



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 16, 2026 – 10:35 AM UTC

PDB ID : 3MM5 / pdb_00003mm5
Title : Dissimilatory sulfite reductase in complex with the substrate sulfite
Authors : Parey, K.; Warkentin, E.; Kroneck, P.M.H.; Ermler, U.
Deposited on : 2010-04-19
Resolution : 1.80 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

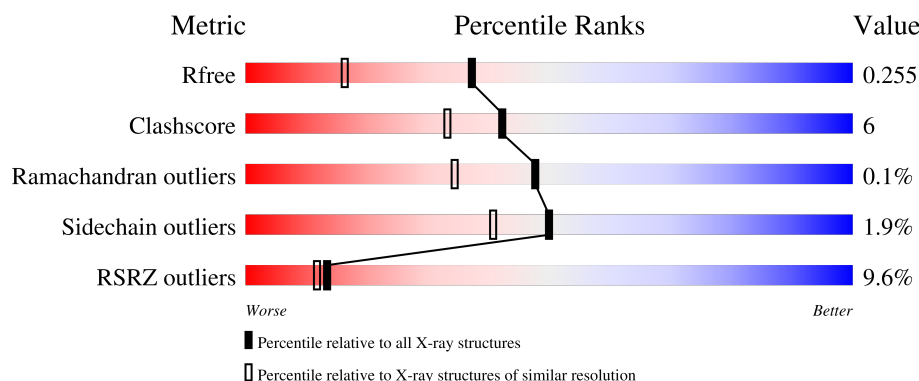
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	418	3% 89% 11%
1	D	418	22% 87% 11% .
2	B	366	% 89% 9% ..
2	E	366	12% 84% 13% ..

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
3	SRM	A	580	X	-	-	-
3	SRM	B	570	X	-	-	-
3	SRM	D	580	X	-	-	-
3	SRM	E	570	X	-	-	-
4	SF4	E	585	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13810 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.

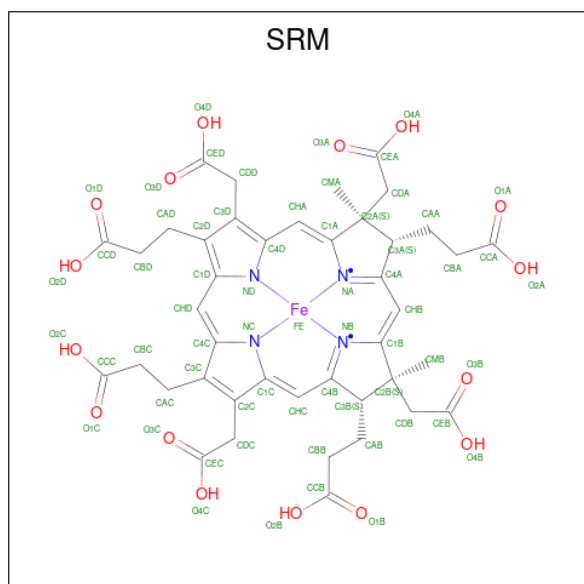
- Molecule 1 is a protein called Sulfite reductase, dissimilatory-type subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	3	0
			3348	2146	557	619	26			
1	D	417	Total	C	N	O	S	0	1	0
			3336	2139	558	613	26			

- Molecule 2 is a protein called Sulfite reductase, dissimilatory-type subunit beta.

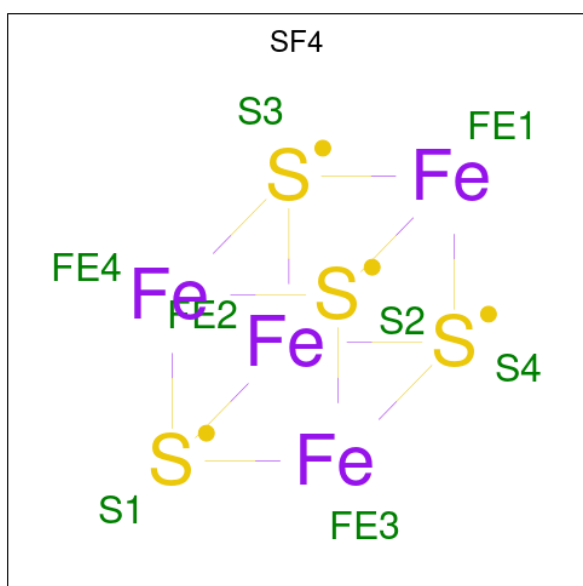
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	363	Total	C	N	O	S	5	5	0
			2930	1883	492	533	22			
2	E	363	Total	C	N	O	S	0	0	0
			2901	1862	491	526	22			

- Molecule 3 is SIROHEME (CCD ID: SRM) (formula: $C_{42}H_{44}FeN_4O_{16}$).



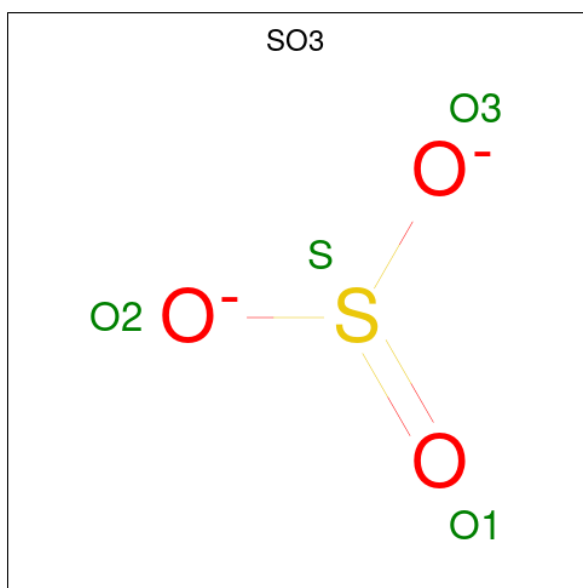
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	
			63	42	1	4	16	
3	B	1	Total	C	Fe	N	O	
			63	42	1	4	16	
3	D	1	Total	C	Fe	N	O	
			63	42	1	4	16	
3	E	1	Total	C	Fe	N	O	
			63	42	1	4	16	

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 5 is SULFITE ION (CCD ID: SO3) (formula: O₃S).



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

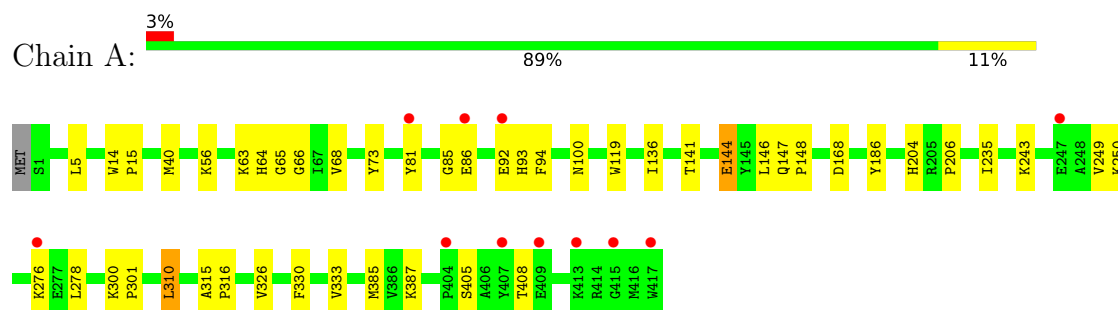
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	229	Total	O	0	0
			229	229		
6	B	565	Total	O	0	0
			565	565		
6	D	92	Total	O	0	0
			92	92		
6	E	85	Total	O	0	0
			85	85		

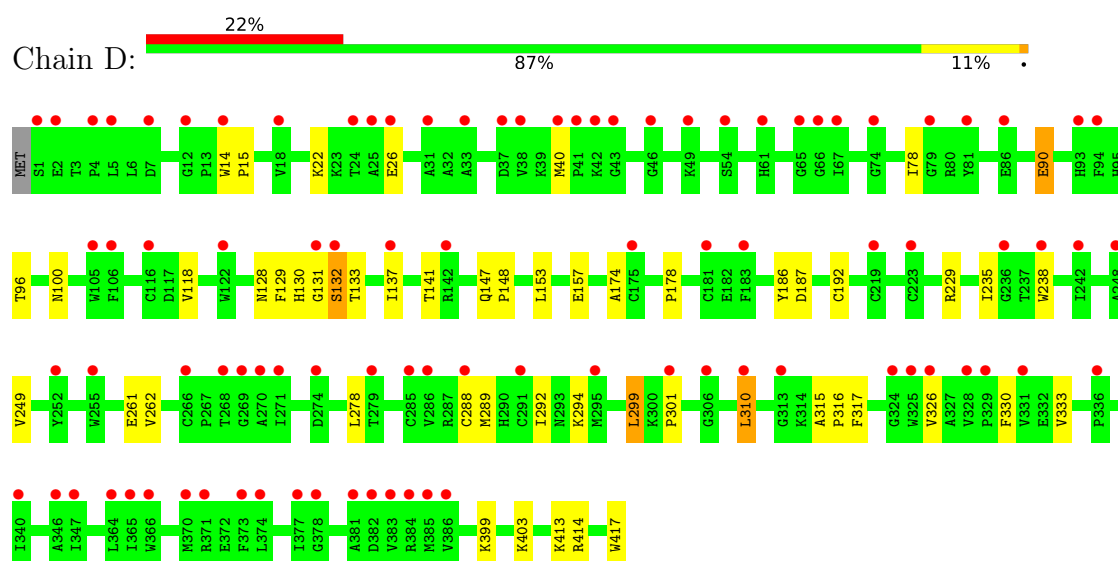
3 Residue-property plots [i](#)

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.

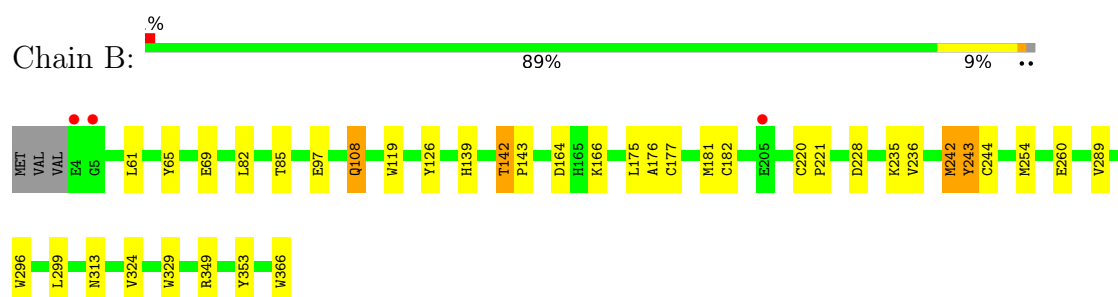
- Molecule 1: Sulfite reductase, dissimilatory-type subunit alpha



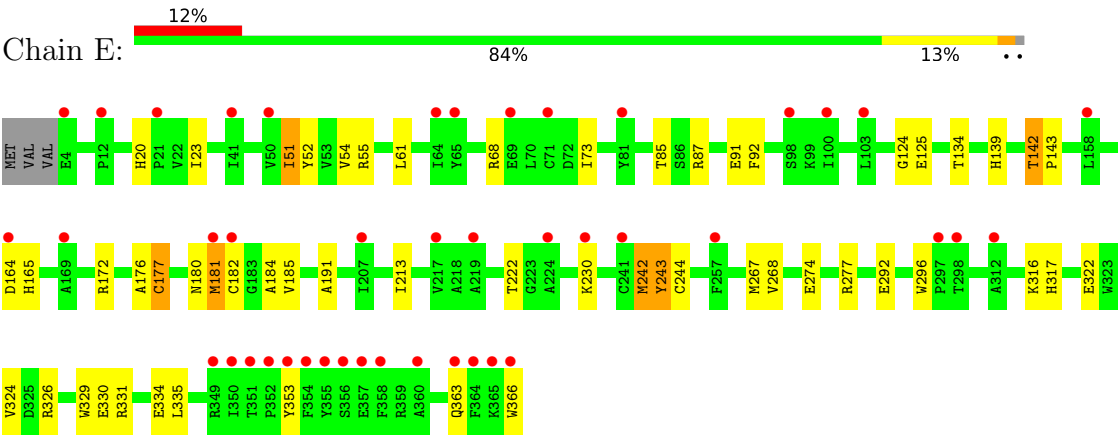
- Molecule 1: Sulfite reductase, dissimilatory-type subunit alpha



- Molecule 2: Sulfite reductase, dissimilatory-type subunit beta



● Molecule 2: Sulfite reductase, dissimilatory-type subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.60Å 68.90Å 145.10Å 90.00° 107.50° 90.00°	Depositor
Resolution (Å)	15.00 – 1.80 15.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-1.80) 99.1 (15.00-1.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.6.0046	Depositor
R, R_{free}	0.158 , 0.188 0.233 , 0.255	Depositor DCC
R_{free} test set	8181 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13810	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SRM, SF4, SO3

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	0.91	0/3444	0.98	2/4646 (0.0%)
1	D	0.56	0/3426	0.82	0/4622
2	B	0.98	2/3025 (0.1%)	1.00	4/4114 (0.1%)
2	E	0.59	2/2984 (0.1%)	0.84	0/4058
All	All	0.78	4/12879 (0.0%)	0.91	6/17440 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	296	TRP	N-CA	5.99	1.50	1.46
2	E	213	ILE	CA-CB	5.80	1.57	1.54
2	E	68	ARG	CZ-NH1	5.41	1.40	1.32
2	B	289	VAL	CA-CB	5.12	1.60	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	108	GLN	CA-CB-CG	6.71	127.52	114.10
2	B	349	ARG	N-CA-C	5.59	117.37	111.28
2	B	254	MET	CA-C-N	-5.58	114.22	119.85
2	B	254	MET	C-N-CA	-5.58	114.22	119.85
1	A	136	ILE	CA-C-N	-5.44	116.44	123.19
1	A	136	ILE	C-N-CA	-5.44	116.44	123.19

There are no chirality outliers.

There are no planarity outliers.

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	3348	0	3294	42	0
1	D	3336	0	3289	40	0
2	B	2930	0	2872	32	0
2	E	2901	0	2837	41	0
3	A	63	0	34	10	0
3	B	63	0	34	1	0
3	D	63	0	34	13	0
3	E	63	0	34	8	0
4	A	16	0	0	0	0
4	B	16	0	0	0	0
4	D	16	0	0	0	0
4	E	16	0	0	3	0
5	A	4	0	0	0	0
5	D	4	0	0	0	0
6	A	229	0	0	5	0
6	B	565	0	0	5	0
6	D	92	0	0	1	0
6	E	85	0	0	1	0
All	All	13810	0	12428	159	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 6.

All (159) 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)
6:B:588:HOH:O	1:D:403[B]:LYS:HE3	1.20	1.30
3:D:580:SRM:HMB2	3:D:580:SRM:HBB2	1.42	0.99
1:A:85:GLY:HA3	1:A:92[A]:GLU:OE2	1.65	0.96
3:D:580:SRM:HBB2	3:D:580:SRM:CMB	1.95	0.95
3:A:580:SRM:O1A	2:B:139:HIS:HD2	1.55	0.88
2:E:134:THR:OG1	2:E:177:CYS:SG	2.32	0.88
1:A:81:TYR:CE2	1:A:93:HIS:CD2	2.63	0.85
1:D:229:ARG:HD2	2:E:184:ALA:HB2	1.61	0.82
3:D:580:SRM:HBD2	3:D:580:SRM:HDD1	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:GLU:HB3	1:D:294:LYS:HE2	1.65	0.76
1:D:399:LYS:HD3	1:D:417:TRP:O	1.86	0.76
1:A:5:LEU:HD11	1:A:56:LYS:HE2	1.68	0.76
1:A:81:TYR:HE2	1:A:93:HIS:CD2	2.03	0.75
1:A:81:TYR:CD2	1:A:93:HIS:CD2	2.77	0.71
3:E:570:SRM:HDD2	3:E:570:SRM:HBD1	1.72	0.71
2:E:85:THR:HB	3:E:570:SRM:HAB2	1.73	0.70
3:D:580:SRM:CMB	3:D:580:SRM:CBB	2.67	0.69
2:E:134:THR:HG21	2:E:182:CYS:HB2	1.74	0.69
1:A:56:LYS:HE3	6:A:709:HOH:O	1.93	0.69
2:B:260:GLU:HB3	1:D:403[B]:LYS:HD2	1.74	0.68
1:D:131:GLY:HA3	3:D:580:SRM:HBB1	1.77	0.67
1:A:66:GLY:H	1:A:81:TYR:HE1	1.42	0.67
2:E:125:GLU:HB3	2:E:165:HIS:HB3	1.77	0.66
3:A:580:SRM:O1A	2:B:139:HIS:CD2	2.45	0.65
3:A:580:SRM:C4C	2:B:182:CYS:HA	2.26	0.65
1:A:64:HIS:HD2	6:A:525:HOH:O	1.80	0.65
1:A:94:PHE:O	2:B:139:HIS:HE1	1.80	0.65
3:D:580:SRM:HMB2	3:D:580:SRM:CBB	2.10	0.63
3:A:580:SRM:CBB	3:A:580:SRM:HMB1	2.28	0.63
2:B:164[B]:ASP:HB3	2:B:166:LYS:HG3	1.80	0.62
1:D:235:ILE:HD12	1:D:310:LEU:HD22	1.81	0.61
1:A:94:PHE:O	2:B:139:HIS:CE1	2.55	0.60
1:A:14:TRP:CD2	1:A:15:PRO:HD2	2.37	0.60
3:A:580:SRM:HMB1	3:A:580:SRM:HBB2	1.83	0.60
1:D:96:THR:HG23	2:E:139:HIS:CE1	2.38	0.58
1:D:315:ALA:HB1	1:D:316:PRO:CD	2.33	0.58
1:D:288:CYS:O	1:D:289:MET:HB2	2.02	0.58
2:E:172:ARG:HH21	3:E:570:SRM:C2C	2.17	0.58
6:A:511:HOH:O	2:E:331:ARG:HD2	2.03	0.57
2:E:20:HIS:HB3	2:E:23:ILE:HD12	1.86	0.57
2:B:313:ASN:HB3	6:B:420:HOH:O	2.04	0.57
2:B:175:LEU:CD2	6:B:508:HOH:O	2.53	0.56
2:B:175:LEU:C	2:B:175:LEU:HD23	2.30	0.56
1:A:65:GLY:HA2	1:A:81:TYR:HD1	1.70	0.56
2:E:176:ALA:HB2	2:E:185:VAL:HG21	1.87	0.55
2:E:134:THR:CG2	2:E:182:CYS:HB2	2.37	0.55
1:A:235:ILE:HD12	1:A:310:LEU:HD22	1.88	0.54
1:A:243:LYS:HE3	1:A:301:PRO:O	2.07	0.53
1:A:315:ALA:HB1	1:A:316:PRO:CD	2.38	0.53
1:D:22:LYS:O	1:D:26:GLU:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:ALA:HB1	1:D:316:PRO:HD3	1.90	0.53
2:E:134:THR:HB	4:E:585:SF4:S4	2.50	0.52
3:E:570:SRM:HDD2	3:E:570:SRM:CBD	2.40	0.52
1:D:249:VAL:HG11	1:D:278:LEU:HB2	1.93	0.51
1:A:65:GLY:CA	1:A:81:TYR:HD1	2.23	0.51
2:B:85:THR:HB	3:B:570:SRM:HAB1	1.93	0.51
1:D:261:GLU:CB	1:D:294:LYS:HE2	2.37	0.51
1:D:316:PRO:HG2	2:E:181:MET:HE3	1.92	0.51
2:E:324:VAL:HG11	2:E:329:TRP:CE2	2.45	0.51
1:D:238:TRP:CE3	1:D:301:PRO:HB3	2.46	0.50
1:D:40:MET:SD	1:D:141:THR:HA	2.52	0.50
2:E:164:ASP:CG	2:E:165:HIS:H	2.20	0.50
1:A:40:MET:SD	1:A:141:THR:HA	2.51	0.49
3:D:580:SRM:HBB2	3:D:580:SRM:HMB3	1.85	0.49
1:D:316:PRO:HG2	2:E:181:MET:CE	2.42	0.49
1:A:68:VAL:HG22	1:A:146:LEU:CD1	2.42	0.49
1:A:85:GLY:HA3	1:A:92[B]:GLU:HG3	1.95	0.49
1:D:262:VAL:HG22	1:D:294:LYS:HG2	1.93	0.49
1:A:81:TYR:CD2	1:A:93:HIS:HD2	2.30	0.49
2:B:242:MET:C	2:B:243:TYR:CG	2.91	0.49
2:E:242:MET:C	2:E:243:TYR:CG	2.91	0.49
2:E:326:ARG:HD2	6:E:793:HOH:O	2.12	0.49
1:D:90:GLU:CD	1:D:90:GLU:H	2.20	0.48
2:B:324:VAL:HG11	2:B:329:TRP:CE2	2.48	0.48
1:D:78:ILE:HB	1:D:96:THR:OG1	2.13	0.48
3:A:580:SRM:C3C	2:B:182:CYS:HA	2.43	0.48
1:D:128:ASN:HD22	2:E:61:LEU:HA	1.78	0.48
1:A:250:LYS:NZ	1:A:276:LYS:O	2.46	0.48
1:A:243:LYS:HD2	1:A:300:LYS:HE3	1.94	0.47
1:A:186:TYR:CD1	1:A:333:VAL:HG11	2.50	0.47
1:A:81:TYR:HD2	1:A:93:HIS:HD2	1.61	0.47
2:E:51:ILE:HG13	2:E:52:TYR:N	2.30	0.47
2:E:142:THR:N	2:E:143:PRO:CD	2.77	0.47
1:A:147:GLN:HB3	1:A:148:PRO:HD3	1.97	0.47
2:E:87:ARG:HG3	3:E:570:SRM:HBB2	1.97	0.47
1:A:81:TYR:CE2	1:A:93:HIS:CG	3.01	0.46
1:D:14:TRP:CD2	1:D:15:PRO:HD2	2.50	0.46
2:E:177:CYS:HB2	4:E:585:SF4:S3	2.55	0.46
1:A:63:LYS:HG2	1:A:81:TYR:O	2.15	0.46
1:D:330:PHE:HB2	2:E:366:TRP:CH2	2.51	0.46
1:D:310:LEU:HD12	1:D:326:VAL:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144[A]:GLU:H	1:A:144[A]:GLU:CD	2.22	0.46
1:A:315:ALA:HB1	1:A:316:PRO:HD2	1.98	0.45
1:A:330:PHE:HB2	2:B:366:TRP:CH2	2.52	0.45
3:A:580:SRM:C1C	2:B:182:CYS:HA	2.46	0.45
3:A:580:SRM:NC	2:B:182:CYS:HA	2.31	0.45
1:D:128:ASN:HB2	1:D:137:ILE:HB	1.97	0.45
1:D:414:ARG:HD3	6:D:771:HOH:O	2.16	0.45
2:B:175:LEU:HD22	6:B:508:HOH:O	2.14	0.45
2:E:73:ILE:HG22	2:E:92:PHE:CE2	2.51	0.45
3:D:580:SRM:HDA2	4:E:585:SF4:S1	2.57	0.45
1:A:81:TYR:HD2	1:A:93:HIS:CD2	2.31	0.45
2:B:175:LEU:HD23	6:B:508:HOH:O	2.14	0.45
2:B:228:ASP:HB2	2:B:235:LYS:HG3	1.99	0.45
3:A:580:SRM:CBB	3:A:580:SRM:CMB	2.95	0.44
3:E:570:SRM:HHA	3:E:570:SRM:O4D	2.17	0.44
2:B:82:LEU:N	2:B:82:LEU:HD23	2.33	0.44
3:E:570:SRM:HCD1	3:E:570:SRM:HAC2	1.76	0.44
1:A:81:TYR:HE2	1:A:93:HIS:CG	2.33	0.44
1:D:317:PHE:HD2	2:E:180:ASN:HD22	1.65	0.44
1:A:65:GLY:HA2	1:A:81:TYR:CD1	2.51	0.44
1:A:119:TRP:CH2	1:A:141:THR:HB	2.53	0.44
1:A:168:ASP:HB3	1:A:206:PRO:HG3	2.00	0.44
2:E:330:GLU:O	2:E:334:GLU:HG3	2.17	0.44
1:D:129:PHE:HA	1:D:130:HIS:HA	1.81	0.43
2:B:142:THR:N	2:B:143:PRO:CD	2.81	0.43
3:D:580:SRM:HDD1	3:D:580:SRM:CBD	2.45	0.43
3:A:580:SRM:HBA1	3:A:580:SRM:HHB	2.00	0.43
1:D:131:GLY:CA	3:D:580:SRM:HBB1	2.45	0.43
2:B:242:MET:SD	2:B:244:CYS:HB3	2.59	0.43
1:D:133:THR:H	3:D:580:SRM:HAB2	1.84	0.43
3:D:580:SRM:HHB	3:D:580:SRM:HDB1	1.84	0.42
2:E:316:LYS:HG2	2:E:317:HIS:CD2	2.54	0.42
2:B:353:TYR:HA	2:E:353:TYR:HA	2.00	0.42
2:E:54:VAL:O	2:E:91:GLU:HA	2.19	0.42
1:A:249:VAL:HG11	1:A:278:LEU:HB2	2.01	0.42
2:B:164[A]:ASP:HB3	2:B:166:LYS:HG3	2.01	0.42
2:B:299:LEU:HD23	2:B:299:LEU:C	2.45	0.42
2:B:65:TYR:O	2:B:69[A]:GLU:HG3	2.20	0.41
1:D:178:PRO:HG3	1:D:187:ASP:HA	2.02	0.41
1:D:186:TYR:CD1	1:D:333:VAL:HG11	2.55	0.41
1:D:147:GLN:HB3	1:D:148:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:SER:OG	1:A:408:THR:HG23	2.19	0.41
1:D:118:VAL:HG11	1:D:153:LEU:HG	2.01	0.41
1:A:56:LYS:CE	6:A:709:HOH:O	2.62	0.41
2:B:119:TRP:HB2	2:B:126:TYR:CD2	2.56	0.41
1:D:292:ILE:HG12	1:D:299:LEU:HB3	2.03	0.41
2:E:55:ARG:HH22	3:E:570:SRM:HBA2	1.86	0.41
2:E:274:GLU:O	2:E:363:GLN:NE2	2.53	0.41
1:A:63:LYS:HE2	1:A:81:TYR:HB3	2.03	0.41
1:A:326:VAL:HB	1:A:385:MET:HA	2.02	0.41
2:B:176:ALA:HB1	2:B:181:MET:HA	2.02	0.41
1:D:174:ALA:HB2	1:D:192:CYS:HB2	2.03	0.41
2:E:191:ALA:HB3	2:E:267:MET:HB2	2.03	0.41
2:E:124:GLY:HA3	2:E:316:LYS:CD	2.51	0.41
2:E:164:ASP:CG	2:E:165:HIS:N	2.79	0.41
1:A:73:TYR:CD1	1:A:204:HIS:HB3	2.56	0.41
2:E:277:ARG:HG2	2:E:322:GLU:HG2	2.03	0.40
2:B:260:GLU:HB3	1:D:403[B]:LYS:CD	2.46	0.40
1:A:387:LYS:NZ	6:A:1082:HOH:O	2.53	0.40
2:B:220:CYS:HA	2:B:221:PRO:HD3	1.96	0.40
1:D:78:ILE:HB	1:D:96:THR:HG1	1.85	0.40
1:D:132:SER:HB3	3:D:580:SRM:HCD2	2.02	0.40
2:E:242:MET:SD	2:E:244:CYS:HB3	2.62	0.40
2:E:142:THR:N	2:E:143:PRO:HD3	2.37	0.40
2:E:176:ALA:HB1	2:E:181:MET:HA	2.04	0.40
2:E:222:THR:HG23	2:E:242:MET:HE3	2.04	0.40
2:E:292:GLU:HB2	2:E:296:TRP:HA	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	418/418 (100%)	408 (98%)	10 (2%)	0	100	100
1	D	416/418 (100%)	404 (97%)	12 (3%)	0	100	100
2	B	366/366 (100%)	353 (96%)	12 (3%)	1 (0%)	36	25
2	E	361/366 (99%)	347 (96%)	13 (4%)	1 (0%)	36	25
All	All	1561/1568 (100%)	1512 (97%)	47 (3%)	2 (0%)	48	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	142	THR
2	E	142	THR

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	356/354 (101%)	351 (99%)	5 (1%)	59	52
1	D	354/354 (100%)	347 (98%)	7 (2%)	48	38
2	B	319/317 (101%)	311 (98%)	8 (2%)	42	30
2	E	314/317 (99%)	306 (98%)	8 (2%)	42	30
All	All	1343/1342 (100%)	1315 (98%)	28 (2%)	50	36

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

Mol	Chain	Res	Type
1	A	86	GLU
1	A	100	ASN
1	A	144[A]	GLU
1	A	144[B]	GLU
1	A	310	LEU
2	B	97[A]	GLU
2	B	97[B]	GLU
2	B	108	GLN
2	B	177	CYS

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Mol	Chain	Res	Type
2	B	236[A]	VAL
2	B	236[B]	VAL
2	B	242	MET
2	B	243	TYR
1	D	90	GLU
1	D	100	ASN
1	D	132	SER
1	D	157	GLU
1	D	299	LEU
1	D	310	LEU
1	D	413	LYS
2	E	51	ILE
2	E	177	CYS
2	E	181	MET
2	E	230	LYS
2	E	242	MET
2	E	243	TYR
2	E	268	VAL
2	E	335	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	64	HIS
1	A	100	ASN
1	A	128	ASN
2	B	135	GLN
2	B	139	HIS
1	D	50	GLN
1	D	61	HIS
1	D	100	ASN
1	D	128	ASN
2	E	108	GLN
2	E	135	GLN
2	E	180	ASN
2	E	363	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 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	$\# Z > 2$
4	SF4	D	575	1	0,12,12	-	-	-		
4	SF4	D	576	1	0,12,12	-	-	-		
4	SF4	B	585	2	0,12,12	-	-	-		
3	SRM	A	580	5,2	68,70,70	1.69	10 (14%)	86,112,112	2.50	31 (36%)
4	SF4	A	576	1	0,12,12	-	-	-		
4	SF4	E	586	2	0,12,12	-	-	-		
4	SF4	A	575	1	0,12,12	-	-	-		
5	SO3	A	590	3	1,3,3	0.25	0	0,3,3	-	-
5	SO3	D	590	3	1,3,3	0.48	0	0,3,3	-	-
3	SRM	B	570	1	68,70,70	1.99	16 (23%)	86,112,112	2.77	35 (40%)
3	SRM	D	580	5,2	68,70,70	2.12	16 (23%)	86,112,112	2.63	29 (33%)
4	SF4	B	586	2	0,12,12	-	-	-		
4	SF4	E	585	2	0,12,12	-	-	-		
3	SRM	E	570	1	68,70,70	2.32	13 (19%)	86,112,112	2.88	33 (38%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	D	575	1	-	-	0/6/5/5
4	SF4	D	576	1	-	-	0/6/5/5
4	SF4	B	585	2	-	-	0/6/5/5
3	SRM	A	580	5,2	1/1/19/23	11/38/126/126	-
4	SF4	A	576	1	-	-	0/6/5/5
4	SF4	E	586	2	-	-	0/6/5/5
4	SF4	A	575	1	-	-	0/6/5/5
3	SRM	B	570	1	1/1/19/23	15/38/126/126	-
3	SRM	D	580	5,2	2/2/19/23	13/38/126/126	-
4	SF4	B	586	2	-	-	0/6/5/5
4	SF4	E	585	2	-	-	0/6/5/5
3	SRM	E	570	1	1/1/19/23	17/38/126/126	-

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	570	SRM	C4A-NA	-10.37	1.27	1.35
3	E	570	SRM	C3C-C2C	7.21	1.51	1.36
3	D	580	SRM	C3C-C2C	6.03	1.49	1.36
3	B	570	SRM	C4A-NA	-5.78	1.31	1.35
3	E	570	SRM	C1C-NC	-5.64	1.29	1.39
3	E	570	SRM	C4C-NC	-5.61	1.29	1.39
3	B	570	SRM	C3C-C2C	5.59	1.48	1.36
3	D	580	SRM	C3A-C4A	-5.44	1.39	1.51
3	D	580	SRM	C3B-C4B	-5.36	1.39	1.51
3	A	580	SRM	C3C-C2C	5.09	1.47	1.36
3	A	580	SRM	C3A-C4A	-5.02	1.40	1.51
3	B	570	SRM	C1D-C2D	4.69	1.54	1.44
3	A	580	SRM	C3B-C4B	-4.64	1.41	1.51
3	B	570	SRM	C1C-C2C	4.59	1.53	1.45
3	D	580	SRM	FE-NA	4.53	2.08	1.94
3	D	580	SRM	FE-NB	4.28	2.08	1.94
3	D	580	SRM	FE-NC	4.25	2.09	1.95
3	B	570	SRM	C4C-NC	-3.99	1.32	1.39
3	D	580	SRM	C1D-C2D	3.84	1.52	1.44
3	B	570	SRM	C4C-C3C	3.67	1.51	1.45
3	E	570	SRM	C4D-C3D	3.65	1.51	1.44
3	A	580	SRM	FE-NB	3.62	2.06	1.94
3	D	580	SRM	C4A-NA	-3.61	1.32	1.35
3	B	570	SRM	C3B-C4B	-3.58	1.43	1.51
3	B	570	SRM	C4B-NB	3.51	1.37	1.35
3	E	570	SRM	C1D-C2D	3.40	1.51	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	580	SRM	FE-NA	3.31	2.05	1.94
3	D	580	SRM	C4D-C3D	3.27	1.51	1.44
3	A	580	SRM	C1D-C2D	3.21	1.51	1.44
3	B	570	SRM	C1C-NC	-3.15	1.33	1.39
3	D	580	SRM	C3D-C2D	3.14	1.54	1.40
3	D	580	SRM	C1C-C2C	3.10	1.50	1.45
3	B	570	SRM	C2B-C3B	-3.00	1.47	1.55
3	E	570	SRM	C3D-C2D	3.00	1.53	1.40
3	E	570	SRM	C1C-C2C	2.97	1.50	1.45
3	D	580	SRM	C4C-NC	-2.91	1.34	1.39
3	D	580	SRM	C1C-NC	-2.79	1.34	1.39
3	D	580	SRM	C1D-ND	-2.77	1.34	1.39
3	D	580	SRM	C4C-C3C	2.59	1.49	1.45
3	B	570	SRM	O2C-CCC	-2.56	1.22	1.30
3	D	580	SRM	C4D-ND	-2.55	1.34	1.39
3	E	570	SRM	C4C-C3C	2.55	1.49	1.45
3	E	570	SRM	C2B-C3B	-2.54	1.48	1.55
3	E	570	SRM	CDD-C3D	2.49	1.54	1.51
3	E	570	SRM	C4D-ND	-2.42	1.35	1.39
3	A	580	SRM	CDD-C3D	2.38	1.54	1.51
3	E	570	SRM	C1D-ND	-2.37	1.35	1.39
3	B	570	SRM	CDD-C3D	2.26	1.54	1.51
3	A	580	SRM	C2A-C1A	-2.23	1.49	1.54
3	B	570	SRM	CDC-CEC	2.18	1.54	1.51
3	A	580	SRM	C4C-NC	-2.17	1.35	1.39
3	B	570	SRM	C4D-C3D	2.16	1.48	1.44
3	A	580	SRM	C4D-ND	-2.16	1.35	1.39
3	B	570	SRM	FE-NA	2.03	2.01	1.94
3	B	570	SRM	C3D-C2D	2.03	1.49	1.40

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	580	SRM	C2A-C3A-C4A	9.88	113.41	100.89
3	D	580	SRM	CAA-C3A-C4A	9.51	127.78	111.19
3	E	570	SRM	C1D-C2D-C3D	-9.48	96.87	106.81
3	A	580	SRM	C2A-C3A-C4A	8.70	111.92	100.89
3	E	570	SRM	CAB-C3B-C4B	8.56	126.12	111.19
3	B	570	SRM	C2B-C3B-C4B	8.35	111.47	100.89
3	A	580	SRM	CAA-C3A-C4A	7.91	124.99	111.19
3	A	580	SRM	CMB-C2B-C3B	7.61	126.09	112.05
3	E	570	SRM	C4C-C3C-C2C	-7.41	98.55	106.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	570	SRM	C2D-C1D-ND	7.12	118.06	110.15
3	B	570	SRM	C1D-C2D-C3D	-6.98	99.49	106.81
3	E	570	SRM	C2B-C1B-CHB	-6.97	117.28	123.54
3	D	580	SRM	C2B-C3B-C4B	5.99	108.48	100.89
3	B	570	SRM	CBC-CAC-C3C	-5.97	96.04	112.53
3	A	580	SRM	C1A-NA-C4A	5.65	112.32	105.34
3	E	570	SRM	C3C-C4C-NC	5.64	115.76	110.32
3	B	570	SRM	C2A-C1A-CHA	-5.57	118.54	123.54
3	D	580	SRM	C3C-C4C-NC	5.53	115.66	110.32
3	B	570	SRM	C3B-C2B-C1B	-5.46	91.66	100.92
3	D	580	SRM	C4D-C3D-C2D	-5.39	101.16	106.81
3	B	570	SRM	CMB-C2B-C3B	5.38	121.98	112.05
3	B	570	SRM	C3C-C4C-NC	5.34	115.47	110.32
3	B	570	SRM	CHC-C1C-NC	5.28	130.20	124.45
3	B	570	SRM	CHD-C4C-C3C	-5.20	116.65	124.86
3	E	570	SRM	C2A-C1A-CHA	-5.06	118.99	123.54
3	E	570	SRM	C2B-C3B-C4B	4.96	107.17	100.89
3	B	570	SRM	C4C-C3C-C2C	-4.93	101.33	106.84
3	B	570	SRM	CHC-C1C-C2C	-4.92	117.10	124.86
3	E	570	SRM	CDA-C2A-C1A	4.85	122.13	107.11
3	E	570	SRM	CAC-C3C-C2C	-4.84	117.88	129.24
3	B	570	SRM	C2B-C1B-CHB	-4.79	119.24	123.54
3	D	580	SRM	C4D-ND-C1D	4.79	113.62	105.82
3	D	580	SRM	C1A-NA-C4A	4.48	110.87	105.34
3	D	580	SRM	C4C-C3C-C2C	-4.47	101.84	106.84
3	D	580	SRM	C2C-C1C-NC	4.34	114.51	110.32
3	B	570	SRM	C2D-C1D-ND	4.22	114.83	110.15
3	A	580	SRM	CAB-C3B-C4B	-4.15	103.95	111.19
3	A	580	SRM	CHC-C1C-NC	4.12	128.94	124.45
3	E	570	SRM	CAC-C3C-C4C	-4.05	116.62	124.85
3	B	570	SRM	C1C-CHC-C4B	-4.04	116.88	126.62
3	B	570	SRM	C3A-C4A-NA	3.94	118.51	110.83
3	E	570	SRM	C3A-C4A-NA	3.84	118.32	110.83
3	D	580	SRM	CBD-CAD-C2D	3.81	123.08	112.53
3	E	570	SRM	C1C-C2C-C3C	-3.80	102.59	106.84
3	B	570	SRM	C4D-CHA-C1A	-3.77	118.92	125.87
3	A	580	SRM	C2B-C3B-C4B	3.73	105.62	100.89
3	E	570	SRM	CAB-C3B-C2B	3.72	124.43	114.19
3	D	580	SRM	CBB-CAB-C3B	3.69	125.11	114.65
3	E	570	SRM	CMB-C2B-C3B	3.69	118.86	112.05
3	D	580	SRM	C1C-C2C-C3C	-3.68	102.73	106.84
3	E	570	SRM	CHC-C1C-C2C	-3.65	119.10	124.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	570	SRM	CBD-CAD-C2D	3.64	122.58	112.53
3	E	570	SRM	C4D-CHA-C1A	-3.63	119.19	125.87
3	A	580	SRM	CBD-CAD-C2D	3.61	122.52	112.53
3	A	580	SRM	CAB-C3B-C2B	-3.61	104.26	114.19
3	A	580	SRM	CHD-C1D-ND	3.57	130.34	123.86
3	D	580	SRM	CHC-C1C-NC	-3.55	120.58	124.45
3	D	580	SRM	C3A-C2A-C1A	-3.55	94.89	100.92
3	A	580	SRM	O3D-CED-CDD	-3.47	112.24	122.11
3	A	580	SRM	CHC-C1C-C2C	-3.47	119.39	124.86
3	D	580	SRM	C3A-C4A-CHB	3.40	130.56	123.33
3	E	570	SRM	C3B-C2B-C1B	-3.38	95.18	100.92
3	A	580	SRM	CDA-C2A-C1A	3.36	117.53	107.11
3	B	570	SRM	CAB-C3B-C4B	3.36	117.05	111.19
3	E	570	SRM	CAD-C2D-C1D	-3.25	118.58	124.94
3	B	570	SRM	CHA-C4D-C3D	-3.21	118.27	125.30
3	D	580	SRM	CMA-C2A-CDA	3.21	116.19	110.74
3	A	580	SRM	CMA-C2A-C3A	-3.20	106.13	112.05
3	B	570	SRM	CHA-C4D-ND	3.16	129.59	123.86
3	B	570	SRM	C1C-C2C-C3C	-3.11	103.36	106.84
3	B	570	SRM	C3B-C4B-NB	-3.08	104.81	110.83
3	E	570	SRM	C3A-C4A-CHB	-3.05	116.84	123.33
3	A	580	SRM	CMA-C2A-CDA	3.04	115.90	110.74
3	B	570	SRM	CHD-C4C-NC	3.02	127.74	124.45
3	D	580	SRM	CAD-C2D-C1D	-2.99	119.09	124.94
3	E	570	SRM	CHC-C1C-NC	2.99	127.71	124.45
3	E	570	SRM	C2C-C1C-NC	2.97	113.19	110.32
3	B	570	SRM	CAB-CBB-CCB	-2.95	104.62	112.49
3	E	570	SRM	CAA-C3A-C4A	-2.93	106.08	111.19
3	D	580	SRM	CDA-C2A-C1A	2.92	116.17	107.11
3	D	580	SRM	CHD-C4C-NC	-2.92	121.27	124.45
3	E	570	SRM	CHD-C4C-C3C	-2.89	120.30	124.86
3	E	570	SRM	CBC-CAC-C3C	-2.88	104.57	112.53
3	D	580	SRM	C2D-C1D-ND	-2.87	106.97	110.15
3	B	570	SRM	O1D-CCD-CBD	-2.83	114.11	123.09
3	A	580	SRM	CAD-CBD-CCD	-2.82	106.20	113.67
3	B	570	SRM	CEC-CDC-C2C	-2.80	106.73	113.76
3	B	570	SRM	CAA-C3A-C4A	-2.72	106.45	111.19
3	E	570	SRM	CAB-CBB-CCB	2.67	119.62	112.49
3	B	570	SRM	CAD-C2D-C1D	2.62	130.05	124.94
3	A	580	SRM	C2A-C1A-CHA	-2.60	121.20	123.54
3	E	570	SRM	C1C-CHC-C4B	-2.57	120.42	126.62
3	E	570	SRM	CEC-CDC-C2C	-2.55	107.34	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	580	SRM	C1D-C2D-C3D	-2.55	104.14	106.81
3	A	580	SRM	CHD-C1D-C2D	-2.52	119.78	125.30
3	A	580	SRM	CDB-C2B-C3B	-2.51	101.74	108.37
3	A	580	SRM	C3A-C4A-NA	-2.51	105.94	110.83
3	A	580	SRM	O4D-CED-CDD	2.50	122.25	114.51
3	A	580	SRM	CDA-C2A-C3A	2.49	114.95	108.37
3	A	580	SRM	C3A-C2A-C1A	-2.48	96.70	100.92
3	E	570	SRM	O1C-CCC-CBC	-2.48	115.24	123.09
3	D	580	SRM	C1D-C2D-C3D	-2.44	104.25	106.81
3	B	570	SRM	C2C-C1C-NC	2.43	112.67	110.32
3	D	580	SRM	C2A-C1A-CHA	2.37	125.67	123.54
3	D	580	SRM	O2A-CCA-CBA	2.33	121.36	114.00
3	E	570	SRM	CED-CDD-C3D	2.32	119.60	113.76
3	B	570	SRM	O2D-CCD-CBD	2.32	121.32	114.00
3	B	570	SRM	CHD-C1D-C2D	-2.31	120.25	125.30
3	D	580	SRM	CAC-C3C-C4C	2.31	129.54	124.85
3	E	570	SRM	CHD-C1D-C2D	-2.30	120.25	125.30
3	B	570	SRM	C3A-C4A-CHB	-2.28	118.49	123.33
3	A	580	SRM	CBA-CAA-C3A	2.27	121.08	114.65
3	B	570	SRM	CBB-CAB-C3B	2.27	121.08	114.65
3	D	580	SRM	C2B-C1B-CHB	-2.26	121.51	123.54
3	A	580	SRM	CHD-C4C-NC	-2.26	121.99	124.45
3	D	580	SRM	CMB-C2B-C3B	2.25	116.19	112.05
3	A	580	SRM	C1C-C2C-C3C	-2.23	104.34	106.84
3	D	580	SRM	O3B-CEB-CDB	-2.16	116.84	122.95
3	A	580	SRM	C4D-ND-C1D	2.14	109.31	105.82
3	A	580	SRM	CHA-C4D-C3D	-2.13	120.65	125.30
3	E	570	SRM	CMA-C2A-CDA	-2.12	107.14	110.74
3	B	570	SRM	C1A-NA-C4A	-2.10	102.74	105.34
3	D	580	SRM	C3B-C2B-C1B	-2.08	97.38	100.92
3	D	580	SRM	O1A-CCA-CBA	-2.06	116.56	123.09
3	E	570	SRM	O4B-CEB-CDB	2.03	120.77	114.35
3	B	570	SRM	C4B-NB-C1B	2.02	107.83	105.34
3	A	580	SRM	C4D-C3D-C2D	-2.02	104.69	106.81
3	A	580	SRM	C4D-CHA-C1A	-2.01	122.17	125.87

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	580	SRM	NC
3	B	570	SRM	NC
3	D	580	SRM	NC

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Mol	Chain	Res	Type	Atom
3	D	580	SRM	C3A
3	E	570	SRM	NC

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	580	SRM	C1B-C2B-CDB-CEB
3	D	580	SRM	CMB-C2B-CDB-CEB
3	D	580	SRM	C3B-C2B-CDB-CEB
3	D	580	SRM	C2B-C3B-CAB-CBB
3	D	580	SRM	C2D-C3D-CDD-CED
3	E	570	SRM	C4A-C3A-CAA-CBA
3	E	570	SRM	C4D-C3D-CDD-CED
3	E	570	SRM	C4C-C3C-CAC-CBC
3	E	570	SRM	C1D-C2D-CAD-CBD
3	E	570	SRM	C2B-C3B-CAB-CBB
3	B	570	SRM	C4A-C3A-CAA-CBA
3	E	570	SRM	C3C-CAC-CBC-CCC
3	E	570	SRM	C3B-CAB-CBB-CCB
3	B	570	SRM	C4D-C3D-CDD-CED
3	D	580	SRM	C2A-C3A-CAA-CBA
3	A	580	SRM	C3B-CAB-CBB-CCB
3	A	580	SRM	C2A-C3A-CAA-CBA
3	E	570	SRM	C4B-C3B-CAB-CBB
3	B	570	SRM	C3D-CDD-CED-O3D
3	E	570	SRM	C3D-CDD-CED-O3D
3	E	570	SRM	C3D-CDD-CED-O4D
3	B	570	SRM	C2B-CDB-CEB-O3B
3	A	580	SRM	C3D-CDD-CED-O3D
3	B	570	SRM	C3D-CDD-CED-O4D
3	D	580	SRM	C2B-CDB-CEB-O4B
3	A	580	SRM	C3D-CDD-CED-O4D
3	D	580	SRM	C2B-CDB-CEB-O3B
3	E	570	SRM	C2B-CDB-CEB-O4B
3	B	570	SRM	CAB-CBB-CCB-O2B
3	B	570	SRM	CAB-CBB-CCB-O1B
3	E	570	SRM	CAA-CBA-CCA-O1A
3	A	580	SRM	C3B-C2B-CDB-CEB
3	A	580	SRM	CAB-CBB-CCB-O1B
3	B	570	SRM	CAA-CBA-CCA-O2A
3	A	580	SRM	CAB-CBB-CCB-O2B
3	E	570	SRM	CAD-CBD-CCD-O2D

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Mol	Chain	Res	Type	Atoms
3	B	570	SRM	CAC-CBC-CCC-O1C
3	E	570	SRM	CAD-CBD-CCD-O1D
3	E	570	SRM	C2B-CDB-CEB-O3B
3	B	570	SRM	CAA-CBA-CCA-O1A
3	A	580	SRM	CAC-CBC-CCC-O2C
3	B	570	SRM	CAC-CBC-CCC-O2C
3	E	570	SRM	CAA-CBA-CCA-O2A
3	D	580	SRM	CAC-CBC-CCC-O2C
3	D	580	SRM	CAC-CBC-CCC-O1C
3	B	570	SRM	C2B-CDB-CEB-O4B
3	E	570	SRM	C3A-CAA-CBA-CCA
3	D	580	SRM	CAB-CBB-CCB-O2B
3	A	580	SRM	CAC-CBC-CCC-O1C
3	D	580	SRM	CAB-CBB-CCB-O1B
3	B	570	SRM	CAD-CBD-CCD-O1D
3	D	580	SRM	C3D-C2D-CAD-CBD
3	B	570	SRM	C3B-C2B-CDB-CEB
3	B	570	SRM	CAD-CBD-CCD-O2D
3	A	580	SRM	C1D-C2D-CAD-CBD
3	A	580	SRM	CAA-CBA-CCA-O1A

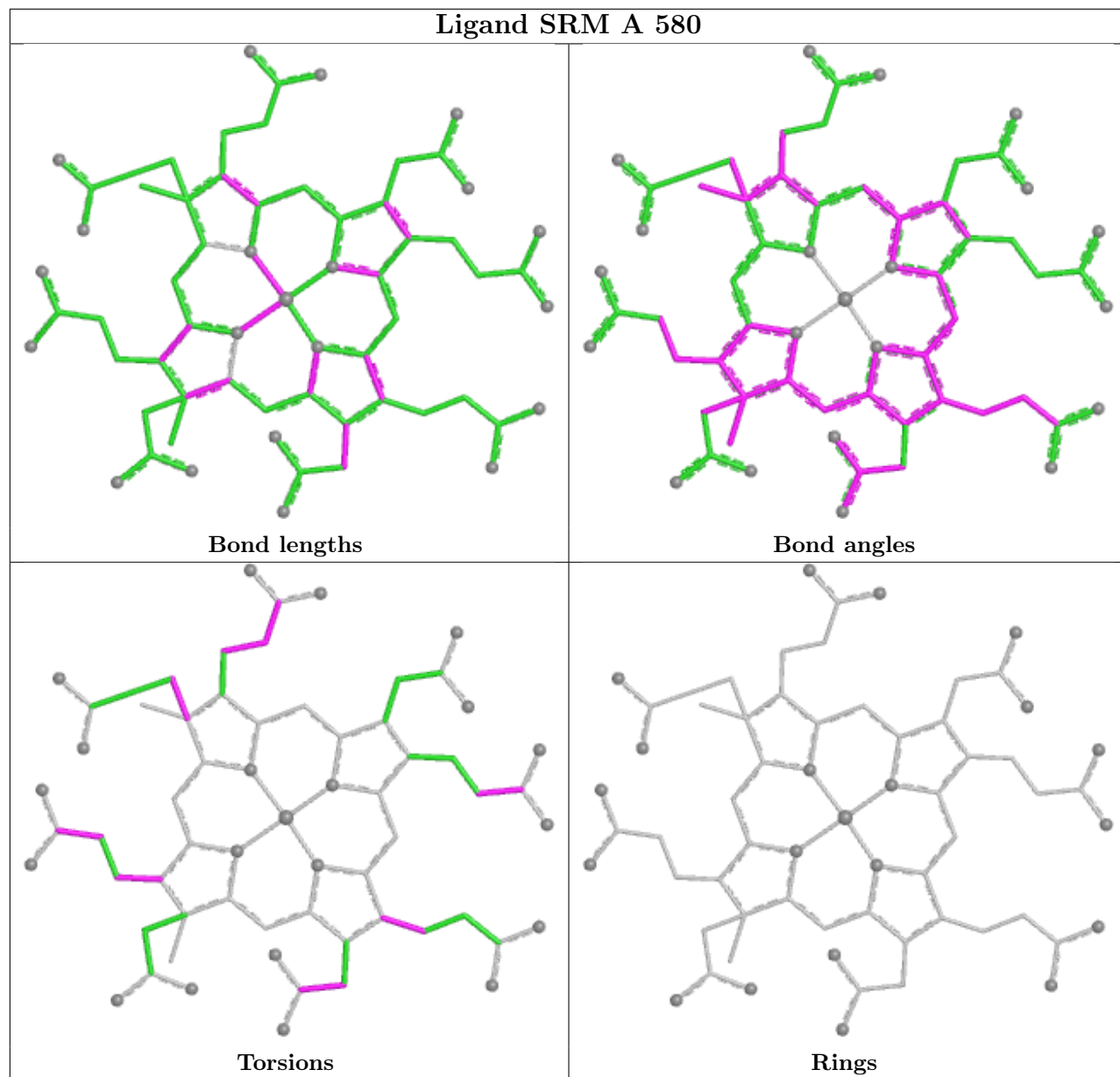
There are no ring outliers.

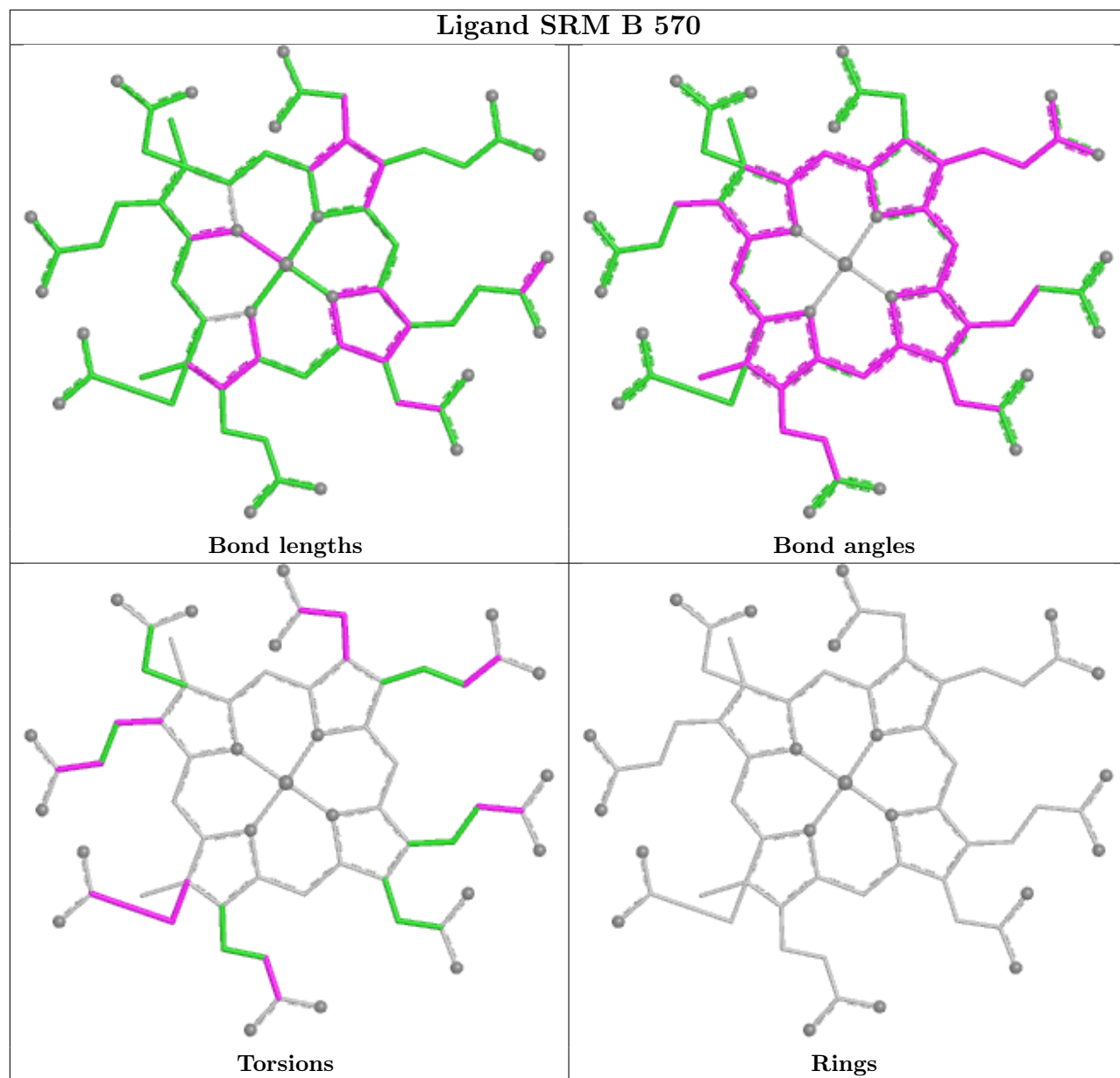
5 monomers are involved in 34 short contacts:

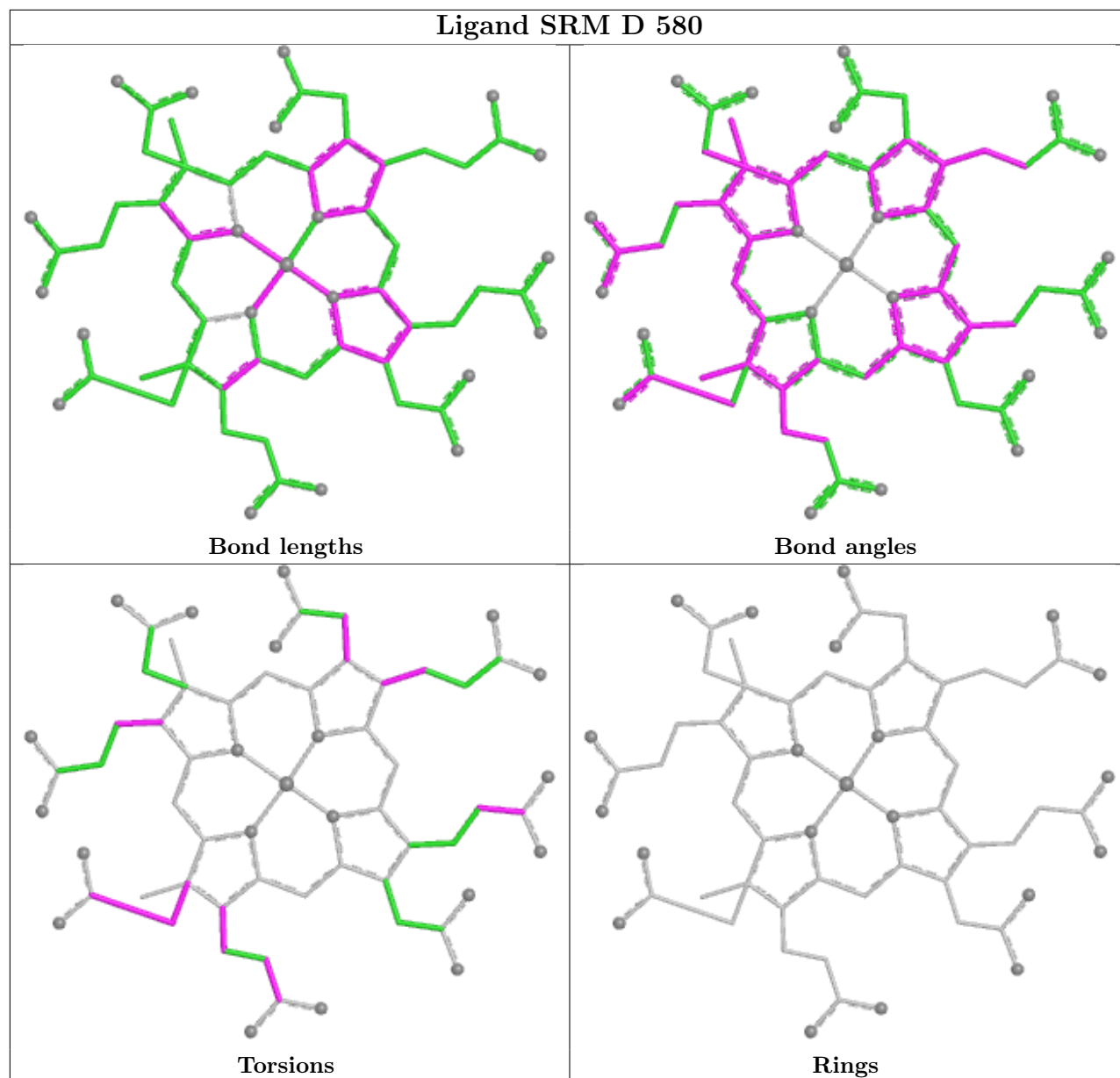
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	580	SRM	10	0
3	B	570	SRM	1	0
3	D	580	SRM	13	0
4	E	585	SF4	3	0
3	E	570	SRM	8	0

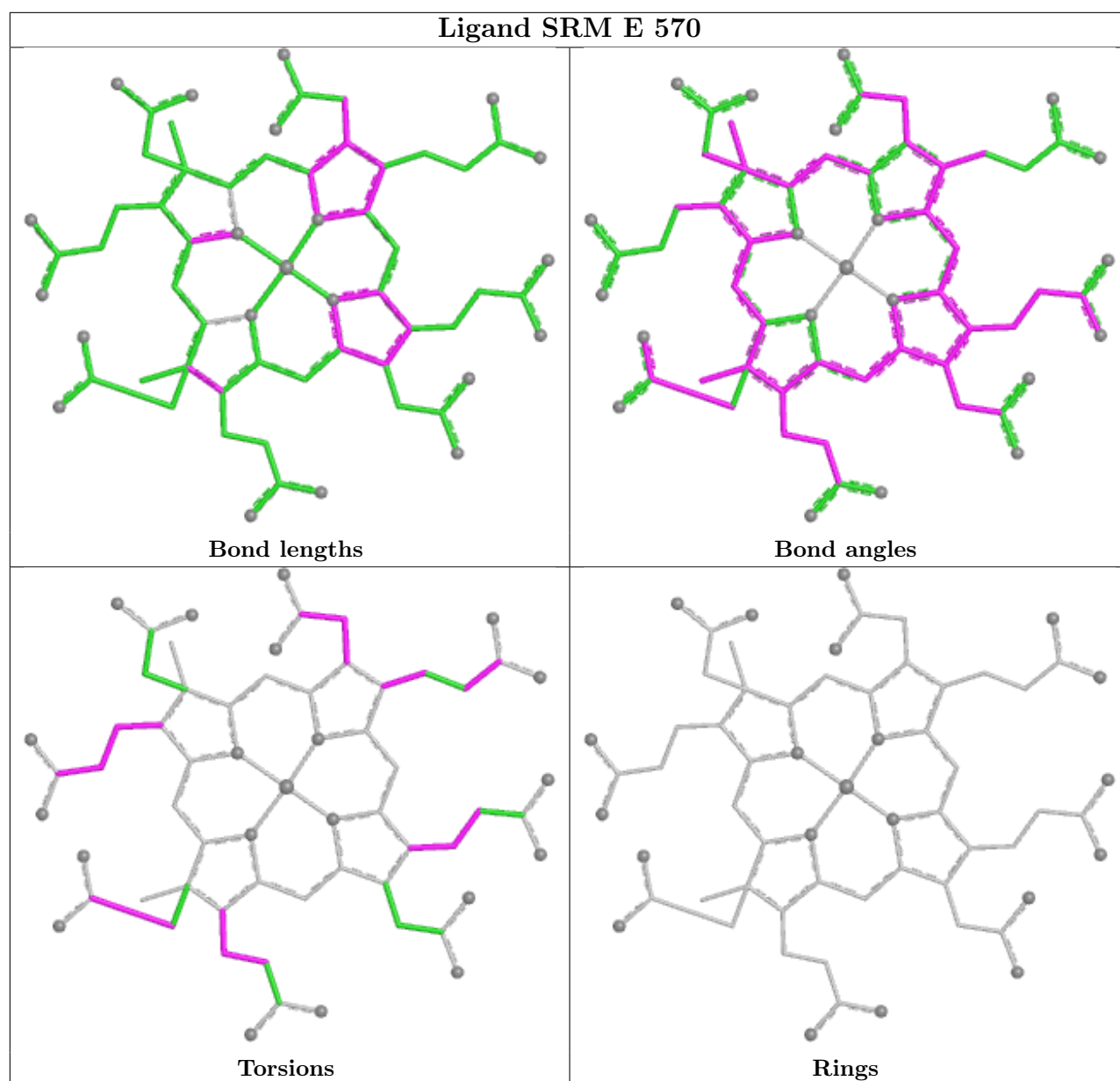
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	417/418 (99%)	-0.12	11 (2%) 57 57	6, 9, 20, 38	3 (0%)
1	D	417/418 (99%)	1.37	92 (22%) 2 2	4, 10, 18, 25	1 (0%)
2	B	363/366 (99%)	-0.28	3 (0%) 82 83	5, 9, 16, 46	5 (1%)
2	E	363/366 (99%)	1.04	43 (11%) 9 7	6, 10, 20, 36	0
All	All	1560/1568 (99%)	0.51	149 (9%) 13 12	4, 9, 19, 46	9 (0%)

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	383	VAL	6.2
1	D	81	TYR	5.5
1	D	285	CYS	5.2
1	D	266	CYS	5.0
1	D	43	GLY	5.0
1	D	386	VAL	4.9
1	D	286	VAL	4.6
2	E	354	PHE	4.6
1	D	181	CYS	4.3
1	D	86	GLU	4.3
2	E	365	LYS	4.2
1	A	415	GLY	4.2
2	E	353	TYR	4.1
1	D	291	CYS	4.1
1	D	381	ALA	4.1
1	D	25	ALA	4.0
1	D	54	SER	3.8
2	E	366	TRP	3.8
1	D	1	SER	3.8
1	D	269	GLY	3.8
1	D	4	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	374	LEU	3.7
2	E	182	CYS	3.7
1	D	365	ILE	3.7
2	E	100	ILE	3.7
1	D	93	HIS	3.6
1	A	407	TYR	3.6
1	D	26	GLU	3.6
1	A	81	TYR	3.6
1	D	223	CYS	3.6
1	A	417	TRP	3.5
1	D	38	VAL	3.5
1	D	79	GLY	3.4
1	D	37	ASP	3.4
1	D	270	ALA	3.4
1	D	252	TYR	3.4
2	E	352	PRO	3.4
2	E	4	GLU	3.3
1	D	18	VAL	3.3
1	D	66	GLY	3.3
2	E	21	PRO	3.3
1	D	41	PRO	3.3
2	E	356	SER	3.3
1	D	268	THR	3.2
2	E	357	GLU	3.2
1	D	377	ILE	3.1
1	D	5	LEU	3.1
1	D	12	GLY	3.1
2	E	364	PHE	3.1
1	D	33	ALA	3.1
1	D	238	TRP	3.1
2	B	4	GLU	3.0
1	D	378	GLY	3.0
2	E	181	MET	2.9
1	A	409	GLU	2.9
1	D	325	TRP	2.9
1	D	288	CYS	2.9
1	D	271	ILE	2.9
2	E	350	ILE	2.9
1	D	384	ARG	2.9
1	D	366	TRP	2.9
1	D	326	VAL	2.9
2	E	207	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	67	ILE	2.8
2	E	351	THR	2.8
1	D	328	VAL	2.8
1	A	413	LYS	2.8
1	D	175	CYS	2.8
2	B	205	GLU	2.8
1	D	31	ALA	2.8
2	E	230	LYS	2.8
1	D	248	ALA	2.7
1	D	49	LYS	2.7
2	E	358	PHE	2.7
1	D	382	ASP	2.7
1	D	131	GLY	2.7
1	D	183	PHE	2.7
1	D	24	THR	2.7
2	E	257	PHE	2.5
1	D	105	TRP	2.5
1	D	74	GLY	2.5
2	B	5	GLY	2.5
1	D	132	SER	2.5
2	E	98	SER	2.5
2	E	349	ARG	2.5
1	D	364	LEU	2.5
1	D	373	PHE	2.5
1	D	340	ILE	2.5
1	D	14	TRP	2.5
1	D	42	LYS	2.5
1	D	40	MET	2.4
2	E	360	ALA	2.4
1	D	65	GLY	2.4
1	D	324	GLY	2.4
1	A	247	GLU	2.4
1	D	94	PHE	2.4
1	D	242	ILE	2.4
2	E	12	PRO	2.4
1	D	385	MET	2.4
1	D	219	CYS	2.4
2	E	103	LEU	2.3
2	E	64	ILE	2.3
1	D	346	ALA	2.3
2	E	219	ALA	2.3
1	D	236	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	347	ILE	2.3
1	D	371	ARG	2.3
2	E	158	LEU	2.3
1	D	46	GLY	2.2
1	D	336	PRO	2.2
1	D	370	MET	2.2
1	D	2	GLU	2.2
1	D	279	THR	2.2
2	E	71	CYS	2.2
1	D	313	GLY	2.2
2	E	41	ILE	2.2
1	D	61	HIS	2.2
1	D	306	GLY	2.2
1	D	310	LEU	2.2
1	A	404	PRO	2.2
1	D	329	PRO	2.2
2	E	169	ALA	2.2
1	A	86	GLU	2.1
1	A	92[A]	GLU	2.1
2	E	355	TYR	2.1
1	D	255	TRP	2.1
2	E	363	GLN	2.1
1	D	7	ASP	2.1
1	D	274	ASP	2.1
1	D	122	TRP	2.1
2	E	50	VAL	2.1
1	D	116	CYS	2.1
1	D	301	PRO	2.1
2	E	81	TYR	2.1
2	E	164	ASP	2.1
1	A	276	LYS	2.1
2	E	298	THR	2.1
1	D	295	MET	2.1
2	E	297	PRO	2.1
2	E	224	ALA	2.1
2	E	312	ALA	2.1
1	D	142	ARG	2.1
1	D	106	PHE	2.0
2	E	69	GLU	2.0
2	E	65	TYR	2.0
2	E	217	VAL	2.0
2	E	241	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	137	ILE	2.0
1	D	331	VAL	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](#)

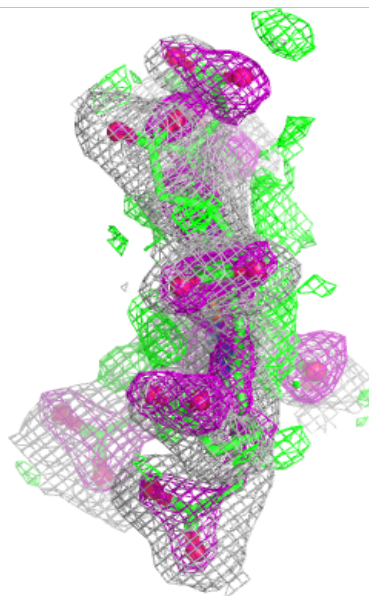
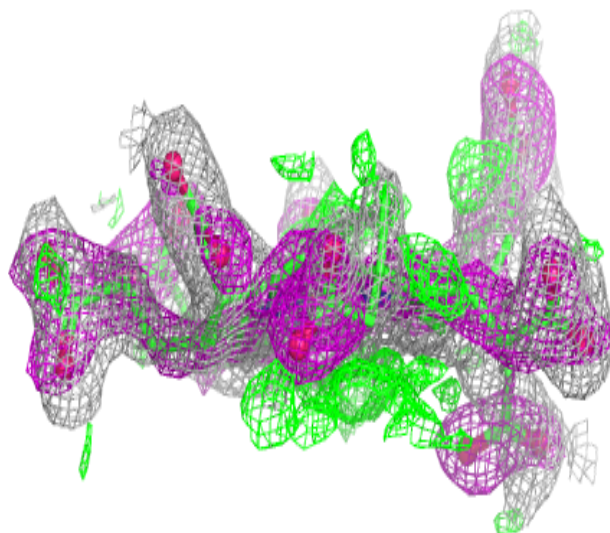
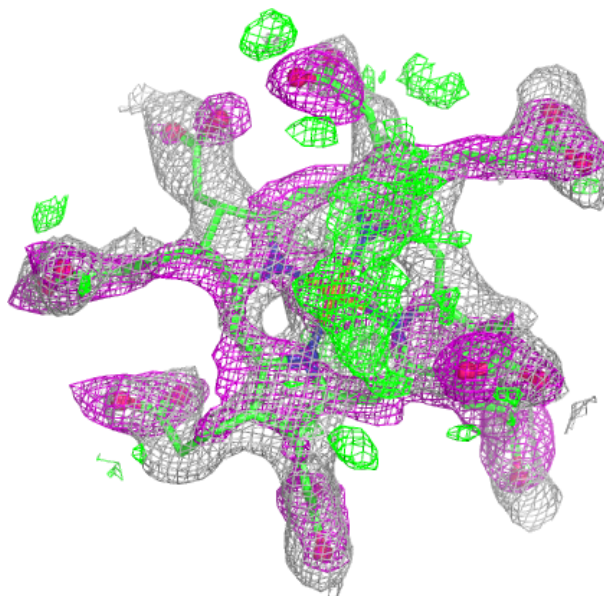
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SRM	D	580	63/63	0.85	0.12	12,17,25,26	0
3	SRM	E	570	63/63	0.85	0.11	8,9,11,13	0
5	SO3	D	590	4/4	0.86	0.26	48,50,52,56	4
4	SF4	E	585	8/8	0.94	0.27	9,10,11,12	0
4	SF4	D	575	8/8	0.95	0.27	6,6,7,7	0
4	SF4	D	576	8/8	0.96	0.24	6,6,7,7	0
3	SRM	B	570	63/63	0.96	0.06	6,8,11,13	0
4	SF4	E	586	8/8	0.96	0.20	9,9,10,10	0
3	SRM	A	580	63/63	0.96	0.07	8,10,15,18	0
4	SF4	B	586	8/8	0.98	0.04	7,7,8,8	0
5	SO3	A	590	4/4	0.98	0.09	18,23,30,30	0
4	SF4	A	576	8/8	0.98	0.10	5,7,8,8	0
4	SF4	B	585	8/8	0.99	0.03	8,10,13,13	0
4	SF4	A	575	8/8	0.99	0.03	7,8,8,9	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.

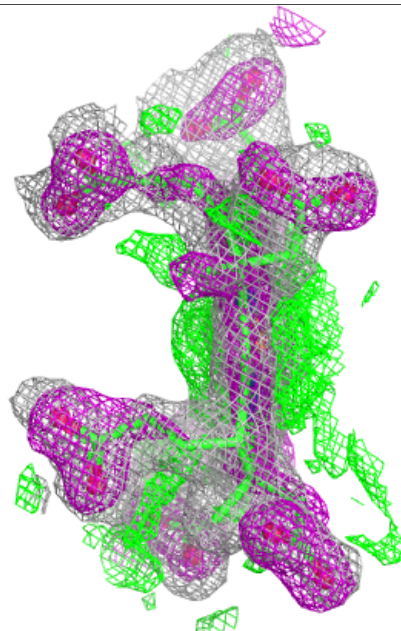
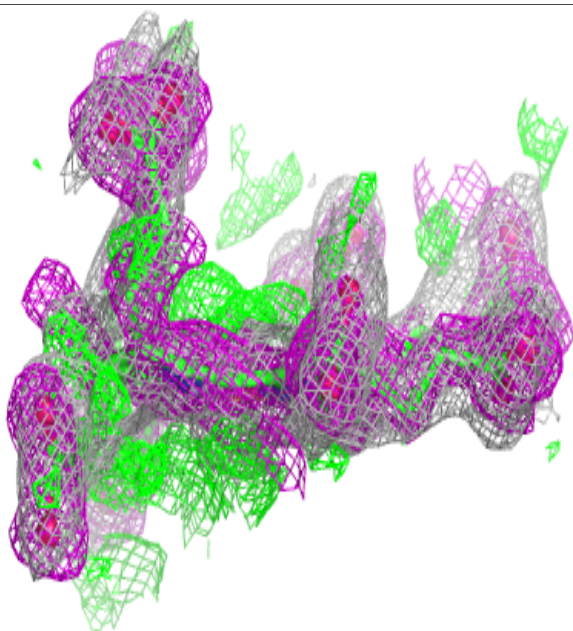
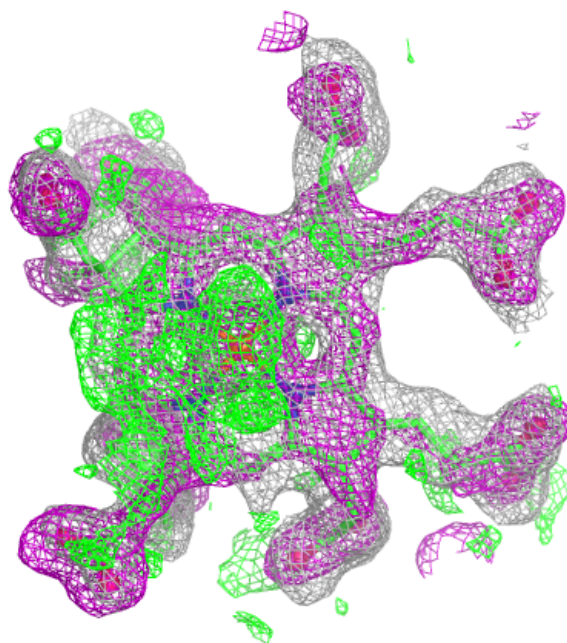
Electron density around SRM D 580:

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



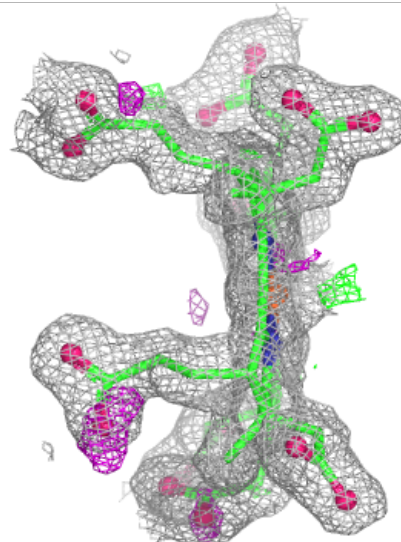
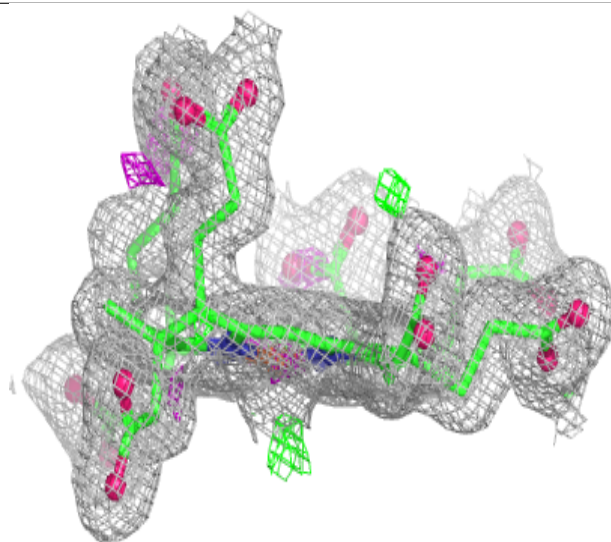
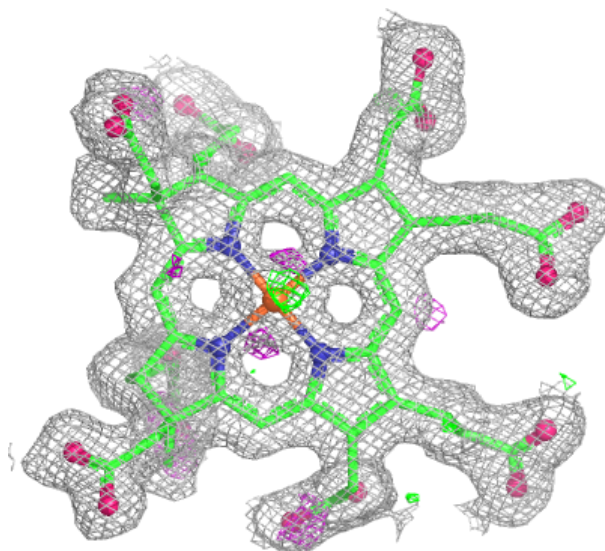
Electron density around SRM E 570:

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



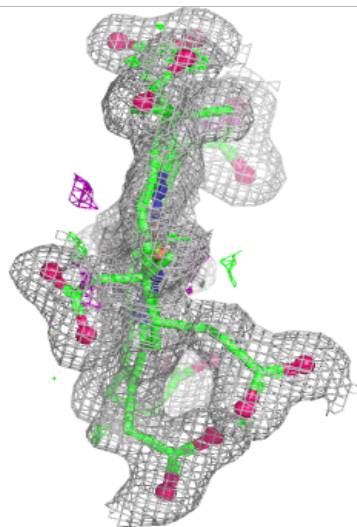
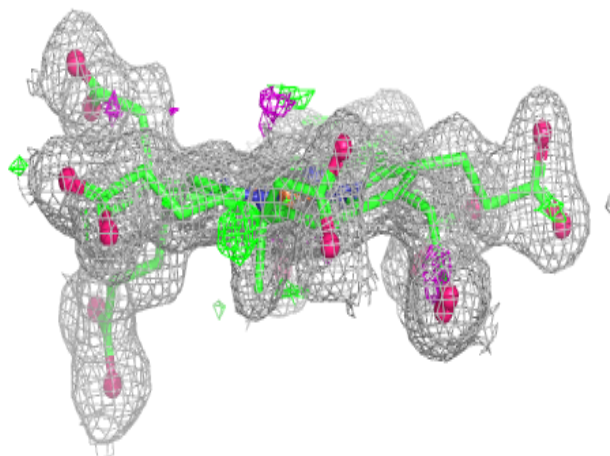
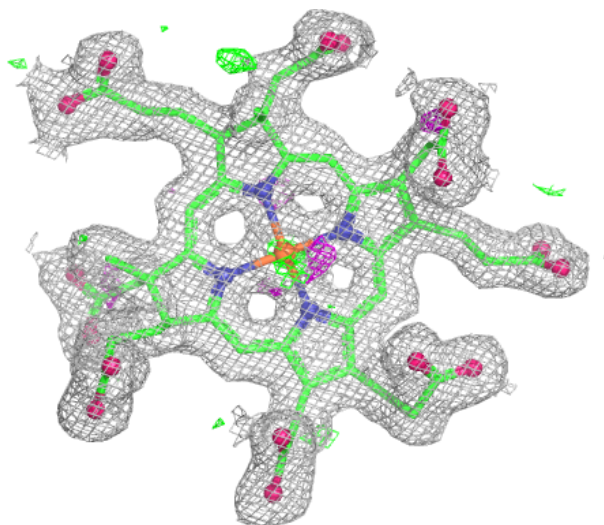
Electron density around SRM B 570:

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



Electron density around SRM A 580:

$2mF_o-DF_c$ (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.