



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 25, 2020 – 03:35 PM BST

PDB ID : 5H8Y
Title : Crystal structure of the complex between maize sulfite reductase and ferredoxin in the form-2 crystal
Authors : Kurisu, G.; Nakayama, M.; Hase, T.
Deposited on : 2015-12-25
Resolution : 2.20 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 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 : 2.13
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) : 2.13

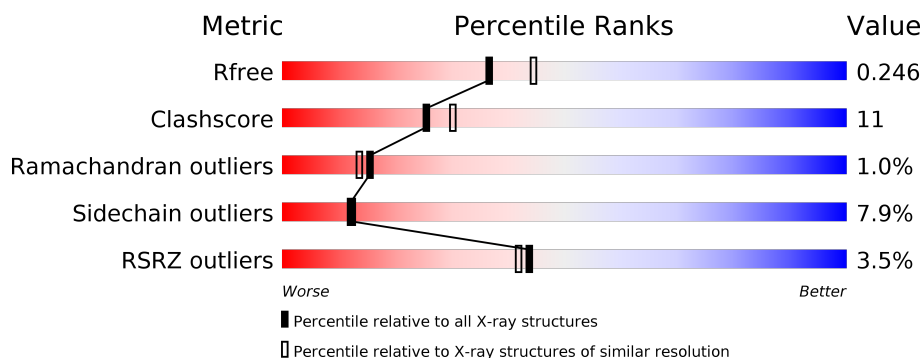
1 Overall quality at a glance ⓘ

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 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	583	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 76% 16% • • • </div> </div>
1	B	583	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 78% 14% • • • </div> </div>
1	C	583	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 77% 14% 5% • • </div> </div>
1	D	583	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 77% 13% • • 5% </div> </div>
2	E	98	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 78% 17% • • </div> </div>
2	F	98	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 51% 23% • • 26% </div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 19620 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.

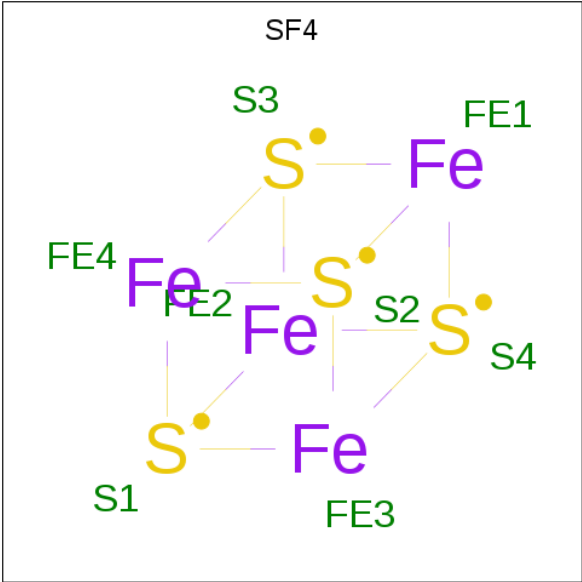
- Molecule 1 is a protein called Sulfite reductase [ferredoxin], chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	567	Total	C	N	O	S	0	0	0
			4458	2831	770	840	17			
1	B	565	Total	C	N	O	S	0	0	0
			4455	2829	772	838	16			
1	C	563	Total	C	N	O	S	0	0	0
			4429	2816	768	828	17			
1	D	554	Total	C	N	O	S	0	0	0
			4365	2777	754	818	16			

- Molecule 2 is a protein called Ferredoxin-1, chloroplastic.

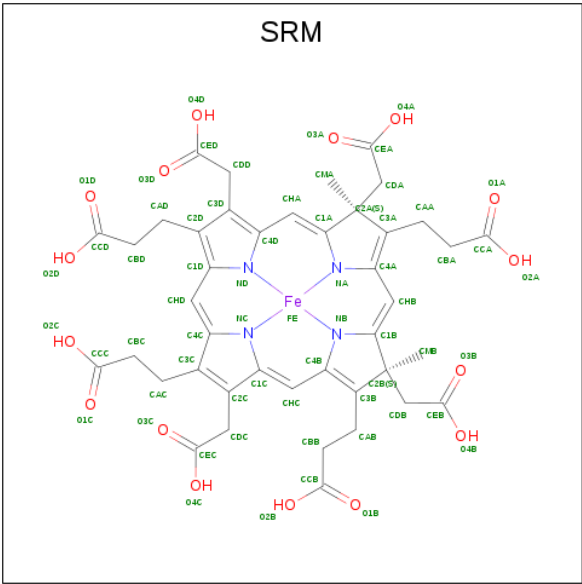
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	96	Total	C	N	O	S	0	0	0
			726	447	113	162	4			
2	F	73	Total	C	N	O	S	0	0	0
			495	302	86	103	4			

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 4 is SIROHEME (three-letter code: SRM) (formula: $C_{42}H_{42}FeN_4O_{16}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		
4	B	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		
4	C	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		
4	D	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		

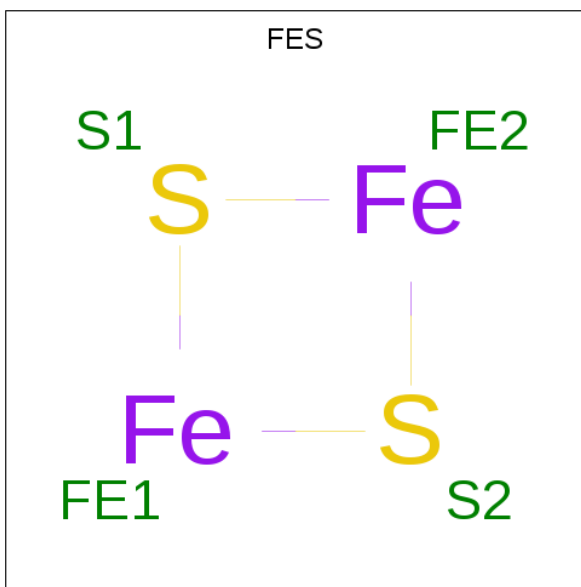
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

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

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

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).




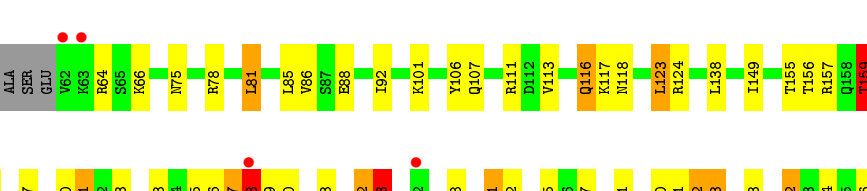
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	E	1	Total	Fe	S	0	0
			4	2	2		
7	F	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	118	Total	O	0	0
			118	118		
8	B	124	Total	O	0	0
			124	124		
8	C	77	Total	O	0	0
			77	77		
8	D	66	Total	O	0	0
			66	66		
8	E	7	Total	O	0	0
			7	7		

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.

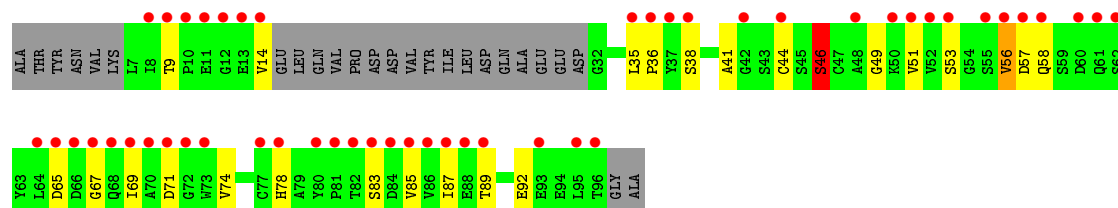
- Chain A: 



Residue	Percentage (%)
C540	76%
R364	76%
K365	76%
M369	76%
M372	76%
I373	76%
R374	76%
R375	76%
W376	76%
D379	76%
R380	76%
F381	76%
R382	76%
V385	76%
K392	76%
W402	76%
K417	76%
H423	76%
G431	76%
Q432	76%
R438	76%
P486	76%
A491	76%
L497	76%
P498	76%
L499	76%
A503	76%
Q504	76%
T505	76%
I511	76%
L512	76%
K516	76%
R517	76%
I518	76%
R519	76%
K528	76%
D529	76%
S532	76%
V533	76%
V534	76%
V535	76%
C188	76%
G189	76%
D190	76%
L191	76%
A197	76%
I217	76%
L220	76%
L221	76%
T222	76%
P223	76%
V233	76%
D234	76%
G235	76%
E236	76%
P237	76%
L238	76%
M239	76%
S240	76%
E243	76%
N252	76%
D253	76%
D262	76%
Y268	76%
Q271	76%
Y272	76%
R275	76%
E276	76%
F277	76%
V281	76%
D290	76%
I291	76%
L292	76%
T293	76%
D303	76%
T322	76%
H323	76%
R324	76%
V325	76%
E326	76%
L332	76%
I348	76%
Q355	76%
R356	76%
ALA	16%
PRO	16%
ALA	16%
LVS	16%
LVS	16%
ASP	16%
ALA	16%
SER	16%
GLU	16%
V62	16%
V63	16%
R64	16%
S65	16%
R66	16%
N75	16%
R78	16%
L81	16%
L85	16%
V86	16%
S87	16%
E88	16%
I92	16%
K101	16%
Y106	16%
Q107	16%
R111	16%
D112	16%
V113	16%
Q116	16%
K117	16%
N118	16%
L123	16%
R124	16%
L138	16%
I149	16%
T155	16%
T156	16%
R157	16%
Q158	16%
T159	16%
F160	16%
L170	16%
T184	16%
L185	16%

- Chain B: 
- | Label | Color |
|-------|--------|
| K365 | Yellow |
| G567 | Green |
| G568 | Green |
| T569 | Green |
| P570 | Green |
| T571 | Green |
| Q572 | Green |
| S573 | Green |
| T574 | Green |
| L575 | Green |
| I588 | Green |
| E589 | Green |
| W599 | Green |
| N600 | Red |
| S608 | Green |
| F609 | Green |
| F612 | Green |
| T616 | Orange |
| K627 | Red |
| ALA | Grey |
| GLU | Grey |
| SER | Grey |
| PRO | Grey |
| ALA | Grey |
| ALA | Grey |
| ALA | Grey |
| K365 | Yellow |
| I178 | Yellow |
| T184 | Yellow |
| L185 | Orange |
| C188 | Yellow |
| G189 | Yellow |
| D190 | Yellow |
| L191 | Yellow |
| A197 | Yellow |
| L220 | Yellow |
| L221 | Yellow |
| T222 | Yellow |
| P223 | Yellow |
| D230 | Yellow |
| V233 | Yellow |
| D234 | Green |
| GLY | Grey |
| E236 | Yellow |
| K237 | Yellow |
| I238 | Red |
| M239 | Yellow |
| S240 | Yellow |
| A241 | Green |
| E242 | Yellow |
| N252 | Yellow |
| D253 | Red |
| N254 | Yellow |
| S255 | Yellow |
| H256 | Yellow |
| G257 | Yellow |
| T258 | Yellow |
| I511 | Yellow |
| D262 | Green |
| L512 | Orange |
| V281 | Yellow |
| D290 | Yellow |
| I291 | Green |
| L292 | Yellow |
| D303 | Yellow |
| R321 | Yellow |
| V332 | Yellow |
| V533 | Yellow |
| V534 | Green |
| V535 | Yellow |
| C540 | Yellow |
| R546 | Orange |
| L552 | Yellow |
| G553 | Green |
| R554 | Orange |
| I178 | Yellow |
| T184 | Yellow |
| L185 | Orange |
| C188 | Yellow |
| G189 | Yellow |
| D190 | Yellow |
| L191 | Yellow |
| A197 | Yellow |
| L220 | Yellow |
| L221 | Yellow |
| T222 | Yellow |
| P223 | Yellow |
| D230 | Yellow |
| V233 | Yellow |
| D234 | Green |
| GLY | Grey |
| E236 | Yellow |
| K237 | Yellow |
| I238 | Red |
| M239 | Yellow |
| S240 | Yellow |
| A241 | Green |
| E242 | Yellow |
| N252 | Yellow |
| D253 | Red |
| N254 | Yellow |
| S255 | Yellow |
| H256 | Yellow |
| G257 | Yellow |
| T258 | Yellow |
| I511 | Yellow |
| D262 | Green |
| L512 | Orange |
| V281 | Yellow |
| D290 | Yellow |
| I291 | Green |
| L292 | Yellow |
| D303 | Yellow |
| R321 | Yellow |
| V332 | Yellow |
| V533 | Yellow |
| V534 | Green |
| V535 | Yellow |
| C540 | Yellow |
| R546 | Orange |
| L552 | Yellow |
| G553 | Green |
| R554 | Orange |
| T155 | Yellow |
| T156 | Yellow |
| R157 | Yellow |
| Q158 | Green |
| T159 | Yellow |
| F160 | Orange |
| G164 | Yellow |
| L170 | Yellow |
| L174 | Yellow |

- Chain C: 77% 14% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	176.22Å 176.22Å 195.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.07 – 2.20 30.06 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.07-2.20) 100.0 (30.06-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.218 , 0.247 0.219 , 0.246	Depositor DCC
R_{free} test set	8681 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 15.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.229 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19620	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% 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: MG, SRM, SF4, FES, CL

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	0.88	4/4554 (0.1%)	1.01	26/6173 (0.4%)
1	B	0.88	3/4550 (0.1%)	1.02	22/6165 (0.4%)
1	C	0.78	3/4524 (0.1%)	0.98	23/6131 (0.4%)
1	D	0.72	0/4456	0.95	19/6036 (0.3%)
2	E	0.71	0/738	0.80	0/1008
2	F	0.74	1/502 (0.2%)	0.79	0/684
All	All	0.81	11/19324 (0.1%)	0.98	90/26197 (0.3%)

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	A	0	2
1	B	0	4
1	C	0	5
1	D	0	2
2	F	0	1
All	All	0	14

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	285	GLY	N-CA	6.76	1.56	1.46
1	B	600	ASN	N-CA	5.86	1.58	1.46
1	A	578	SER	CB-OG	-5.84	1.34	1.42
1	A	111	ARG	CD-NE	-5.76	1.36	1.46
1	C	321	ARG	CD-NE	-5.53	1.37	1.46

The worst 5 of 90 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	364	ARG	NE-CZ-NH2	-13.94	113.33	120.30
1	B	546	ARG	NE-CZ-NH2	-13.19	113.70	120.30
1	B	364	ARG	NE-CZ-NH2	-13.06	113.77	120.30
1	C	364	ARG	NE-CZ-NH2	-12.07	114.26	120.30
1	D	546	ARG	NE-CZ-NH2	-11.48	114.56	120.30

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	236	GLU	Peptide
1	A	238	ILE	Peptide
1	B	238	ILE	Peptide
1	B	239	MET	Peptide
1	B	256	HIS	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	4458	0	4430	107	0
1	B	4455	0	4437	78	0
1	C	4429	0	4413	94	0
1	D	4365	0	4349	84	0
2	E	726	0	671	15	0
2	F	495	0	431	16	0
3	A	8	0	0	0	0
3	B	8	0	0	0	0
3	C	8	0	0	0	0
3	D	8	0	0	0	0
4	A	63	0	34	9	0
4	B	63	0	34	10	0
4	C	63	0	34	7	0
4	D	63	0	34	11	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	E	4	0	0	0	0
7	F	4	0	0	0	0
8	A	118	0	0	8	0
8	B	124	0	0	3	0
8	C	77	0	0	10	0
8	D	66	0	0	2	0
8	E	7	0	0	1	0
All	All	19620	0	18867	404	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 11.

The worst 5 of 404 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:106:TYR:HE1	1:A:188:CYS:SG	1.11	1.66
1:C:106:TYR:HE1	1:C:188:CYS:SG	1.17	1.65
1:D:106:TYR:HE1	1:D:188:CYS:SG	1.17	1.64
1:A:106:TYR:CE1	1:A:188:CYS:SG	2.03	1.50
1:C:255:SER:C	1:C:257:GLY:HA3	1.36	1.39

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	565/583 (97%)	546 (97%)	14 (2%)	5 (1%)	17 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	561/583 (96%)	545 (97%)	10 (2%)	6 (1%)	14	12
1	C	559/583 (96%)	544 (97%)	9 (2%)	6 (1%)	14	12
1	D	544/583 (93%)	529 (97%)	10 (2%)	5 (1%)	17	16
2	E	94/98 (96%)	90 (96%)	4 (4%)	0	100	100
2	F	69/98 (70%)	61 (88%)	5 (7%)	3 (4%)	2	1
All	All	2392/2528 (95%)	2315 (97%)	52 (2%)	25 (1%)	15	14

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	432	GLN
1	B	238	ILE
1	B	432	GLN
1	B	600	ASN
1	C	256	HIS

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	479/493 (97%)	440 (92%)	39 (8%)	11	12
1	B	480/493 (97%)	443 (92%)	37 (8%)	13	13
1	C	475/493 (96%)	437 (92%)	38 (8%)	12	12
1	D	470/493 (95%)	433 (92%)	37 (8%)	12	12
2	E	83/83 (100%)	78 (94%)	5 (6%)	19	22
2	F	49/83 (59%)	44 (90%)	5 (10%)	7	6
All	All	2036/2138 (95%)	1875 (92%)	161 (8%)	12	12

5 of 161 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	574	THR

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Mol	Chain	Res	Type
1	C	245	PRO
1	D	590	LYS
1	B	616	THR
1	C	159	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	454	GLN
1	C	224	GLN
1	D	454	GLN
1	B	504	GLN
1	B	572	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 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	SRM	D	702	1	34,70,70	2.68	17 (50%)	38,112,112	3.75	12 (31%)
7	FES	E	101	2	0,4,4	0.00	-	-		
7	FES	F	101	2	0,4,4	0.00	-	-		
3	SF4	B	701	1	0,12,12	0.00	-	-		
3	SF4	A	701	1	0,12,12	0.00	-	-		
3	SF4	D	701	1	0,12,12	0.00	-	-		
3	SF4	C	701	1	0,12,12	0.00	-	-		
4	SRM	C	702	1	34,70,70	2.76	17 (50%)	38,112,112	4.14	14 (36%)
4	SRM	B	702	1	34,70,70	2.69	15 (44%)	38,112,112	4.20	18 (47%)
4	SRM	A	702	1	34,70,70	2.67	15 (44%)	38,112,112	4.08	24 (63%)

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	SRM	D	702	1	-	8/22/126/126	-
7	FES	E	101	2	-	-	0/1/1/1
7	FES	F	101	2	-	-	0/1/1/1
3	SF4	B	701	1	-	-	0/6/5/5
3	SF4	A	701	1	-	-	0/6/5/5
3	SF4	D	701	1	-	-	0/6/5/5
3	SF4	C	701	1	-	-	0/6/5/5
4	SRM	C	702	1	-	7/22/126/126	-
4	SRM	B	702	1	-	7/22/126/126	-
4	SRM	A	702	1	-	7/22/126/126	-

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	702	SRM	CAB-C3B	-7.65	1.39	1.51
4	C	702	SRM	C4B-NB	-7.60	1.25	1.39
4	D	702	SRM	CHA-C1A	7.29	1.47	1.36
4	B	702	SRM	CHA-C1A	6.95	1.47	1.36
4	D	702	SRM	C4B-NB	-6.44	1.27	1.39

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	702	SRM	CAB-CBB-CCB	17.77	142.48	112.67
4	A	702	SRM	CAB-CBB-CCB	16.76	140.79	112.67
4	C	702	SRM	CAB-CBB-CCB	16.44	140.25	112.67
4	D	702	SRM	CAB-CBB-CCB	15.15	138.09	112.67
4	C	702	SRM	CBB-CAB-C3B	-10.83	87.92	113.40

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

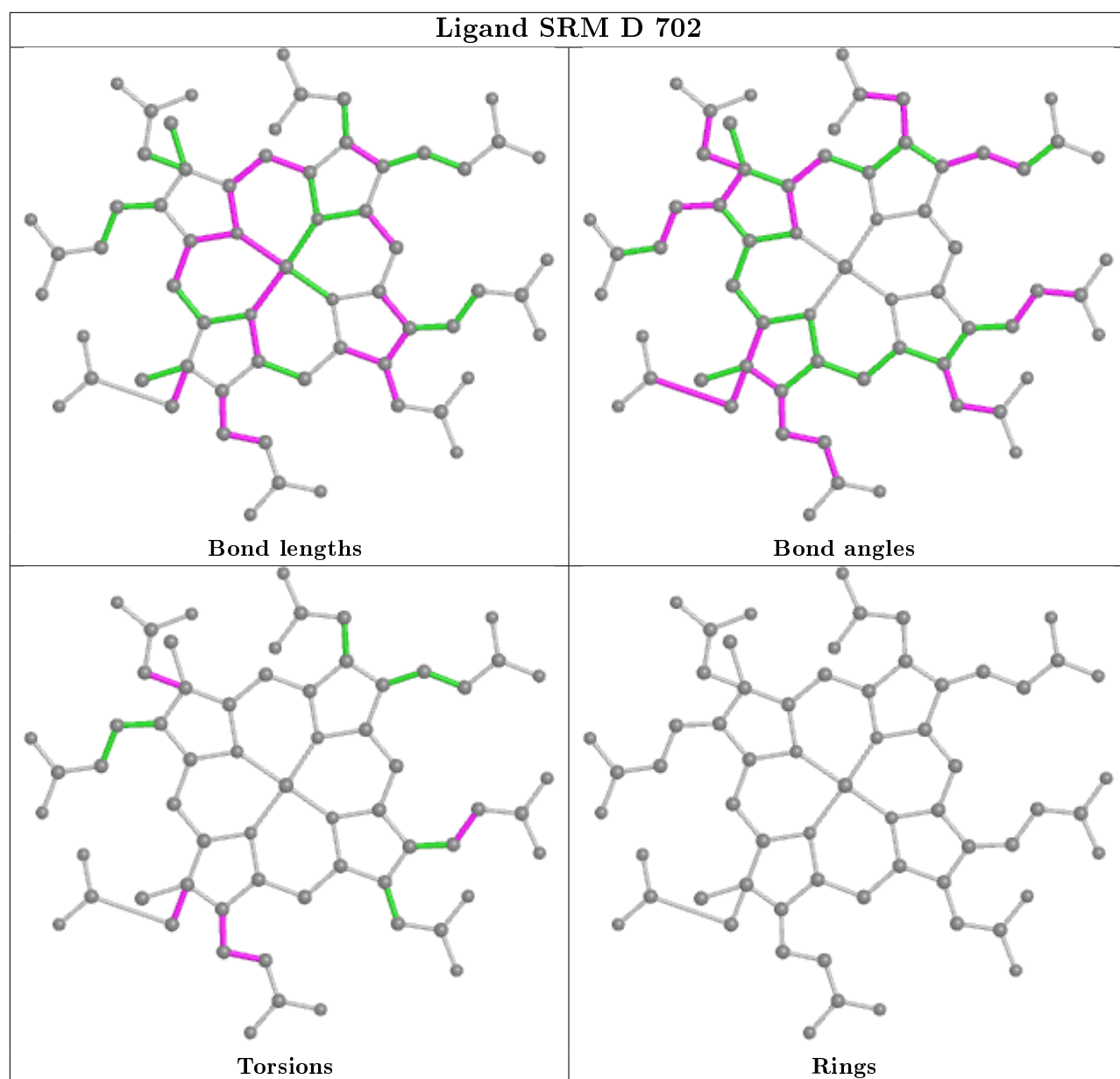
Mol	Chain	Res	Type	Atoms
4	D	702	SRM	C1A-C2A-CDA-CEA
4	D	702	SRM	CMA-C2A-CDA-CEA
4	D	702	SRM	C3A-C2A-CDA-CEA
4	D	702	SRM	C3B-C2B-CDB-CEB
4	C	702	SRM	C1A-C2A-CDA-CEA

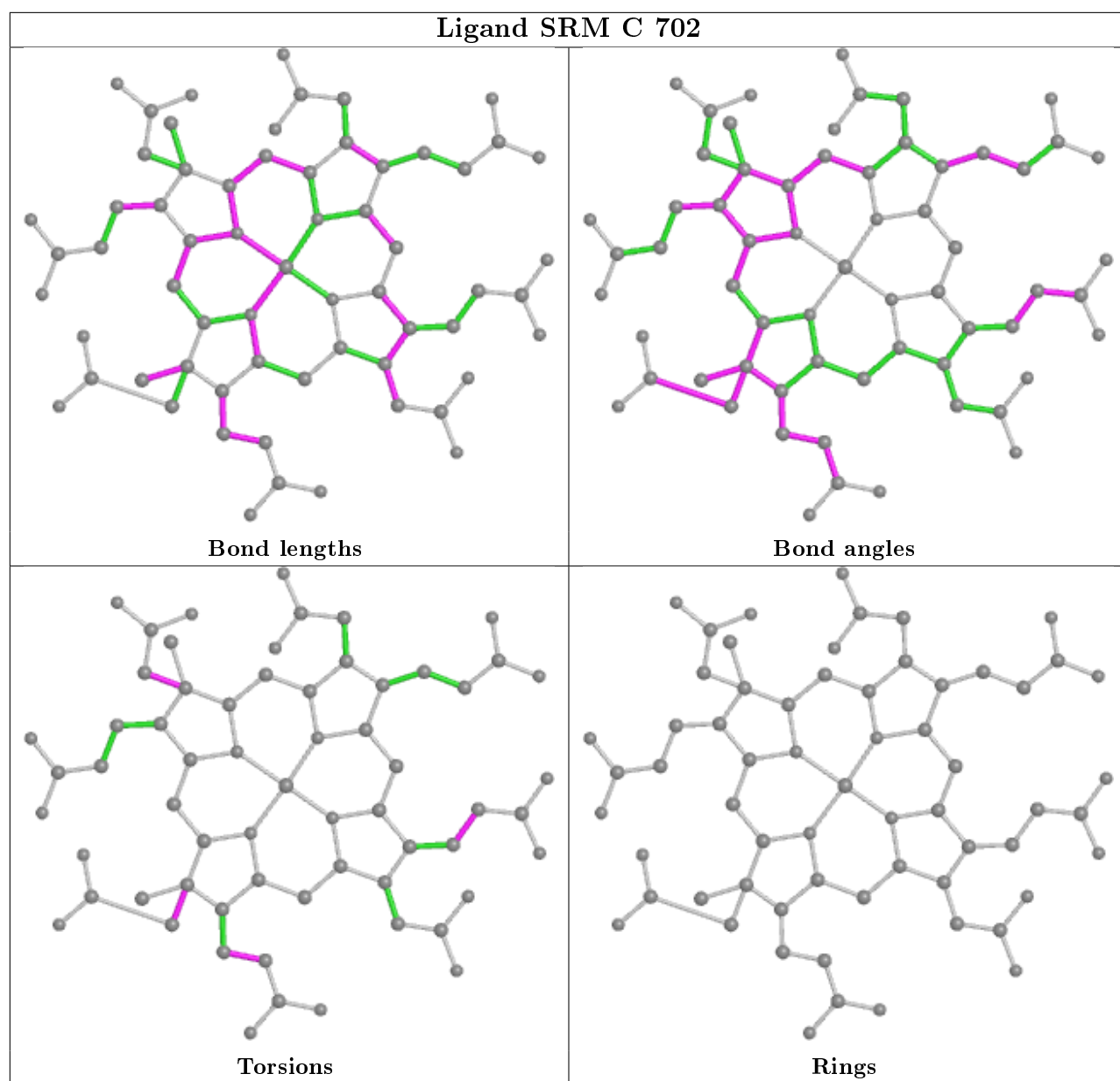
There are no ring outliers.

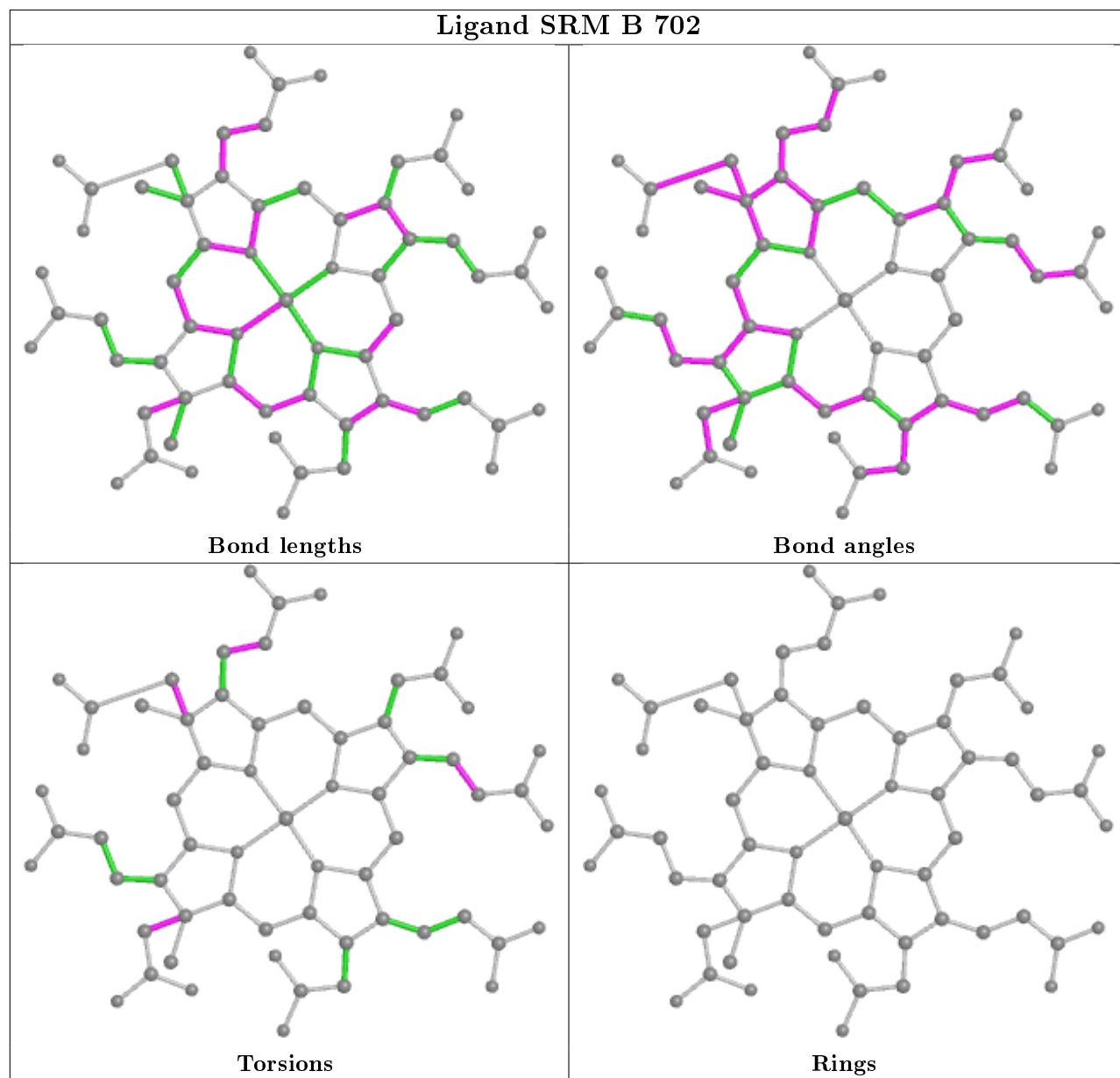
4 monomers are involved in 37 short contacts:

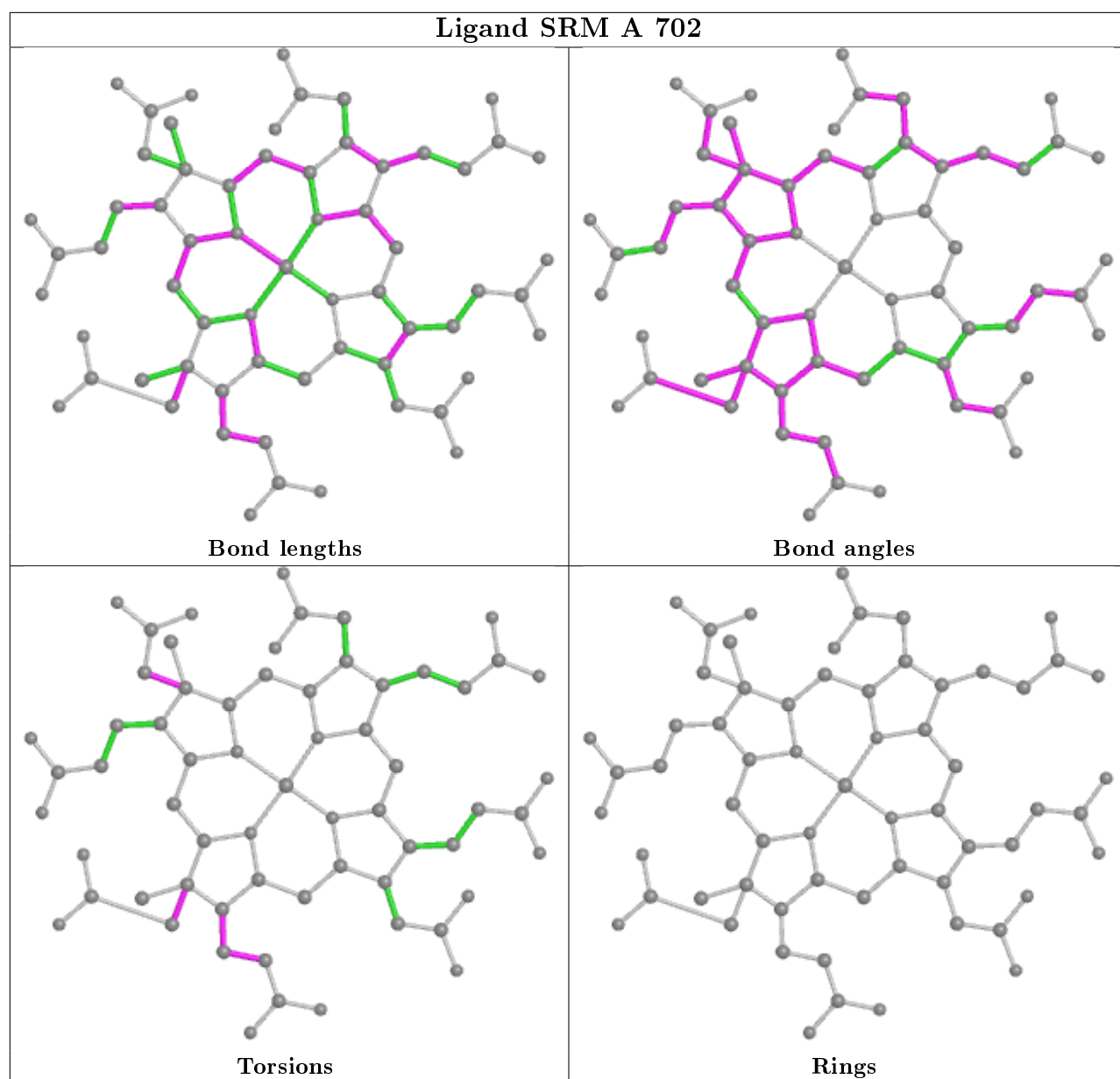
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	702	SRM	11	0
4	C	702	SRM	7	0
4	B	702	SRM	10	0
4	A	702	SRM	9	0

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	567/583 (97%)	-0.56	5 (0%) 84 83	17, 27, 43, 77	0
1	B	565/583 (96%)	-0.54	4 (0%) 87 86	17, 27, 43, 66	0
1	C	563/583 (96%)	-0.37	7 (1%) 79 77	18, 35, 61, 84	0
1	D	554/583 (95%)	-0.22	15 (2%) 54 52	20, 43, 70, 90	0
2	E	96/98 (97%)	0.13	4 (4%) 36 34	32, 47, 72, 86	0
2	F	73/98 (74%)	3.38	50 (68%) 0 0	48, 75, 104, 119	0
All	All	2418/2528 (95%)	-0.29	85 (3%) 44 42	17, 32, 67, 119	0

The worst 5 of 85 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	69	ILE	9.5
2	F	51	VAL	9.4
2	F	70	ALA	9.2
2	E	96	THR	8.2
2	F	48	ALA	8.1

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

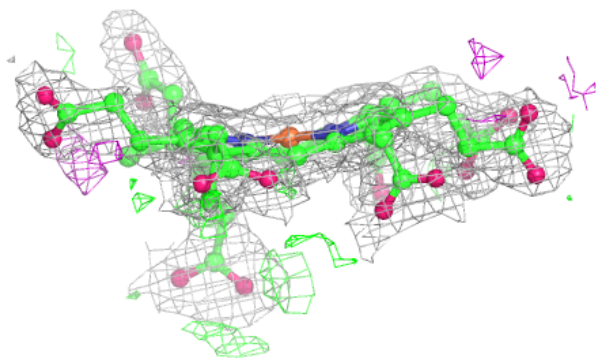
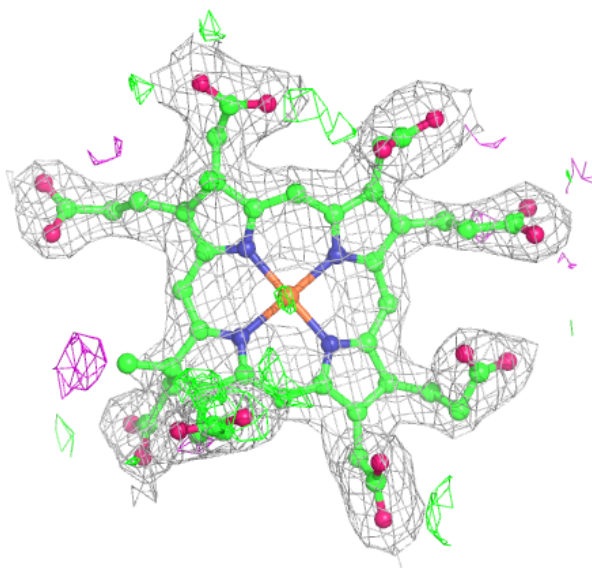
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SRM	D	702	63/63	0.95	0.11	24,34,41,46	0
4	SRM	C	702	63/63	0.95	0.13	23,28,36,44	0
6	CL	A	704	1/1	0.96	0.14	34,34,34,34	0
4	SRM	B	702	63/63	0.96	0.11	18,22,29,43	0
3	SF4	D	701	8/8	0.97	0.05	25,27,29,29	0
7	FES	F	101	4/4	0.97	0.06	41,42,47,47	0
6	CL	C	704	1/1	0.97	0.25	44,44,44,44	0
4	SRM	A	702	63/63	0.97	0.12	17,23,29,40	0
6	CL	B	704	1/1	0.98	0.19	40,40,40,40	0
3	SF4	A	701	8/8	0.98	0.06	19,20,23,23	0
3	SF4	C	701	8/8	0.98	0.06	22,24,24,25	0
6	CL	D	704	1/1	0.98	0.23	43,43,43,43	0
3	SF4	B	701	8/8	0.99	0.05	20,21,22,22	0
5	MG	C	703	1/1	0.99	0.20	12,12,12,12	0
7	FES	E	101	4/4	0.99	0.04	31,34,35,37	0
5	MG	A	703	1/1	1.00	0.17	8,8,8,8	0
5	MG	B	703	1/1	1.00	0.14	8,8,8,8	0
5	MG	D	703	1/1	1.00	0.21	16,16,16,16	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.

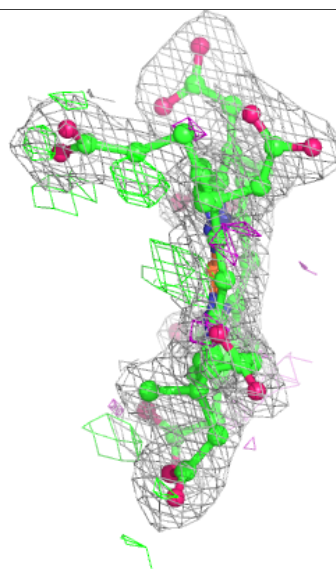
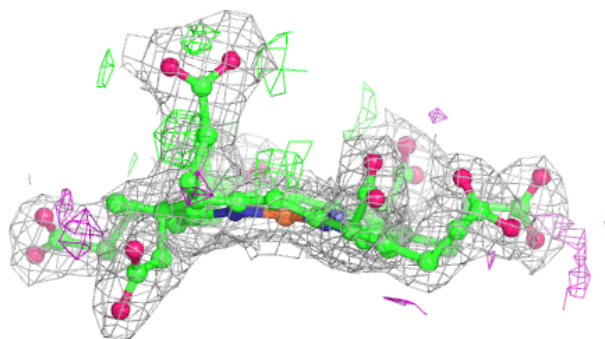
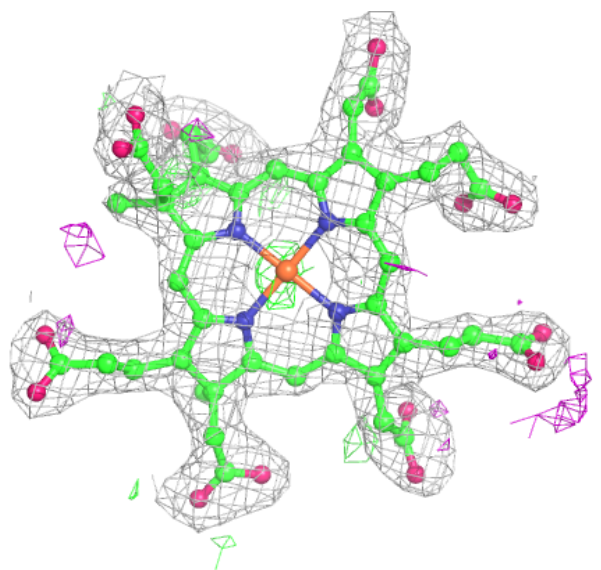
Electron density around SRM D 702:

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



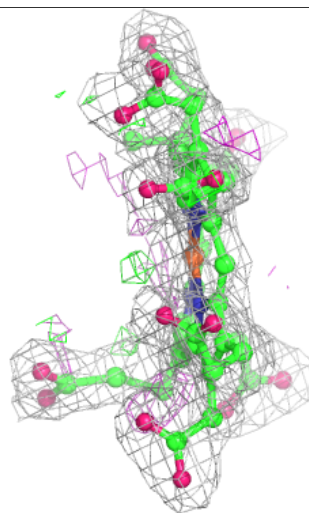
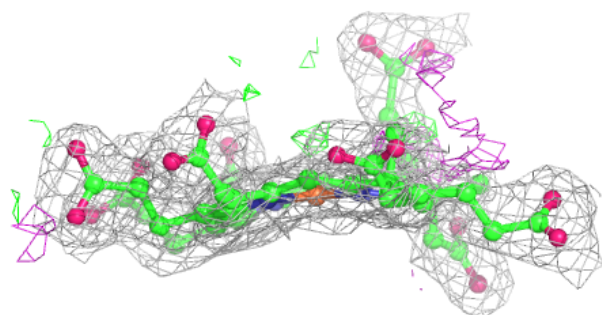
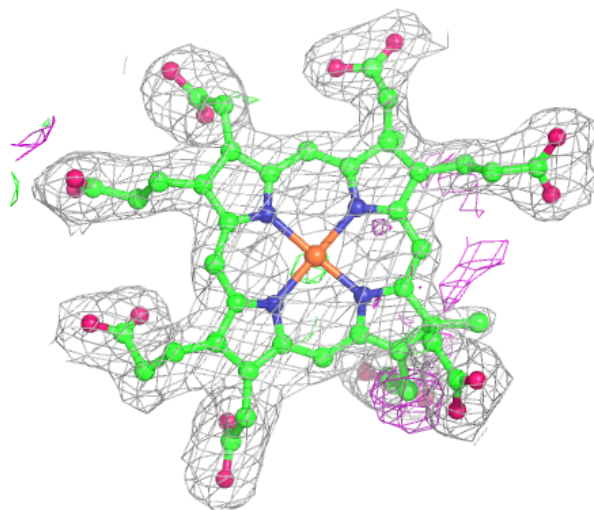
Electron density around SRM C 702:

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



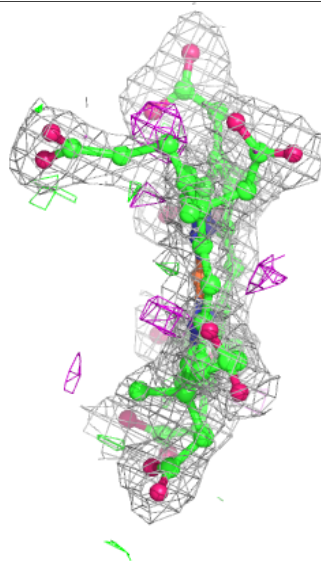
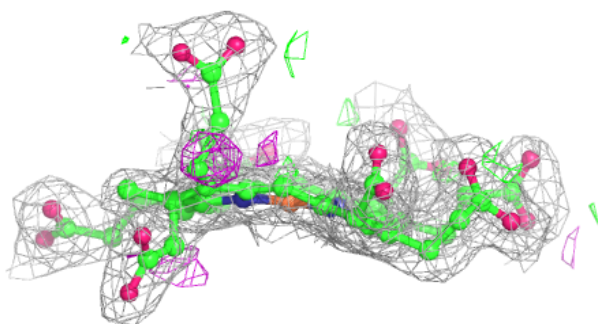
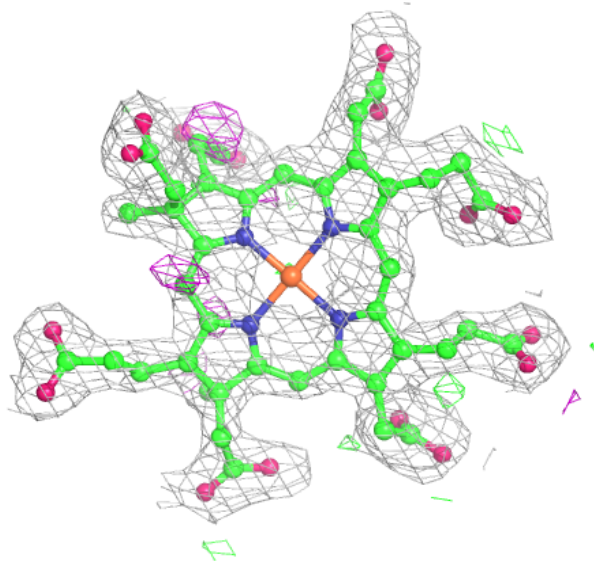
Electron density around SRM B 702:

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



Electron density around SRM A 702:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.