



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 07:48 am BST

PDB ID : 2W0D
Title : Does a Fast Nuclear Magnetic Resonance Spectroscopy- and X-Ray Crystallography Hybrid Approach Provide Reliable Structural Information of Ligand-Protein Complexes? A Case Study of Metalloproteinases.
Authors : Isaksson, J.; Nystrom, S.; Derbyshire, D.J.; Wallberg, H.; Agback, T.; Kovacs, H.; Bertini, I.; Felli, I.C.
Deposited on : 2008-08-13
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

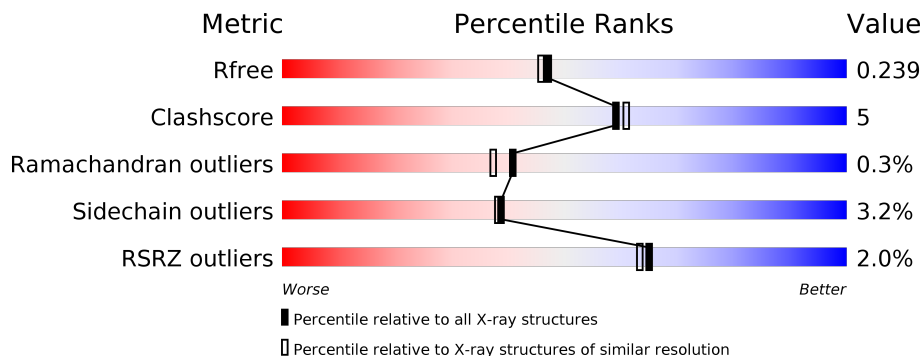
1 Overall quality at a glance i

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))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	164	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">2% 81% 13% ••</p>
1	B	164	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 88%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">3% 88% 8% ••</p>
1	C	164	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 91%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">% 91% 6% •</p>
1	D	164	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 91%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">% 91% 6% ••</p>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5911 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 MACROPHAGE METALLOELASTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	159	1276	820	222	230	4	0	9	1
1	B	159	1275	822	220	230	3	0	8	1
1	C	160	1263	808	221	230	4	0	3	1
1	D	160	1253	803	218	227	5	0	2	1

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	MET	-	expression tag	UNP P39900
A	264	HIS	-	expression tag	UNP P39900
A	265	HIS	-	expression tag	UNP P39900
A	266	HIS	-	expression tag	UNP P39900
A	267	HIS	-	expression tag	UNP P39900
A	268	HIS	-	expression tag	UNP P39900
A	219	ALA	GLU	engineered mutation	UNP P39900
B	105	MET	-	expression tag	UNP P39900
B	264	HIS	-	expression tag	UNP P39900
B	265	HIS	-	expression tag	UNP P39900
B	266	HIS	-	expression tag	UNP P39900
B	267	HIS	-	expression tag	UNP P39900
B	268	HIS	-	expression tag	UNP P39900
B	219	ALA	GLU	engineered mutation	UNP P39900
C	105	MET	-	expression tag	UNP P39900
C	264	HIS	-	expression tag	UNP P39900
C	265	HIS	-	expression tag	UNP P39900
C	266	HIS	-	expression tag	UNP P39900
C	267	HIS	-	expression tag	UNP P39900
C	268	HIS	-	expression tag	UNP P39900
C	219	ALA	GLU	engineered mutation	UNP P39900

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Chain	Residue	Modelled	Actual	Comment	Reference
D	105	MET	-	expression tag	UNP P39900
D	264	HIS	-	expression tag	UNP P39900
D	265	HIS	-	expression tag	UNP P39900
D	266	HIS	-	expression tag	UNP P39900
D	267	HIS	-	expression tag	UNP P39900
D	268	HIS	-	expression tag	UNP P39900
D	219	ALA	GLU	engineered mutation	UNP P39900

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total 2	Zn 2	0	0
2	A	3	Total 3	Zn 3	0	0
2	D	2	Total 2	Zn 2	0	0
2	C	3	Total 3	Zn 3	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

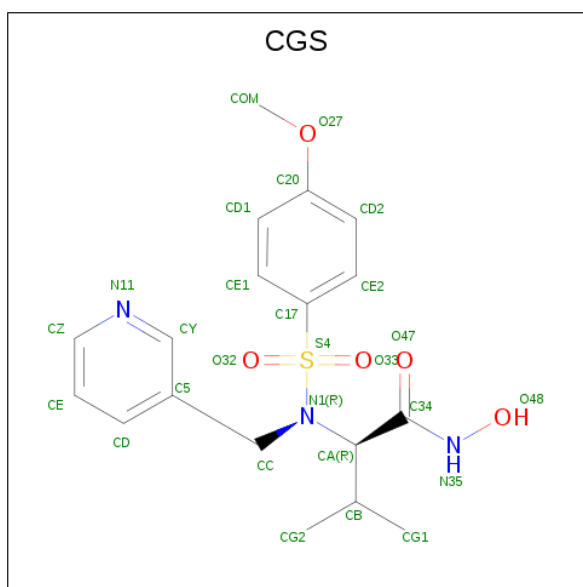
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total 3	Ca 3	0	0
3	A	3	Total 3	Ca 3	0	0
3	D	3	Total 3	Ca 3	0	0
3	C	3	Total 3	Ca 3	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

- Molecule 5 is N-HYDROXY-2(R)-[[[4-METHOXYPHENYL)SULFONYL](3-PICOLYL)AMINO]-3-METHYLBUTANAMIDE HYDROCHLORIDE (three-letter code: CGS) (formula: C₁₈H₂₃N₃O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			27	18	3	5	1		
5	B	1	Total	C	N	O	S	0	0
			27	18	3	5	1		
5	C	1	Total	C	N	O	S	0	0
			27	18	3	5	1		
5	D	1	Total	C	N	O	S	0	0
			27	18	3	5	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Cl	0	0
			1	1		
6	C	1	Total	Cl	0	0
			1	1		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Na	0	0
			1	1		

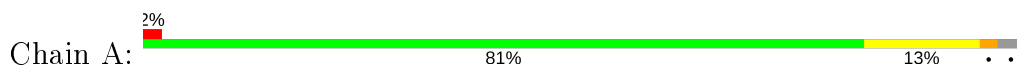
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	197	Total 197	O 197	0	0
8	B	170	Total 170	O 170	0	0
8	C	145	Total 145	O 145	0	0
8	D	171	Total 171	O 171	0	0

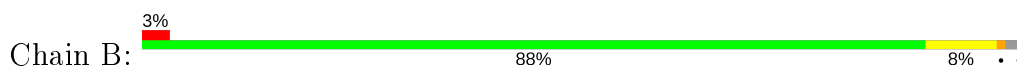
3 Residue-property plots [i](#)

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

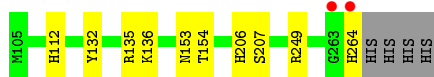
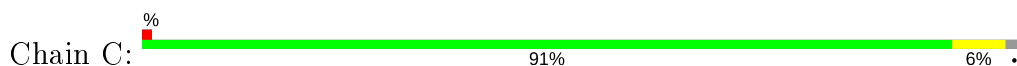
- Molecule 1: MACROPHAGE METALLOELASTASE



- Molecule 1: MACROPHAGE METALLOELASTASE



- Molecule 1: MACROPHAGE METALLOELASTASE



- Molecule 1: MACROPHAGE METALLOELASTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	38.16Å 99.94Å 79.42Å 90.00° 96.59° 90.00°	Depositor
Resolution (Å)	33.71 – 2.00 33.71 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (33.71-2.00) 97.3 (33.71-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.65 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.179 , 0.237 0.181 , 0.239	Depositor DCC
R_{free} test set	1948 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	12.0	Xtrriage
Anisotropy	0.148	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5911	wwPDB-VP
Average B, all atoms (Å ²)	5.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.98% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CL, NA, CA, ACT, CGS

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	0.51	0/1336	0.65	1/1810 (0.1%)
1	B	0.55	0/1339	0.64	0/1816
1	C	0.54	0/1308	0.61	1/1775 (0.1%)
1	D	0.54	0/1297	0.64	0/1758
All	All	0.54	0/5280	0.63	2/7159 (0.0%)

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	GLY	O-C-N	-5.20	114.38	122.70
1	C	249	ARG	CA-CB-CG	5.09	124.60	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	106	GLY	Peptide

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	1276	0	1229	18	0
1	B	1275	0	1227	19	0
1	C	1263	0	1196	6	0
1	D	1253	0	1194	5	0
2	A	3	0	0	0	0
2	B	2	0	0	0	0
2	C	3	0	0	0	0
2	D	2	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
4	A	12	0	9	1	0
4	C	8	0	6	0	0
4	D	8	0	6	0	0
5	A	27	0	22	0	0
5	B	27	0	22	0	0
5	C	27	0	22	0	0
5	D	27	0	22	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	D	1	0	0	0	0
8	A	197	0	0	9	0
8	B	170	0	0	7	0
8	C	145	0	0	4	0
8	D	171	0	0	3	0
All	All	5911	0	4955	48	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 5.

All (48) 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:D:126:ASN:HB3	8:D:2026:HOH:O	1.40	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235[A]:VAL:HG23	8:B:2127:HOH:O	1.50	1.10
1:B:112[A]:HIS:CD2	1:B:113[A]:TYR:CE1	2.45	1.03
1:B:112[A]:HIS:CD2	1:B:113[A]:TYR:CD1	2.52	0.97
1:A:150[A]:SER:OG	8:A:2048:HOH:O	1.83	0.93
1:B:112[A]:HIS:HD2	1:B:113[A]:TYR:CE1	1.91	0.84
1:A:262:TYR:O	1:A:264:HIS:N	2.21	0.74
1:B:113[A]:TYR:CZ	8:B:2006:HOH:O	2.42	0.72
1:B:112[A]:HIS:HD2	1:B:113[A]:TYR:HE1	1.41	0.69
1:A:153:ASN:ND2	8:A:2052:HOH:O	2.29	0.66
1:B:110:ARG:NH2	8:B:2004:HOH:O	2.30	0.64
1:C:135:ARG:NH1	8:C:2027:HOH:O	2.33	0.61
1:A:112[B]:HIS:HD2	8:A:2011:HOH:O	1.85	0.60
1:B:244:ASP:OD1	1:B:246:ASN:HB3	2.03	0.58
1:B:112[A]:HIS:NE2	1:B:113[A]:TYR:CE1	2.72	0.57
1:B:112[A]:HIS:CD2	1:B:113[A]:TYR:HE1	2.10	0.56
1:A:177[A]:LYS:HD2	8:A:2101:HOH:O	2.06	0.55
1:A:231:ASP:OD2	1:A:233:LYS:HG2	2.07	0.54
1:A:165:ARG:NH2	8:A:2075:HOH:O	2.39	0.53
1:A:191:ILE:HD13	4:A:1270:ACT:H2	1.91	0.53
1:B:249:ARG:HD3	8:B:2156:HOH:O	2.08	0.52
1:B:150[A]:SER:OG	8:B:2046:HOH:O	2.18	0.51
1:A:145:THR:HB	1:A:146:PRO:HD2	1.94	0.51
1:A:177[A]:LYS:HG3	1:A:200:ASP:O	2.11	0.50
1:B:177[A]:LYS:HD3	1:B:200:ASP:O	2.12	0.49
1:C:153:ASN:O	8:C:2043:HOH:O	2.19	0.49
1:A:208[B]:GLY:O	1:A:209[B]:GLY:C	2.51	0.49
1:B:112[A]:HIS:CD2	1:B:113[A]:TYR:HD1	2.22	0.49
1:D:264:HIS:N	8:D:2164:HOH:O	2.47	0.48
1:B:113[A]:TYR:CE1	8:B:2006:HOH:O	2.65	0.47
1:C:112:HIS:ND1	8:C:2014:HOH:O	2.18	0.47
1:A:106:GLY:N	8:A:2002:HOH:O	2.48	0.47
1:A:213:PHE:CD1	1:A:245:ILE:HG12	2.51	0.46
1:D:117:ARG:HD2	1:D:155:GLY:O	2.15	0.46
1:D:251:SER:HB2	8:D:2130:HOH:O	2.15	0.46
1:B:112[A]:HIS:HD2	1:B:113[A]:TYR:CD1	2.15	0.45
1:D:156[B]:MET:HE1	1:D:160:LEU:HD22	1.98	0.45
1:B:151:LYS:NZ	1:B:153:ASN:OD1	2.52	0.42
1:C:264:HIS:N	8:C:2139:HOH:O	2.52	0.42
1:A:177[A]:LYS:NZ	8:A:2102:HOH:O	0.70	0.41
1:C:206[B]:HIS:H	1:C:206[B]:HIS:CD2	2.37	0.41
1:C:132:TYR:CE1	1:C:136:LYS:HE3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ARG:NH2	8:A:2029:HOH:O	2.54	0.41
1:A:177[B]:LYS:HD3	8:A:2131:HOH:O	2.20	0.41
1:A:235[B]:VAL:HG11	1:A:250:LEU:HD23	2.03	0.41
1:B:235[A]:VAL:CG2	8:B:2127:HOH:O	2.31	0.41
1:A:233:LYS:HG2	1:A:233:LYS:HZ2	1.82	0.41
1:B:247:THR:HG22	1:B:247:THR:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	166/164 (101%)	158 (95%)	7 (4%)	1 (1%)	25	19
1	B	165/164 (101%)	161 (98%)	4 (2%)	0	100	100
1	C	161/164 (98%)	157 (98%)	4 (2%)	0	100	100
1	D	160/164 (98%)	156 (98%)	3 (2%)	1 (1%)	25	19
All	All	652/656 (99%)	632 (97%)	18 (3%)	2 (0%)	41	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	GLY
1	D	244	ASP

5.3.2 Protein sidechains [i](#)

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	133/132 (101%)	124 (93%)	9 (7%)	16	11
1	B	134/132 (102%)	130 (97%)	4 (3%)	41	41
1	C	130/132 (98%)	128 (98%)	2 (2%)	65	69
1	D	129/132 (98%)	125 (97%)	4 (3%)	40	40
All	All	526/528 (100%)	507 (96%)	19 (4%)	39	34

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	ASN
1	A	150[A]	SER
1	A	150[B]	SER
1	A	154	THR
1	A	230[A]	SER
1	A	230[B]	SER
1	A	233	LYS
1	A	244	ASP
1	A	245	ILE
1	B	150[A]	SER
1	B	150[B]	SER
1	B	245	ILE
1	B	249	ARG
1	C	154	THR
1	C	207	SER
1	D	117	ARG
1	D	127	ARG
1	D	154	THR
1	D	245	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	ASN
1	A	246	ASN
1	B	119	ASN
1	C	139	GLN
1	C	153	ASN
1	D	206	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 25 are monoatomic - leaving 11 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	ACT	C	1272	2	1,3,3	1.59	0	0,3,3	0.00	-
5	CGS	A	1273	2	28,28,28	0.77	1 (3%)	37,39,39	1.11	1 (2%)
5	CGS	D	1273	2	28,28,28	0.83	1 (3%)	37,39,39	1.00	2 (5%)
5	CGS	C	1273	2	28,28,28	0.84	1 (3%)	37,39,39	1.34	4 (10%)
4	ACT	C	1270	2	1,3,3	0.83	0	0,3,3	0.00	-
4	ACT	A	1270	2	1,3,3	1.35	0	0,3,3	0.00	-
4	ACT	D	1272	-	1,3,3	1.40	0	0,3,3	0.00	-
4	ACT	A	1271	2	1,3,3	1.46	0	0,3,3	0.00	-
4	ACT	D	1271	-	1,3,3	2.01	1 (100%)	0,3,3	0.00	-
5	CGS	B	1269	2	28,28,28	0.82	1 (3%)	37,39,39	1.07	3 (8%)
4	ACT	A	1272	-	1,3,3	1.36	0	0,3,3	0.00	-

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
5	CGS	A	1273	2	-	1/32/32/32	0/2/2/2
5	CGS	C	1273	2	-	0/32/32/32	0/2/2/2
5	CGS	B	1269	2	-	1/32/32/32	0/2/2/2
5	CGS	D	1273	2	-	1/32/32/32	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1273	CGS	CY-N11	2.44	1.39	1.34
5	A	1273	CGS	CY-N11	2.36	1.39	1.34
5	C	1273	CGS	CY-N11	2.23	1.39	1.34
5	B	1269	CGS	CY-N11	2.21	1.39	1.34
4	D	1271	ACT	CH3-C	2.01	1.51	1.48

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1273	CGS	CC-N1-S4	4.28	124.89	117.89
5	A	1273	CGS	CC-N1-S4	4.12	124.63	117.89
5	D	1273	CGS	CC-N1-S4	3.21	123.14	117.89
5	B	1269	CGS	CC-N1-S4	3.10	122.96	117.89
5	C	1273	CGS	COM-O27-C20	2.97	123.97	117.51
5	B	1269	CGS	C5-CC-N1	2.83	118.34	113.48
5	B	1269	CGS	COM-O27-C20	2.69	123.35	117.51
5	C	1273	CGS	C5-CC-N1	2.66	118.05	113.48
5	C	1273	CGS	O33-S4-O32	-2.44	115.56	119.52
5	D	1273	CGS	COM-O27-C20	2.02	121.89	117.51

There are no chirality outliers.

All (3) torsion outliers are listed below:

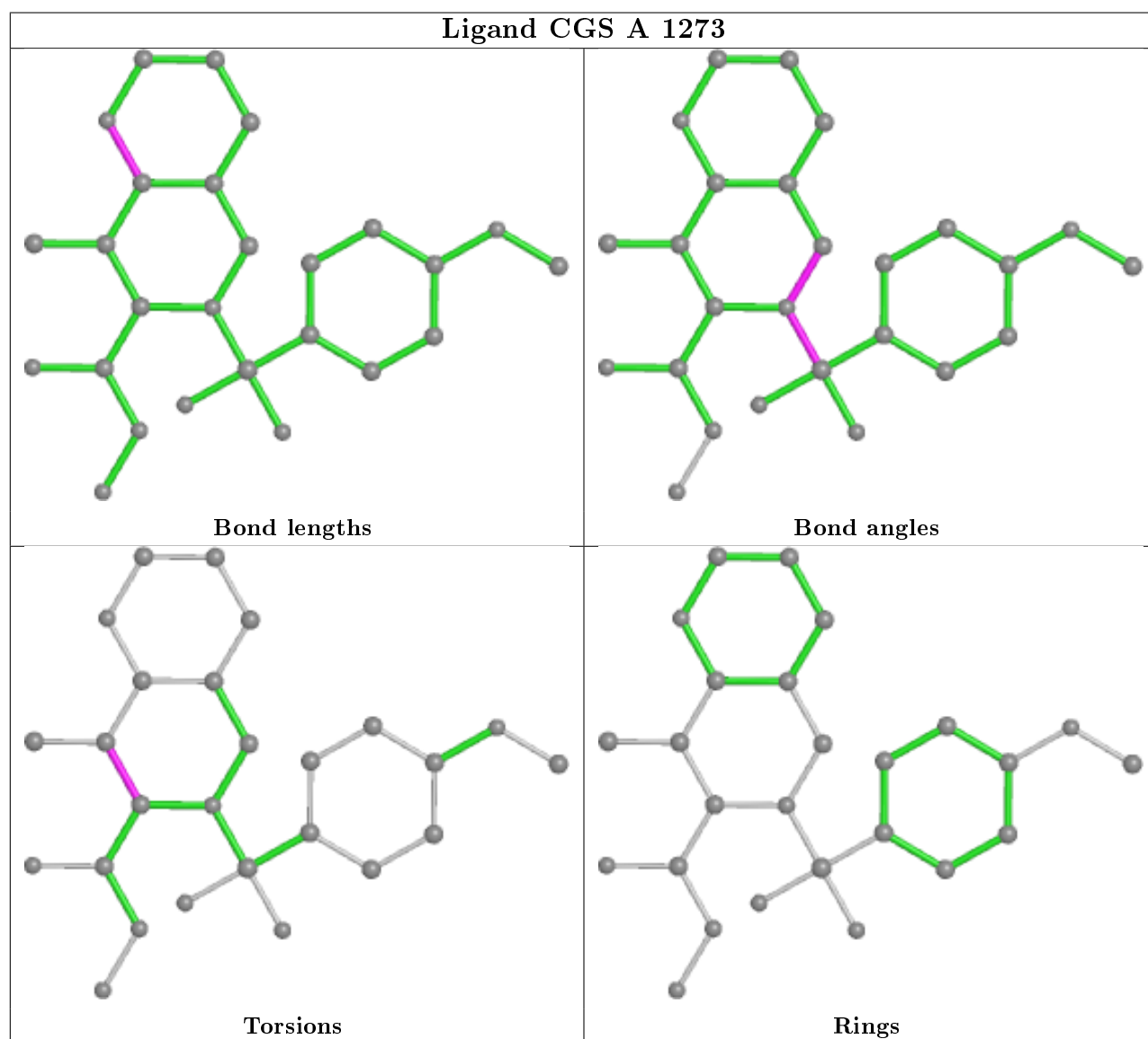
Mol	Chain	Res	Type	Atoms
5	D	1273	CGS	C34-CA-CB-CG1
5	B	1269	CGS	C34-CA-CB-CG1
5	A	1273	CGS	C34-CA-CB-CG1

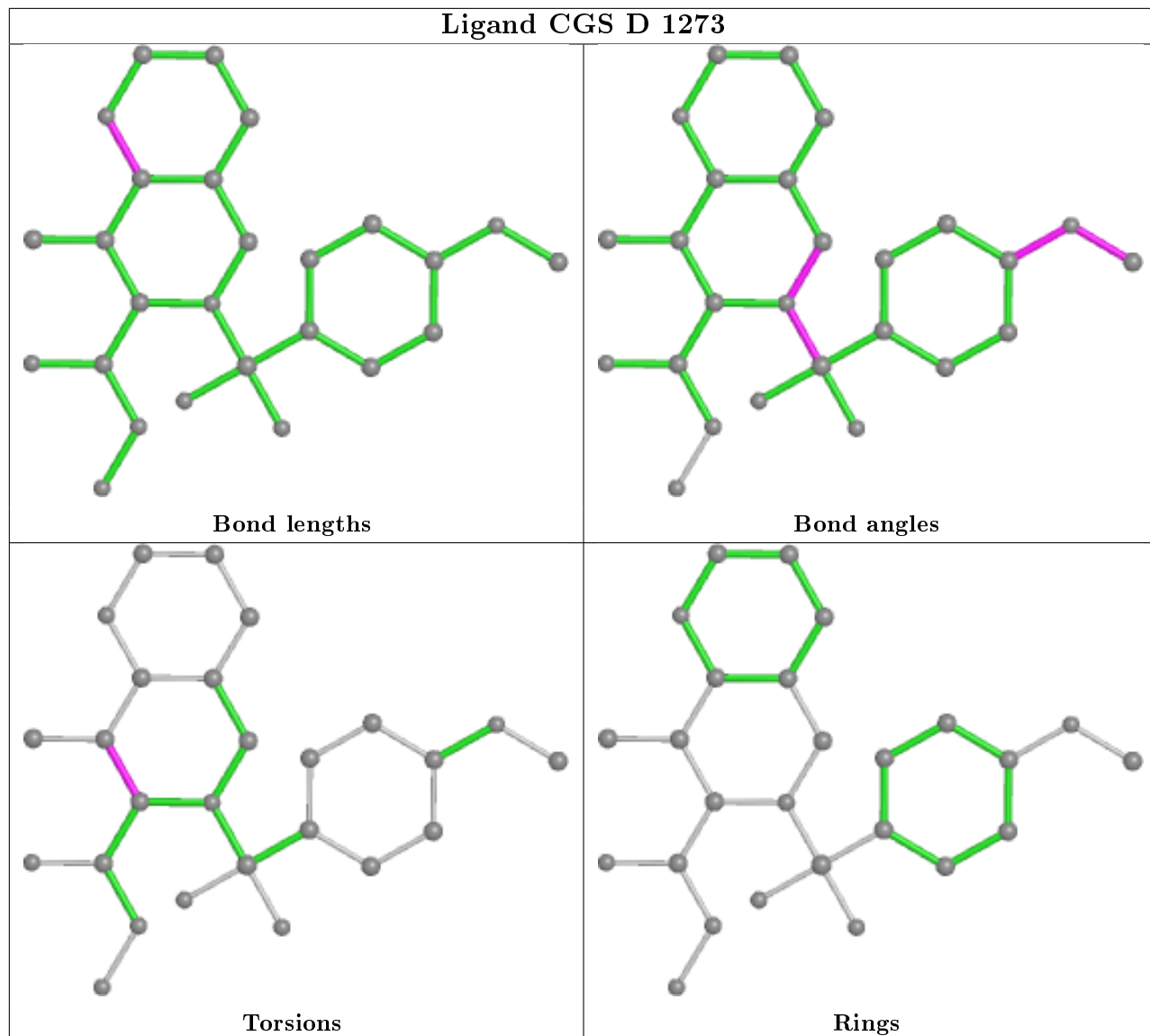
There are no ring outliers.

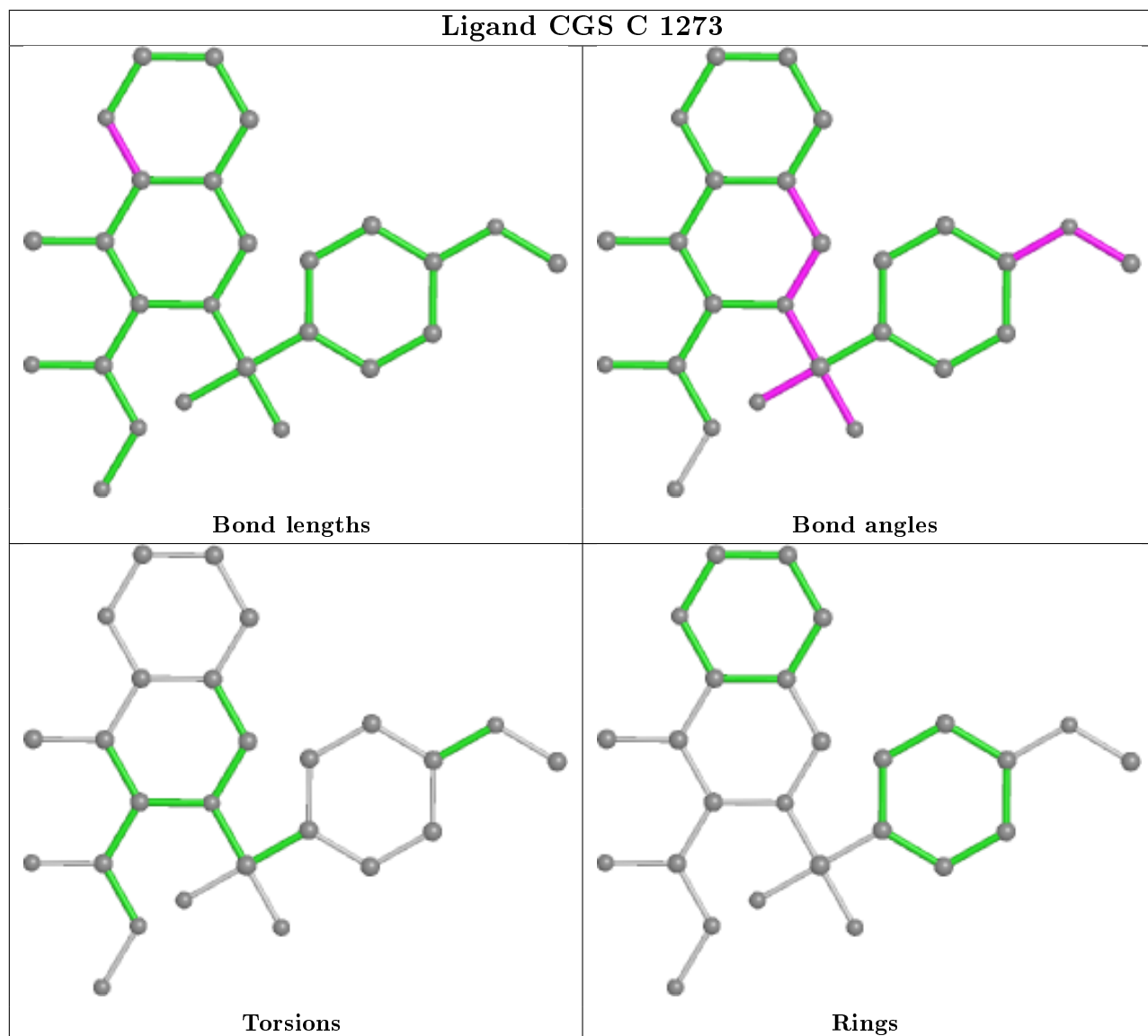
1 monomer is involved in 1 short contact:

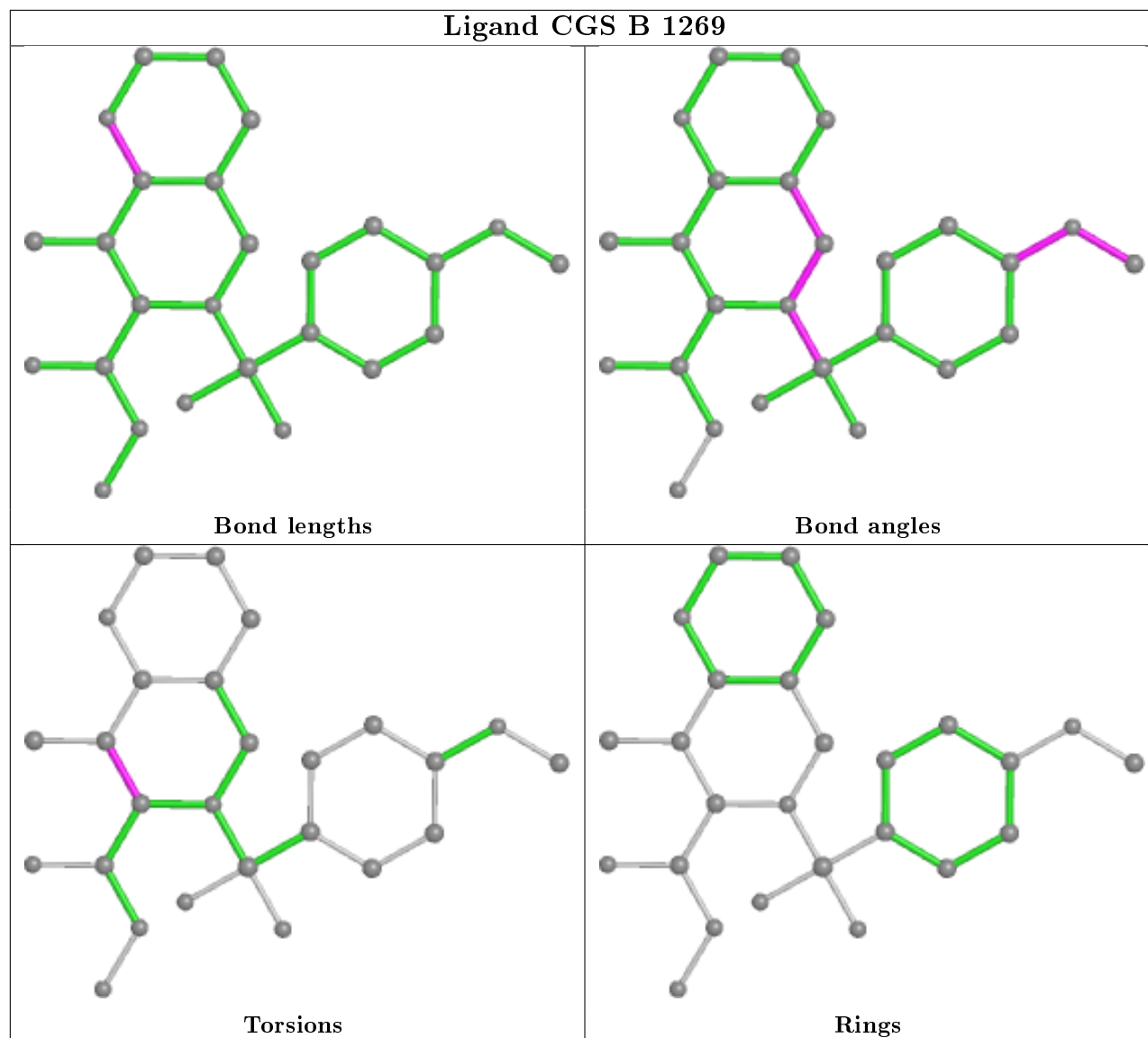
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1270	ACT	1	0

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.









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	159/164 (96%)	-0.03	4 (2%) 57 56	3, 5, 9, 12	0
1	B	159/164 (96%)	-0.19	5 (3%) 49 48	3, 5, 10, 12	0
1	C	160/164 (97%)	-0.06	2 (1%) 77 76	2, 5, 10, 13	0
1	D	160/164 (97%)	-0.28	2 (1%) 77 76	3, 5, 9, 11	0
All	All	638/656 (97%)	-0.14	13 (2%) 65 63	2, 5, 10, 13	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	264	HIS	9.1
1	D	264	HIS	6.2
1	B	106	GLY	5.4
1	A	264	HIS	5.1
1	A	263	GLY	4.8
1	A	245	ILE	4.5
1	B	263	GLY	3.5
1	B	264	HIS	3.3
1	C	263	GLY	2.8
1	A	247	THR	2.5
1	B	110	ARG	2.3
1	D	249	ARG	2.1
1	B	246	ASN	2.0

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 carbohydrates 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.

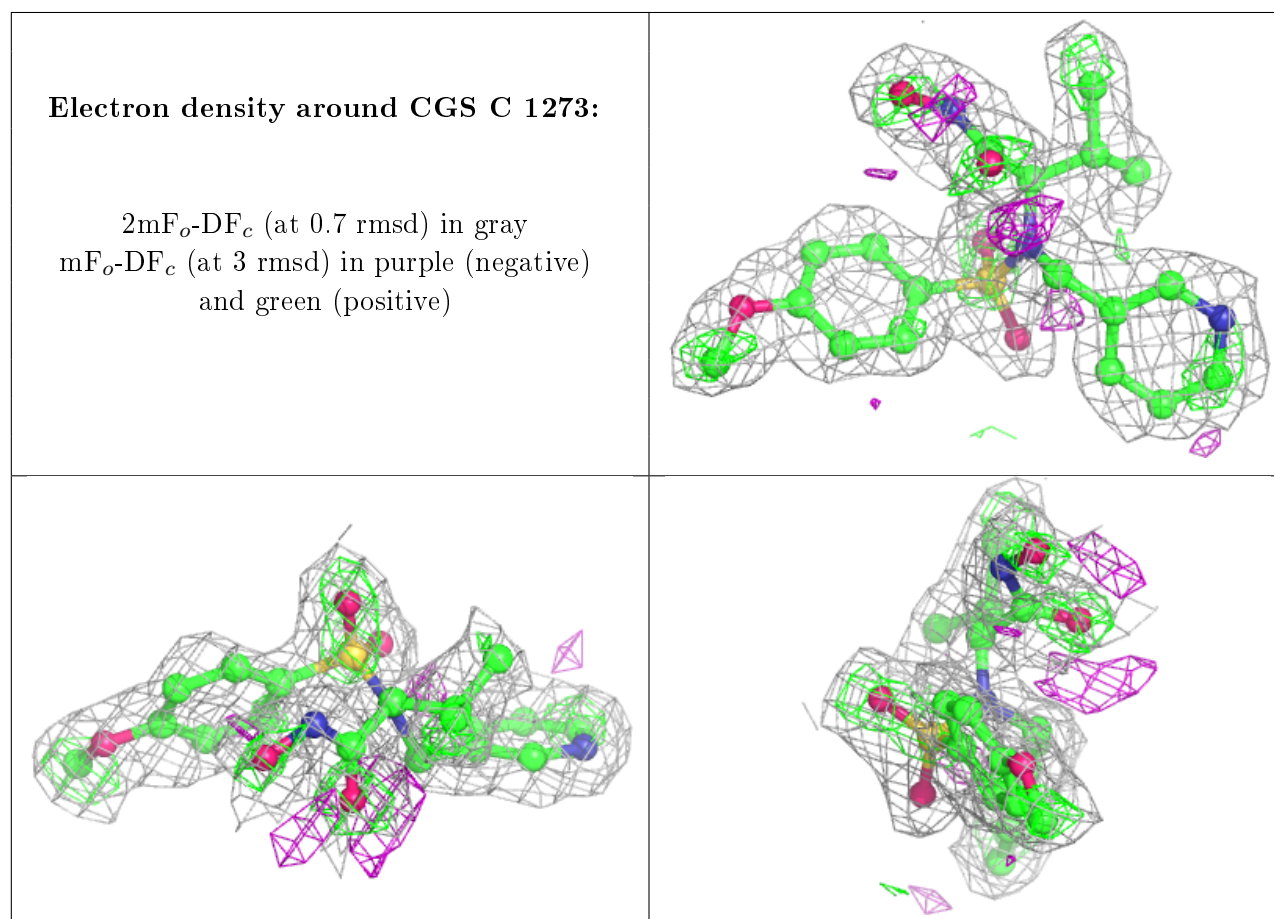
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	CGS	C	1273	27/27	0.89	0.24	3,4,5,5	0
4	ACT	A	1272	4/4	0.90	0.13	17,17,17,17	0
5	CGS	A	1273	27/27	0.92	0.20	2,4,5,5	0
4	ACT	D	1271	4/4	0.93	0.17	10,10,10,10	0
5	CGS	D	1273	27/27	0.94	0.13	3,4,5,6	0
5	CGS	B	1269	27/27	0.95	0.13	3,4,5,6	0
4	ACT	C	1272	4/4	0.95	0.16	11,12,12,13	0
4	ACT	D	1272	4/4	0.95	0.13	2,2,2,2	0
4	ACT	A	1271	4/4	0.96	0.10	7,7,8,8	0
4	ACT	C	1270	4/4	0.97	0.10	2,2,2,2	0
6	CL	C	1271	1/1	0.98	0.06	2,2,2,2	0
7	NA	D	1270	1/1	0.98	0.12	8,8,8,8	0
6	CL	D	1269	1/1	0.98	0.11	2,2,2,2	0
3	CA	A	1267	1/1	0.99	0.16	4,4,4,4	0
3	CA	C	1268	1/1	0.99	0.07	4,4,4,4	0
3	CA	D	1268	1/1	0.99	0.04	5,5,5,5	0
3	CA	B	1268	1/1	0.99	0.11	6,6,6,6	0
3	CA	A	1268	1/1	0.99	0.16	6,6,6,6	0
3	CA	A	1266	1/1	0.99	0.04	4,4,4,4	0
3	CA	B	1267	1/1	0.99	0.02	5,5,5,5	0
3	CA	C	1266	1/1	0.99	0.03	4,4,4,4	0
4	ACT	A	1270	4/4	0.99	0.06	3,3,3,3	0
2	ZN	A	1264	1/1	1.00	0.01	5,5,5,5	0
2	ZN	B	1265	1/1	1.00	0.01	5,5,5,5	0
2	ZN	C	1265	1/1	1.00	0.01	6,6,6,6	0
2	ZN	C	1269	1/1	1.00	0.06	3,3,3,3	0
2	ZN	B	1264	1/1	1.00	0.01	6,6,6,6	0
2	ZN	D	1265	1/1	1.00	0.01	5,5,5,5	0
2	ZN	A	1269	1/1	1.00	0.05	3,3,3,3	0
3	CA	B	1266	1/1	1.00	0.03	4,4,4,4	0
2	ZN	D	1264	1/1	1.00	0.01	6,6,6,6	0
3	CA	D	1267	1/1	1.00	0.02	5,5,5,5	0

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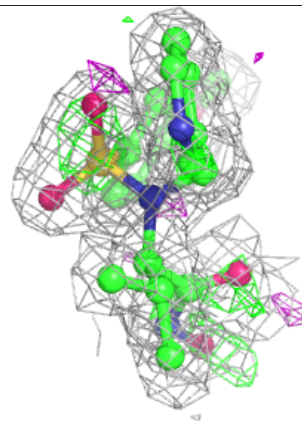
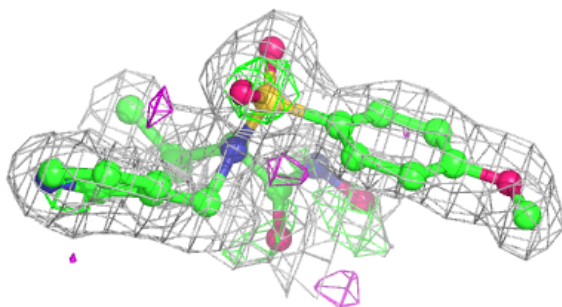
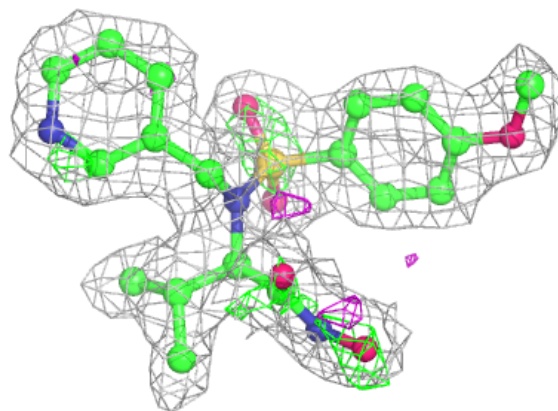
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CA	C	1267	1/1	1.00	0.12	5,5,5,5	0
2	ZN	C	1264	1/1	1.00	0.02	5,5,5,5	0
3	CA	D	1266	1/1	1.00	0.01	4,4,4,4	0
2	ZN	A	1265	1/1	1.00	0.01	5,5,5,5	0

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.



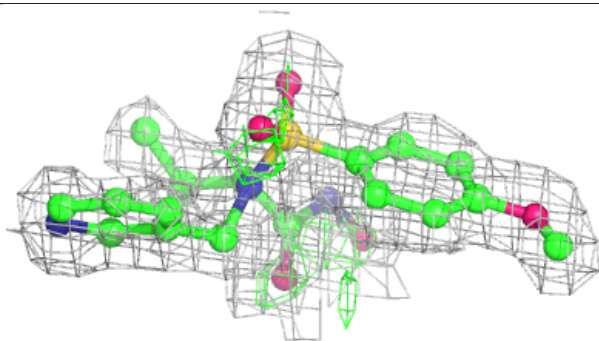
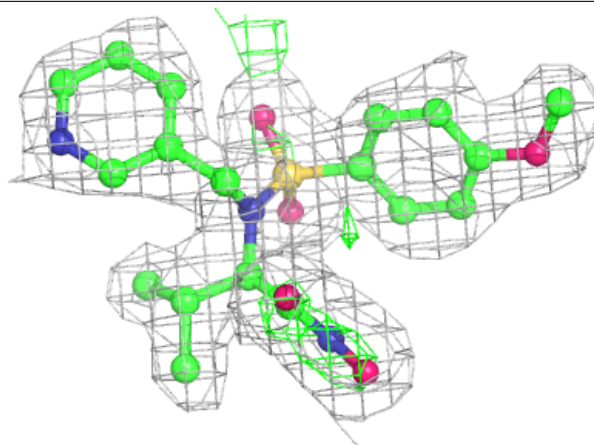
Electron density around CGS A 1273:

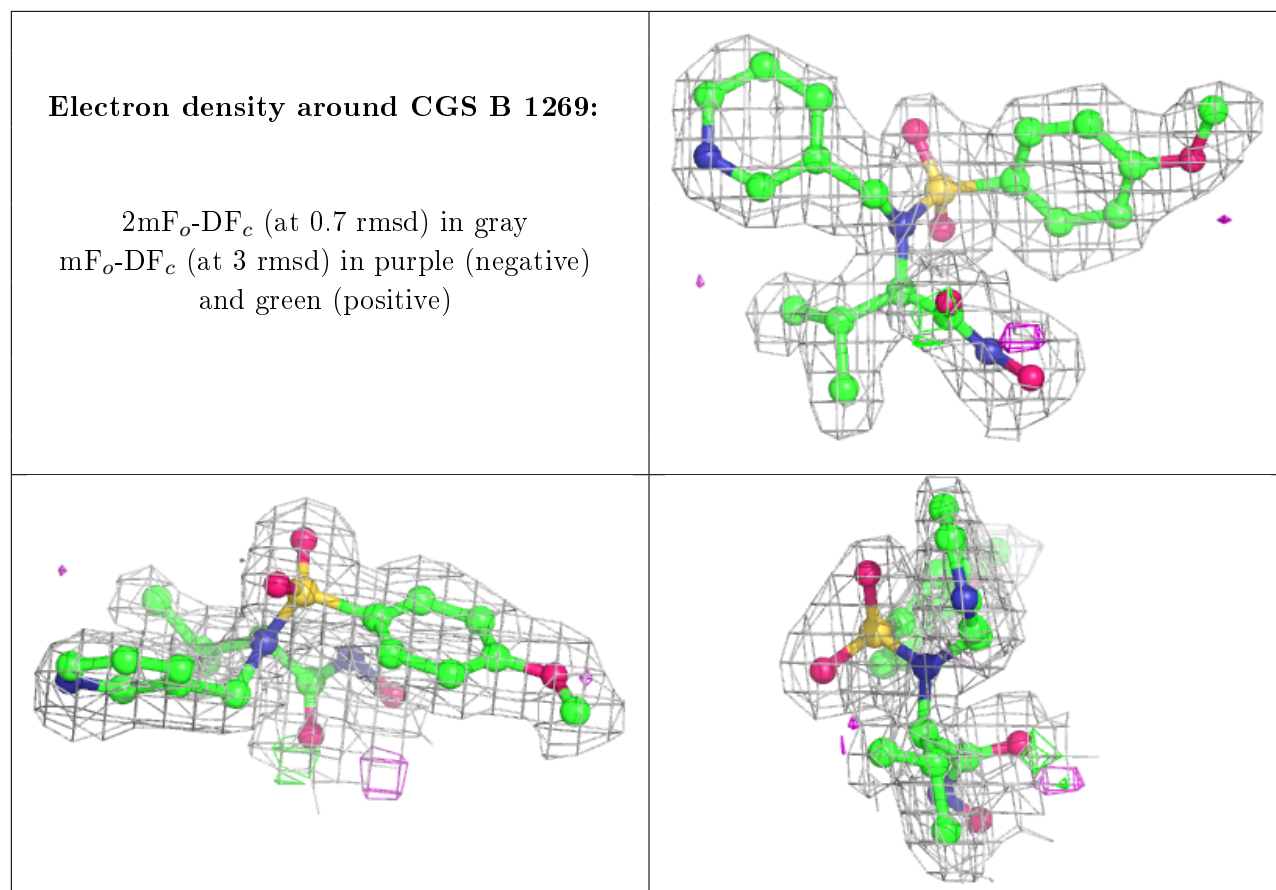
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CGS D 1273:

$2mF_o-DF_c$ (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.