



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2026 – 09:21 PM EDT

PDB ID : 1R27 / pdb_00001r27
Title : Crystal Structure of NarGH complex
Authors : Jormakka, M.; Richardson, D.; Byrne, B.; Iwata, S.
Deposited on : 2003-09-26
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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)	:	2.50

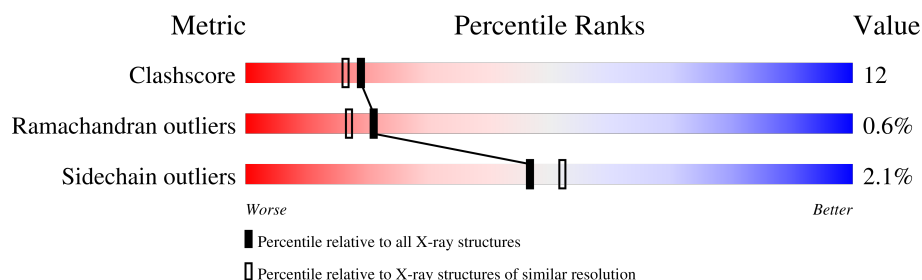
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	1246	73% 22% • •
1	C	1246	75% 21% • •
2	B	512	75% 13% • 9%
2	D	512	71% 17% • 9%

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
4	SF4	B	5800	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 29331 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 Respiratory nitrate reductase 1 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1218	Total	C	N	O	S	0	0	0
			9660	6100	1691	1821	48			
1	C	1218	Total	C	N	O	S	0	0	0
			9660	6100	1691	1821	48			

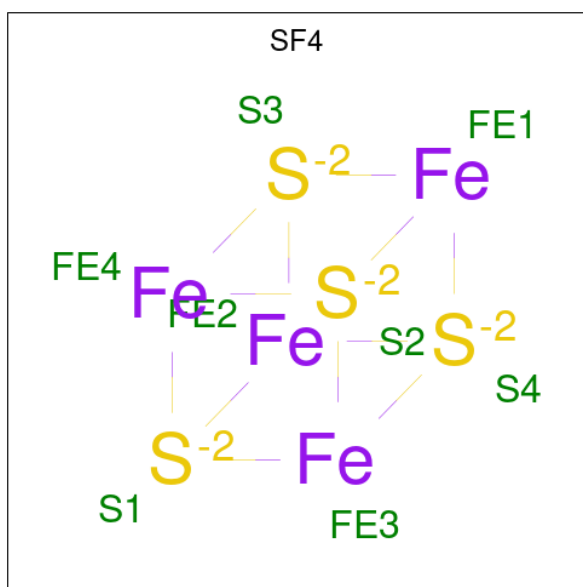
- Molecule 2 is a protein called Respiratory nitrate reductase 1 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	465	Total	C	N	O	S	0	0	0
			3711	2354	640	687	30			
2	D	465	Total	C	N	O	S	0	0	0
			3711	2354	640	687	30			

- Molecule 3 is MOLYBDENUM ATOM (CCD ID: MO) (formula: Mo).

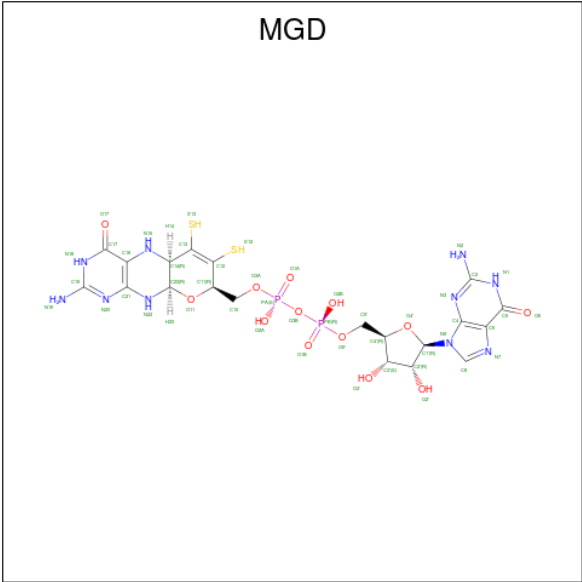
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mo	0	0
			1	1		
3	C	1	Total	Mo	0	0
			1	1		

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



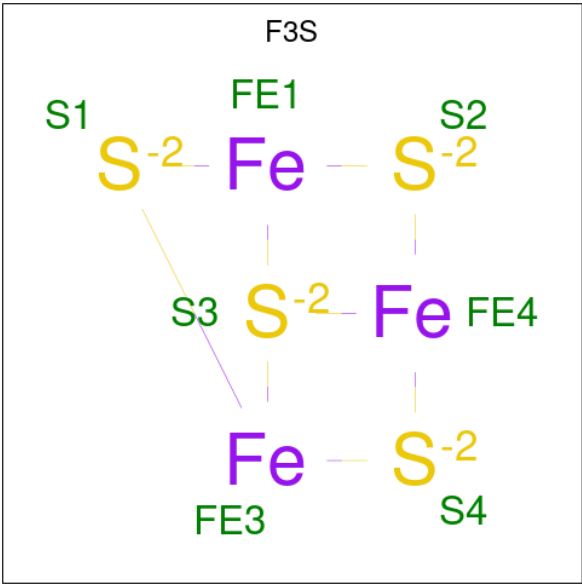
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	C	1	Total	Fe	S	0	0
			8	4	4		
4	D	1	Total	Fe	S	0	0
			8	4	4		
4	D	1	Total	Fe	S	0	0
			8	4	4		
4	D	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: MGD) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 6 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe₃S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total 7	Fe 3	S 4	0	0
6	D	1	Total 7	Fe 3	S 4	0	0

- Molecule 7 is water.

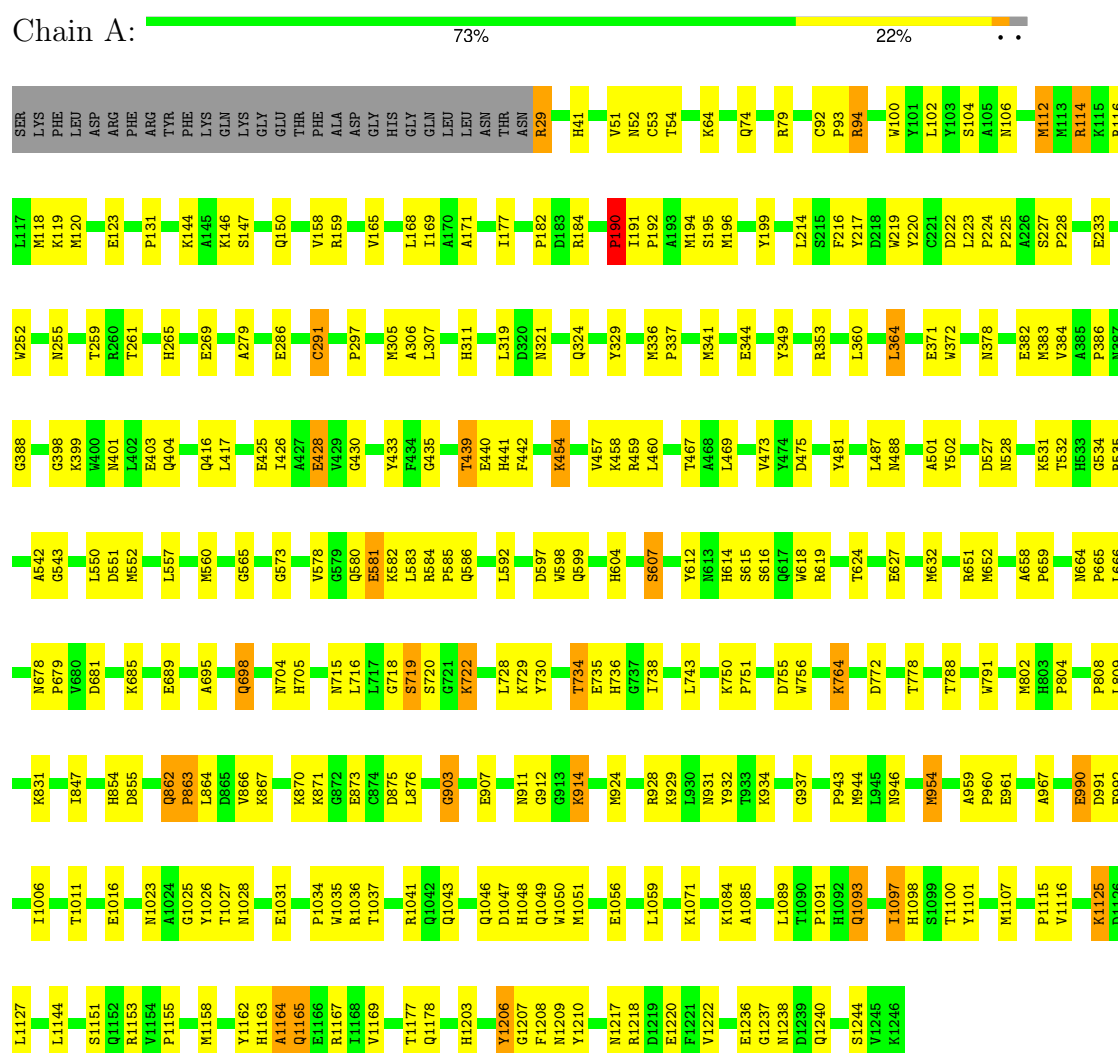
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	815	Total 815	O 815	0	0
7	B	376	Total 376	O 376	0	0
7	C	784	Total 784	O 784	0	0
7	D	346	Total 346	O 346	0	0

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.

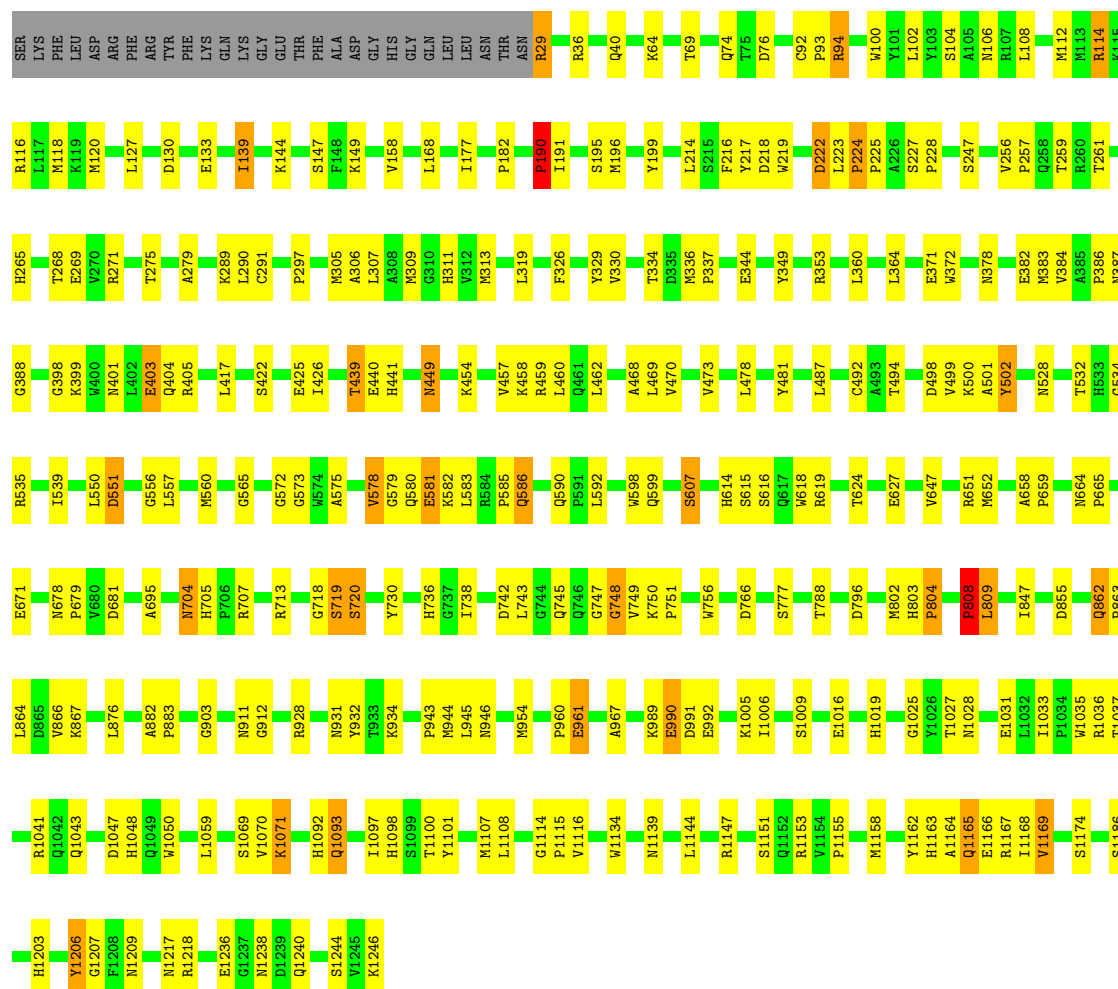
Note EDS was not executed.

- Molecule 1: Respiratory nitrate reductase 1 alpha chain



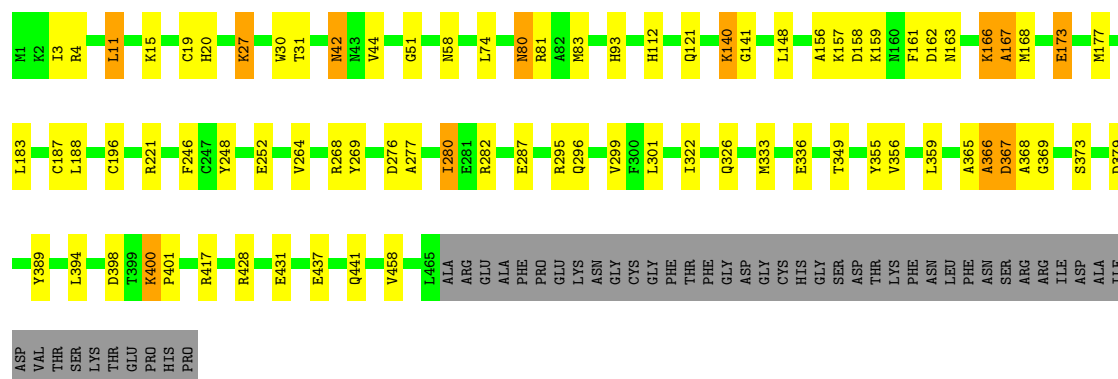
- Molecule 1: Respiratory nitrate reductase 1 alpha chain





• Molecule 2: Respiratory nitrate reductase 1 beta chain

Chain B: 75% 13% 9%



• Molecule 2: Respiratory nitrate reductase 1 beta chain

Chain D: 71% 17% 9%

PRO	GLU	L319	L148	M1
LYS	ASP	E323	K157	K2
ASN	GLY	K333	F161	I3
CYS	GLY	E336	Q165	Q6
PHE	THR	K337	K166	L11
PHE	THR	K338	A167	K15
GLY	GLY	T349	E173	C19
ASP	GLY	L350	F176	H20
CYS	HIS	L359	M177	K27
HIS	GLY	S360	L183	W30
SER	GLY	P361	C187	T31
ASP	THR	A365	C196	V44
LYS	LYS	A366	D207	P48
PHE	ASN	E370	R221	G51
ASN	LEU	L371	F234	N58
PHE	ASN	G372	F246	G59
ASN	SER	S373	C247	E60
SER	SER	D379	Y248	I67
SER	ARG	R384	P249	L74
ARG	ILE	L394	E252	Q75
ASP	ALA	T395	V264	G79
ILE	ASP	K400	R268	N80
ASP	THR	P401	Y269	R81
SER	SER	V402	D276	A82
LYS	LYS	L403	A277	N83
THR	THR	L406	D278	L84
GLU	GLU	K407	A279	L85
PRO	PRO	R408	L280	G86
HIS	HIS	M409	E281	K87
PRO	PRO	R417	R282	I88
		K424	S285	P103
		R428	T286	F106
		T436	E287	H112
		Q439	R295	T113
		A440	Q296	A114
		Q441	V299	K119
		L465	F300	S120
		ALA	L301	Q121
		ARG	K307	I130
		GLU		E133
		ALA		
		PHE		

4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	127.40 Å 298.30 Å 296.85 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.86 – 2.00	Depositor
% Data completeness (in resolution range)	88.2 (39.86-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.204 , 0.230	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	29331	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, MGD, F3S, MO

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	0.39	1/9914 (0.0%)	0.93	40/13462 (0.3%)
1	C	0.37	0/9914	0.92	41/13462 (0.3%)
2	B	0.38	0/3800	0.91	15/5145 (0.3%)
2	D	0.38	0/3800	0.93	14/5145 (0.3%)
All	All	0.38	1/27428 (0.0%)	0.93	110/37214 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	954	MET	SD-CE	-7.39	1.61	1.79

The worst 5 of 110 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	990	GLU	N-CA-C	-10.61	96.54	110.43
1	A	607	SER	N-CA-C	10.23	122.43	111.28
1	C	607	SER	N-CA-C	10.00	122.18	111.28
1	C	1163	HIS	N-CA-C	8.60	122.88	110.24
1	A	809	LEU	N-CA-C	-8.56	95.73	109.76

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9660	0	9330	260	0
1	C	9660	0	9330	245	0
2	B	3711	0	3659	64	0
2	D	3711	0	3659	80	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	8	0	0	0	0
4	B	24	0	0	2	0
4	C	8	0	0	0	0
4	D	24	0	0	1	0
5	A	94	0	44	6	0
5	C	94	0	44	7	0
6	B	7	0	0	0	0
6	D	7	0	0	0	0
7	A	815	0	0	39	0
7	B	376	0	0	7	0
7	C	784	0	0	25	0
7	D	346	0	0	9	0
All	All	29331	0	26066	628	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 12.

The worst 5 of 628 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:1098:HIS:O	1:A:1164:ALA:HB1	1.50	1.11
1:A:592:LEU:HB2	1:A:954:MET:HE3	1.37	1.05
1:A:454:LYS:HD3	1:A:487:LEU:HB3	1.40	1.00
1:C:990:GLU:O	1:C:991:ASP:HB2	1.66	0.96
1:C:652:MET:HE1	1:C:866:VAL:HG13	1.47	0.94

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	1216/1246 (98%)	1150 (95%)	59 (5%)	7 (1%)	21	17
1	C	1216/1246 (98%)	1144 (94%)	62 (5%)	10 (1%)	16	11
2	B	463/512 (90%)	450 (97%)	10 (2%)	3 (1%)	21	17
2	D	463/512 (90%)	448 (97%)	14 (3%)	1 (0%)	43	42
All	All	3358/3516 (96%)	3192 (95%)	145 (4%)	21 (1%)	21	17

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1164	ALA
1	A	1244	SER
1	C	748	GLY
1	A	578	VAL
1	A	719	SER

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	1019/1043 (98%)	997 (98%)	22 (2%)	45	50
1	C	1019/1043 (98%)	1000 (98%)	19 (2%)	50	56
2	B	400/439 (91%)	391 (98%)	9 (2%)	44	49
2	D	400/439 (91%)	391 (98%)	9 (2%)	44	49
All	All	2838/2964 (96%)	2779 (98%)	59 (2%)	47	52

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	173	GLU
2	D	165	GLN
1	C	139	ILE

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Mol	Chain	Res	Type
2	D	161	PHE
1	C	1238	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	404	GLN
1	C	984	HIS
1	C	480	ASN
1	C	708	ASN
1	C	1082	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SF4	C	7807	1	0,12,12	-	-	-		
4	SF4	B	5800	2	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SF4	B	5805	2	0,12,12	-	-	-		
4	SF4	A	5807	1	0,12,12	-	-	-		
4	SF4	B	5806	2	0,12,12	-	-	-		
4	SF4	D	7805	2	0,12,12	-	-	-		
6	F3S	B	5808	2	0,9,9	-	-	-		
5	MGD	C	7802	3	47,52,52	2.08	11 (23%)	58,81,81	1.97	5 (8%)
6	F3S	D	7808	2	0,9,9	-	-	-		
4	SF4	D	7800	2	0,12,12	-	-	-		
4	SF4	D	7806	2	0,12,12	-	-	-		
5	MGD	A	5802	3	47,52,52	2.03	9 (19%)	58,81,81	1.92	3 (5%)
5	MGD	C	7801	3	47,52,52	2.29	15 (31%)	58,81,81	1.59	6 (10%)
5	MGD	A	5801	3	47,52,52	2.46	16 (34%)	58,81,81	1.70	6 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	C	7807	1	-	-	0/6/5/5
4	SF4	B	5800	2	-	-	0/6/5/5
4	SF4	B	5805	2	-	-	0/6/5/5
4	SF4	A	5807	1	-	-	0/6/5/5
4	SF4	B	5806	2	-	-	0/6/5/5
4	SF4	D	7805	2	-	-	0/6/5/5
6	F3S	B	5808	2	-	-	0/3/3/3
5	MGD	C	7802	3	-	4/22/66/66	0/6/6/6
6	F3S	D	7808	2	-	-	0/3/3/3
4	SF4	D	7800	2	-	-	0/6/5/5
4	SF4	D	7806	2	-	-	0/6/5/5
5	MGD	A	5802	3	-	4/22/66/66	0/6/6/6
5	MGD	C	7801	3	-	5/22/66/66	0/6/6/6
5	MGD	A	5801	3	-	5/22/66/66	0/6/6/6

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	7802	MGD	C14-N15	7.95	1.55	1.46
5	A	5801	MGD	C21-N22	7.29	1.43	1.35
5	A	5802	MGD	C14-N15	7.05	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	7801	MGD	PA-O3B	5.63	1.65	1.59
5	A	5801	MGD	PA-O3B	5.48	1.65	1.59

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	7802	MGD	O11-C23-C14	-11.57	101.25	108.96
5	A	5802	MGD	O11-C23-C14	-10.98	101.64	108.96
5	A	5801	MGD	O11-C23-N22	7.09	115.04	108.61
5	C	7801	MGD	O11-C23-N22	6.47	114.48	108.61
5	C	7802	MGD	O11-C23-N22	-6.16	103.02	108.61

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	5801	MGD	C5'-O5'-PB-O1B
5	A	5801	MGD	C5'-O5'-PB-O3B
5	A	5802	MGD	C5'-O5'-PB-O1B
5	A	5802	MGD	C5'-O5'-PB-O3B
5	C	7801	MGD	C5'-O5'-PB-O1B

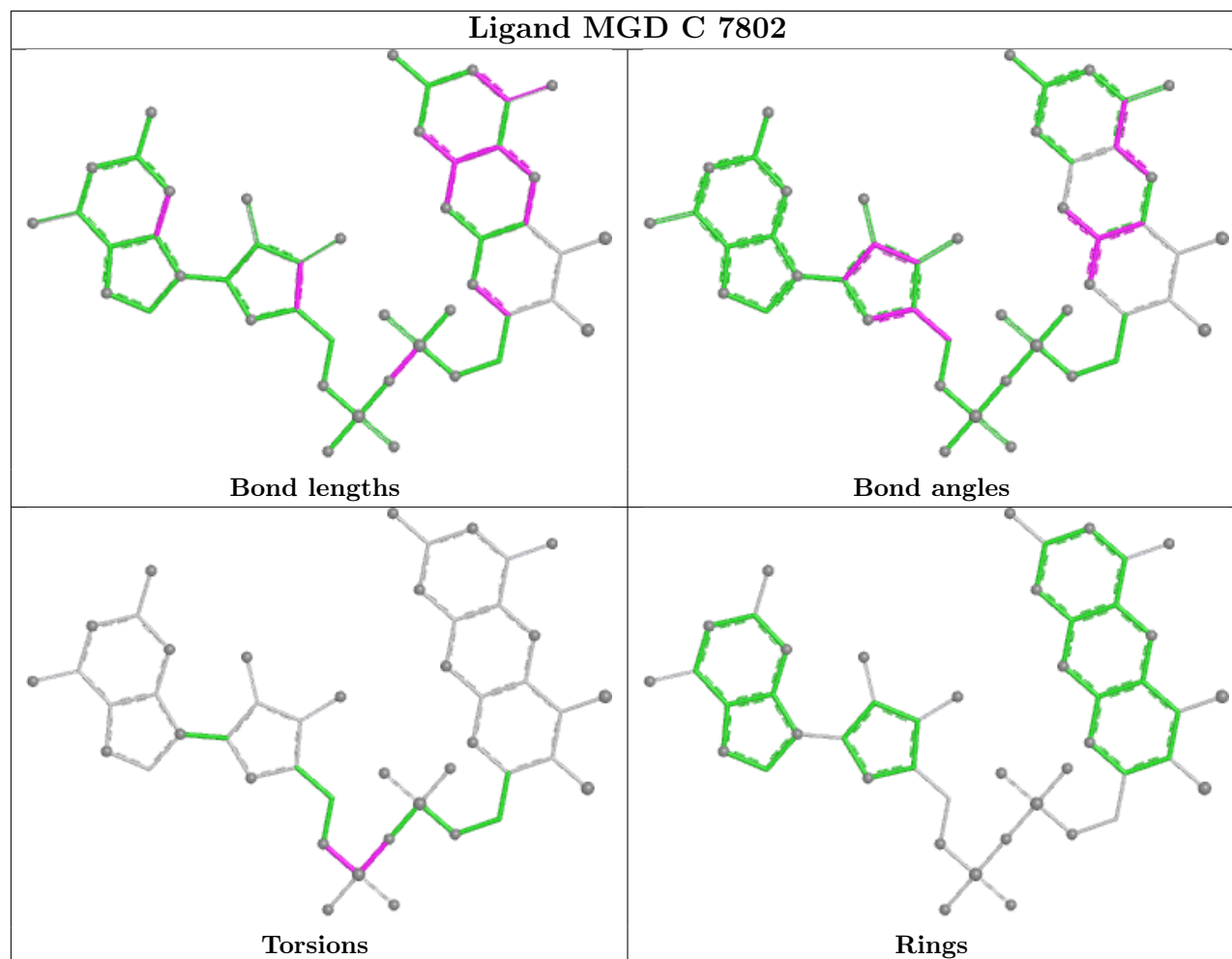
There are no ring outliers.

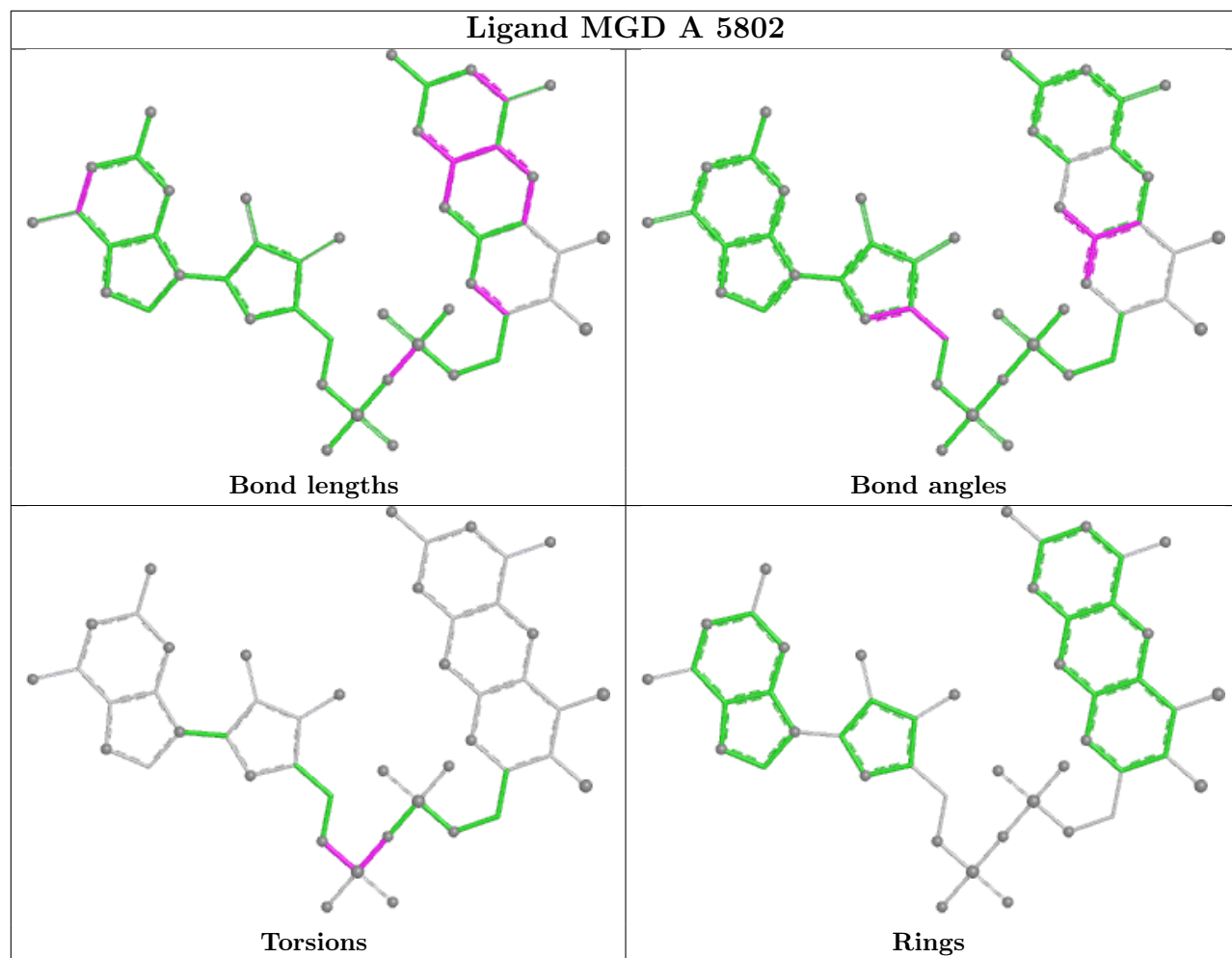
6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	5800	SF4	2	0
5	C	7802	MGD	4	0
4	D	7800	SF4	1	0
5	A	5802	MGD	5	0
5	C	7801	MGD	3	0
5	A	5801	MGD	1	0

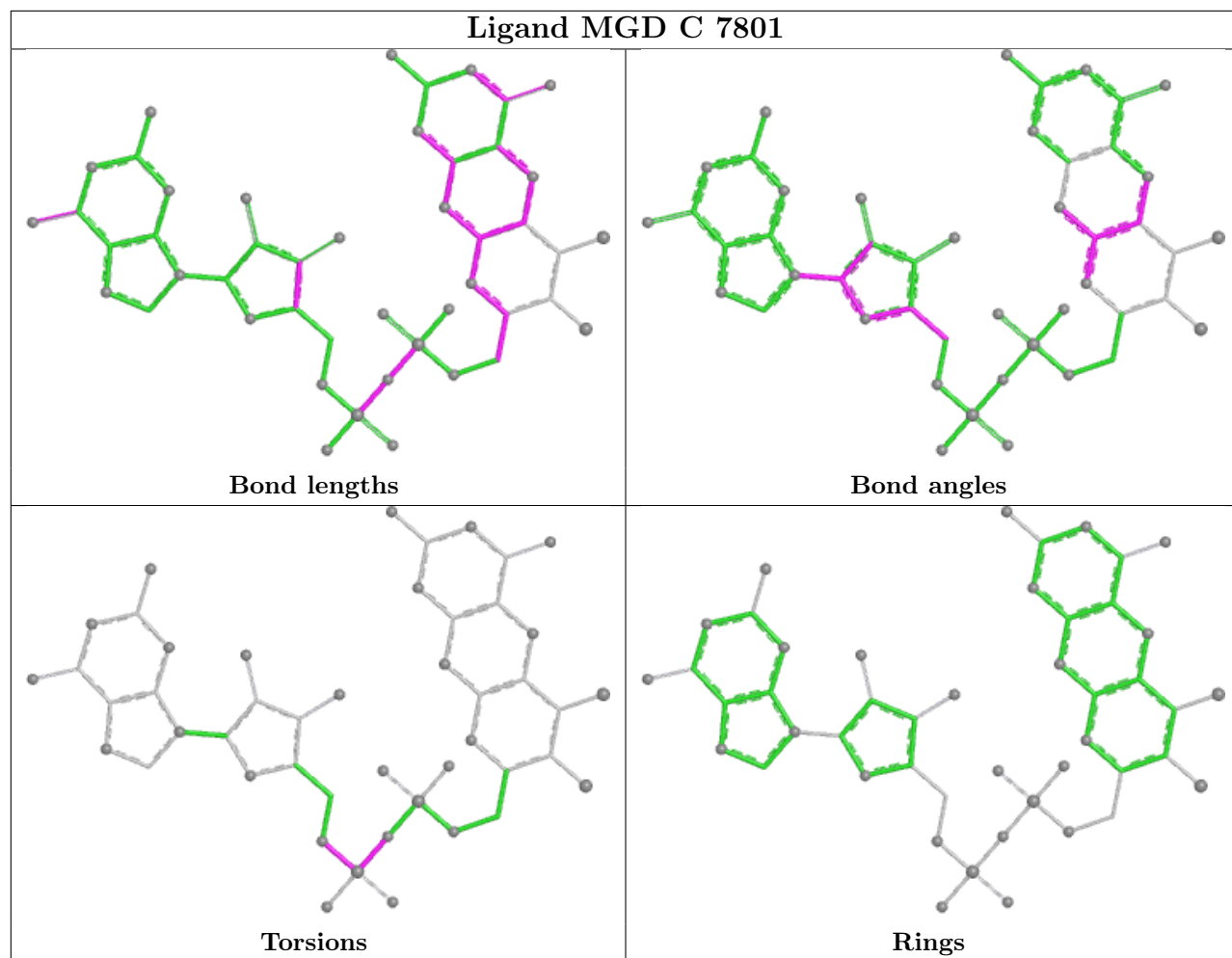
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

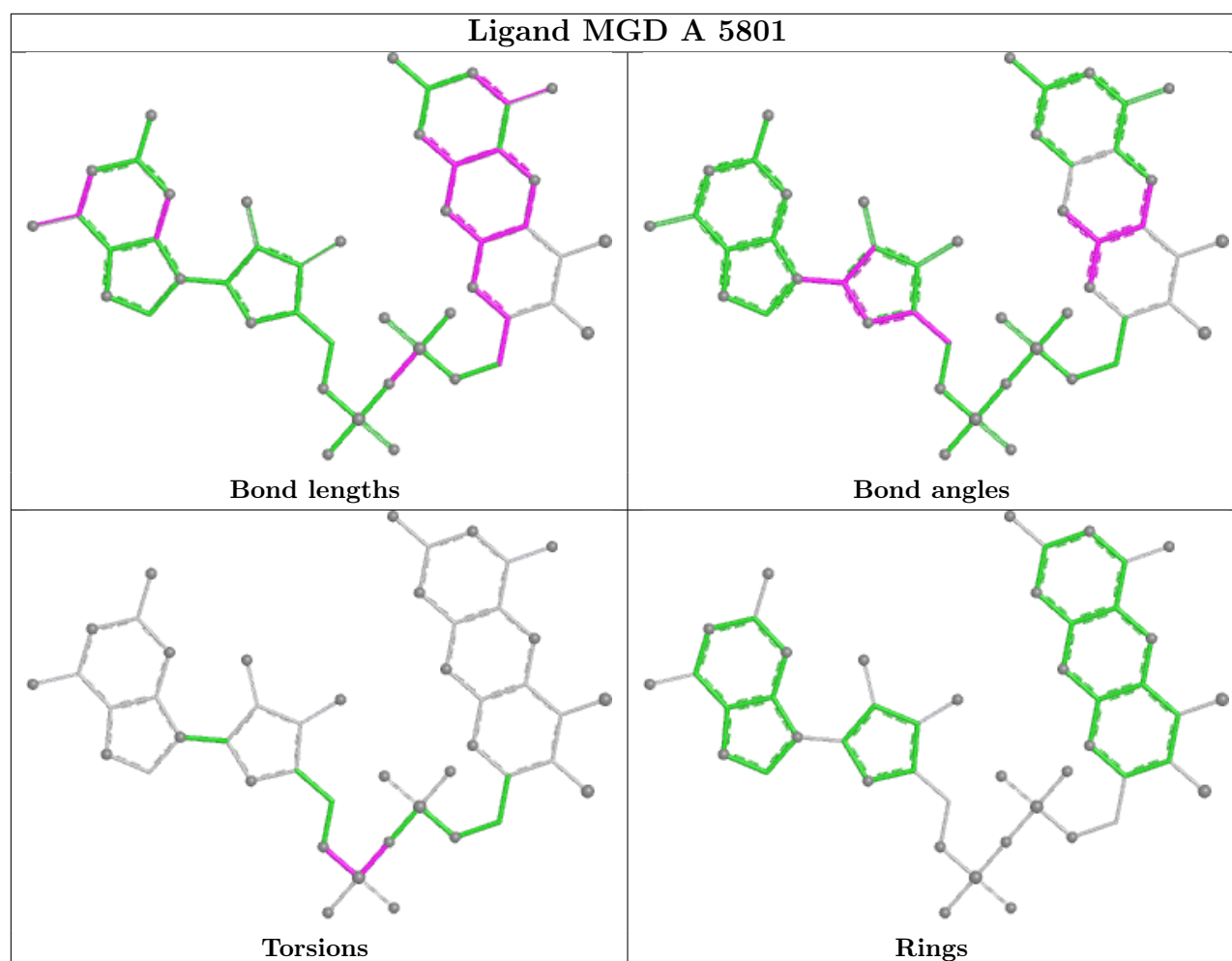
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





Ligand MGD C 7801





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.