



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:09 PM UTC

PDB ID : 2XWQ / pdb_00002xwq
Title : Anaerobic cobalt chelatase from *Archeaoglobus fulgidus* (CbiX) in complex with metalated sirohydrochlorin product
Authors : Ladakis, D.; Brindley, A.A.; Deery, E.; Warren, M.J.; Pickersgill, R.W.
Deposited on : 2010-11-04
Resolution : 2.01 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

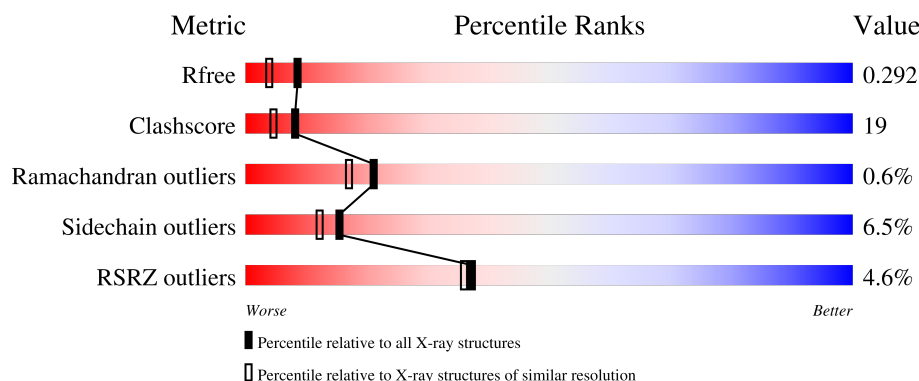
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 $\leq 5\%$. 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	133	2% 68% 21% 5% 5%
1	B	133	71% 19% • 6%
1	C	133	11% 64% 26% 5% 5%
1	D	133	5% 60% 28% 5% • 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SIR	B	1126[A]	X	-	-	-
2	SIR	B	1126[B]	X	-	-	-
2	SIR	D	1126[A]	X	-	X	-
2	SIR	D	1126[B]	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4475 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.

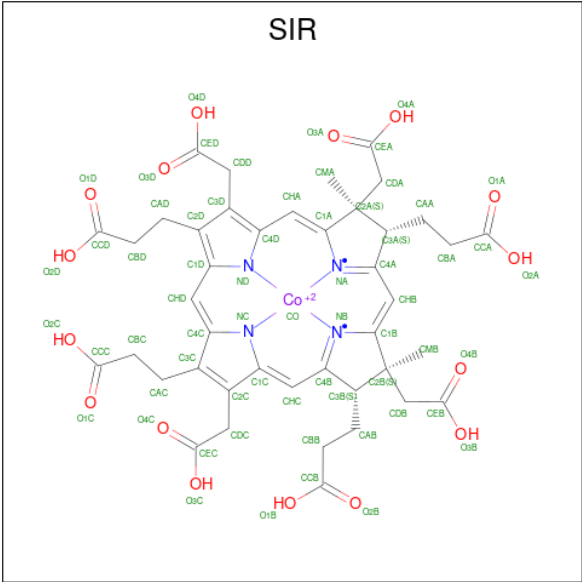
- Molecule 1 is a protein called SIROHYDROCHLORIN COBALTOCHELATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	126	Total	C	N	O	S	0	0	0
			1012	647	180	179	6			
1	B	125	Total	C	N	O	S	0	0	0
			1008	645	179	178	6			
1	C	126	Total	C	N	O	S	0	0	0
			1012	647	180	179	6			
1	D	125	Total	C	N	O	S	0	0	0
			1008	645	179	178	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP O29537
B	0	GLY	-	expression tag	UNP O29537
C	0	GLY	-	expression tag	UNP O29537
D	0	GLY	-	expression tag	UNP O29537

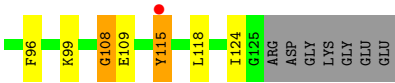
- Molecule 2 is COBALT SIROHYDROCHLORIN (CCD ID: SIR) (formula: $C_{42}H_{44}CoN_4O_{16}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Co	N	O	0	1
			126	84	2	8	32		
2	D	1	Total	C	Co	N	O	0	1
			126	84	2	8	32		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	49	Total	O	0	0
			49	49		
3	B	59	Total	O	0	0
			59	59		
3	C	26	Total	O	0	0
			26	26		
3	D	49	Total	O	0	0
			49	49		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.01Å 99.00Å 116.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.57 – 2.01 45.57 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.57-2.01) 99.9 (45.57-2.01)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.217 , 0.282 (Not available) , 0.292	Depositor DCC
R_{free} test set	1842 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4475	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% 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: SIR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.29	4/1033 (0.4%)	1.29	3/1388 (0.2%)
1	B	1.33	3/1029 (0.3%)	1.19	3/1383 (0.2%)
1	C	1.04	3/1033 (0.3%)	1.16	5/1388 (0.4%)
1	D	1.24	1/1029 (0.1%)	1.24	3/1383 (0.2%)
All	All	1.23	11/4124 (0.3%)	1.22	14/5542 (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	C	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	77	GLU	CA-C	6.10	1.57	1.52
1	C	11	GLY	N-CA	5.98	1.50	1.44
1	A	67	LEU	C-O	-5.94	1.17	1.23
1	D	90	GLY	N-CA	5.43	1.50	1.45
1	A	20	VAL	CA-CB	5.39	1.60	1.54
1	B	20	VAL	CA-CB	5.34	1.61	1.54
1	C	121	VAL	C-O	5.23	1.29	1.24
1	C	116	ALA	C-O	5.17	1.30	1.24
1	B	72	GLY	C-O	-5.11	1.19	1.24
1	B	28	ILE	N-CA	5.05	1.52	1.46
1	A	69	ILE	CA-CB	5.05	1.61	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	LEU	CA-C-N	-8.74	109.92	119.19
1	A	79	LEU	C-N-CA	-8.74	109.92	119.19
1	C	11	GLY	N-CA-C	-7.45	102.37	112.57
1	D	108	GLY	N-CA-C	7.39	121.59	112.64
1	D	78	ASP	N-CA-C	6.90	118.46	111.07
1	B	68	PHE	N-CA-C	-6.39	98.96	108.99
1	D	115	TYR	N-CA-C	5.75	118.49	111.82
1	B	13	GLN	N-CA-C	5.67	118.19	111.33
1	C	44	ARG	CB-CA-C	-5.64	110.06	116.54
1	B	85	PHE	N-CA-C	-5.50	102.14	110.50
1	C	44	ARG	CA-C-N	-5.28	115.36	122.86
1	C	44	ARG	C-N-CA	-5.28	115.36	122.86
1	A	57	MET	N-CA-C	5.20	118.29	109.76
1	C	108	GLY	N-CA-C	5.17	119.14	112.83

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	10	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	1012	0	1021	29	0
1	B	1008	0	1018	33	0
1	C	1012	0	1021	39	0
1	D	1008	0	1018	47	0
2	B	126	0	70	12	0
2	D	126	0	70	40	0
3	A	49	0	0	0	0
3	B	59	0	0	5	0
3	C	26	0	0	0	0
3	D	49	0	0	1	0
All	All	4475	0	4218	165	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 19.

All (165) 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)
2:D:1126[A]:SIR:CEA	2:D:1126[A]:SIR:CDA	1.75	1.62
2:D:1126[A]:SIR:HBD2	2:D:1126[A]:SIR:O4D	1.36	1.23
2:D:1126[A]:SIR:HMA2	2:D:1126[A]:SIR:O4A	1.39	1.20
2:D:1126[A]:SIR:O4D	2:D:1126[A]:SIR:CBD	1.96	1.14
1:A:16:HIS:CD2	1:B:71:TYR:H	1.70	1.08
2:D:1126[A]:SIR:HMA3	2:D:1126[A]:SIR:O1A	1.53	1.06
2:D:1126[A]:SIR:HBC1	2:D:1126[A]:SIR:HDC2	1.38	1.04
2:D:1126[A]:SIR:HMA3	2:D:1126[A]:SIR:CCA	1.85	1.04
2:D:1126[A]:SIR:C3B	2:D:1126[A]:SIR:O3B	2.08	1.00
2:B:1126[A]:SIR:O4B	2:B:1126[A]:SIR:CMB	2.12	0.97
2:D:1126[B]:SIR:CHC	2:D:1126[B]:SIR:CBB	2.40	0.97
1:A:47:ARG:HH11	1:A:47:ARG:HG3	1.27	0.96
2:B:1126[A]:SIR:O4B	2:B:1126[A]:SIR:HMB3	1.63	0.96
1:A:71:TYR:H	1:B:16:HIS:HD2	1.02	0.95
1:C:45:LYS:HD3	1:C:45:LYS:C	1.94	0.92
1:C:71:TYR:H	1:D:16:HIS:HD2	1.07	0.92
1:A:71:TYR:H	1:B:16:HIS:CD2	1.89	0.90
2:D:1126[B]:SIR:O4B	2:D:1126[B]:SIR:C1B	2.16	0.90
1:A:49:MET:HE3	1:A:82:LEU:HD12	1.55	0.89
1:A:16:HIS:HD2	1:B:71:TYR:H	0.90	0.89
1:A:16:HIS:HD2	1:B:71:TYR:N	1.70	0.89
2:D:1126[B]:SIR:CHC	2:D:1126[B]:SIR:HBB1	2.02	0.88
1:D:46:ARG:NH2	2:D:1126[B]:SIR:O1B	2.07	0.87
1:B:26:LYS:NZ	1:B:30:GLU:OE2	2.07	0.87
2:D:1126[A]:SIR:O4A	2:D:1126[A]:SIR:CMA	2.24	0.86
2:D:1126[A]:SIR:HBD2	2:D:1126[A]:SIR:CED	2.05	0.85
1:B:3:ARG:NH1	1:D:32:GLY:O	2.10	0.85
2:D:1126[A]:SIR:CCA	2:D:1126[A]:SIR:CMA	2.55	0.84
1:C:71:TYR:H	1:D:16:HIS:CD2	1.95	0.83
2:D:1126[A]:SIR:CEA	2:D:1126[A]:SIR:C2A	2.57	0.83
1:C:25:ARG:HG2	1:C:25:ARG:HH11	1.46	0.80
1:A:47:ARG:HH11	1:A:47:ARG:CG	1.95	0.79
2:D:1126[A]:SIR:O4D	2:D:1126[A]:SIR:HBD1	1.84	0.77
1:B:49:MET:HE3	1:B:82:LEU:HD11	1.66	0.77
2:D:1126[B]:SIR:HHA	2:D:1126[B]:SIR:CEA	2.15	0.76
2:B:1126[A]:SIR:HBC2	2:B:1126[A]:SIR:HHD	1.66	0.76
1:C:45:LYS:HD3	1:C:46:ARG:N	2.00	0.76
2:D:1126[B]:SIR:O4B	2:D:1126[B]:SIR:CHB	2.34	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:TYR:N	1:B:16:HIS:HD2	1.83	0.74
1:A:10:HIS:HD2	1:A:11:GLY:O	1.71	0.73
2:D:1126[B]:SIR:O2A	2:D:1126[B]:SIR:H3A	1.88	0.73
1:D:12:SER:O	1:D:13:GLN:HG2	1.89	0.73
1:B:49:MET:HE2	1:B:82:LEU:HD12	1.70	0.72
1:B:18:ARG:NH1	3:B:2009:HOH:O	2.19	0.71
1:D:68:PHE:HD2	2:D:1126[B]:SIR:HBD2	1.55	0.71
1:A:69:ILE:O	1:A:108:GLY:HA3	1.90	0.71
1:B:49:MET:CE	1:B:82:LEU:HD11	2.20	0.71
1:B:49:MET:CE	1:B:82:LEU:CD1	2.70	0.70
2:D:1126[B]:SIR:CEA	2:D:1126[B]:SIR:CHA	2.70	0.70
1:D:44:ARG:O	1:D:45:LYS:HB2	1.91	0.70
2:D:1126[A]:SIR:CEA	2:D:1126[A]:SIR:HMA2	2.21	0.69
1:D:15:ASN:O	1:D:19:GLU:HG3	1.93	0.68
2:D:1126[B]:SIR:CBB	2:D:1126[B]:SIR:HHC	2.22	0.68
1:B:46:ARG:NH2	2:B:1126[A]:SIR:O1B	2.24	0.68
1:B:49:MET:HE2	1:B:82:LEU:CD1	2.22	0.68
2:D:1126[B]:SIR:CHC	2:D:1126[B]:SIR:HBB2	2.23	0.68
2:D:1126[B]:SIR:HHC	2:D:1126[B]:SIR:HBB2	1.76	0.67
1:C:25:ARG:HG2	1:C:25:ARG:NH1	2.07	0.67
1:C:10:HIS:HD2	1:C:11:GLY:HA2	1.61	0.66
1:D:12:SER:O	1:D:13:GLN:CB	2.43	0.66
1:A:3:ARG:NH2	1:C:3:ARG:HH22	1.94	0.65
2:D:1126[A]:SIR:HDC2	2:D:1126[A]:SIR:CBC	2.22	0.65
1:A:47:ARG:HG3	1:A:47:ARG:NH1	2.02	0.64
1:C:69:ILE:O	1:C:108:GLY:HA3	1.98	0.64
1:C:71:TYR:N	1:D:16:HIS:HD2	1.89	0.64
1:B:18:ARG:NE	3:B:2008:HOH:O	1.88	0.64
1:B:10:HIS:HD2	1:B:11:GLY:O	1.81	0.63
1:B:69:ILE:O	1:B:108:GLY:HA3	1.97	0.63
2:D:1126[A]:SIR:HMA3	2:D:1126[A]:SIR:CBA	2.29	0.62
1:C:16:HIS:CD2	1:D:71:TYR:H	2.18	0.62
1:C:45:LYS:C	1:C:45:LYS:CD	2.63	0.61
2:B:1126[A]:SIR:O2B	2:B:1126[A]:SIR:CHC	2.49	0.60
1:D:77:GLU:HG3	1:D:87:ARG:HE	1.65	0.60
2:D:1126[B]:SIR:HBD1	2:D:1126[B]:SIR:HHD	1.83	0.60
1:D:12:SER:O	1:D:13:GLN:CG	2.49	0.60
1:D:45:LYS:HZ2	1:D:47:ARG:NH1	2.00	0.60
1:C:36:GLU:HG2	1:C:57:MET:HE3	1.84	0.59
1:A:109:GLU:OE2	1:B:16:HIS:HE1	1.84	0.59
2:D:1126[A]:SIR:CEA	2:D:1126[A]:SIR:CMA	2.80	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:SER:O	1:D:13:GLN:HB3	2.04	0.57
1:A:35:ASP:OD1	1:C:0:GLY:HA2	2.05	0.57
1:D:22:GLU:OE2	1:D:25:ARG:NH2	2.26	0.57
1:C:77:GLU:HG2	1:C:87:ARG:HD3	1.87	0.57
2:D:1126[A]:SIR:CMA	2:D:1126[A]:SIR:CBA	2.78	0.57
1:C:46:ARG:NH2	2:D:1126[B]:SIR:O3A	2.39	0.56
2:B:1126[A]:SIR:HHD	2:B:1126[A]:SIR:CBC	2.36	0.55
1:D:69:ILE:O	1:D:108:GLY:HA3	2.05	0.55
1:C:50:PRO:O	1:C:54:ILE:HG13	2.05	0.55
1:D:68:PHE:CD2	2:D:1126[B]:SIR:HBD2	2.38	0.55
1:C:28:ILE:HG22	1:C:37:VAL:HG21	1.88	0.54
1:D:53:ALA:O	1:D:57:MET:HG3	2.08	0.54
1:C:10:HIS:HD2	1:C:11:GLY:CA	2.21	0.53
1:A:21:MET:HE2	1:A:39:ILE:HB	1.90	0.53
2:B:1126[A]:SIR:O4B	2:B:1126[A]:SIR:HMB2	2.06	0.53
1:C:16:HIS:HD2	1:D:71:TYR:H	1.56	0.52
1:C:71:TYR:CG	1:C:89:ARG:HD2	2.45	0.52
1:A:16:HIS:HA	1:A:19:GLU:HG3	1.91	0.51
1:A:47:ARG:CG	1:A:47:ARG:NH1	2.65	0.51
1:A:49:MET:HE3	1:A:82:LEU:CD1	2.33	0.50
1:C:89:ARG:HH11	1:C:89:ARG:HB3	1.76	0.50
1:B:115:TYR:CE1	1:D:115:TYR:CD1	3.00	0.50
1:A:3:ARG:HH21	1:C:3:ARG:HH22	1.60	0.50
1:D:38:LYS:HD2	1:D:57:MET:HG2	1.94	0.50
1:A:51:ASP:OD1	1:A:52:GLU:N	2.46	0.49
2:B:1126[B]:SIR:HHD	2:B:1126[B]:SIR:HBD2	1.94	0.49
1:D:45:LYS:NZ	1:D:47:ARG:CZ	2.75	0.48
1:D:45:LYS:HZ2	1:D:47:ARG:HD3	1.79	0.48
1:D:45:LYS:O	1:D:45:LYS:HD3	2.13	0.48
2:D:1126[A]:SIR:C1A	2:D:1126[A]:SIR:HBA1	2.44	0.48
1:A:74:HIS:ND1	2:B:1126[B]:SIR:O3D	2.46	0.48
1:D:2:ARG:O	1:D:59:CYS:HB3	2.14	0.48
2:B:1126[B]:SIR:HMA1	2:B:1126[B]:SIR:HAA2	1.58	0.48
1:C:74:HIS:ND1	2:D:1126[B]:SIR:O3C	2.20	0.48
1:C:10:HIS:CD2	1:C:10:HIS:C	2.90	0.47
1:A:16:HIS:CD2	1:B:71:TYR:N	2.56	0.47
1:A:111:TYR:HB3	1:A:115:TYR:CE2	2.50	0.47
1:B:115:TYR:CD1	1:D:115:TYR:CE1	3.03	0.47
1:A:18:ARG:NH2	1:A:47:ARG:O	2.39	0.46
2:B:1126[A]:SIR:HHB	2:B:1126[A]:SIR:CEB	2.46	0.46
1:D:77:GLU:HG3	1:D:87:ARG:HH21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1126[A]:SIR:HBC1	2:D:1126[A]:SIR:CDC	2.23	0.46
1:B:49:MET:CE	1:B:82:LEU:HD12	2.37	0.45
1:C:109:GLU:OE2	1:D:16:HIS:CE1	2.69	0.45
2:D:1126[A]:SIR:O1A	2:D:1126[A]:SIR:CMA	2.44	0.45
1:C:83:LEU:HD12	1:C:103:ILE:HD11	1.98	0.45
1:D:79:LEU:HB3	1:D:80:PRO:HD3	1.97	0.45
1:D:2:ARG:HB2	1:D:59:CYS:HA	1.98	0.45
1:D:74:HIS:ND1	2:D:1126[B]:SIR:O4D	2.39	0.45
1:A:16:HIS:HE1	1:B:109:GLU:OE2	1.99	0.45
1:B:18:ARG:NH2	3:B:2008:HOH:O	2.50	0.45
1:B:18:ARG:HH11	1:B:18:ARG:HB2	1.81	0.45
1:D:45:LYS:NZ	1:D:47:ARG:NH1	2.65	0.44
1:D:72:GLY:O	1:D:76:THR:HG23	2.17	0.44
1:D:99:LYS:NZ	3:D:2040:HOH:O	2.50	0.44
1:D:115:TYR:CE1	1:D:118:LEU:HD12	2.52	0.44
1:C:16:HIS:HE1	1:D:109:GLU:OE2	2.01	0.44
1:D:25:ARG:O	1:D:29:GLU:HB2	2.18	0.44
1:C:109:GLU:OE2	1:D:16:HIS:HE1	2.01	0.44
1:D:47:ARG:HA	1:D:48:PRO:C	2.43	0.44
2:D:1126[A]:SIR:CBC	2:D:1126[A]:SIR:CDC	2.92	0.44
1:B:122:PHE:HB3	1:C:31:SER:HB2	2.00	0.43
2:D:1126[A]:SIR:CDA	2:D:1126[A]:SIR:O3A	2.51	0.43
1:B:118:LEU:HD23	1:B:118:LEU:HA	1.70	0.43
1:D:115:TYR:CD1	1:D:118:LEU:HD12	2.54	0.43
1:C:5:LEU:HD23	1:C:37:VAL:HG13	2.01	0.43
1:A:111:TYR:O	1:A:115:TYR:CD2	2.72	0.43
1:C:72:GLY:HA2	1:D:14:LEU:HD13	2.01	0.42
1:B:25:ARG:HD3	3:B:2012:HOH:O	2.18	0.42
1:C:49:MET:HB3	1:C:50:PRO:CD	2.49	0.42
1:C:73:LEU:HD23	1:C:73:LEU:HA	1.72	0.42
1:A:31:SER:HB3	1:D:124:ILE:HD11	2.02	0.41
1:C:42:ALA:O	1:C:74:HIS:HD2	2.03	0.41
1:D:86:PRO:O	1:D:92:LYS:HE2	2.20	0.41
1:B:44:ARG:NH1	3:B:2056:HOH:O	2.53	0.41
1:D:49:MET:HE3	1:D:82:LEU:CD1	2.50	0.41
1:C:21:MET:HE2	1:C:39:ILE:HB	2.02	0.41
2:B:1126[A]:SIR:HHC	2:B:1126[A]:SIR:CCB	2.50	0.41
1:C:2:ARG:HB2	1:C:60:ASP:H	1.86	0.41
1:A:120:SER:OG	1:B:104:CYS:HB3	2.21	0.41
1:B:2:ARG:HA	1:B:35:ASP:OD2	2.20	0.41
1:B:15:ASN:O	1:B:16:HIS:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:ALA:H	1:D:78:ASP:HB3	1.86	0.41
1:D:51:ASP:HB2	1:D:96:PHE:CZ	2.56	0.41
1:C:77:GLU:CG	1:C:87:ARG:HD3	2.50	0.40
1:C:53:ALA:O	1:C:57:MET:HG3	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	124/133 (93%)	119 (96%)	5 (4%)	0	100	100
1	B	123/133 (92%)	120 (98%)	3 (2%)	0	100	100
1	C	124/133 (93%)	113 (91%)	11 (9%)	0	100	100
1	D	123/133 (92%)	116 (94%)	4 (3%)	3 (2%)	4	2
All	All	494/532 (93%)	468 (95%)	23 (5%)	3 (1%)	21	17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	45	LYS
1	D	13	GLN
1	D	44	ARG

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	107/112 (96%)	94 (88%)	13 (12%)	5	3
1	B	107/112 (96%)	101 (94%)	6 (6%)	19	16
1	C	107/112 (96%)	101 (94%)	6 (6%)	19	16
1	D	107/112 (96%)	104 (97%)	3 (3%)	38	41
All	All	428/448 (96%)	400 (94%)	28 (6%)	15	12

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	ARG
1	A	3	ARG
1	A	14	LEU
1	A	18	ARG
1	A	19	GLU
1	A	21	MET
1	A	29	GLU
1	A	44	ARG
1	A	47	ARG
1	A	82	LEU
1	A	89	ARG
1	A	99	LYS
1	B	13	GLN
1	B	18	ARG
1	B	26	LYS
1	B	44	ARG
1	B	45	LYS
1	B	82	LEU
1	C	1	MET
1	C	44	ARG
1	C	45	LYS
1	C	52	GLU
1	C	89	ARG
1	C	97	GLU
1	D	14	LEU
1	D	44	ARG
1	D	82	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	16	HIS
1	A	58	ASN
1	B	15	ASN
1	B	16	HIS
1	C	10	HIS
1	C	16	HIS
1	D	16	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	$\# Z > 2$
2	SIR	B	1126[B]	-	68,70,70	1.81	15 (22%)	90,112,112	2.40	33 (36%)
2	SIR	D	1126[B]	-	68,70,70	1.64	12 (17%)	90,112,112	2.37	33 (36%)
2	SIR	B	1126[A]	-	68,70,70	1.70	13 (19%)	90,112,112	2.18	29 (32%)
2	SIR	D	1126[A]	-	68,70,70	2.03	17 (25%)	90,112,112	2.34	23 (25%)

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	SIR	B	1126[B]	-	3/3/19/23	16/38/126/126	-
2	SIR	D	1126[B]	-	3/3/19/23	18/38/126/126	-
2	SIR	B	1126[A]	-	3/3/19/23	12/38/126/126	-
2	SIR	D	1126[A]	-	3/3/19/23	28/38/126/126	-

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1126[A]	SIR	CDA-CEA	8.25	1.75	1.50
2	B	1126[B]	SIR	CHC-C1C	5.20	1.48	1.38
2	B	1126[B]	SIR	CHD-C4C	5.11	1.48	1.38
2	B	1126[A]	SIR	CHD-C4C	4.72	1.47	1.38
2	D	1126[A]	SIR	CHD-C4C	4.45	1.47	1.38
2	D	1126[A]	SIR	CHC-C1C	4.45	1.47	1.38
2	D	1126[B]	SIR	CHD-C4C	4.39	1.47	1.38
2	B	1126[A]	SIR	CHC-C1C	4.04	1.46	1.38
2	D	1126[B]	SIR	CHA-C4D	3.96	1.48	1.39
2	D	1126[B]	SIR	C1C-C2C	-3.96	1.38	1.45
2	B	1126[A]	SIR	CHD-C1D	3.93	1.48	1.39
2	B	1126[A]	SIR	CHA-C4D	3.81	1.48	1.39
2	B	1126[B]	SIR	CHD-C1D	3.75	1.47	1.39
2	B	1126[A]	SIR	C1C-C2C	-3.67	1.38	1.45
2	B	1126[B]	SIR	C4C-C3C	-3.61	1.38	1.45
2	D	1126[B]	SIR	CHD-C1D	3.56	1.47	1.39
2	D	1126[B]	SIR	CHC-C1C	3.56	1.45	1.38
2	B	1126[B]	SIR	CHA-C4D	3.55	1.47	1.39
2	D	1126[A]	SIR	O3A-CEA	3.54	1.33	1.22
2	D	1126[A]	SIR	CHD-C1D	3.50	1.47	1.39
2	D	1126[A]	SIR	CO-NB	-3.35	1.84	1.96
2	B	1126[B]	SIR	C1C-C2C	-3.31	1.39	1.45
2	D	1126[A]	SIR	CHA-C4D	3.27	1.46	1.39
2	D	1126[A]	SIR	C1C-C2C	-3.27	1.39	1.45
2	D	1126[A]	SIR	C4C-C3C	-3.24	1.39	1.45
2	B	1126[B]	SIR	C4D-C3D	-2.91	1.38	1.44
2	D	1126[A]	SIR	CO-NA	-2.86	1.86	1.96
2	D	1126[A]	SIR	C1D-C2D	-2.84	1.38	1.44
2	D	1126[A]	SIR	C4D-C3D	-2.81	1.39	1.44
2	B	1126[B]	SIR	O2C-CCC	-2.75	1.21	1.30
2	B	1126[A]	SIR	C1D-C2D	-2.72	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1126[B]	SIR	O4D-CED	-2.63	1.22	1.30
2	D	1126[B]	SIR	CHC-C4B	-2.60	1.31	1.39
2	D	1126[B]	SIR	C4C-C3C	-2.59	1.40	1.45
2	B	1126[B]	SIR	CO-NB	-2.55	1.87	1.96
2	D	1126[B]	SIR	C1C-NC	-2.46	1.34	1.38
2	B	1126[A]	SIR	C4D-C3D	-2.44	1.39	1.44
2	B	1126[A]	SIR	CHC-C4B	-2.44	1.32	1.39
2	B	1126[A]	SIR	C4C-C3C	-2.41	1.41	1.45
2	D	1126[B]	SIR	O3C-CEC	-2.38	1.22	1.30
2	B	1126[B]	SIR	CHB-C4A	-2.38	1.32	1.39
2	B	1126[A]	SIR	CO-NB	-2.37	1.87	1.96
2	D	1126[B]	SIR	CO-NA	-2.37	1.87	1.96
2	D	1126[A]	SIR	C4D-ND	-2.29	1.34	1.38
2	D	1126[B]	SIR	CHB-C4A	-2.29	1.32	1.39
2	B	1126[B]	SIR	CBB-CCB	2.27	1.55	1.50
2	B	1126[A]	SIR	CHB-C4A	-2.24	1.32	1.39
2	B	1126[B]	SIR	O4A-CEA	-2.23	1.23	1.30
2	D	1126[A]	SIR	CHB-C4A	-2.22	1.32	1.39
2	B	1126[A]	SIR	CO-NA	-2.18	1.88	1.96
2	B	1126[B]	SIR	CDB-CEB	2.18	1.57	1.50
2	B	1126[B]	SIR	C4A-NA	2.16	1.35	1.30
2	D	1126[A]	SIR	CHC-C4B	-2.13	1.33	1.39
2	D	1126[A]	SIR	C1D-ND	-2.11	1.35	1.38
2	D	1126[A]	SIR	C4C-NC	-2.08	1.35	1.38
2	B	1126[A]	SIR	C2B-C3B	-2.07	1.49	1.55
2	D	1126[B]	SIR	CO-NB	-2.02	1.89	1.96

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1126[B]	SIR	C2C-C1C-NC	8.58	117.56	110.89
2	B	1126[B]	SIR	C4A-CHB-C1B	-8.03	114.03	125.84
2	D	1126[A]	SIR	C4A-CHB-C1B	-8.02	114.04	125.84
2	B	1126[A]	SIR	C2C-C1C-NC	8.02	117.12	110.89
2	D	1126[A]	SIR	C2C-C1C-NC	6.86	116.23	110.89
2	B	1126[B]	SIR	C2C-C1C-NC	6.52	115.95	110.89
2	D	1126[B]	SIR	C3C-C4C-NC	6.21	115.72	110.89
2	D	1126[B]	SIR	C3D-C4D-ND	6.18	116.22	110.73
2	D	1126[A]	SIR	C3C-C4C-NC	6.07	115.60	110.89
2	B	1126[B]	SIR	C3C-C4C-NC	6.02	115.57	110.89
2	D	1126[B]	SIR	C2D-C1D-ND	5.78	115.86	110.73
2	D	1126[A]	SIR	C3D-C4D-ND	5.78	115.86	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1126[B]	SIR	CAD-C2D-C1D	5.39	135.47	124.94
2	B	1126[A]	SIR	C3D-C4D-ND	5.32	115.45	110.73
2	D	1126[A]	SIR	O3A-CEA-CDA	-5.31	107.93	122.95
2	D	1126[B]	SIR	CAD-C2D-C1D	5.26	135.21	124.94
2	D	1126[A]	SIR	C2D-C1D-ND	5.18	115.33	110.73
2	B	1126[A]	SIR	C3C-C4C-NC	5.16	114.90	110.89
2	D	1126[A]	SIR	CHC-C1C-NC	-4.94	119.00	124.85
2	B	1126[A]	SIR	C2D-C1D-ND	4.90	115.08	110.73
2	D	1126[A]	SIR	O4A-CEA-O3A	4.89	135.91	123.33
2	B	1126[B]	SIR	C3D-C4D-ND	4.77	114.96	110.73
2	D	1126[B]	SIR	C4C-NC-C1C	-4.60	98.33	105.11
2	B	1126[B]	SIR	CAB-C3B-C4B	-4.53	103.28	111.19
2	B	1126[B]	SIR	C2B-C1B-CHB	4.51	127.59	123.54
2	B	1126[B]	SIR	C2D-C1D-ND	4.41	114.64	110.73
2	D	1126[B]	SIR	C4D-ND-C1D	-4.35	98.70	105.11
2	D	1126[A]	SIR	C1C-CHC-C4B	-4.16	116.59	126.62
2	B	1126[A]	SIR	CAC-C3C-C4C	4.14	133.28	124.85
2	B	1126[A]	SIR	C4C-NC-C1C	-4.10	99.07	105.11
2	D	1126[B]	SIR	C2B-C1B-CHB	-4.08	119.88	123.54
2	B	1126[B]	SIR	C2A-C1A-CHA	-4.05	119.91	123.54
2	B	1126[B]	SIR	CHC-C1C-NC	-3.97	120.15	124.85
2	D	1126[A]	SIR	C2B-C1B-CHB	3.90	127.05	123.54
2	B	1126[B]	SIR	C4C-NC-C1C	-3.85	99.45	105.11
2	B	1126[A]	SIR	C2B-C1B-CHB	-3.77	120.16	123.54
2	D	1126[A]	SIR	C4C-NC-C1C	-3.66	99.72	105.11
2	B	1126[A]	SIR	C4A-CHB-C1B	-3.62	120.51	125.84
2	D	1126[B]	SIR	C2A-C1A-CHA	-3.47	120.42	123.54
2	D	1126[B]	SIR	C3B-C4B-CHC	-3.47	115.94	123.33
2	D	1126[A]	SIR	C4D-ND-C1D	-3.42	100.08	105.11
2	B	1126[A]	SIR	CHD-C4C-NC	-3.40	120.83	124.85
2	D	1126[B]	SIR	CAC-C3C-C4C	3.38	131.73	124.85
2	B	1126[B]	SIR	CBD-CAD-C2D	3.38	121.87	112.53
2	B	1126[A]	SIR	C4D-ND-C1D	-3.37	100.15	105.11
2	B	1126[B]	SIR	C2A-C1A-NA	3.31	115.33	111.35
2	D	1126[B]	SIR	C2B-C1B-NB	3.27	115.28	111.35
2	B	1126[B]	SIR	CDB-C2B-C3B	3.26	116.98	108.37
2	B	1126[A]	SIR	CAB-CBB-CCB	-3.25	103.81	112.49
2	B	1126[B]	SIR	CDA-C2A-C1A	3.25	117.17	107.11
2	B	1126[B]	SIR	C4D-ND-C1D	-3.23	100.36	105.11
2	B	1126[B]	SIR	CMA-C2A-CDA	-3.21	105.29	110.74
2	D	1126[A]	SIR	CHC-C4B-NB	-3.18	122.11	125.74
2	B	1126[A]	SIR	CAC-C3C-C2C	-3.17	121.79	129.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1126[B]	SIR	CEC-CDC-C2C	3.14	121.65	113.76
2	B	1126[B]	SIR	C1D-C2D-C3D	-3.11	103.55	106.81
2	B	1126[A]	SIR	CHC-C1C-NC	-3.05	121.25	124.85
2	B	1126[A]	SIR	C2A-C3A-C4A	-3.01	97.08	100.89
2	D	1126[B]	SIR	CBD-CAD-C2D	2.93	120.64	112.53
2	B	1126[B]	SIR	O1B-CCB-O2B	-2.93	115.81	123.33
2	D	1126[B]	SIR	CHA-C4D-ND	-2.92	119.50	124.18
2	D	1126[A]	SIR	CHD-C4C-NC	-2.88	121.44	124.85
2	D	1126[B]	SIR	C3B-C4B-NB	2.87	116.44	110.77
2	B	1126[A]	SIR	CAB-C3B-C2B	-2.83	106.41	114.19
2	D	1126[A]	SIR	C1C-C2C-C3C	-2.82	103.68	106.84
2	D	1126[A]	SIR	CHB-C4A-NA	-2.82	122.53	125.74
2	B	1126[A]	SIR	CED-CDD-C3D	2.80	120.80	113.76
2	D	1126[B]	SIR	CHC-C1C-NC	-2.79	121.55	124.85
2	B	1126[A]	SIR	CAC-CBC-CCC	-2.78	106.30	113.67
2	B	1126[A]	SIR	C2B-C1B-NB	2.77	114.68	111.35
2	D	1126[B]	SIR	C4C-C3C-C2C	-2.73	103.78	106.84
2	D	1126[A]	SIR	CAD-CBD-CCD	-2.67	106.59	113.67
2	D	1126[B]	SIR	CHD-C4C-NC	-2.67	121.69	124.85
2	D	1126[A]	SIR	C4D-C3D-C2D	-2.65	104.03	106.81
2	D	1126[B]	SIR	CMB-C2B-CDB	2.64	115.22	110.74
2	B	1126[B]	SIR	CHB-C4A-NA	-2.61	122.76	125.74
2	B	1126[B]	SIR	C3B-C2B-C1B	-2.59	96.52	100.92
2	D	1126[A]	SIR	C4D-CHA-C1A	-2.58	121.11	125.87
2	B	1126[B]	SIR	C1C-CHC-C4B	-2.58	120.39	126.62
2	B	1126[B]	SIR	C3A-C4A-NA	2.55	115.80	110.77
2	D	1126[B]	SIR	CHC-C1C-C2C	-2.54	120.85	124.86
2	B	1126[A]	SIR	C1C-C2C-C3C	-2.53	104.01	106.84
2	B	1126[B]	SIR	O3B-CEB-O4B	-2.52	116.85	123.33
2	B	1126[B]	SIR	CHD-C4C-C3C	-2.51	120.90	124.86
2	D	1126[B]	SIR	C1D-C2D-C3D	-2.50	104.19	106.81
2	B	1126[B]	SIR	O3B-CEB-CDB	2.48	122.19	114.35
2	B	1126[B]	SIR	CAA-C3A-C4A	2.48	115.50	111.19
2	B	1126[A]	SIR	C4D-C3D-C2D	-2.46	104.24	106.81
2	D	1126[B]	SIR	CAA-C3A-C4A	2.46	115.47	111.19
2	D	1126[B]	SIR	C3A-C4A-NA	2.44	115.59	110.77
2	D	1126[A]	SIR	CHB-C1B-NB	-2.42	120.99	124.92
2	B	1126[A]	SIR	C3B-C4B-CHC	-2.42	118.19	123.33
2	D	1126[A]	SIR	C2A-C1A-CHA	-2.38	121.41	123.54
2	B	1126[A]	SIR	C3B-C4B-NB	2.34	115.39	110.77
2	B	1126[B]	SIR	C1C-C2C-C3C	-2.32	104.24	106.84
2	D	1126[B]	SIR	O3C-CEC-CDC	2.32	121.70	114.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1126[A]	SIR	CHA-C4D-ND	-2.30	120.50	124.18
2	B	1126[A]	SIR	O4B-CEB-CDB	-2.27	116.52	122.95
2	D	1126[B]	SIR	O2D-CCD-CBD	2.24	121.08	114.00
2	B	1126[B]	SIR	O1B-CCB-CBB	2.24	121.07	114.00
2	B	1126[B]	SIR	CAB-C3B-C2B	2.23	120.33	114.19
2	B	1126[A]	SIR	O2A-CCA-CBA	2.22	121.00	114.00
2	D	1126[B]	SIR	O4B-CEB-CDB	-2.21	116.70	122.95
2	B	1126[B]	SIR	CAB-CBB-CCB	2.19	118.33	112.49
2	B	1126[A]	SIR	O3C-CEC-CDC	2.18	121.25	114.51
2	D	1126[B]	SIR	O1D-CCD-CBD	-2.15	116.27	123.09
2	D	1126[B]	SIR	C3A-C4A-CHB	-2.13	118.80	123.33
2	B	1126[A]	SIR	CHA-C4D-ND	-2.11	120.79	124.18
2	B	1126[B]	SIR	O3A-CEA-CDA	-2.10	117.01	122.95
2	D	1126[B]	SIR	CAD-CBD-CCD	-2.07	108.18	113.67
2	D	1126[B]	SIR	CDA-C2A-C1A	2.06	113.50	107.11
2	B	1126[A]	SIR	CHC-C1C-C2C	-2.05	121.62	124.86
2	B	1126[A]	SIR	CDB-C2B-C3B	2.04	113.74	108.37
2	D	1126[B]	SIR	CAC-C3C-C2C	-2.03	124.48	129.24
2	D	1126[B]	SIR	CHD-C1D-ND	-2.03	120.93	124.18
2	B	1126[A]	SIR	CHB-C4A-NA	-2.01	123.44	125.74
2	D	1126[A]	SIR	C1D-C2D-C3D	-2.01	104.70	106.81
2	D	1126[B]	SIR	C1C-C2C-C3C	-2.01	104.59	106.84

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1126[A]	SIR	NB
2	B	1126[A]	SIR	NC
2	B	1126[A]	SIR	NA
2	B	1126[B]	SIR	NB
2	B	1126[B]	SIR	NC
2	B	1126[B]	SIR	NA
2	D	1126[A]	SIR	NB
2	D	1126[A]	SIR	NC
2	D	1126[A]	SIR	NA
2	D	1126[B]	SIR	NB
2	D	1126[B]	SIR	NC
2	D	1126[B]	SIR	NA

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1126[A]	SIR	C2C-C3C-CAC-CBC
2	B	1126[A]	SIR	C4C-C3C-CAC-CBC
2	B	1126[B]	SIR	C1A-C2A-CDA-CEA
2	B	1126[B]	SIR	CMA-C2A-CDA-CEA
2	B	1126[B]	SIR	C3A-C2A-CDA-CEA
2	B	1126[B]	SIR	C4A-C3A-CAA-CBA
2	B	1126[B]	SIR	CMB-C2B-CDB-CEB
2	B	1126[B]	SIR	C3B-C2B-CDB-CEB
2	B	1126[B]	SIR	C1B-C2B-CDB-CEB
2	B	1126[B]	SIR	C1D-C2D-CAD-CBD
2	D	1126[A]	SIR	CMB-C2B-CDB-CEB
2	D	1126[A]	SIR	C3B-C2B-CDB-CEB
2	D	1126[A]	SIR	C1B-C2B-CDB-CEB
2	D	1126[A]	SIR	C2B-C3B-CAB-CBB
2	D	1126[A]	SIR	C2C-C3C-CAC-CBC
2	D	1126[B]	SIR	C1A-C2A-CDA-CEA
2	D	1126[B]	SIR	CMA-C2A-CDA-CEA
2	D	1126[B]	SIR	C3A-C2A-CDA-CEA
2	D	1126[B]	SIR	C4B-C3B-CAB-CBB
2	D	1126[A]	SIR	C4C-C3C-CAC-CBC
2	B	1126[A]	SIR	C4B-C3B-CAB-CBB
2	D	1126[B]	SIR	C1D-C2D-CAD-CBD
2	B	1126[B]	SIR	C3D-C2D-CAD-CBD
2	D	1126[B]	SIR	C3D-C2D-CAD-CBD
2	B	1126[B]	SIR	C2A-C3A-CAA-CBA
2	B	1126[B]	SIR	C4B-C3B-CAB-CBB
2	B	1126[B]	SIR	C3B-CAB-CBB-CCB
2	D	1126[A]	SIR	C3A-CAA-CBA-CCA
2	B	1126[A]	SIR	C1B-C2B-CDB-CEB
2	B	1126[A]	SIR	C3A-CAA-CBA-CCA
2	D	1126[A]	SIR	C3B-CAB-CBB-CCB
2	D	1126[A]	SIR	C3D-C2D-CAD-CBD
2	D	1126[A]	SIR	C2C-CDC-CEC-O3C
2	D	1126[A]	SIR	C2C-CDC-CEC-O4C
2	D	1126[B]	SIR	C3B-CAB-CBB-CCB
2	D	1126[A]	SIR	C2A-CDA-CEA-O4A
2	D	1126[A]	SIR	C2B-CDB-CEB-O3B
2	D	1126[A]	SIR	C2B-CDB-CEB-O4B
2	D	1126[A]	SIR	C3D-CDD-CED-O4D
2	D	1126[A]	SIR	C3D-CDD-CED-O3D
2	D	1126[B]	SIR	C2C-C3C-CAC-CBC
2	D	1126[A]	SIR	C1D-C2D-CAD-CBD
2	D	1126[B]	SIR	C2C-CDC-CEC-O4C

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Mol	Chain	Res	Type	Atoms
2	D	1126[B]	SIR	C3D-CDD-CED-O4D
2	B	1126[A]	SIR	C2B-C3B-CAB-CBB
2	D	1126[B]	SIR	CAD-CBD-CCD-O1D
2	B	1126[A]	SIR	CMB-C2B-CDB-CEB
2	D	1126[A]	SIR	CAB-CBB-CCB-O1B
2	D	1126[B]	SIR	CAC-CBC-CCC-O1C
2	D	1126[A]	SIR	CAA-CBA-CCA-O2A
2	B	1126[B]	SIR	CAC-CBC-CCC-O1C
2	D	1126[A]	SIR	CAB-CBB-CCB-O2B
2	D	1126[B]	SIR	CAD-CBD-CCD-O2D
2	D	1126[B]	SIR	C4C-C3C-CAC-CBC
2	B	1126[B]	SIR	CAC-CBC-CCC-O2C
2	D	1126[A]	SIR	C2A-CDA-CEA-O3A
2	B	1126[A]	SIR	C2C-CDC-CEC-O4C
2	D	1126[B]	SIR	C2C-CDC-CEC-O3C
2	B	1126[A]	SIR	CAD-CBD-CCD-O2D
2	D	1126[A]	SIR	C4B-C3B-CAB-CBB
2	B	1126[A]	SIR	CAD-CBD-CCD-O1D
2	B	1126[B]	SIR	CAA-CBA-CCA-O1A
2	D	1126[A]	SIR	CAA-CBA-CCA-O1A
2	B	1126[B]	SIR	CAA-CBA-CCA-O2A
2	D	1126[A]	SIR	CAC-CBC-CCC-O2C
2	D	1126[B]	SIR	CAC-CBC-CCC-O2C
2	D	1126[B]	SIR	CMB-C2B-CDB-CEB
2	D	1126[A]	SIR	CAC-CBC-CCC-O1C
2	B	1126[A]	SIR	C2C-CDC-CEC-O3C
2	D	1126[B]	SIR	C3D-CDD-CED-O3D
2	D	1126[A]	SIR	CAD-CBD-CCD-O1D
2	D	1126[A]	SIR	CAD-CBD-CCD-O2D
2	D	1126[A]	SIR	C2A-C3A-CAA-CBA
2	B	1126[A]	SIR	CAA-CBA-CCA-O2A

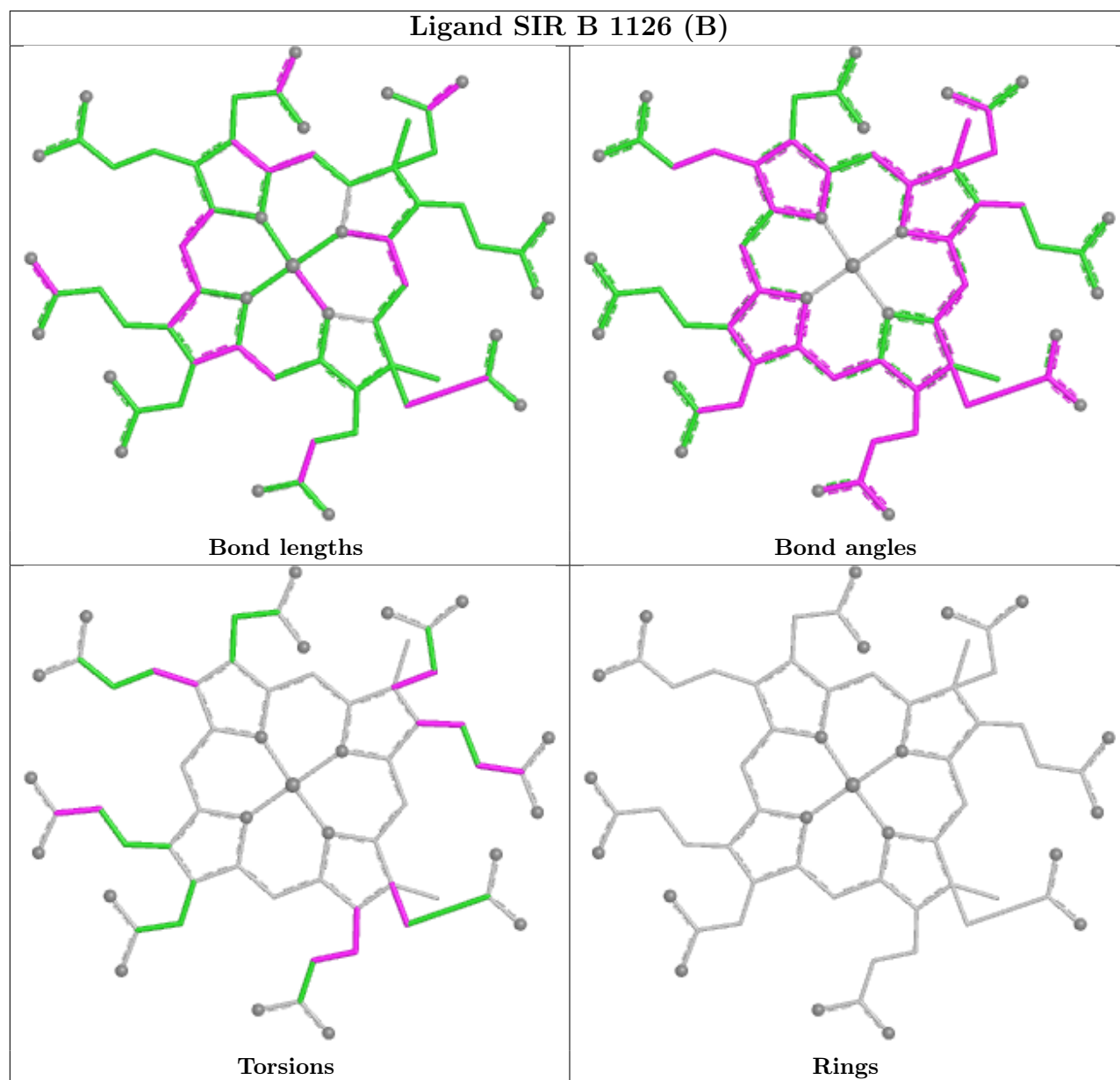
There are no ring outliers.

4 monomers are involved in 52 short contacts:

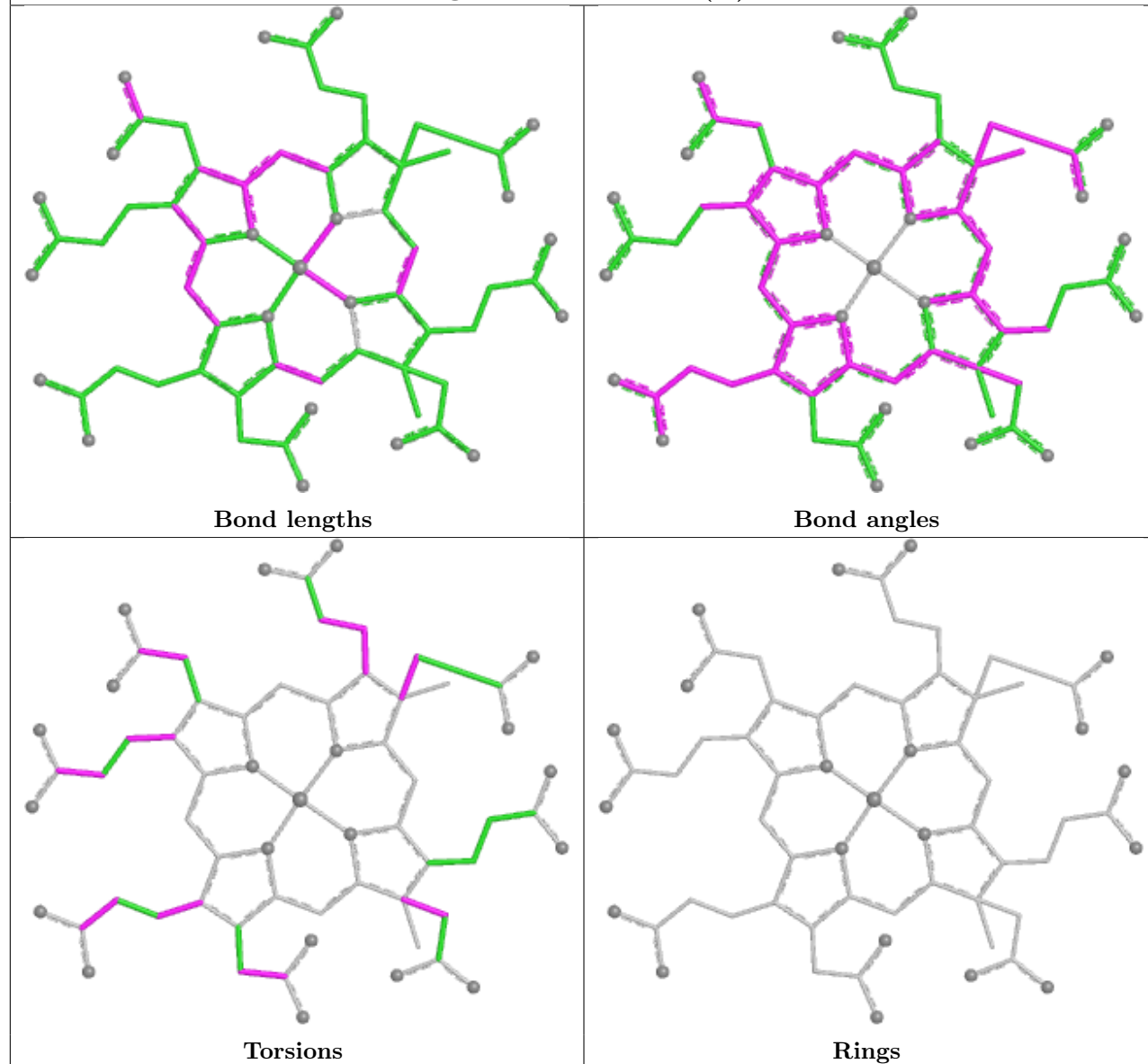
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1126[B]	SIR	3	0
2	D	1126[B]	SIR	17	0
2	B	1126[A]	SIR	9	0
2	D	1126[A]	SIR	23	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

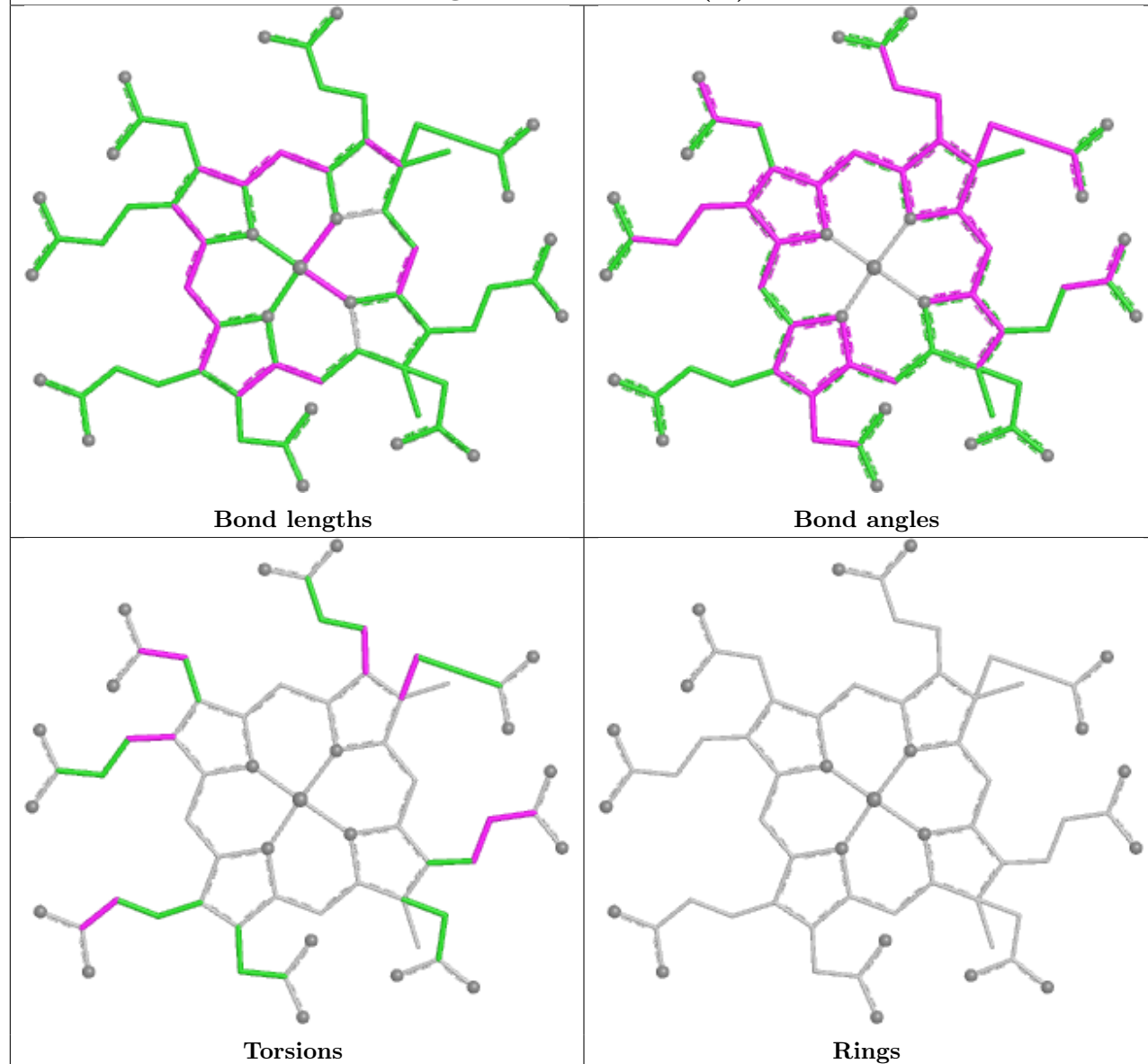
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

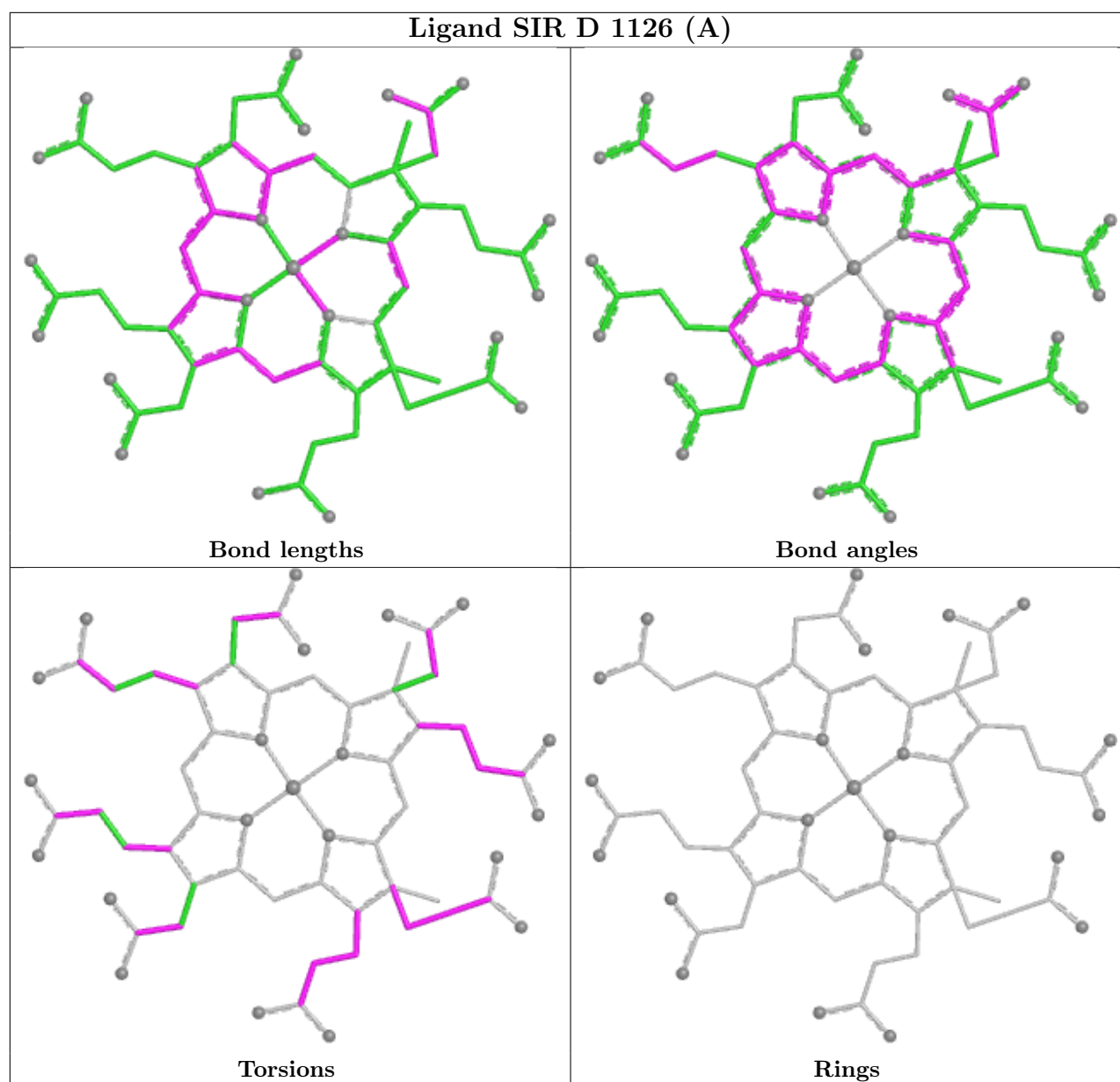


Ligand SIR D 1126 (B)



Ligand SIR B 1126 (A)





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	126/133 (94%)	-0.06	2 (1%) 70 70	12, 25, 39, 57	1 (0%)
1	B	125/133 (93%)	-0.17	0 100 100	14, 21, 40, 52	1 (0%)
1	C	126/133 (94%)	0.79	15 (11%) 9 8	13, 38, 66, 70	1 (0%)
1	D	125/133 (93%)	0.22	6 (4%) 35 34	17, 27, 44, 56	1 (0%)
All	All	502/532 (94%)	0.20	23 (4%) 37 36	12, 27, 57, 70	4 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	43	ALA	5.8
1	A	1	MET	4.3
1	D	44	ARG	3.9
1	C	1	MET	3.6
1	C	91	ILE	3.3
1	C	0	GLY	3.2
1	C	82	LEU	3.1
1	C	85	PHE	3.0
1	C	96	PHE	3.0
1	D	45	LYS	2.9
1	D	115	TYR	2.7
1	C	79	LEU	2.4
1	C	11	GLY	2.4
1	C	86	PRO	2.2
1	C	42	ALA	2.2
1	D	1	MET	2.2
1	C	87	ARG	2.2
1	C	83	LEU	2.1
1	C	84	GLY	2.1
1	A	0	GLY	2.1
1	C	45	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	94	GLY	2.1
1	D	14	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

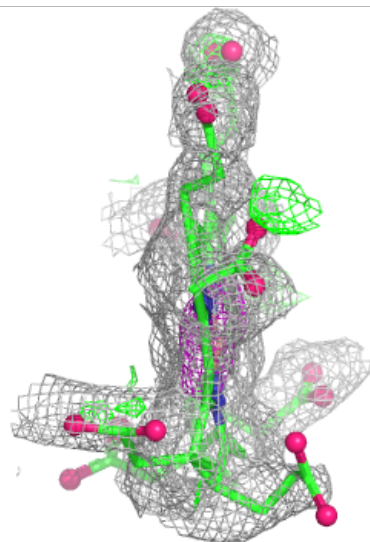
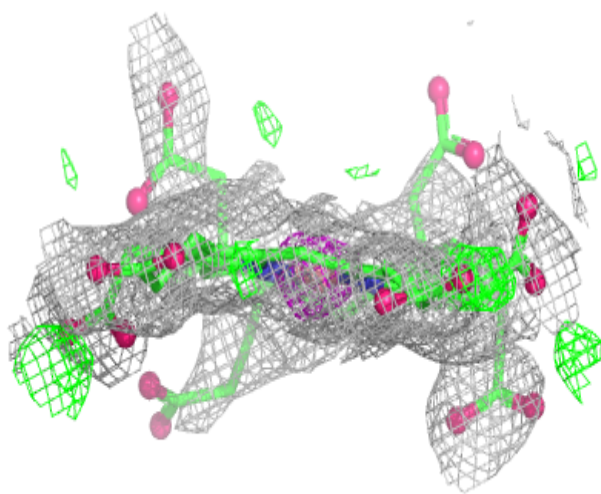
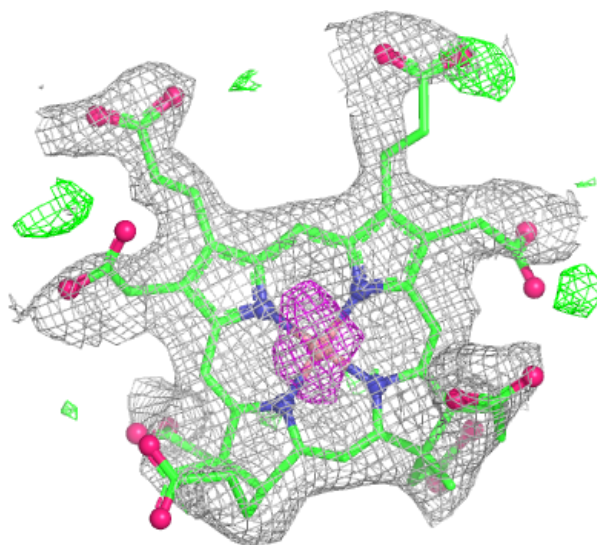
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SIR	D	1126[A]	63/63	0.82	0.33	138,141,142,143	63
2	SIR	D	1126[B]	63/63	0.82	0.33	9,28,36,39	63
2	SIR	B	1126[A]	63/63	0.83	0.16	29,43,47,54	63
2	SIR	B	1126[B]	63/63	0.83	0.16	7,17,29,33	63

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.

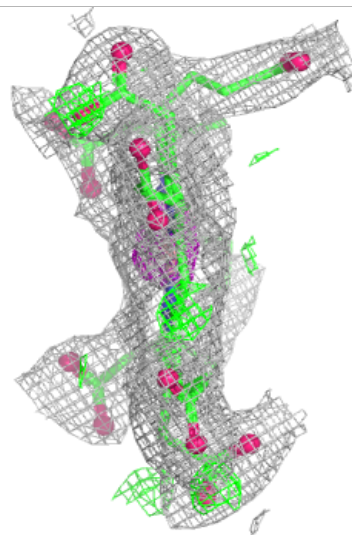
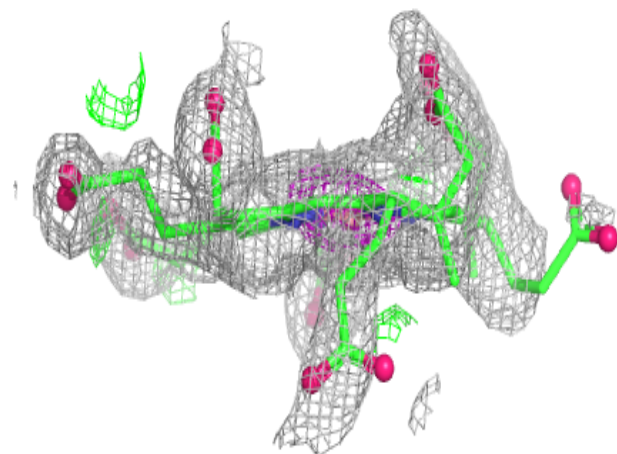
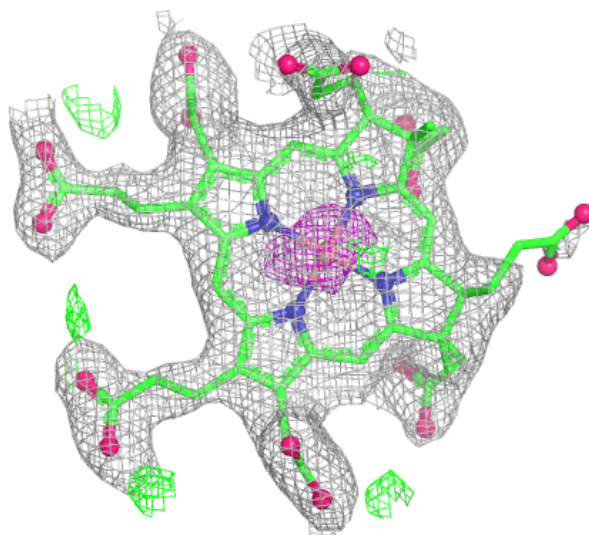
Electron density around SIR D 1126 (A):

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



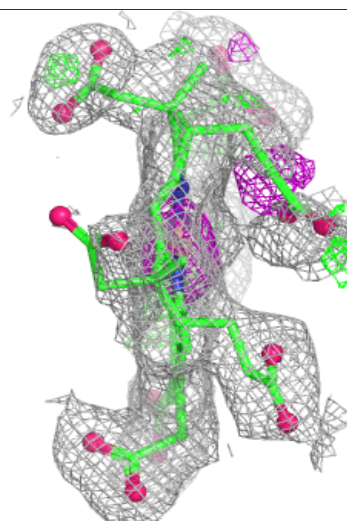
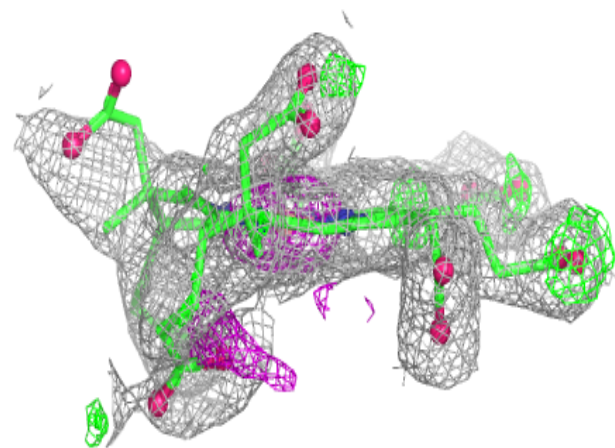
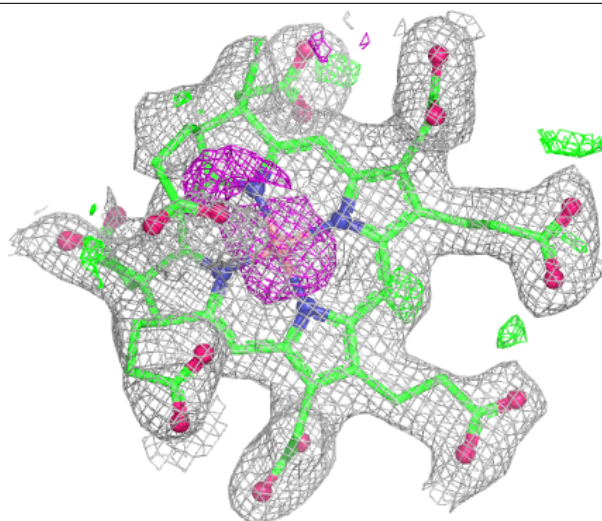
Electron density around SIR D 1126 (B):

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



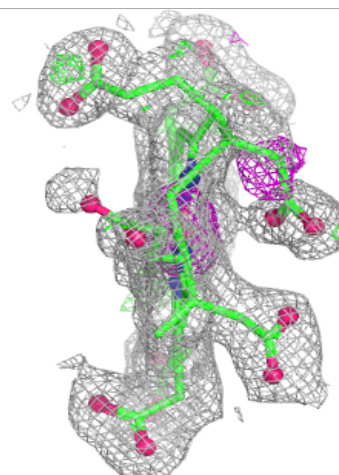
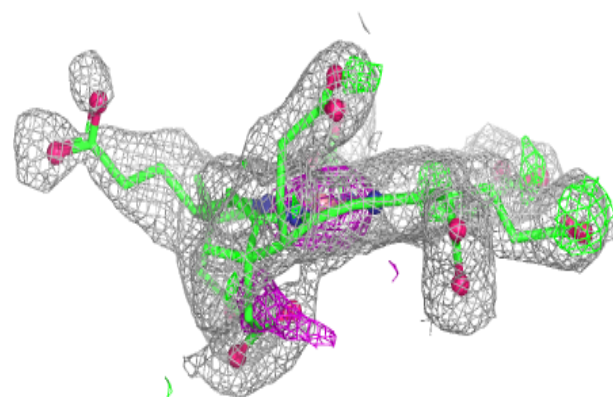
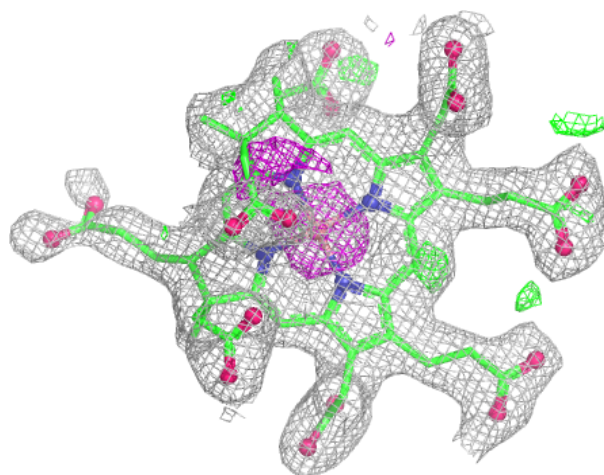
Electron density around SIR B 1126 (A):

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



Electron density around SIR B 1126 (B):

$2mF_o-DF_c$ (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.