OH6-C26
4	B	606	1PE	C12-C22-OH3-C23
5	A	608	PGE	C3-C4-O3-C5
4	A	606	1PE	OH2-C12-C22-OH3
3	B	605	PEG	C4-C3-O2-C2
5	B	607	PGE	C3-C4-O3-C5
4	B	606	1PE	C25-C15-OH6-C26
4	A	607	1PE	OH4-C13-C23-OH3
2	A	604	DIU	O1-C-C1-C2
4	A	606	1PE	C24-C14-OH5-C25
5	A	608	PGE	C1-C2-O2-C3
2	A	602	DIU	O1-C-C1-C2
2	A	602	DIU	O2-C-C1-C2
4	A	606	1PE	C12-C22-OH3-C23
5	A	608	PGE	O1-C1-C2-O2
3	B	605	PEG	C1-C2-O2-C3
4	B	606	1PE	OH2-C12-C22-OH3
4	A	607	1PE	C13-C23-OH3-C22
2	A	604	DIU	O2-C-C1-C2
4	A	607	1PE	OH5-C14-C24-OH4
4	B	606	1PE	OH6-C15-C25-OH5

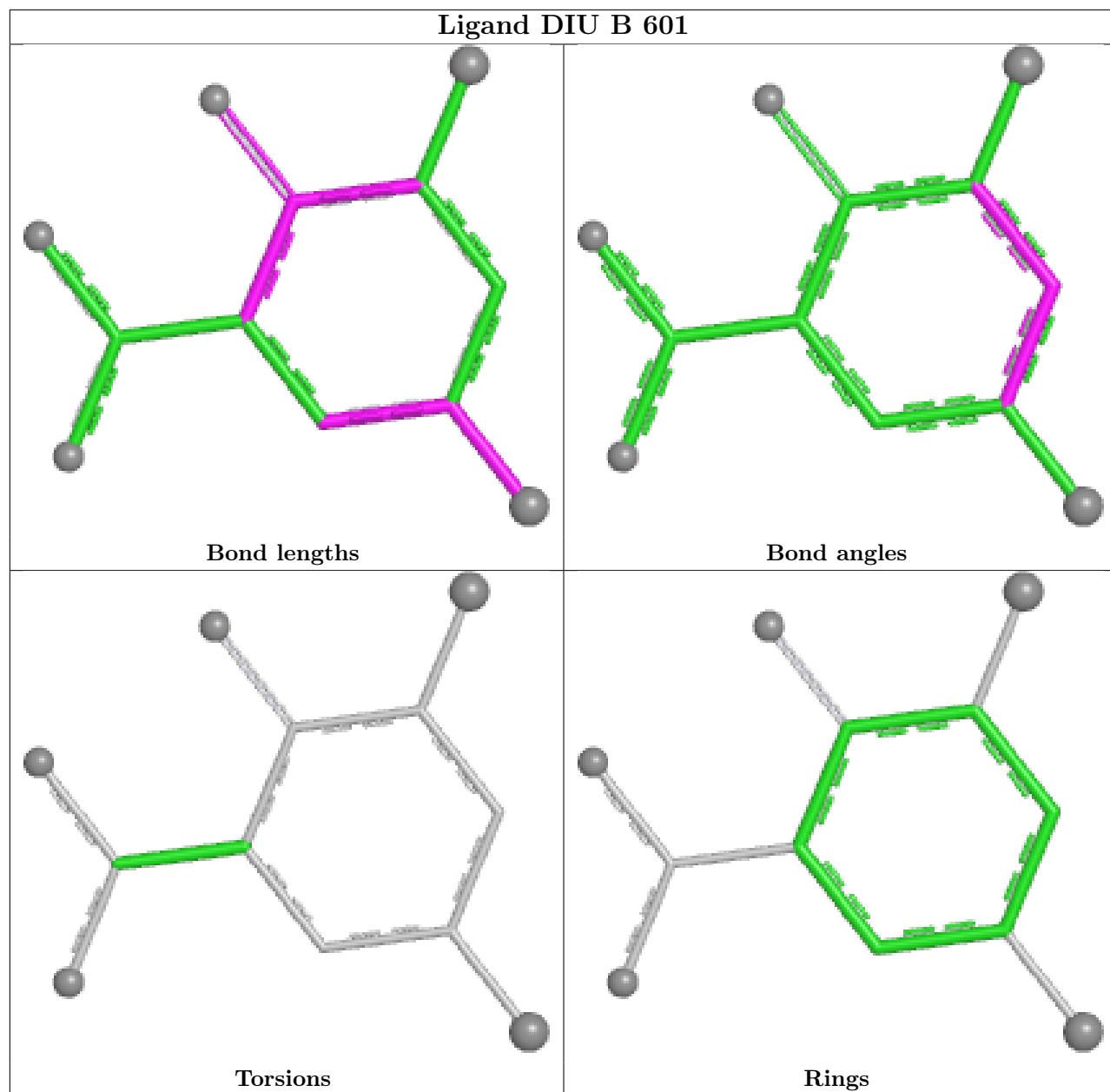
There are no ring outliers.

14 monomers are involved in 25 short contacts:

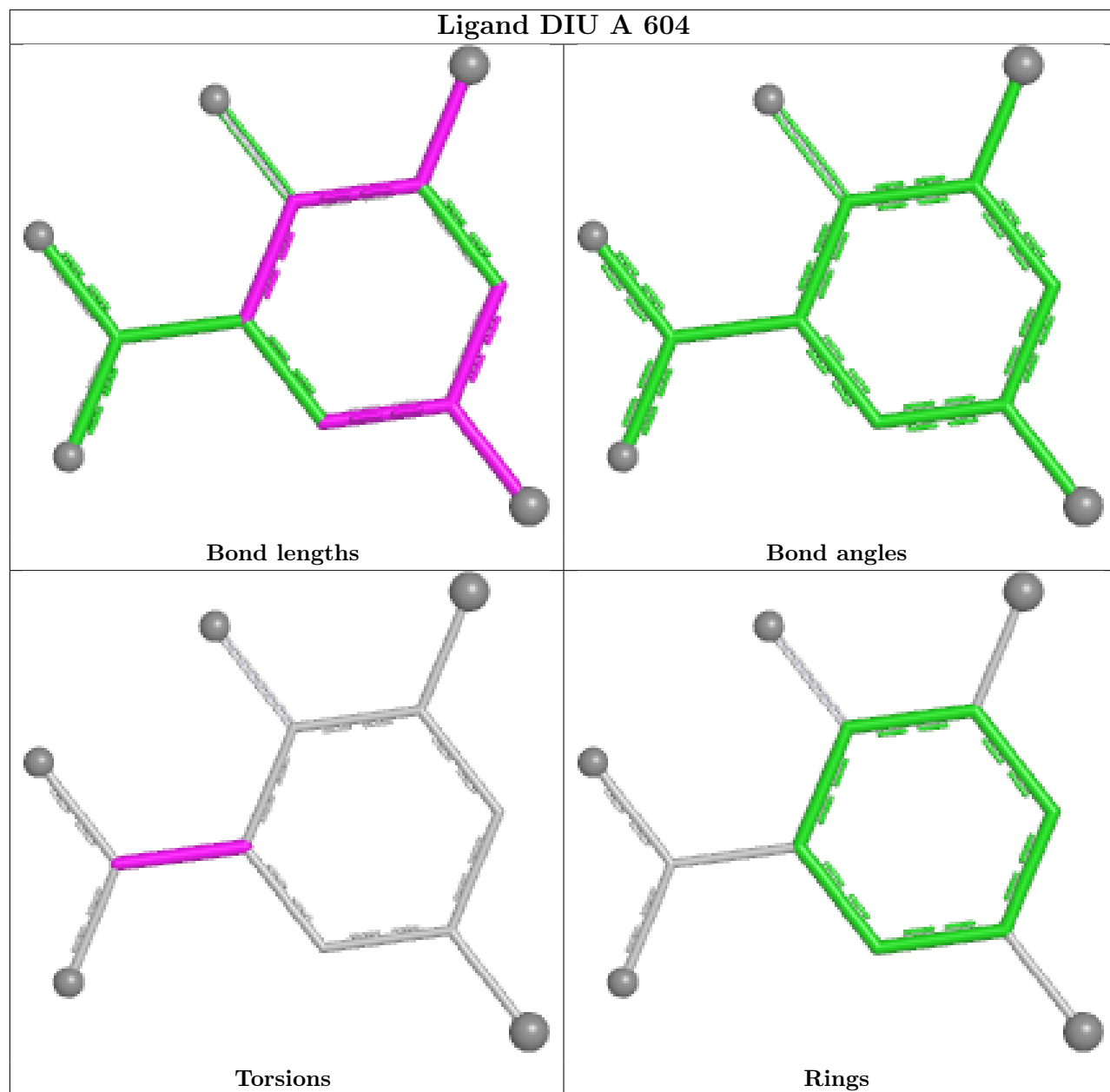
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	DIU	1	0
2	B	601	DIU	2	0
2	A	604	DIU	1	0
2	B	604	DIU	2	0
2	A	602	DIU	2	0
3	B	605	PEG	3	0
4	A	606	1PE	2	0
4	A	607	1PE	1	0
2	B	603	DIU	5	0
2	A	603	DIU	1	0
3	A	605	PEG	2	0
5	B	607	PGE	2	0
5	A	608	PGE	1	0
2	B	602	DIU	1	0

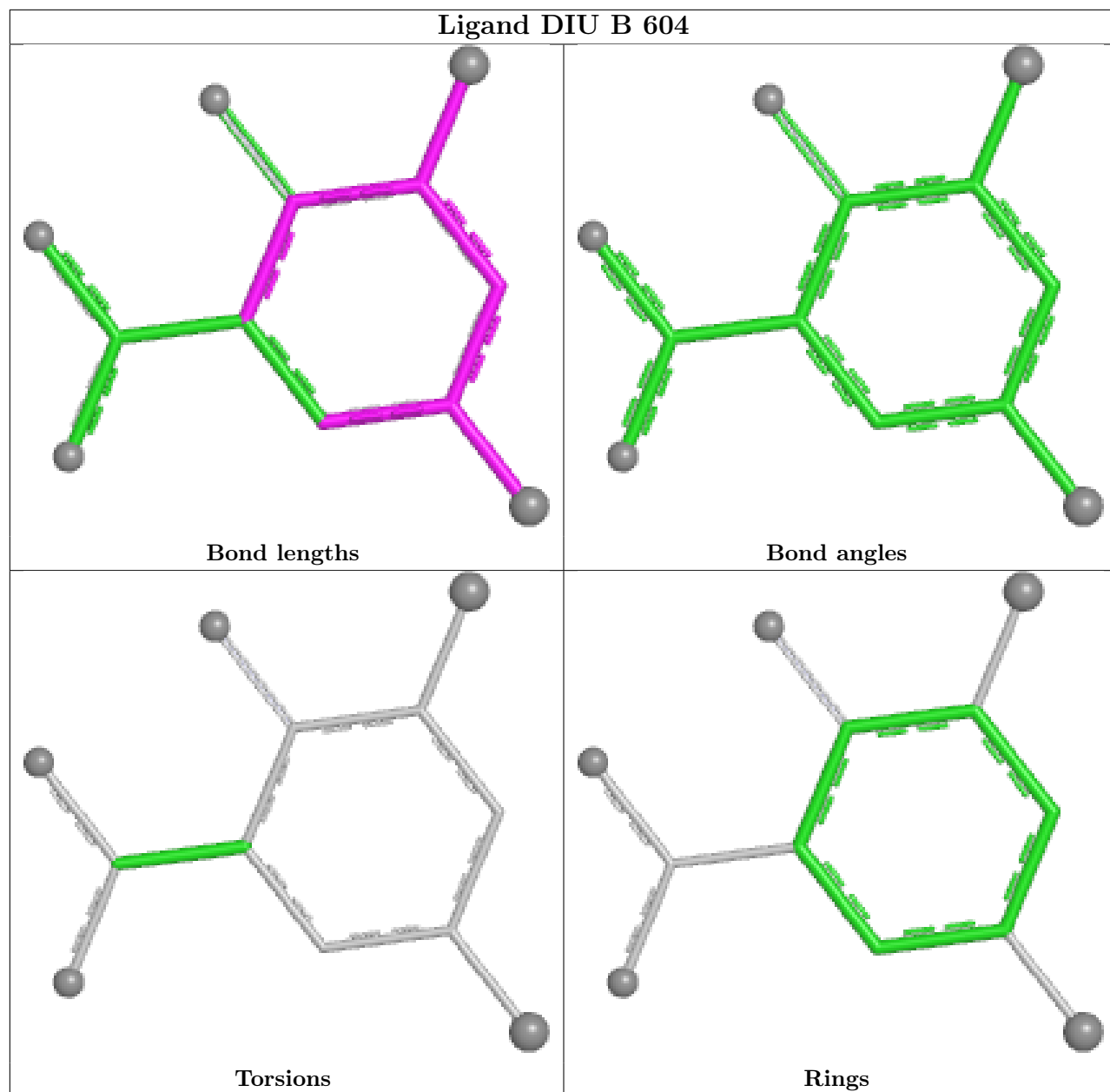
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



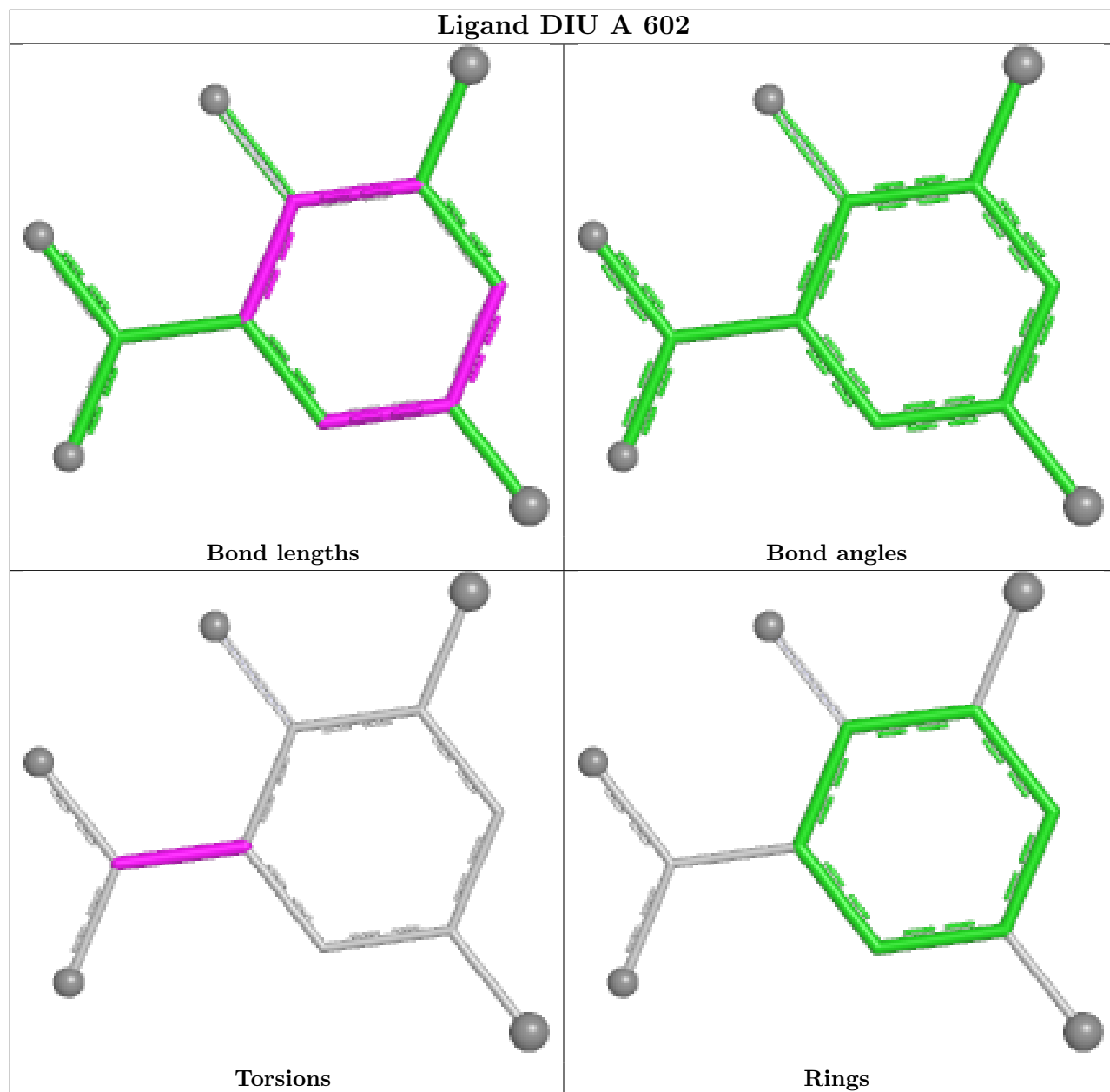


Ligand DIU A 604

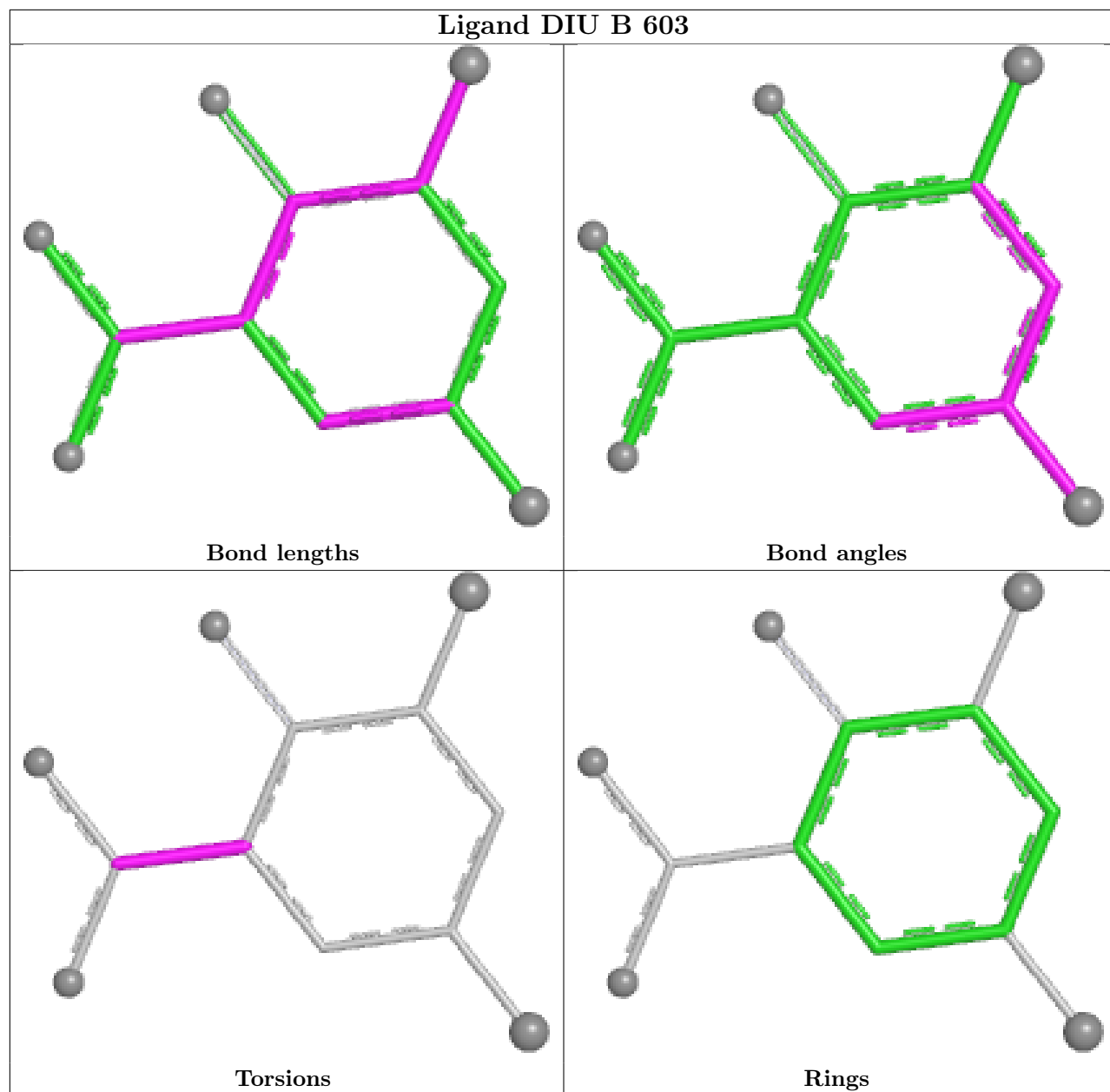




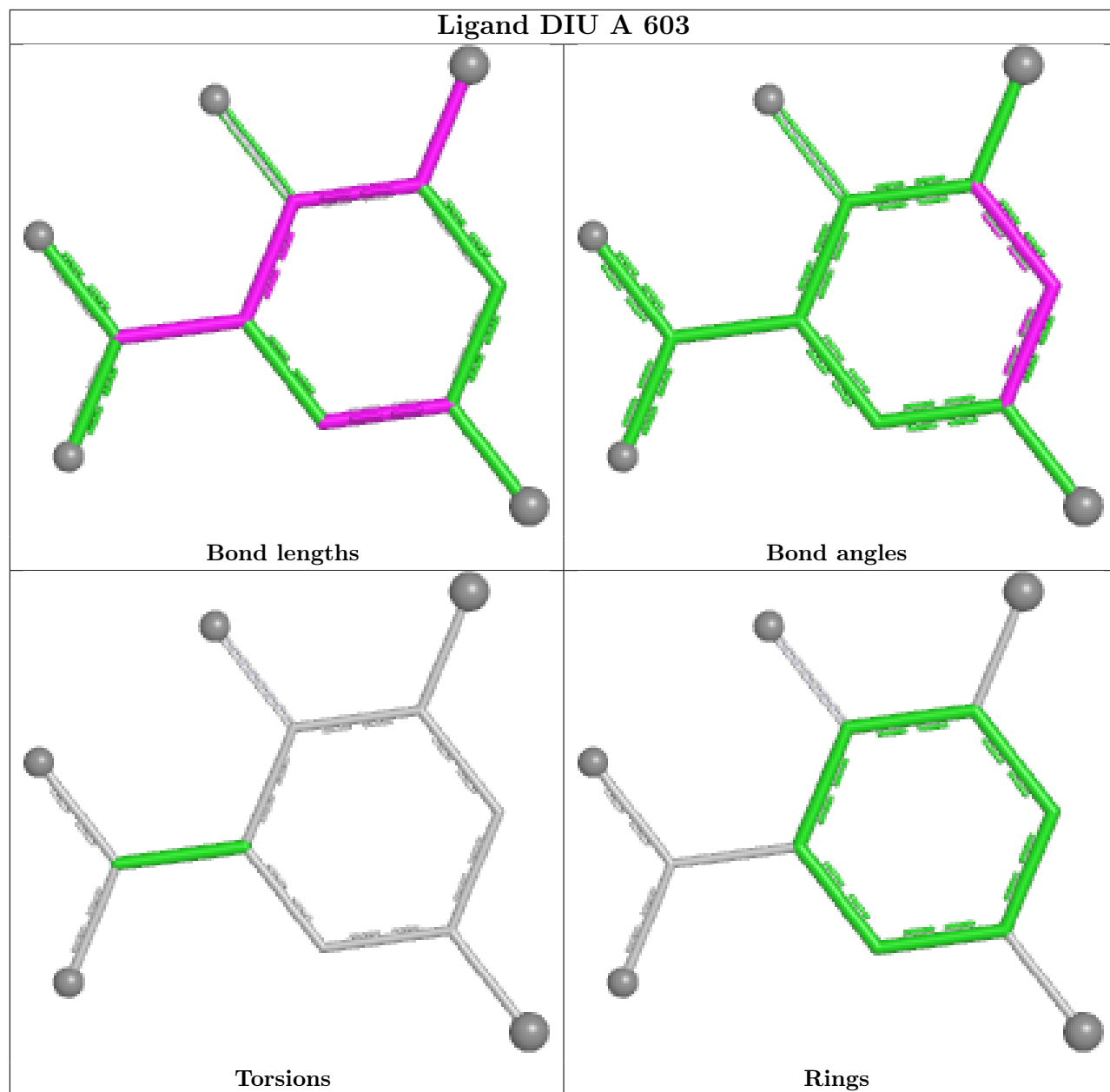
Ligand DIU A 602

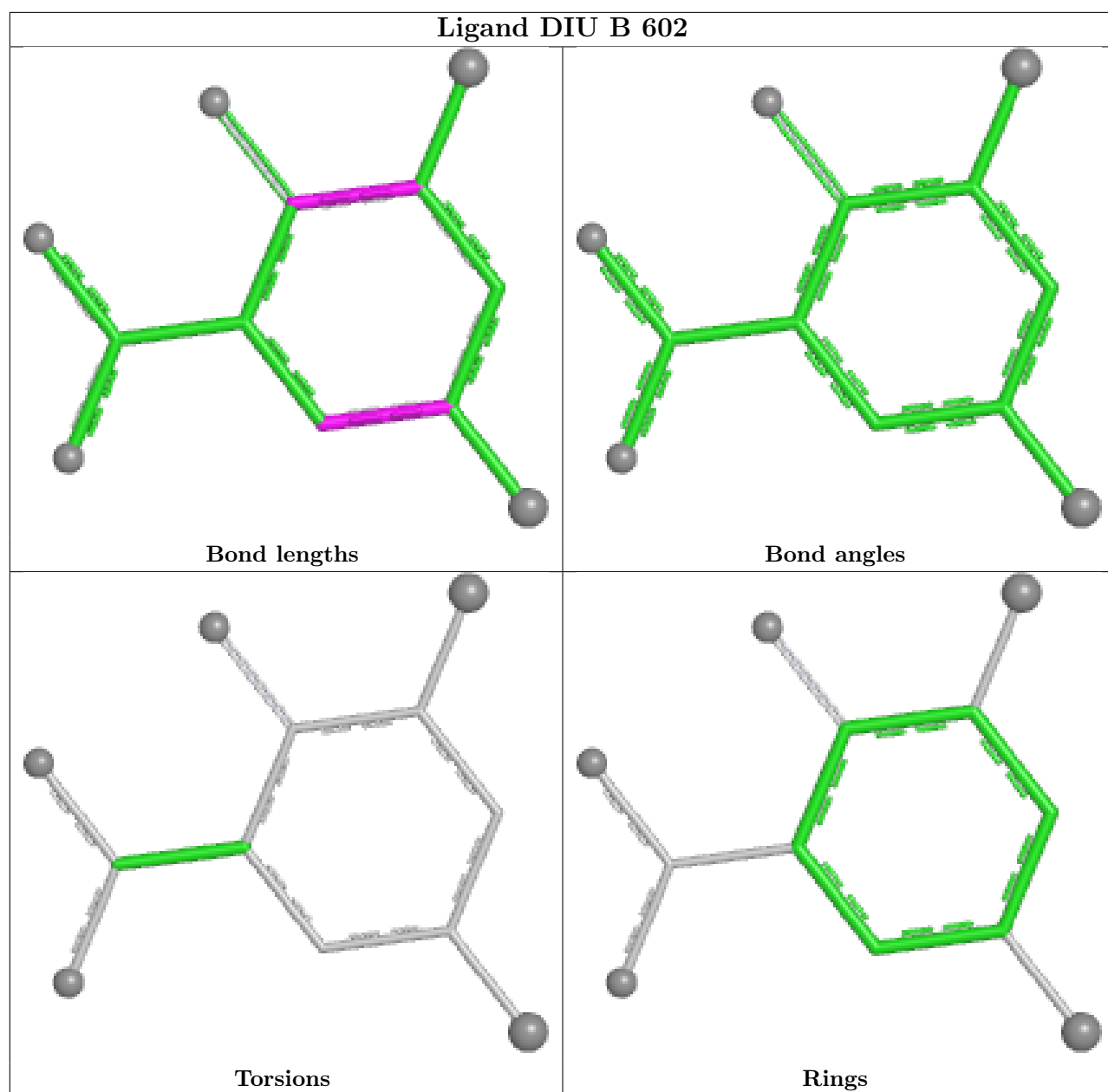


Ligand DIU B 603



Ligand DIU A 603





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	582/583 (99%)	-0.37	0	100 100	14, 40, 71, 101	3 (0%)
1	B	582/583 (99%)	-0.23	1 (0%)	91 90	17, 47, 92, 134	0
All	All	1164/1166 (99%)	-0.30	1 (0%)	92 91	14, 43, 85, 134	3 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	123	CYS	2.4

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	1PE	B	606	16/16	0.80	0.15	52,69,81,81	0
3	PEG	B	605	7/7	0.82	0.14	22,36,58,59	0
2	DIU	B	602	12/12	0.82	0.15	48,50,91,123	12
5	PGE	B	607	10/10	0.84	0.11	62,65,68,69	0

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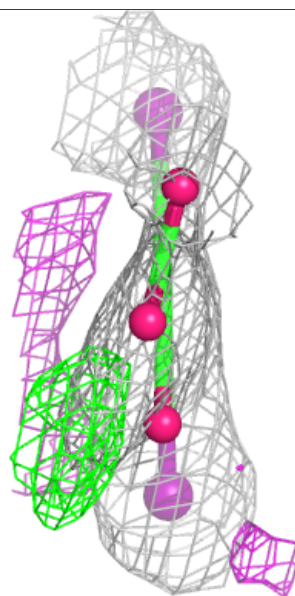
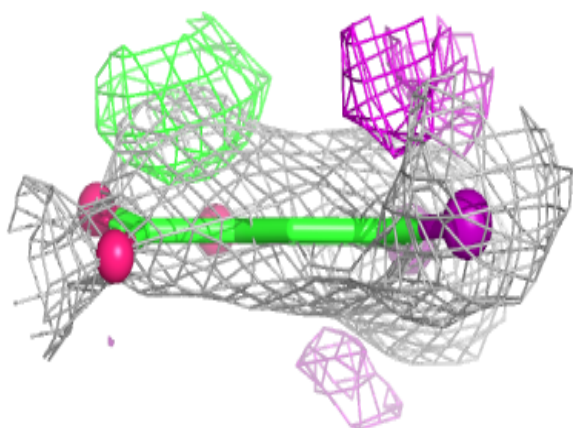
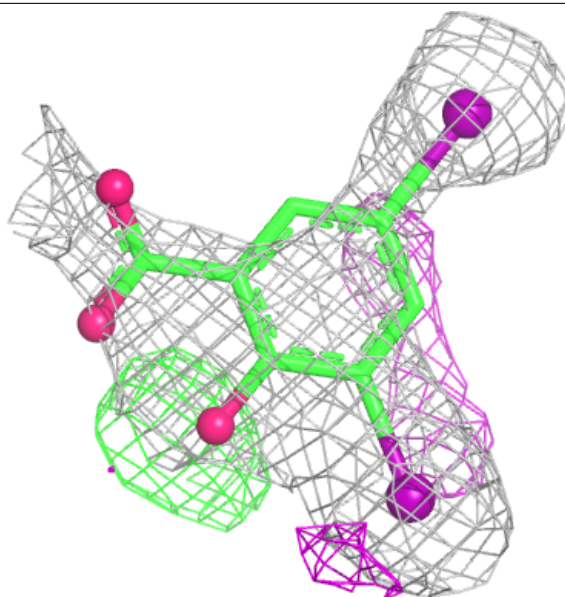
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	1PE	A	607	16/16	0.85	0.12	18,59,66,67	0
6	CA	A	609	1/1	0.88	0.05	62,62,62,62	0
6	CA	A	611	1/1	0.88	0.06	74,74,74,74	0
6	CA	B	610	1/1	0.90	0.07	65,65,65,65	0
4	1PE	A	606	16/16	0.91	0.09	12,31,40,40	0
5	PGE	A	608	10/10	0.91	0.09	40,44,47,49	0
2	DIU	A	602	12/12	0.91	0.10	48,53,96,98	0
3	PEG	A	605	7/7	0.92	0.09	13,26,31,32	0
2	DIU	A	603	12/12	0.93	0.13	61,64,76,120	0
2	DIU	B	603	12/12	0.94	0.10	57,61,78,126	0
6	CA	A	612	1/1	0.95	0.04	48,48,48,48	0
6	CA	B	609	1/1	0.95	0.03	60,60,60,60	0
6	CA	A	610	1/1	0.95	0.04	47,47,47,47	0
2	DIU	B	601	12/12	0.97	0.08	31,38,48,112	0
6	CA	B	608	1/1	0.97	0.08	70,70,70,70	0
2	DIU	B	604	12/12	0.97	0.10	60,94,96,101	0
2	DIU	A	601	12/12	0.97	0.08	25,36,44,116	0
2	DIU	A	604	12/12	0.99	0.07	49,52,62,76	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

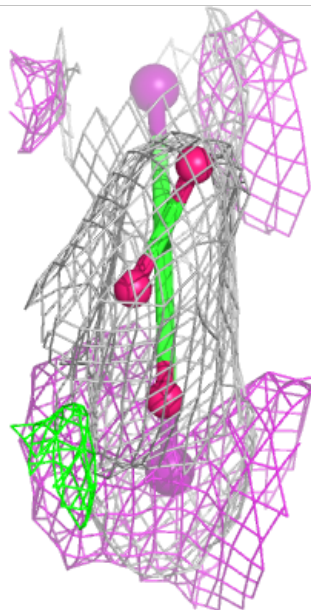
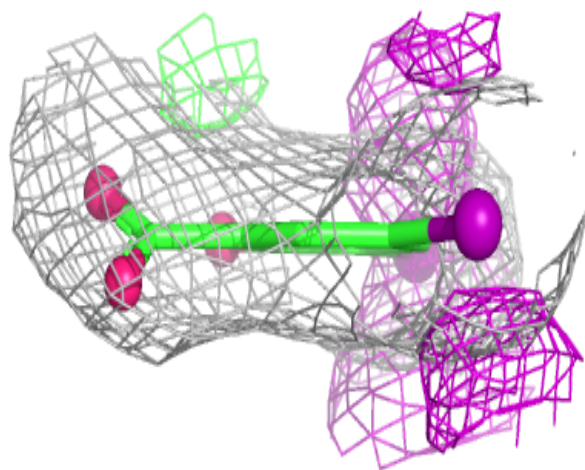
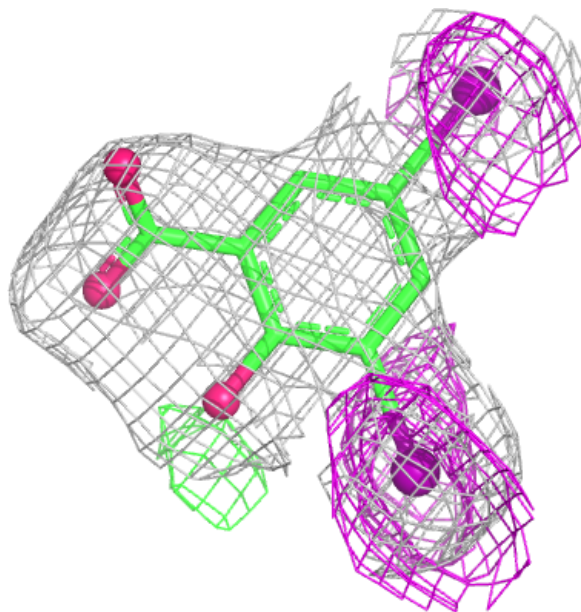
Electron density around DIU B 602:

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



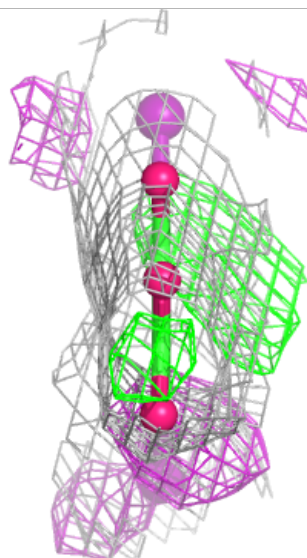
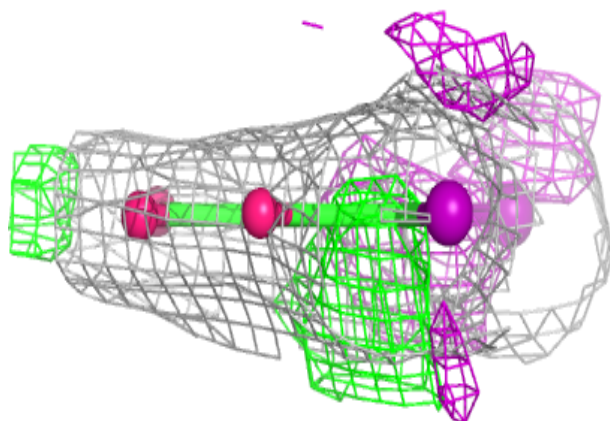
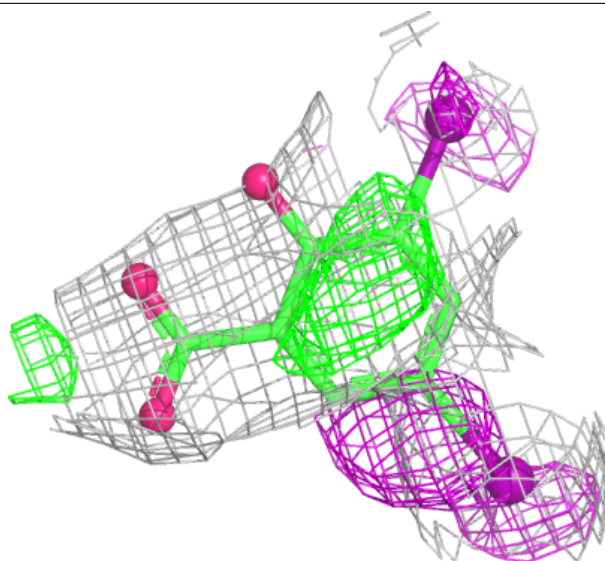
Electron density around DIU A 602:

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and green (positive)



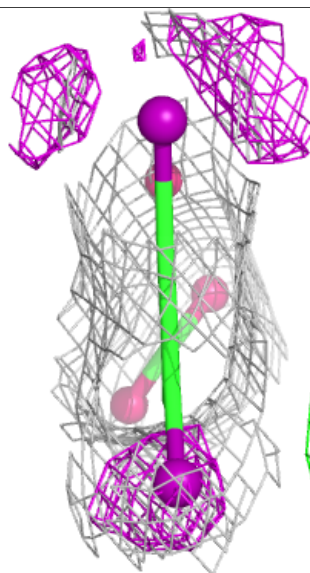
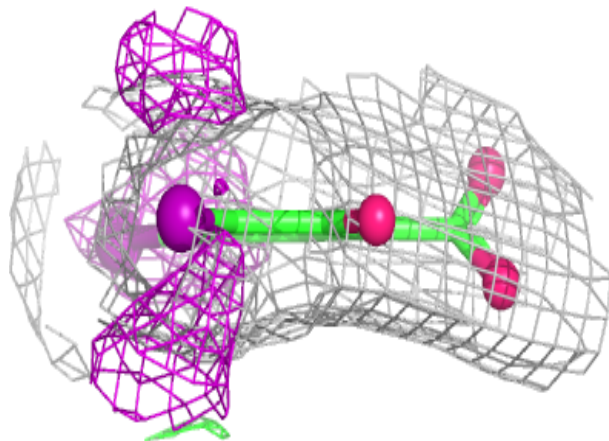
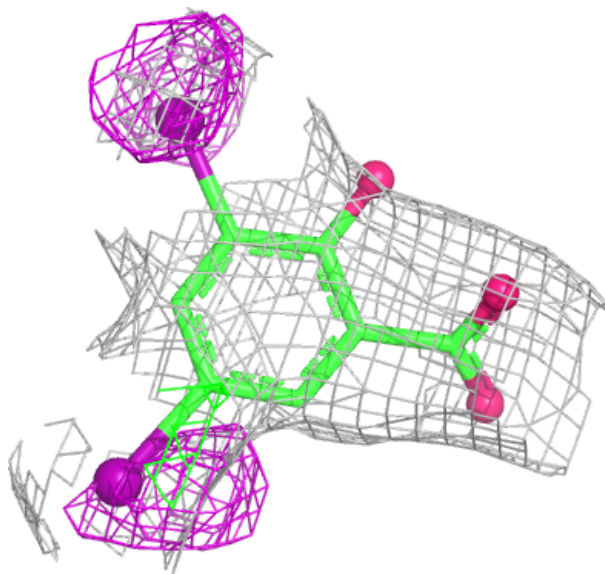
Electron density around DIU A 603:

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and green (positive)



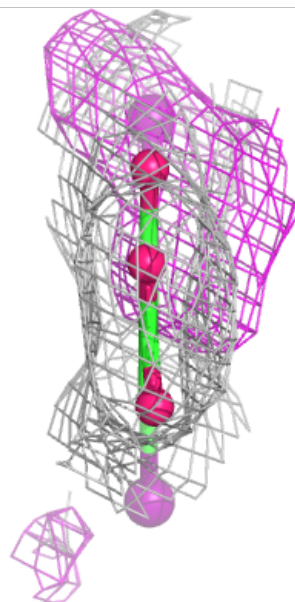
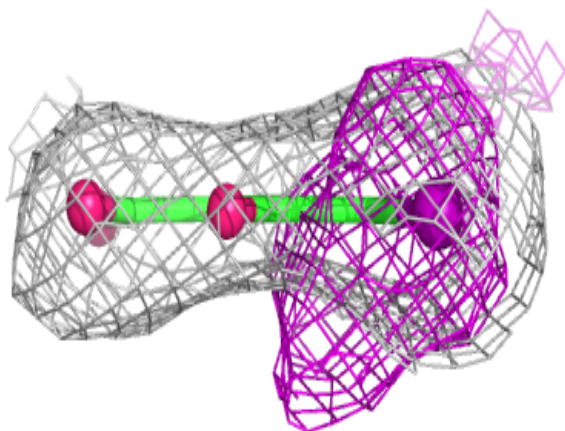
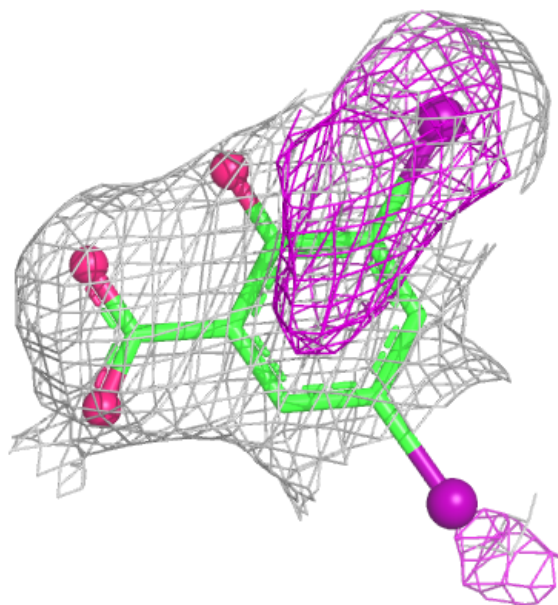
Electron density around DIU B 603:

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



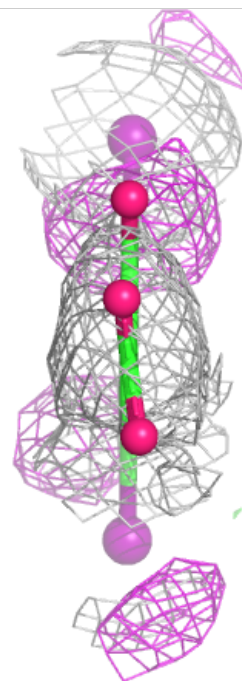
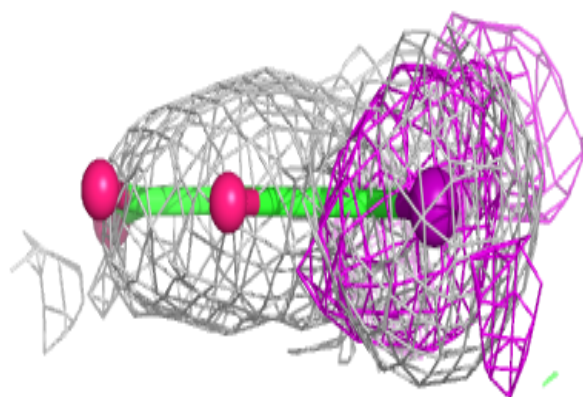
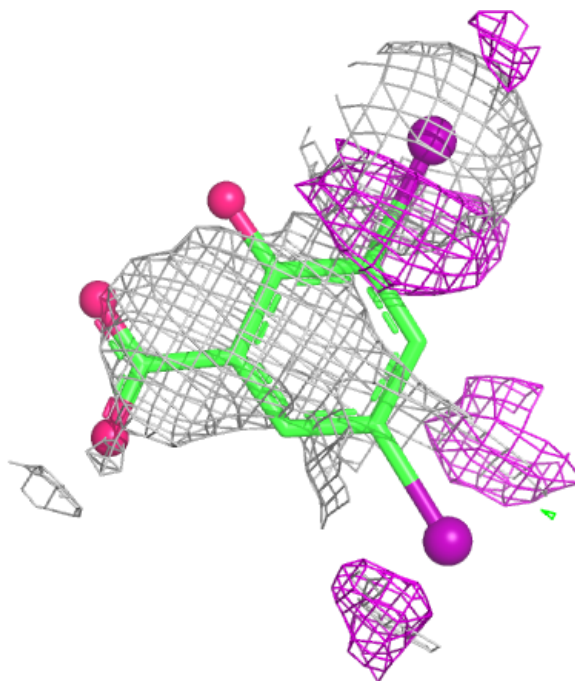
Electron density around DIU B 601:

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and green (positive)



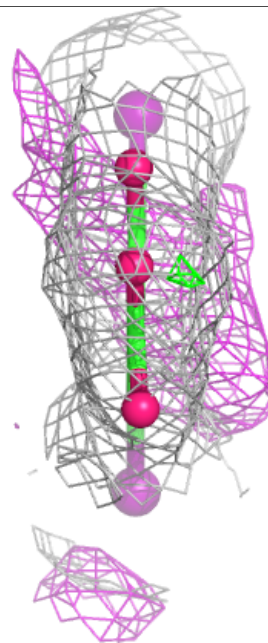
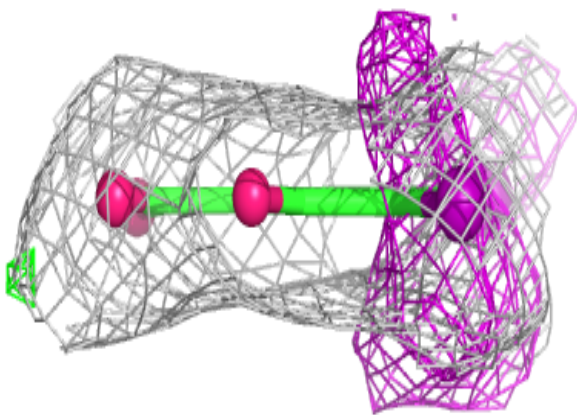
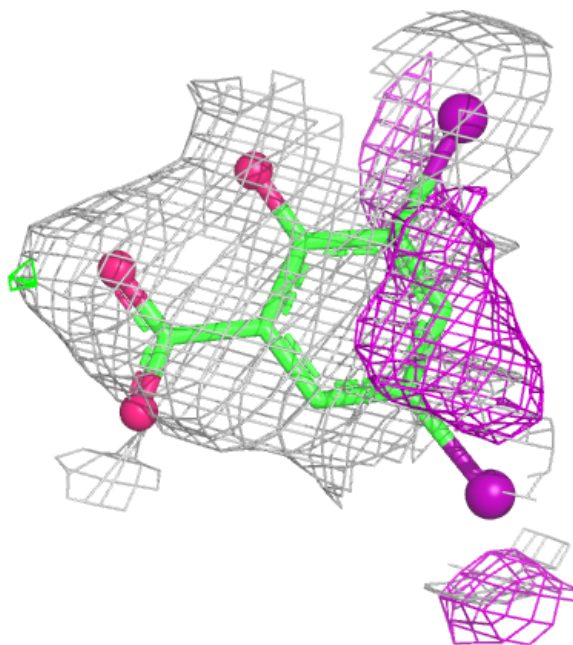
Electron density around DIU B 604:

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and green (positive)



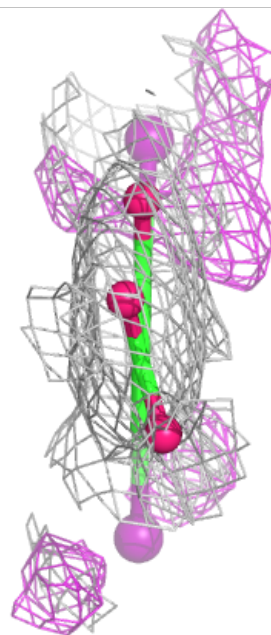
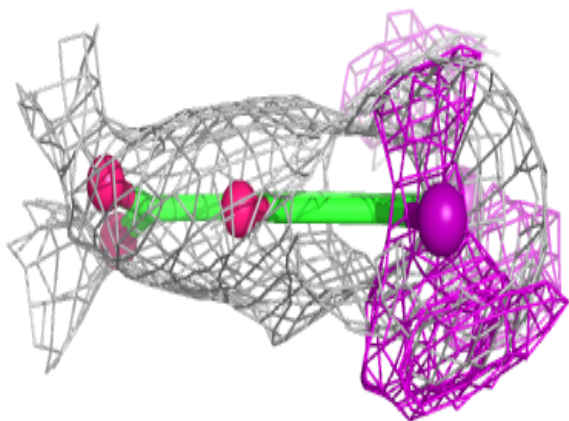
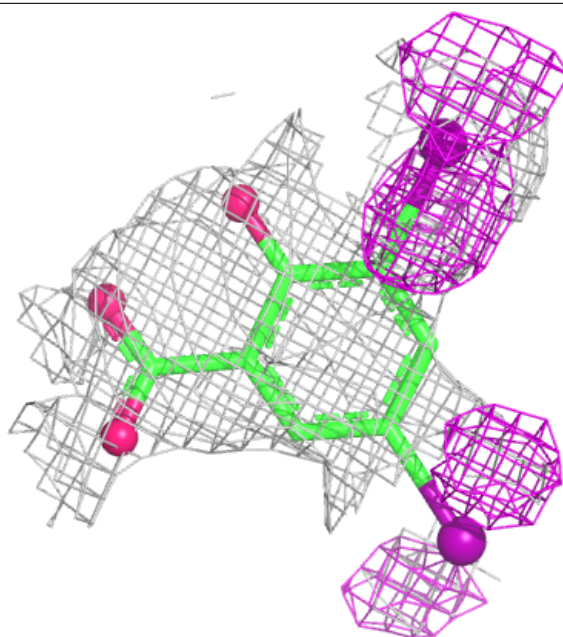
Electron density around DIU A 601:

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



Electron density around DIU A 604:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.