WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Nov 3, 2024 – 02:17 am GMT

PDB ID	:	2VNT
Title	:	Urokinase-Type Plasminogen Activator Inhibitor Complex with a 1-(7- SULP HOAMIDOISOQUINOLINYL)GUANIDINE
Authors	:	Fish, P.V.; Barber, C.G.; Brown, D.G.; Butt, R.; Henry, B.T.; Horne, V.; Huggins, J.P.; McCleverty, D.; Phillips, C.; Webster, R.; Dickinson, R.P.; Collis, M.G.; King, E.; O'Gara, M.; McIntosh, F.
Deposited on	:	2008-02-07
Resolution	:	2.20 Å(reported)

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

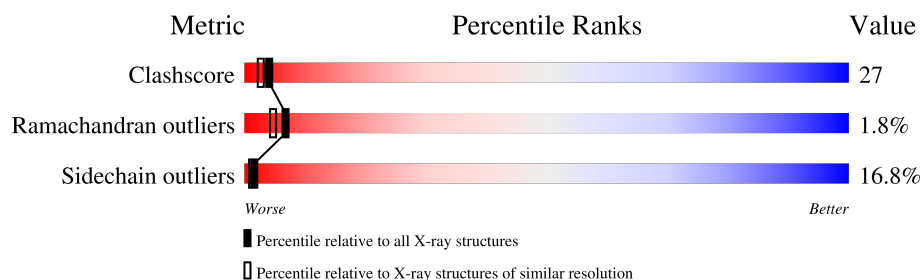|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.20 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	Percentile Ranks	Value
Clashscore		27
Ramachandran outliers		1.8%
Sidechain outliers		16.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	276	58% 27% 9% 7%
1	B	276	52% 29% 12% · 6%
1	C	276	58% 29% 7% 6%
1	D	276	61% 26% 7% 6%
1	E	276	58% 26% 8% · 6%
1	F	276	34% 40% 16% · 7%

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 crite-

ria:

| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	B	1262	-	-	X	-
3	SO4	E	1259	-	-	X	-

2   Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13031 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 UROKINASE-TYPE PLASMINOGEN ACTIVATOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total 2033	C 1280	N 356	O 379	S 18	0	0	1
1	B	259	Total 2041	C 1286	N 357	O 380	S 18	0	0	1
1	C	259	Total 2042	C 1285	N 359	O 380	S 18	0	0	1
1	D	259	Total 2041	C 1286	N 357	O 380	S 18	0	0	1
1	E	259	Total 2041	C 1286	N 357	O 380	S 18	0	0	1
1	F	257	Total 2022	C 1271	N 356	O 377	S 18	0	0	1

- Molecule 2 is 1-({4-CHLORO-1-[(DIAMINOMETHYLIDENE)AMINO]ISOQUINOLIN-7-YL}SULFONYL)-D-PROLINE (three-letter code: QGG) (formula: $C_{15}H_{16}ClN_5O_4S$).

QGG
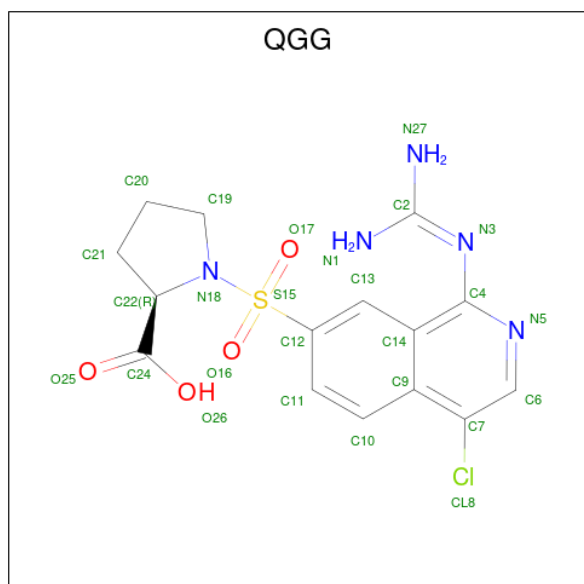
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 26	C 15	Cl 1	N 5	O 4	S 1	0	0
2	B	1	Total 26	C 15	Cl 1	N 5	O 4	S 1	0	0
2	C	1	Total 26	C 15	Cl 1	N 5	O 4	S 1	0	0
2	D	1	Total 26	C 15	Cl 1	N 5	O 4	S 1	0	0
2	E	1	Total 26	C 15	Cl 1	N 5	O 4	S 1	0	0
2	F	1	Total 26	C 15	Cl 1	N 5	O 4	S 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	B	1	Total 5	O 4	S 1	0	0
3	D	1	Total 5	O 4	S 1	0	0
3	D	1	Total 5	O 4	S 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total 5	O 4	S 1	0	0
3	E	1	Total 5	O 4	S 1	0	0
3	E	1	Total 5	O 4	S 1	0	0

- Molecule 4 is water.

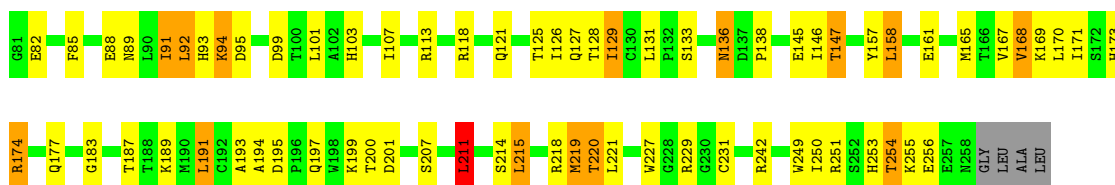| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	90	Total 90	O 90	0	0
4	B	86	Total 86	O 86	0	0
4	C	106	Total 106	O 106	0	0
4	D	113	Total 113	O 113	0	0
4	E	124	Total 124	O 124	0	0
4	F	91	Total 91	O 91	0	0

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.
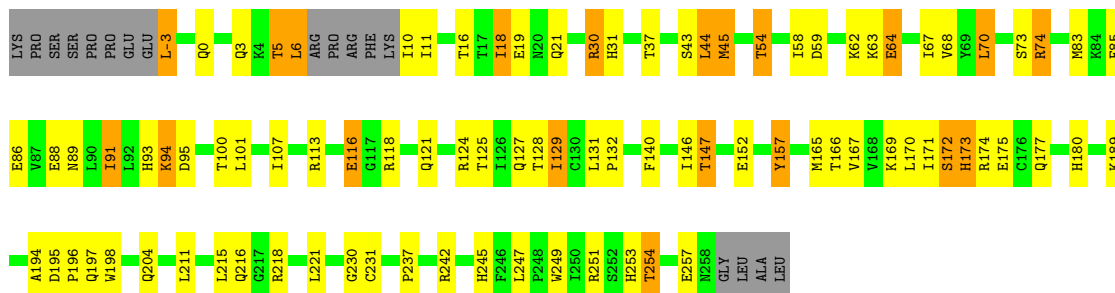
Note EDS was not executed.

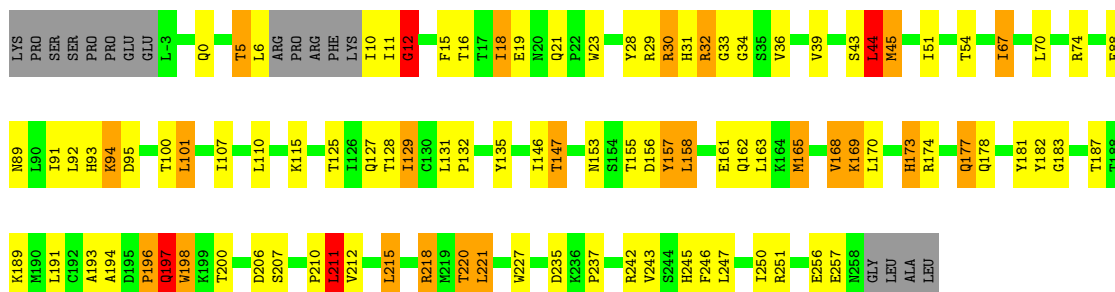• Molecule 1: UROKINASE-TYPE PLASMINOGEN ACTIVATOR

Chain A:

• Molecule 1: UROKINASE-TYPE PLASMINOGEN ACTIVATOR

Chain B:
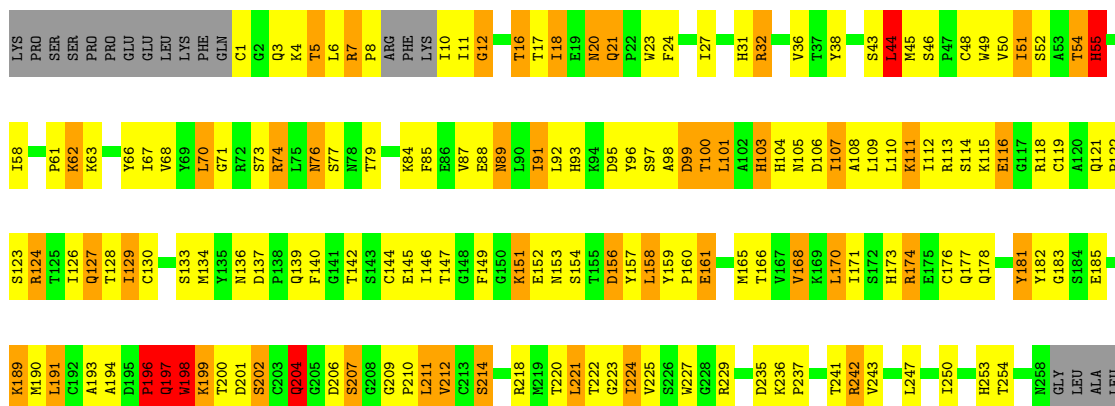

• Molecule 1: UROKINASE-TYPE PLASMINOGEN ACTIVATOR

Chain C:

G81 E82 F85 E88 N89 L90 I91 L92 H93 K94 D95 D99 T100 L101 A102 H103 I107 R113 R118 Q121 T125 I126 Q127 I128 I129 C130 L131 P132 S133 N136 D137 P138 E145 I146 T147 Y157 L158 E161 M165 T166 V167 V168 K169 L170 I171 S172 H173

R174 Q177 G183 T187 T188 K189 M190 L191 C192 A193 A194 D195 P196 Q197 W198 K199 T200 D201 S207 L211 S214 L215 R218 M219 T220 L221 W227 G228 R229 G230 C231 R242 W249 I250 R251 S252 H253 T254 K255 E256 E257 N258 GLY LEU ALA LEU

• Molecule 1: UROKINASE-TYPE PLASMINOGEN ACTIVATOR

Chain D:

61% 26% 7% 6%

LYS PRO SER SER PRO GLU GLU L-3 Q0 Q3 K4 T5 L6 ARG PRO ARG PHE LYS I10 I11 T16 T17 I18 E19 N20 Q21 R30 H31 T37 S43 L44 M45 T54 I58 D59 K62 K63 E64 I67 V68 Y69 L70 S73 R74 M83 K84 F85

E86 V87 E88 N89 L90 I91 L92 H93 K94 D95 T100 L101 I107 R113 E116 G117 R118 Q121 R124 T125 I126 Q127 T128 I129 C130 L131 P132 F140 I146 T147 E152 Y157 M165 T166 V167 V168 K169 L170 I171 S172 H173 R174 E175 C176 Q177 H180 K189

A194 D195 P196 Q197 W198 Q204 L211 L215 Q216 G217 R218 L221 G230 C231 P237 R242 H245 F246 P248 W249 I250 R251 S252 H253 T254 E257 N258 GLY LEU ALA LEU

• Molecule 1: UROKINASE-TYPE PLASMINOGEN ACTIVATOR

Chain E:

58% 26% 8% 6%

LYS PRO SER SER PRO GLU GLU L-3 Q0 T5 L6 ARG PRO ARG PHE LYS I10 I11 G12 F15 T16 T17 I18 E19 N20 Q21 P22 W23 Y28 R29 R30 H31 R32 G33 G34 S35 V36 V39 S43 L44 M45 I51 T54 I67 L70 R74 E88

N89 L90 I91 L92 H93 K94 D95 T100 L101 I107 L110 K115 T125 I126 Q127 T128 I129 C130 L131 P132 Y135 I146 T147 N153 S154 T155 D156 Y157 L158 E161 Q162 L163 K164 M165 V168 K169 L170 H173 R174 Q177 Q178 Y181 Y182 G183 T187 T188

K189 M190 L191 C192 A193 A194 D195 P196 Q197 W198 K199 T200 D206 S207 P210 I211 V212 L215 R218 M219 T220 L221 W227 D235 K236 P237 R242 V243 S244 H245 F246 L247 I250 R251 E256 E257 N258 GLY LEU ALA LEU

• Molecule 1: UROKINASE-TYPE PLASMINOGEN ACTIVATOR

Chain F:

34% 40% 16% 7%

LYS PRO SER SER PRO GLU GLU LEU LYS PHE GLN C1 G2 Q3 K4 T5 L6 R7 P8 ARG PHE LYS I10 I11 G12 T16 T17 I18 E19 N20 Q21 P22 W23 F24 I27 H31 R32 V36 T37 Y38 S43 L44 M45 S46 P47 C48 W49 V50 I51 S52 A53 T54 H55

I58 P61 K62 K63 Y66 I67 V68 Y69 L70 G71 R72 S73 R74 L75 N76 S77 N78 T79 K84 F85 E86 V87 E88 N89 L90 I91 L92 H93 K94 D95 Y96 S97 A98 D99 T100 L101 A102 H103 H104 N105 D106 I107 A108 L109 L110 K111 I112 R113 S114 K115 E116 G117 R118 C119 A120 Q121 P122

S123 R124 T125 I126 Q127 T128 I129 C130 S133 M134 Y135 N136 D137 P138 Q139 F140 G141 T142 S143 C144 E145 I146 T147 G148 F149 G150 K151 E152 N153 S154 T155 D156 Y157 L158 Y159 P160 E161 M165 T166 V167 V168 K169 L170 I171 S172 H173 R174 E175 C176 Q177 Q178 Y181 Y182 G183 S184 E185

K189 M190 L191 C192 A193 A194 D195 P196 Q197 W198 K199 T200 D201 S202 C203 Q204 G205 D206 S207 G208 G209 P210 L211 V212 C213 S214 R218 M219 T220 L221 T222 G223 I224 V225 S226 W227 G228 R229 D235 K236 P237 T241 R242 V243 L247 I250 H253 T254 N258 GLY LEU ALA LEU

4 Data and refinement statistics ⓘ

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	104.56Å 181.11Å 104.36Å 90.00° 94.80° 90.00°	Depositor
Resolution (Å)	35.00 – 2.20	Depositor
% Data completeness (in resolution range)	99.5 (35.00-2.20)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.241 , 0.295	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13031	wwPDB-VP
Average B, all atoms (Å^2)	35.0	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: SO4, QGG

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	0.75	0/2082	0.91	6/2815 (0.2%)
1	B	0.79	1/2090 (0.0%)	0.95	7/2826 (0.2%)
1	C	0.70	0/2092	0.84	2/2830 (0.1%)
1	D	0.83	0/2090	0.97	4/2826 (0.1%)
1	E	0.85	0/2090	0.97	4/2826 (0.1%)
1	F	0.78	0/2071	0.90	4/2802 (0.1%)
All	All	0.78	1/12515 (0.0%)	0.93	27/16925 (0.2%)

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	D	0	1
1	E	0	3
1	F	0	2
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	80	GLN	CG-CD	5.41	1.63	1.51

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	173	HIS	N-CA-C	-11.50	79.94	111.00
1	B	74	ARG	NE-CZ-NH2	-7.97	116.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	211	LEU	CA-CB-CG	7.45	132.42	115.30
1	B	211	LEU	CA-CB-CG	7.11	131.65	115.30
1	D	74	ARG	NE-CZ-NH2	-6.75	116.92	120.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	198	TRP	Peptide
1	D	172	SER	Peptide
1	E	12	GLY	Peptide
1	E	196	PRO	Peptide
1	E	197	GLN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2033	0	1980	83	0
1	B	2041	0	1991	129	0
1	C	2042	0	1987	92	0
1	D	2041	0	1991	88	0
1	E	2041	0	1991	101	0
1	F	2022	0	1970	193	0
2	A	26	0	15	1	0
2	B	26	0	15	4	0
2	C	26	0	15	1	0
2	D	26	0	15	1	0
2	E	26	0	15	1	0
2	F	26	0	15	5	0
3	B	20	0	0	5	0
3	D	15	0	0	1	0
3	E	10	0	0	3	0
4	A	90	0	0	7	0
4	B	86	0	0	20	0
4	C	106	0	0	9	0
4	D	113	0	0	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	124	0	0	12	0
4	F	91	0	0	31	0
All	All	13031	0	12000	661	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 27.

The worst 5 of 661 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:187:THR:OG1	1:A:189:LYS:HD2	1.35	1.24
1:D:94:LYS:H	1:D:94:LYS:CD	1.51	1.20
1:F:21:GLN:HE22	1:F:165:MET:CE	1.53	1.20
1:B:80:GLN:HG2	4:B:2030:HOH:O	1.42	1.20
1:B:45:MET:HE2	1:B:51:ILE:CG2	1.74	1.15

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	254/276 (92%)	234 (92%)	15 (6%)	5 (2%)	6	4
1	B	255/276 (92%)	230 (90%)	19 (8%)	6 (2%)	5	3
1	C	255/276 (92%)	235 (92%)	19 (8%)	1 (0%)	30	34
1	D	255/276 (92%)	232 (91%)	23 (9%)	0	100	100
1	E	255/276 (92%)	238 (93%)	12 (5%)	5 (2%)	6	4
1	F	253/276 (92%)	212 (84%)	31 (12%)	10 (4%)	2	1
All	All	1527/1656 (92%)	1381 (90%)	119 (8%)	27 (2%)	7	5

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	GLY
1	A	197	GLN
1	B	135	TYR
1	C	36	VAL
1	E	12	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	225/242 (93%)	191 (85%)	34 (15%)	2	2
1	B	226/242 (93%)	184 (81%)	42 (19%)	1	1
1	C	226/242 (93%)	194 (86%)	32 (14%)	2	2
1	D	226/242 (93%)	195 (86%)	31 (14%)	3	2
1	E	226/242 (93%)	194 (86%)	32 (14%)	2	2
1	F	224/242 (93%)	168 (75%)	56 (25%)	0	0
All	All	1353/1452 (93%)	1126 (83%)	227 (17%)	1	1

5 of 227 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	54	THR
1	F	204	GLN
1	E	32	ARG
1	F	199	LYS
1	F	111	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	31	HIS
1	D	153	ASN

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Mol	Chain	Res	Type
1	F	253	HIS
1	F	21	GLN
1	D	80	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 ⓘ

There are no oligosaccharides in this entry.

5.6   Ligand geometry ⓘ

15 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	$\#|Z| > 2$
3	SO4	B	1260	-	4,4,4	0.21	0	6,6,6	0.29	0
3	SO4	B	1262	-	4,4,4	0.18	0	6,6,6	0.50	0
2	QGG	A	1258	-	28,28,28	1.60	3 (10%)	40,42,42	2.24	11 (27%)
2	QGG	B	1258	-	28,28,28	1.16	3 (10%)	40,42,42	1.69	10 (25%)
3	SO4	E	1260	-	4,4,4	0.27	0	6,6,6	0.44	0
2	QGG	D	1258	-	28,28,28	1.38	5 (17%)	40,42,42	1.99	12 (30%)
2	QGG	C	1258	-	28,28,28	1.09	2 (7%)	40,42,42	1.45	8 (20%)
3	SO4	B	1259	-	4,4,4	0.23	0	6,6,6	0.30	0
2	QGG	F	1258	-	28,28,28	1.17	3 (10%)	40,42,42	1.98	15 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	QGG	E	1258	-	28,28,28	1.41	4 (14%)	40,42,42	2.02	14 (35%)
3	SO4	B	1261	-	4,4,4	0.23	0	6,6,6	0.39	0
3	SO4	D	1259	-	4,4,4	0.17	0	6,6,6	0.29	0
3	SO4	D	1261	-	4,4,4	0.20	0	6,6,6	0.28	0
3	SO4	E	1259	-	4,4,4	0.26	0	6,6,6	0.51	0
3	SO4	D	1260	-	4,4,4	0.29	0	6,6,6	1.00	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	QGG	A	1258	-	-	1/19/30/30	0/3/3/3
2	QGG	B	1258	-	-	1/19/30/30	0/3/3/3
2	QGG	D	1258	-	-	2/19/30/30	0/3/3/3
2	QGG	C	1258	-	-	0/19/30/30	0/3/3/3
2	QGG	F	1258	-	-	2/19/30/30	0/3/3/3
2	QGG	E	1258	-	-	1/19/30/30	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1258	QGG	O17-S15	-4.87	1.38	1.43
2	E	1258	QGG	C6-C7	-4.72	1.34	1.39
2	D	1258	QGG	C6-C7	-4.64	1.34	1.39
2	A	1258	QGG	S15-N18	3.88	1.69	1.63
2	B	1258	QGG	S15-N18	2.91	1.67	1.63

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1258	QGG	O17-S15-C12	-7.74	98.25	108.05
2	A	1258	QGG	C21-C22-N18	5.98	110.82	102.94
2	D	1258	QGG	O17-S15-C12	-5.19	101.48	108.05
2	F	1258	QGG	C6-C7-C9	-4.86	116.74	121.40
2	E	1258	QGG	O17-S15-C12	-4.82	101.95	108.05

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1258	QGG	C19-N18-S15-O17
2	D	1258	QGG	C19-N18-S15-O17
2	B	1258	QGG	C22-N18-S15-O16
2	E	1258	QGG	C19-N18-S15-O17
2	F	1258	QGG	N18-C22-C24-O25

There are no ring outliers.

11 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1260	SO4	1	0
3	B	1262	SO4	3	0
2	A	1258	QGG	1	0
2	B	1258	QGG	4	0
2	D	1258	QGG	1	0
2	C	1258	QGG	1	0
3	B	1259	SO4	1	0
2	F	1258	QGG	5	0
2	E	1258	QGG	1	0
3	E	1259	SO4	3	0
3	D	1260	SO4	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.
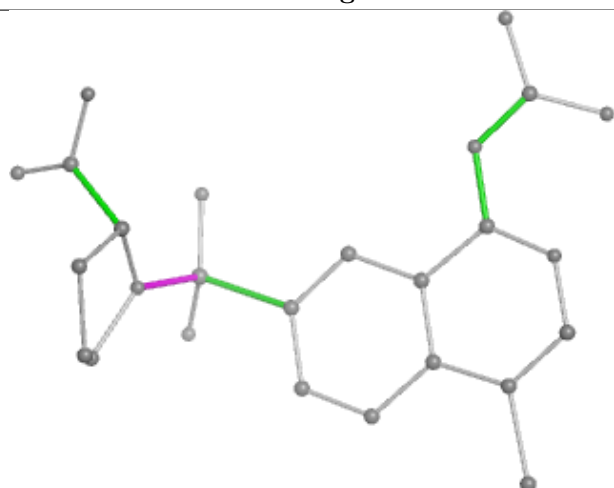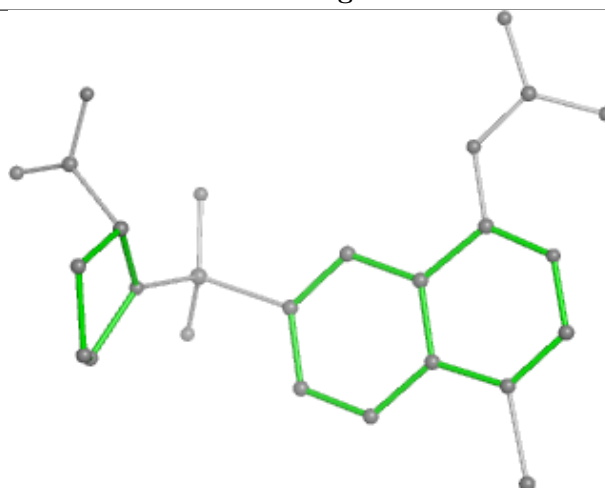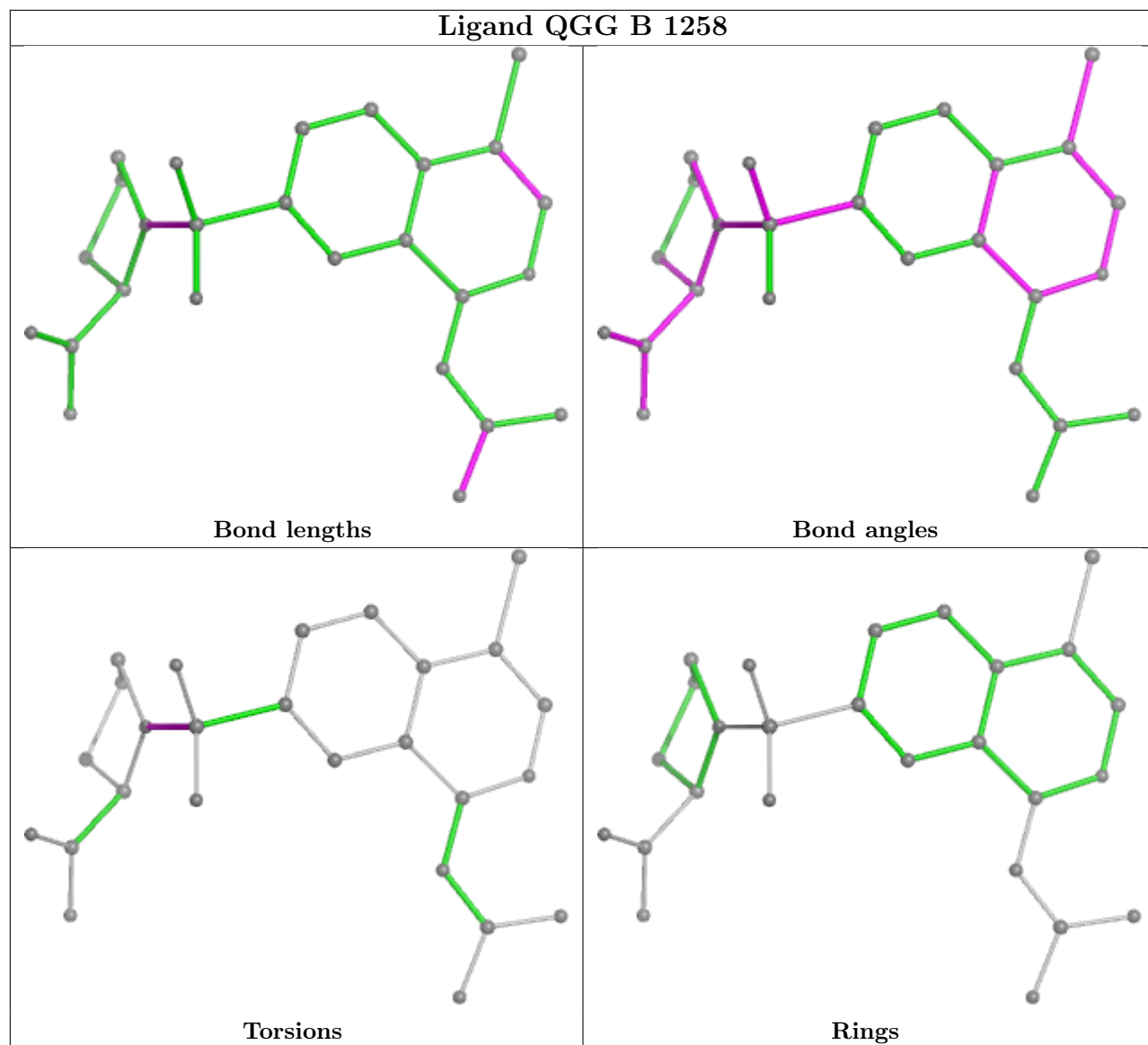
Ligand QGG A 1258
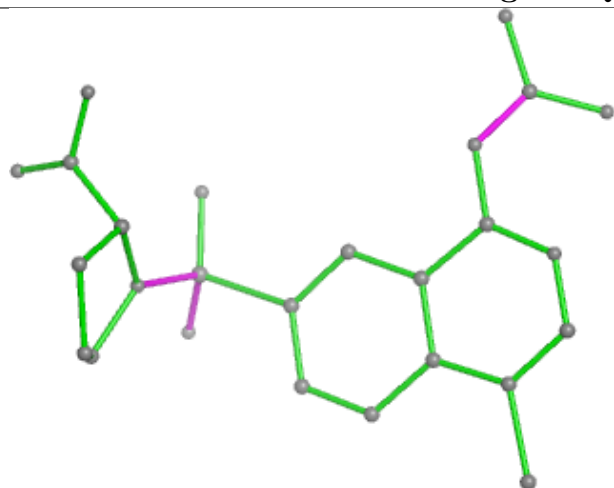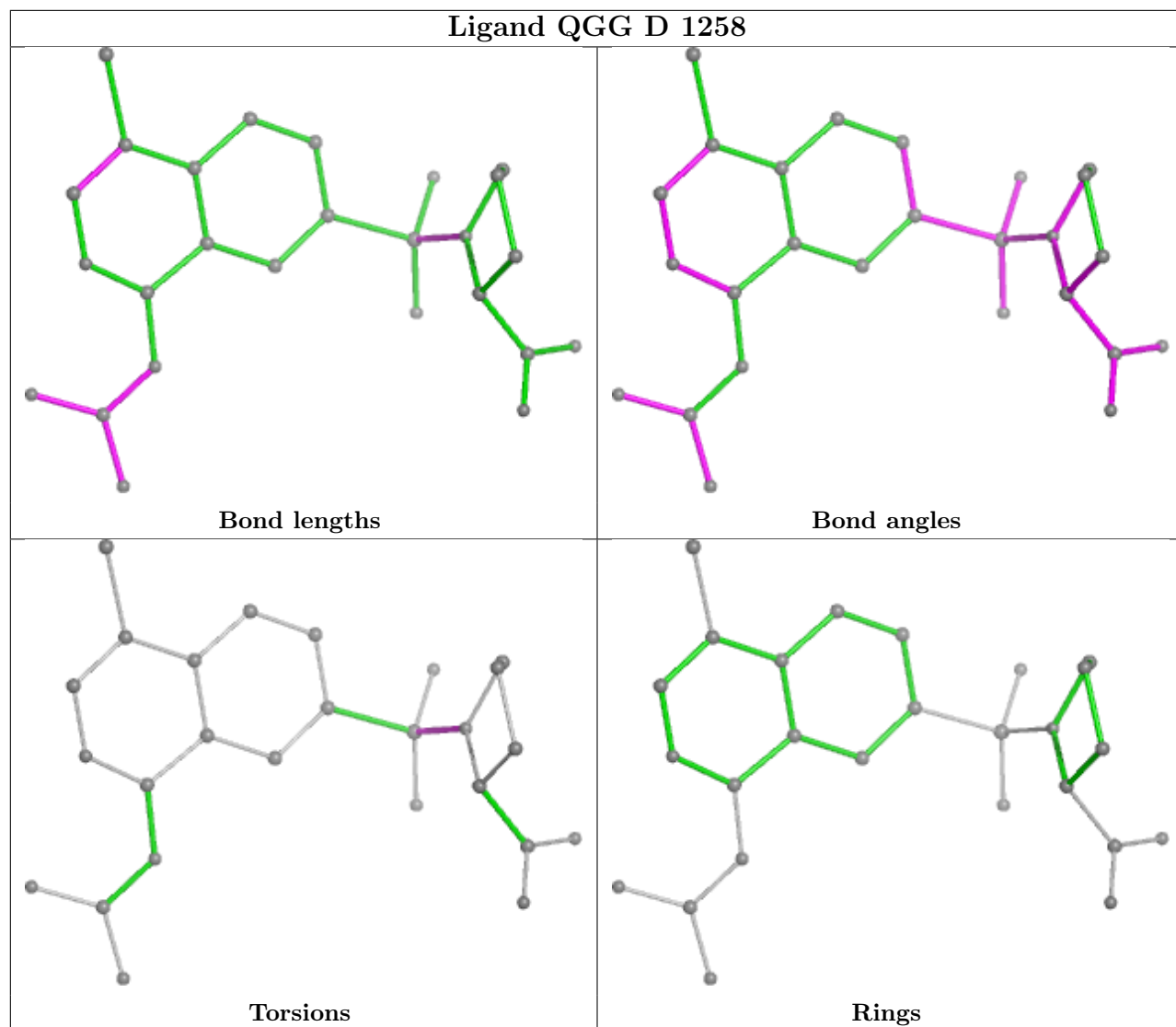

Bond lengths
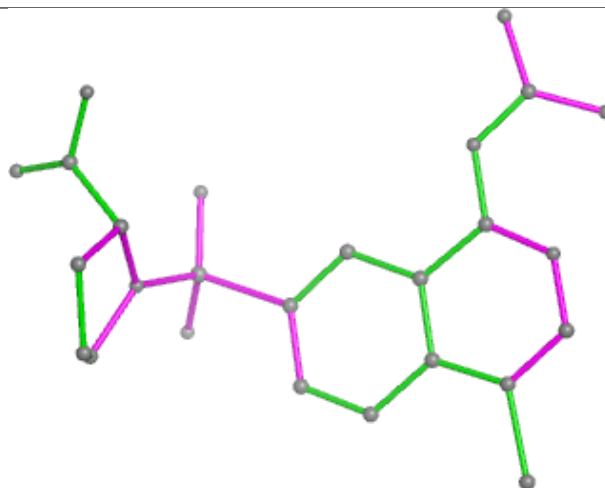
Bond angles

Torsions

Rings

Ligand QGG B 1258

Bond lengths

Bond angles

Torsions

Rings

Ligand QGG D 1258

Bond lengths

Bond angles

Torsions

Rings

Ligand QGG C 1258

Bond lengths

Bond angles

Torsions

Rings

Ligand QGG F 1258

Bond lengths

Bond angles

Torsions

Rings

Ligand QGG E 1258

Bond lengths

Bond angles

Torsions

Rings
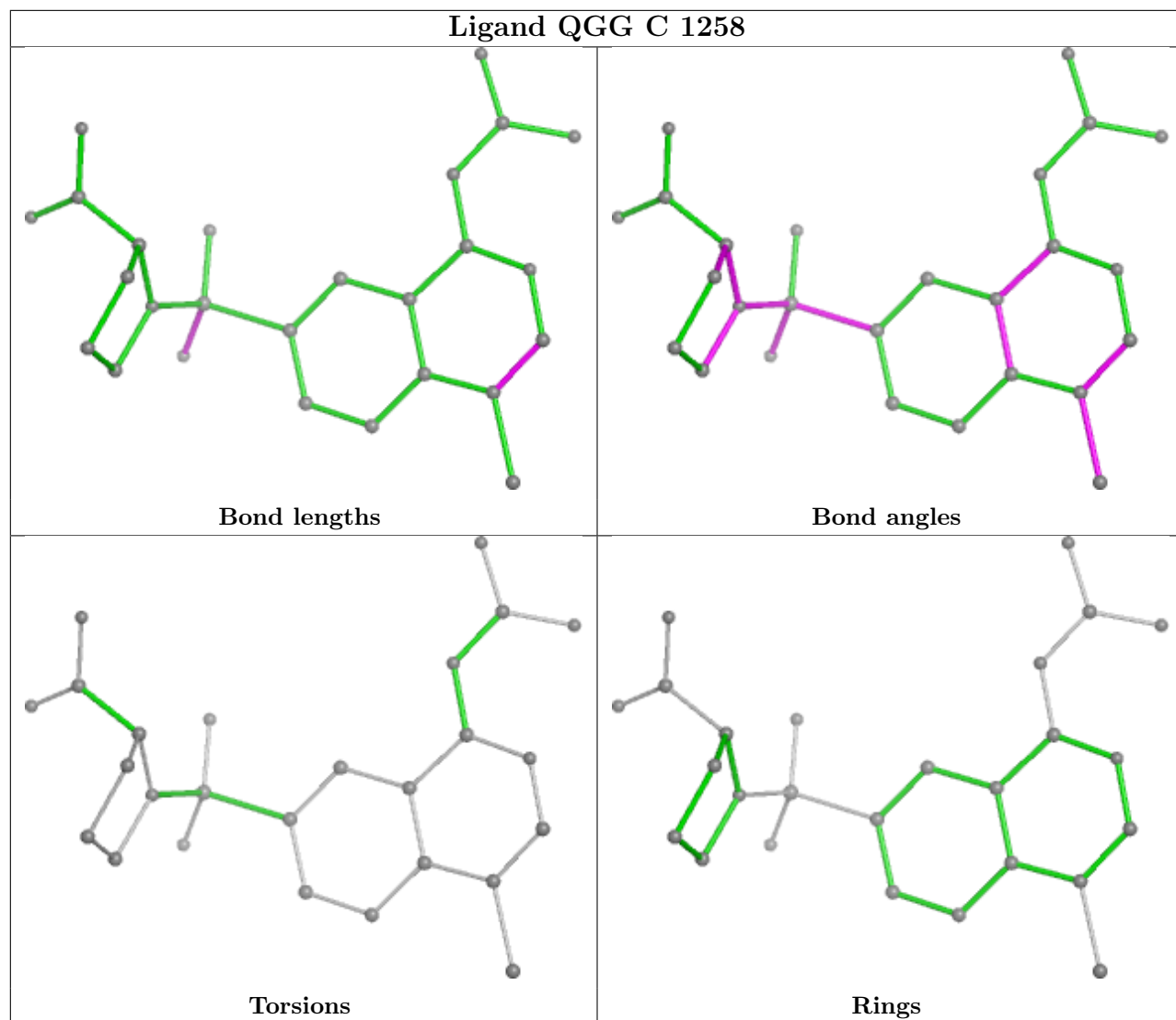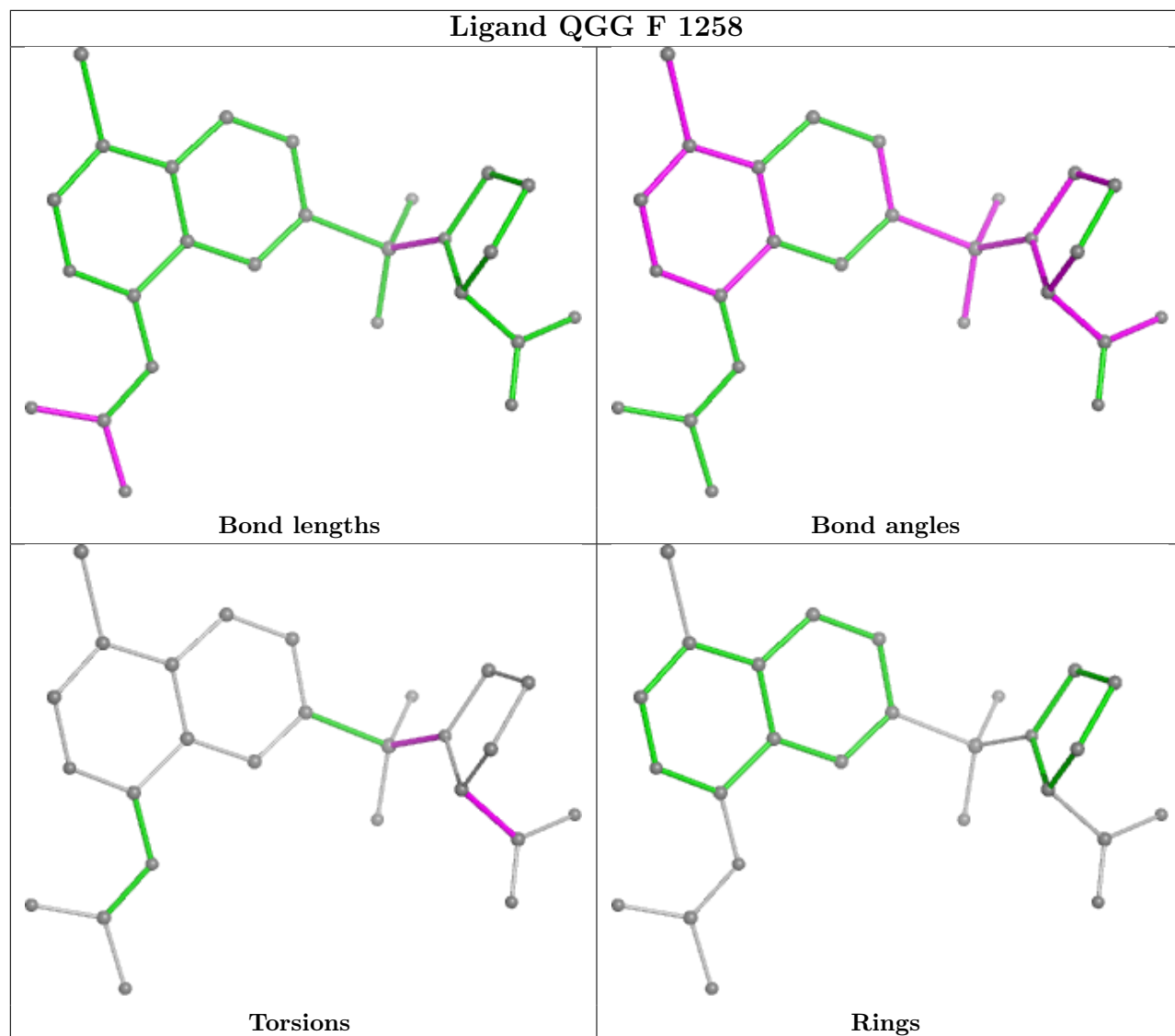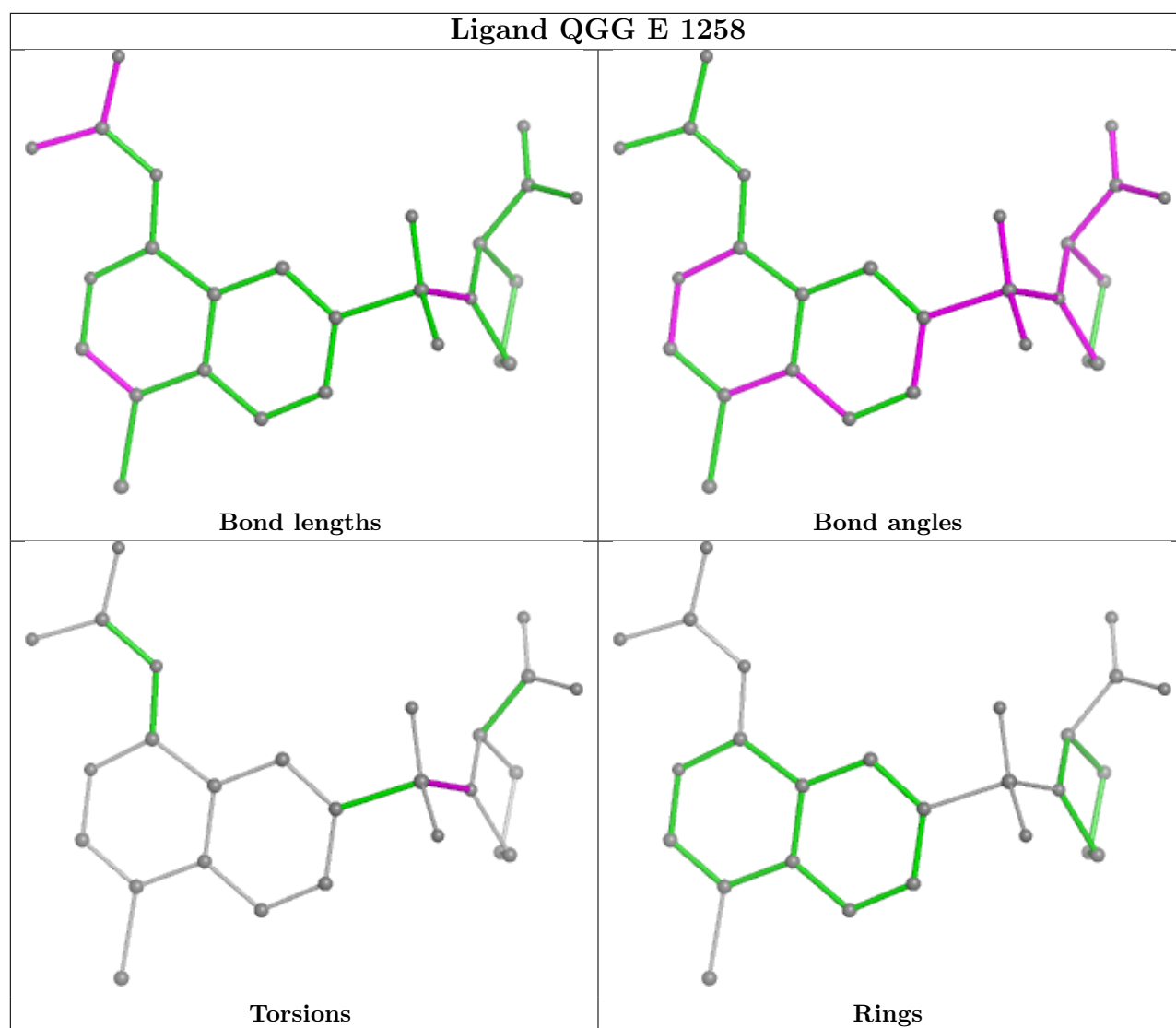
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.