WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Dec 19, 2023 – 01:07 PM EST

PDB ID	:	3MM6
Title	:	Dissimilatory sulfite reductase cyanide complex
Authors	:	Parey, K.; Warkentin, E.; Kroneck, P.M.H.; Ermler, U.
Deposited on	:	2010-04-19
Resolution	:	1.90 Å(reported)

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

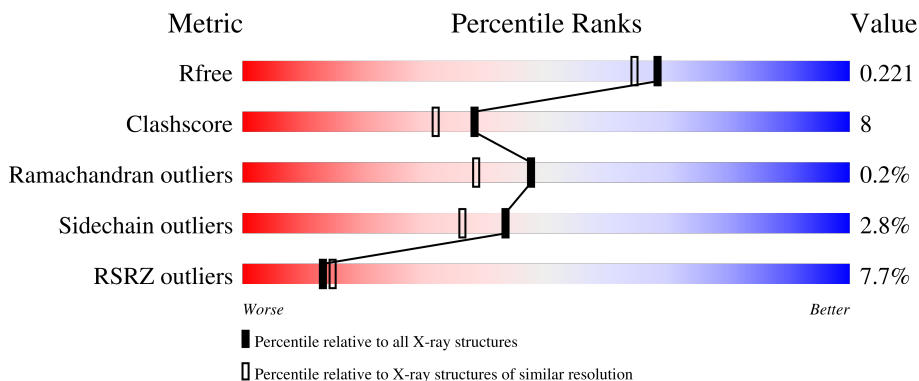|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.90 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.221
Clashscore		8
Ramachandran outliers		0.2%
Sidechain outliers		2.8%
RSRZ outliers		7.7%

Worse ← → *Better*

▮ Percentile relative to all X-ray structures
❚ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	4%　86%　14%
1	D	418	11%　82%　17%　•
2	B	366	2%　87%　12%　••
2	E	366	14%　77%　19%　••

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	-
5	CYN	A	591	-	-	X	-

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 13513 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.
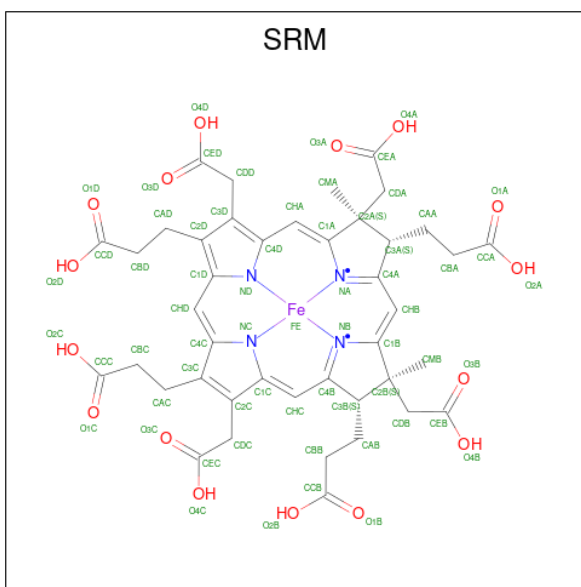
- Molecule 1 is a protein called Sulfite reductase, dissimilatory-type subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3330	2134	557	613	26			
1	D	417	Total	C	N	O	S	0	0	0
			3330	2134	557	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	0	0	0
			2901	1862	491	526	22			
2	E	363	Total	C	N	O	S	0	0	0
			2901	1862	491	526	22			

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

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

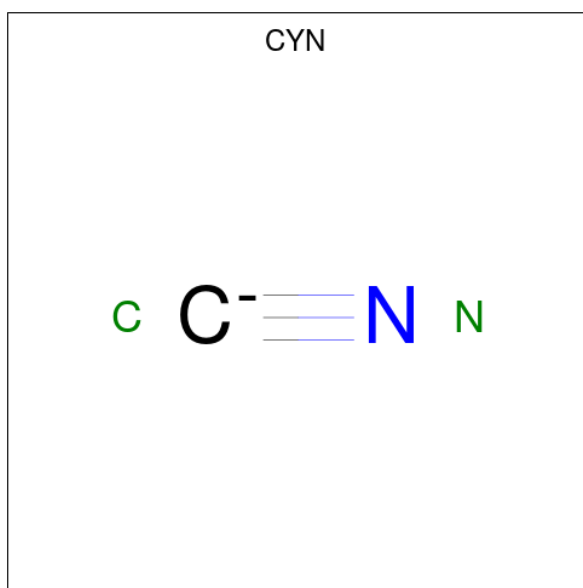- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).
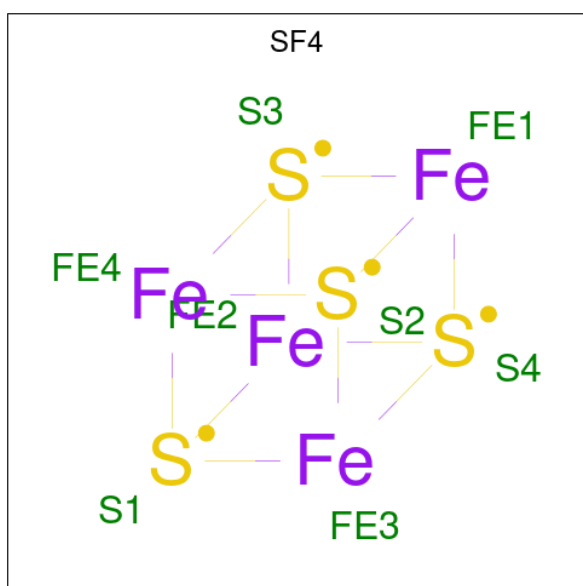
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 8	Fe 4	S 4	0	0
4	A	1	Total 8	Fe 4	S 4	0	0
4	B	1	Total 8	Fe 4	S 4	0	0
4	B	1	Total 8	Fe 4	S 4	0	0
4	D	1	Total 8	Fe 4	S 4	0	0
4	D	1	Total 8	Fe 4	S 4	0	0
4	E	1	Total 8	Fe 4	S 4	0	0
4	E	1	Total 8	Fe 4	S 4	0	0

- Molecule 5 is CYANIDE ION (three-letter code: CYN) (formula: CN).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 2	C 1	N 1	0	0
5	A	1	Total 2	C 1	N 1	0	0
5	D	1	Total 2	C 1	N 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	261	Total 261	O 261	0	0
6	B	299	Total 299	O 299	0	0
6	D	105	Total 105	O 105	0	0
6	E	64	Total 64	O 64	0	0

3 Residue-property plots ⓘ

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

Chain A:

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

Chain D:

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

Chain B:

T249 D258 M267 L272 K283 V286 L299 V300 N313 R319 V324 W329 E330 Y353 F354 Y355 R359 Q363 W366

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

Chain E:

14%

77%   19%

MET VAL VAL E4 G5 V6 K7 R16 H20 P21 V22 I23 N26 Y27 I41 V44 A45 E46 S47 G48 D49 V50 I51 Y52 R55 F56 G57 T58 S63 I64 R68 D72 K76 Y77 S78 D79 G80 Y81 L82 T85 S86 R87 V94 T95 D96 E97 S98 K99

I100 D101 D102 L103 I104 N105 E106 V107 Q108 E109 F113 P114 W119 D120 A121 V122 K123 G124 E125 Y126 T134 H139 T142 P143 A144 I145 S148 G149 I150 V154 E157 E160 M170 C171 R172 L175 A176 C177 M181 C182 G183 A184 V185 H186 A187 S188 A191

I201 P202 N203 D204 E205 A206 I207 R208 K209 T210 C211 E212 I213 P227 D228 M229 K230 N231 K232 T233 I234 K235 M242 Y243 C244 L256 M267 G270 K271 L272 R277 L281 S282 K283 P294 R295 W296 P297 V300 L307 K316 R319 V324 W329 E330

R331 Y353 F354 Y355 W366

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	94.54Å 68.68Å 145.63Å 90.00° 107.57° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 48.39 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.4 (20.00-1.90) 95.4 (48.39-1.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.75 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.6.0046	Depositor
R, R_{free}	0.180 , 0.217 0.181 , 0.221	Depositor DCC
R_{free} test set	6701 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	27.8	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.3	EDS
L-test for twinning [2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.020 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	13513	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: SF4, SRM, CYN

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	0.96	0/3417	0.86	3/4610 (0.1%)
1	D	0.71	5/3417 (0.1%)	0.73	2/4610 (0.0%)
2	B	1.08	3/2984 (0.1%)	0.91	3/4058 (0.1%)
2	E	0.80	9/2984 (0.3%)	0.77	5/4058 (0.1%)
All	All	0.89	17/12802 (0.1%)	0.82	13/17336 (0.1%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	72	ASP	CB-CG	14.12	1.81	1.51
2	E	68	ARG	CZ-NH1	9.98	1.46	1.33
1	D	20	GLU	C-O	8.98	1.40	1.23
2	E	106	GLU	CD-OE1	7.30	1.33	1.25
2	E	96	ASP	C-N	6.91	1.50	1.34
2	E	94	VAL	CB-CG1	6.59	1.66	1.52
2	E	106	GLU	CD-OE2	6.37	1.32	1.25
2	E	96	ASP	C-O	6.27	1.35	1.23
2	E	98	SER	CB-OG	6.03	1.50	1.42
1	D	20	GLU	CG-CD	5.94	1.60	1.51
1	D	113	ARG	CD-NE	5.80	1.56	1.46
1	D	181	CYS	CB-SG	-5.54	1.72	1.81
2	B	108	GLN	CB-CG	5.39	1.67	1.52
2	B	286	VAL	CB-CG1	5.38	1.64	1.52
1	D	20	GLU	C-N	5.28	1.46	1.34
2	E	72	ASP	CG-OD2	5.27	1.37	1.25
2	B	181	MET	C-O	5.15	1.33	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	72	ASP	CB-CG-OD2	9.31	126.68	118.30
1	D	113	ARG	NE-CZ-NH1	7.20	123.90	120.30
2	B	172	ARG	NE-CZ-NH2	-6.46	117.07	120.30
2	E	68	ARG	NE-CZ-NH1	-6.39	117.11	120.30
1	D	181	CYS	CA-CB-SG	-6.27	102.71	114.00
1	A	45	ARG	NE-CZ-NH2	-5.72	117.44	120.30
2	E	277	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	45	ARG	NE-CZ-NH1	5.49	123.04	120.30
2	E	68	ARG	NE-CZ-NH2	5.45	123.03	120.30
2	B	204	ASP	CB-CG-OD1	5.35	123.12	118.30
2	E	277	ARG	NE-CZ-NH2	-5.26	117.67	120.30
2	B	258	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	A	245	ASP	CB-CG-OD1	5.12	122.91	118.30

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	3330	0	3276	46	0
1	D	3330	0	3276	56	0
2	B	2901	0	2837	29	0
2	E	2901	0	2837	67	0
3	A	63	0	34	10	0
3	B	63	0	34	1	0
3	D	63	0	34	7	0
3	E	63	0	34	5	0
4	A	16	0	0	0	0
4	B	16	0	0	0	0
4	D	16	0	0	2	0
4	E	16	0	0	2	0
5	A	4	0	0	5	0
5	D	2	0	0	1	0
6	A	261	0	0	5	0
6	B	299	0	0	3	0
6	D	105	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	64	0	0	1	0
All	All	13513	0	12362	191	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 8.

All (191) 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:E:72:ASP:CB	2:E:72:ASP:CG	1.81	1.49
1:A:81:TYR:CE2	1:A:93:HIS:CD2	2.42	1.08
1:A:81:TYR:HE2	1:A:93:HIS:CD2	1.72	1.08
2:E:85:THR:HB	3:E:570:SRM:HAB2	1.39	1.04
2:E:185:VAL:HG23	6:E:683:HOH:O	1.62	0.97
2:B:108:GLN:HE21	2:B:115:CYS:H	1.15	0.92
2:E:230:LYS:CB	2:E:231:ASN:HB2	1.99	0.92
1:A:81:TYR:CD2	1:A:93:HIS:HD2	1.89	0.89
1:A:371:ARG:NH1	6:A:771:HOH:O	2.05	0.88
2:E:230:LYS:HB2	2:E:231:ASN:HB2	1.55	0.86
1:D:170:ARG:HH12	5:D:592:CYN:C	1.90	0.84
4:D:576:SF4:S1	6:D:774:HOH:O	2.37	0.81
1:A:81:TYR:CE2	1:A:93:HIS:HD2	1.95	0.78
2:E:134:THR:HG21	2:E:182:CYS:HB3	1.65	0.77
2:E:134:THR:HG21	2:E:182:CYS:CB	2.15	0.76
1:A:66:GLY:H	1:A:81:TYR:HE1	1.32	0.73
1:D:94:PHE:O	2:E:139:HIS:HE1	1.71	0.72
3:A:580:SRM:C4C	2:B:182:CYS:HA	2.21	0.70
1:D:288:CYS:O	1:D:289:MET:HB2	1.92	0.69
1:A:94:PHE:O	2:B:139:HIS:HE1	1.76	0.68
1:A:133:THR:OG1	5:A:591:CYN:C	2.41	0.68
1:A:229:ARG:HD3	2:B:184:ALA:HB2	1.77	0.67
2:E:55:ARG:HH22	3:E:570:SRM:HBA2	1.59	0.66
1:A:93:HIS:ND1	6:A:652:HOH:O	2.29	0.65
2:B:85:THR:HB	3:B:570:SRM:HAB1	1.82	0.62
1:A:170:ARG:HH11	5:A:591:CYN:C	2.12	0.62
1:A:14:TRP:CD2	1:A:15:PRO:HD2	2.35	0.62
1:A:81:TYR:CD2	1:A:93:HIS:CD2	2.74	0.62
1:D:63:LYS:HE2	1:D:81:TYR:HB3	1.81	0.62
1:A:229:ARG:NH1	3:A:580:SRM:O4C	2.34	0.61
1:D:16:SER:HB3	1:D:19:LYS:HB3	1.82	0.61
1:D:400:ASP:OD1	6:D:579:HOH:O	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:ASN:HB2	1:D:137:ILE:HB	1.84	0.60
1:D:14:TRP:CD2	1:D:15:PRO:HD2	2.38	0.59
3:A:580:SRM:NC	2:B:182:CYS:HA	2.18	0.59
2:E:272:LEU:HB2	3:E:570:SRM:CCC	2.33	0.59
2:E:296:TRP:N	2:E:297:PRO:HD3	2.17	0.58
3:A:580:SRM:CBB	3:A:580:SRM:CMB	2.82	0.58
2:E:150:ILE:O	2:E:154:VAL:HG23	2.04	0.58
2:E:230:LYS:CA	2:E:231:ASN:HB2	2.33	0.58
2:E:72:ASP:CG	2:E:72:ASP:CA	2.69	0.58
1:D:112:LEU:HD11	2:E:82:LEU:HD11	1.86	0.58
2:E:170:MET:O	2:E:319:ARG:HG2	2.03	0.57
1:D:73:TYR:CD1	1:D:204:HIS:HB3	2.40	0.57
1:A:94:PHE:O	2:B:139:HIS:CE1	2.56	0.56
1:D:81:TYR:CE2	1:D:93:HIS:HD2	2.24	0.56
1:A:65:GLY:HA2	1:A:81:TYR:HD1	1.70	0.56
2:E:134:THR:HG21	2:E:182:CYS:HB2	1.87	0.56
2:E:142:THR:N	2:E:143:PRO:CD	2.70	0.55
1:D:62:TRP:HB3	1:D:80:ARG:HD2	1.88	0.55
3:A:580:SRM:C1C	2:B:182:CYS:HA	2.37	0.55
1:D:247:GLU:HA	1:D:250:LYS:HD2	1.88	0.55
3:E:570:SRM:HDD2	3:E:570:SRM:HBD2	1.88	0.54
1:A:219:CYS:HB2	1:A:220:PRO:CD	2.37	0.54
1:D:45:ARG:HG3	1:D:45:ARG:HH11	1.71	0.54
3:D:580:SRM:CMB	3:D:580:SRM:HBB2	2.38	0.54
3:D:580:SRM:HBB2	3:D:580:SRM:HMB1	1.89	0.53
2:E:267:MET:HA	2:E:283:LYS:O	2.08	0.53
2:B:108:GLN:NE2	2:B:115:CYS:H	1.95	0.53
2:B:299:LEU:C	2:B:299:LEU:HD23	2.29	0.53
3:A:580:SRM:O1A	2:B:139:HIS:HD2	1.91	0.53
2:E:182:CYS:HB2	4:E:585:SF4:S2	2.47	0.53
2:E:296:TRP:N	2:E:297:PRO:CD	2.72	0.53
1:D:215:LYS:HE2	1:D:229:ARG:HG3	1.90	0.53
1:A:81:TYR:HD2	1:A:93:HIS:HD2	1.48	0.52
1:D:94:PHE:O	2:E:139:HIS:CE1	2.59	0.52
2:B:170:MET:O	2:B:319:ARG:HG2	2.10	0.52
1:D:387:LYS:NZ	6:D:737:HOH:O	2.43	0.52
1:A:66:GLY:N	1:A:81:TYR:HE1	2.04	0.52
1:A:219:CYS:HB2	1:A:220:PRO:HD2	1.91	0.52
2:B:175:LEU:C	2:B:175:LEU:HD23	2.30	0.52
2:B:184:ALA:HB3	6:B:499:HOH:O	2.10	0.51
2:E:120:ASP:OD1	2:E:122:VAL:HB	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:ALA:HB3	1:D:229:ARG:HE	1.75	0.51
1:D:286:VAL:HG22	6:D:774:HOH:O	2.10	0.51
3:A:580:SRM:CMB	3:A:580:SRM:HBB2	2.41	0.51
1:D:315:ALA:HB1	1:D:316:PRO:CD	2.41	0.51
1:A:222:ASP:OD2	1:A:227:LYS:NZ	2.42	0.51
1:D:343:ILE:HD11	1:D:379:ARG:NH2	2.26	0.51
1:D:127:THR:HA	1:D:137:ILE:O	2.11	0.50
2:E:176:ALA:HB2	2:E:185:VAL:HG21	1.92	0.50
1:A:170:ARG:HH12	5:A:590:CYN:C	2.25	0.50
1:D:63:LYS:HE2	1:D:81:TYR:CB	2.42	0.50
1:A:79:GLY:HA2	1:A:95:HIS:ND1	2.27	0.50
2:E:271:LYS:NZ	2:E:277:ARG:O	2.41	0.50
2:E:105:ASN:O	2:E:109:GLU:HB2	2.12	0.49
1:D:14:TRP:CG	1:D:15:PRO:HD2	2.47	0.49
1:D:100:ASN:HD22	1:D:101:GLN:N	2.11	0.49
1:D:174:ALA:HB1	1:D:188:THR:HB	1.94	0.48
1:A:225:ALA:O	1:A:229:ARG:HG2	2.14	0.48
1:A:235:ILE:HD12	1:A:310:LEU:HD22	1.94	0.48
1:A:399:LYS:HB2	1:A:417:TRP:CZ2	2.48	0.48
1:A:147:GLN:HB3	1:A:148:PRO:HD3	1.96	0.48
1:D:187:ASP:OD2	2:E:16:ARG:NH2	2.46	0.48
3:D:580:SRM:O1A	2:E:139:HIS:HD2	1.96	0.48
1:D:155:ASN:OD1	2:E:7:LYS:HE3	2.14	0.48
2:B:157:GLU:HG3	2:B:300:VAL:HG11	1.95	0.48
2:E:126:TYR:N	2:E:126:TYR:CD1	2.81	0.48
1:A:213:LYS:HE2	5:A:591:CYN:C	2.44	0.48
3:A:580:SRM:HBB2	3:A:580:SRM:HMB3	1.94	0.48
1:A:178:PRO:HG3	1:A:187:ASP:HA	1.96	0.48
1:D:147:GLN:HB3	1:D:148:PRO:HD3	1.95	0.48
2:B:228:ASP:HB2	2:B:235:LYS:HG3	1.96	0.48
1:D:267:PRO:HG2	6:D:774:HOH:O	2.13	0.48
1:A:133:THR:HG21	5:A:591:CYN:C	2.44	0.47
3:D:580:SRM:HHB	3:D:580:SRM:HBA1	1.95	0.47
3:D:580:SRM:HDB1	2:E:134:THR:HG22	1.96	0.47
2:E:134:THR:HB	4:E:585:SF4:S4	2.54	0.47
1:D:9:LEU:HD21	2:E:294:PRO:O	2.15	0.47
1:A:56:LYS:NZ	6:A:526:HOH:O	2.42	0.47
1:D:79:GLY:HA2	1:D:95:HIS:ND1	2.30	0.46
1:D:294:LYS:HB3	1:D:294:LYS:HE2	1.61	0.46
1:D:316:PRO:HA	1:D:321:ALA:N	2.30	0.46
2:E:175:LEU:C	2:E:175:LEU:HD23	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:ALA:HB1	1:D:316:PRO:HD2	1.98	0.46
1:D:179:ALA:O	2:E:23:ILE:HG23	2.16	0.46
1:D:45:ARG:HG3	1:D:45:ARG:NH1	2.30	0.45
1:D:310:LEU:HD12	1:D:326:VAL:HA	1.97	0.45
2:E:52:TYR:CE1	2:E:97:GLU:HB3	2.51	0.45
1:D:187:ASP:OD1	2:E:27:TYR:OH	2.34	0.45
2:E:124:GLY:HA3	2:E:316:LYS:HD3	1.99	0.45
2:E:185:VAL:HG13	2:E:191:ALA:HB1	1.97	0.45
2:B:146:ASP:O	2:B:150:ILE:HD12	2.17	0.45
2:B:353:TYR:HA	2:E:353:TYR:HA	1.97	0.45
1:D:129:PHE:HA	1:D:130:HIS:HA	1.66	0.45
1:D:350:TRP:CG	1:D:376:VAL:HG21	2.51	0.45
1:D:81:TYR:CE2	1:D:93:HIS:CD2	3.03	0.45
1:A:99:ILE:HB	1:A:136:ILE:HB	1.99	0.45
2:E:76:LYS:HD3	2:E:77:TYR:CZ	2.52	0.45
2:B:324:VAL:HG11	2:B:329:TRP:CE2	2.52	0.45
2:E:44:VAL:HG22	2:E:50:VAL:HG22	1.99	0.45
2:E:157:GLU:HG3	2:E:300:VAL:CG1	2.47	0.44
1:A:173:SER:OG	1:A:215:LYS:HG2	2.18	0.44
2:E:58:THR:HG22	2:E:113:PHE:CE2	2.53	0.44
1:A:145:TYR:C	1:A:148:PRO:HD2	2.37	0.44
2:B:176:ALA:HB1	2:B:181:MET:HA	1.99	0.44
1:D:219:CYS:HB2	1:D:220:PRO:CD	2.48	0.44
1:D:135:ASP:OD2	1:D:163:GLY:HA3	2.18	0.44
2:E:87:ARG:CZ	2:E:172:ARG:HD2	2.47	0.43
3:E:570:SRM:HAC2	3:E:570:SRM:HCD1	1.85	0.43
3:A:580:SRM:HDD2	3:A:580:SRM:HAD1	1.79	0.43
2:E:20:HIS:HA	2:E:21:PRO:HD2	1.64	0.43
1:A:96:THR:HG21	6:A:553:HOH:O	2.17	0.43
1:D:24:THR:OG1	2:E:63:SER:HB2	2.19	0.43
1:A:288:CYS:O	1:A:289:MET:HB2	2.18	0.43
1:D:112:LEU:CD1	2:E:82:LEU:HD11	2.48	0.43
3:D:580:SRM:CMB	3:D:580:SRM:CBB	2.96	0.43
1:A:96:THR:HG23	2:B:139:HIS:NE2	2.33	0.43
1:A:316:PRO:HA	1:A:321:ALA:N	2.34	0.43
2:E:58:THR:HG22	2:E:113:PHE:CD2	2.53	0.43
2:E:113:PHE:HA	2:E:114:PRO:HD2	1.61	0.43
2:B:359:ARG:HD3	2:B:363:GLN:O	2.19	0.43
1:A:269:GLY:HA2	6:A:589:HOH:O	2.19	0.43
2:B:191:ALA:HB3	2:B:267:MET:HB2	2.01	0.42
2:E:324:VAL:HG11	2:E:329:TRP:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:580:SRM:C3C	2:B:182:CYS:HA	2.49	0.42
1:D:86:GLU:H	1:D:86:GLU:HG2	1.69	0.42
1:D:65:GLY:HA2	1:D:81:TYR:CD1	2.53	0.42
2:E:20:HIS:HB3	2:E:23:ILE:HG13	2.02	0.42
2:E:52:TYR:HB2	2:E:94:VAL:O	2.18	0.42
1:D:50:GLN:HE22	1:D:82:SER:HB2	1.85	0.42
2:E:242:MET:SD	2:E:244:CYS:HB3	2.59	0.42
2:B:313:ASN:HB3	6:B:478:HOH:O	2.19	0.42
2:E:230:LYS:HE3	2:E:230:LYS:HA	2.02	0.42
1:D:178:PRO:HG3	1:D:187:ASP:HA	2.01	0.41
1:A:259:GLU:OE2	1:A:264:LYS:HE3	2.19	0.41
1:D:218:GLY:HA3	4:D:575:SF4:S2	2.60	0.41
1:D:316:PRO:HG2	2:E:181:MET:HE3	2.01	0.41
1:D:317:PHE:HA	1:D:318:VAL:HA	1.80	0.41
3:D:580:SRM:HDD2	3:D:580:SRM:HAD1	1.91	0.41
2:E:145:ILE:HG12	2:E:177:CYS:HA	2.01	0.41
2:E:175:LEU:HD23	2:E:176:ALA:N	2.35	0.41
2:E:20:HIS:CD2	2:E:79:ASP:HB2	2.55	0.41
1:A:115:LEU:HD21	1:A:160:PHE:CG	2.54	0.41
2:B:57:GLY:HA2	2:B:89:ASN:OD1	2.21	0.41
1:D:109:THR:N	2:E:80:GLY:O	2.52	0.41
2:E:46:GLU:C	2:E:48:GLY:H	2.22	0.41
1:A:62:TRP:HB3	1:A:80:ARG:HD2	2.03	0.41
1:A:219:CYS:CB	1:A:220:PRO:CD	2.98	0.41
1:D:108:SER:HA	2:E:80:GLY:O	2.21	0.40
1:D:93:HIS:HB2	1:D:142:ARG:HG2	2.03	0.40
1:A:252:TYR:CD2	1:A:295:MET:HG2	2.56	0.40
2:B:220:CYS:HA	2:B:221:PRO:HD3	1.76	0.40
2:B:330:GLU:HB2	6:B:369:HOH:O	2.21	0.40
2:E:134:THR:CG2	2:E:182:CYS:HB3	2.43	0.40
2:E:331:ARG:HA	2:E:331:ARG:HD3	1.94	0.40
1:A:64:HIS:HE1	2:B:249:THR:O	2.05	0.40
1:A:326:VAL:HB	1:A:385:MET:HA	2.03	0.40
2:E:4:GLU:HG3	2:E:5:GLY:H	1.87	0.40
2:E:108:GLN:HE21	2:E:108:GLN:N	2.20	0.40
2:E:119:TRP:CE2	2:E:170:MET:CE	3.04	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	415/418 (99%)	405 (98%)	10 (2%)	0	100	100
1	D	415/418 (99%)	391 (94%)	24 (6%)	0	100	100
2	B	361/366 (99%)	350 (97%)	10 (3%)	1 (0%)	41	31
2	E	361/366 (99%)	333 (92%)	26 (7%)	2 (1%)	25	15
All	All	1552/1568 (99%)	1479 (95%)	70 (4%)	3 (0%)	47	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	231	ASN
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	353/354 (100%)	346 (98%)	7 (2%)	55	51
1	D	353/354 (100%)	345 (98%)	8 (2%)	50	45
2	B	314/317 (99%)	305 (97%)	9 (3%)	42	35
2	E	314/317 (99%)	301 (96%)	13 (4%)	30	21
All	All	1334/1342 (99%)	1297 (97%)	37 (3%)	43	36

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	54	SER
1	A	68	VAL
1	A	100	ASN
1	A	210	TYR
1	A	224	VAL
1	A	310	LEU
2	B	4	GLU
2	B	78	SER
2	B	97	GLU
2	B	177	CYS
2	B	188	SER
2	B	229	MET
2	B	242	MET
2	B	243	TYR
2	B	283	LYS
1	D	19	LYS
1	D	100	ASN
1	D	132	SER
1	D	133	THR
1	D	210	TYR
1	D	294	LYS
1	D	310	LEU
1	D	332	GLU
2	E	41	ILE
2	E	82	LEU
2	E	97	GLU
2	E	108	GLN
2	E	148	SER
2	E	160	GLU
2	E	177	CYS
2	E	182	CYS
2	E	230	LYS
2	E	242	MET
2	E	243	TYR
2	E	256	LEU
2	E	307	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	93	HIS

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Mol	Chain	Res	Type
1	A	100	ASN
2	B	108	GLN
2	B	139	HIS
1	D	50	GLN
1	D	93	HIS
1	D	100	ASN
2	E	108	GLN
2	E	139	HIS
2	E	180	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
5	CYN	D	592	3	0,1,1	-	-	-		
5	CYN	A	590	3	0,1,1	-	-	-		
3	SRM	D	580	5,2	68,70,70	2.14	17 (25%)	81,112,112	2.75	25 (30%)
3	SRM	E	570	1	68,70,70	2.21	11 (16%)	81,112,112	3.06	37 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	SRM	B	570	1	68,70,70	2.22	15 (22%)	81,112,112	2.88	35 (43%)
4	SF4	B	585	2	0,12,12	-	-	-		
4	SF4	A	576	1	0,12,12	-	-	-		
4	SF4	E	585	2	0,12,12	-	-	-		
4	SF4	B	586	2	0,12,12	-	-	-		
3	SRM	A	580	5,2	68,70,70	1.88	12 (17%)	81,112,112	2.82	33 (40%)
4	SF4	A	575	1	0,12,12	-	-	-		
4	SF4	E	586	2	0,12,12	-	-	-		
4	SF4	D	576	1,6	0,12,12	-	-	-		
5	CYN	A	591	-	0,1,1	-	-	-		
4	SF4	D	575	1	0,12,12	-	-	-		

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
3	SRM	D	580	5,2	1/1/19/23	12/38/126/126	-
3	SRM	E	570	1	1/1/19/23	14/38/126/126	-
3	SRM	B	570	1	1/1/19/23	14/38/126/126	-
4	SF4	B	585	2	-	-	0/6/5/5
4	SF4	A	576	1	-	-	0/6/5/5
4	SF4	E	585	2	-	-	0/6/5/5
4	SF4	B	586	2	-	-	0/6/5/5
3	SRM	A	580	5,2	1/1/19/23	10/38/126/126	-
4	SF4	A	575	1	-	-	0/6/5/5
4	SF4	E	586	2	-	-	0/6/5/5
4	SF4	D	576	1,6	-	-	0/6/5/5
4	SF4	D	575	1	-	-	0/6/5/5

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	570	SRM	C4A-NA	-9.55	1.28	1.35
3	B	570	SRM	C4A-NA	-8.52	1.29	1.35
3	D	580	SRM	C3D-C2D	7.12	1.55	1.39
3	E	570	SRM	C3C-C2C	6.66	1.51	1.36
3	D	580	SRM	C3C-C2C	6.28	1.50	1.36
3	E	570	SRM	C3D-C2D	6.11	1.53	1.39
3	A	580	SRM	C3A-C4A	-5.97	1.38	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	570	SRM	C3D-C2D	5.74	1.52	1.39
3	B	570	SRM	C4C-NC	-5.73	1.28	1.39
3	A	580	SRM	C3C-C2C	5.73	1.49	1.36
3	D	580	SRM	C3A-C4A	-5.66	1.39	1.51
3	B	570	SRM	C4B-NB	5.45	1.39	1.35
3	B	570	SRM	C3C-C2C	5.43	1.48	1.36
3	A	580	SRM	C3B-C4B	-5.06	1.40	1.51
3	D	580	SRM	C3B-C4B	-5.05	1.40	1.51
3	E	570	SRM	C1C-NC	-4.82	1.30	1.39
3	A	580	SRM	C3D-C2D	4.64	1.50	1.39
3	E	570	SRM	C1C-C2C	4.38	1.53	1.45
3	E	570	SRM	C4C-NC	-4.14	1.31	1.39
3	D	580	SRM	C4A-NA	-4.10	1.32	1.35
3	B	570	SRM	C4C-C3C	4.09	1.52	1.45
3	B	570	SRM	CDC-CEC	3.74	1.56	1.51
3	D	580	SRM	FE-NC	3.63	2.09	1.95
3	D	580	SRM	CAD-C2D	3.41	1.57	1.52
3	D	580	SRM	CHD-C4C	3.34	1.40	1.35
3	D	580	SRM	C4C-NC	-3.07	1.33	1.39
3	A	580	SRM	CHA-C1A	2.94	1.40	1.35
3	E	570	SRM	C4C-C3C	2.83	1.50	1.45
3	E	570	SRM	CAD-C2D	2.70	1.56	1.52
3	D	580	SRM	C1C-C2C	2.69	1.50	1.45
3	E	570	SRM	CHA-C1A	2.67	1.40	1.35
3	A	580	SRM	CHD-C4C	2.67	1.39	1.35
3	B	570	SRM	C1C-NC	-2.66	1.34	1.39
3	A	580	SRM	C1C-C2C	2.66	1.49	1.45
3	A	580	SRM	CAD-C2D	2.62	1.55	1.52
3	D	580	SRM	C4C-C3C	2.60	1.49	1.45
3	D	580	SRM	C1C-NC	-2.53	1.34	1.39
3	B	570	SRM	CHA-C1A	2.51	1.40	1.35
3	B	570	SRM	C2B-C3B	-2.47	1.48	1.55
3	D	580	SRM	FE-NB	2.43	2.10	1.97
3	D	580	SRM	CBD-CCD	2.40	1.56	1.50
3	A	580	SRM	C1D-ND	2.37	1.41	1.36
3	B	570	SRM	O4A-CEA	-2.34	1.22	1.30
3	B	570	SRM	C1C-C2C	2.32	1.49	1.45
3	D	580	SRM	FE-NA	2.31	2.09	1.97
3	E	570	SRM	C2B-C3B	-2.31	1.48	1.55
3	A	580	SRM	C4C-NC	-2.30	1.35	1.39
3	B	570	SRM	CAA-CBA	2.29	1.60	1.52
3	A	580	SRM	O3B-CEB	2.22	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	580	SRM	CAA-C3A	-2.21	1.49	1.54
3	D	580	SRM	CHA-C1A	2.20	1.39	1.35
3	E	570	SRM	CDC-C2C	2.13	1.54	1.51
3	B	570	SRM	CAD-C2D	2.13	1.55	1.52
3	B	570	SRM	C3B-C4B	-2.08	1.46	1.51
3	A	580	SRM	C2B-C1B	-2.05	1.49	1.54

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	580	SRM	C2A-C3A-C4A	10.11	113.84	100.90
3	B	570	SRM	C2B-C3B-C4B	8.93	112.33	100.90
3	A	580	SRM	C2A-C3A-C4A	8.72	112.07	100.90
3	A	580	SRM	CMB-C2B-C3B	8.54	127.86	112.08
3	D	580	SRM	CBD-CAD-C2D	8.42	126.99	112.62
3	E	570	SRM	CBD-CAD-C2D	8.20	126.61	112.62
3	A	580	SRM	CAA-C3A-C4A	7.31	124.07	111.19
3	E	570	SRM	C2A-C1A-CHA	-7.04	117.11	123.54
3	D	580	SRM	CAA-C3A-C4A	7.01	123.56	111.19
3	A	580	SRM	C2B-C1B-CHB	-6.86	117.28	123.54
3	E	570	SRM	C3D-CDD-CED	6.75	122.29	114.21
3	E	570	SRM	C2B-C3B-C4B	6.67	109.44	100.90
3	B	570	SRM	C3C-C4C-NC	6.64	116.78	110.32
3	B	570	SRM	CMB-C2B-C3B	6.63	124.32	112.08
3	E	570	SRM	C2B-C1B-CHB	-6.45	117.65	123.54
3	B	570	SRM	C4C-C3C-C2C	-6.21	99.68	106.86
3	B	570	SRM	C2A-C1A-CHA	-6.16	117.92	123.54
3	A	580	SRM	C2B-C3B-C4B	6.13	108.75	100.90
3	E	570	SRM	CAB-C3B-C4B	6.06	121.88	111.19
3	A	580	SRM	CMA-C2A-C3A	-5.89	101.19	112.08
3	E	570	SRM	C4C-C3C-C2C	-5.71	100.25	106.86
3	B	570	SRM	CBC-CAC-C3C	-5.70	96.79	112.63
3	D	580	SRM	C3D-CDD-CED	5.67	120.99	114.21
3	B	570	SRM	C2B-C1B-CHB	-5.56	118.46	123.54
3	D	580	SRM	C2B-C3B-C4B	5.50	107.94	100.90
3	E	570	SRM	C3C-C4C-NC	5.43	115.61	110.32
3	A	580	SRM	C3C-C4C-NC	5.43	115.61	110.32
3	E	570	SRM	C4D-CHA-C1A	-5.39	119.45	130.12
3	B	570	SRM	CHD-C4C-C3C	-5.37	116.25	124.93
3	E	570	SRM	CAC-C3C-C2C	-5.34	118.26	129.51
3	B	570	SRM	C3B-C2B-C1B	-5.28	91.86	100.92
3	D	580	SRM	C1A-NA-C4A	5.23	111.16	105.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	570	SRM	CBD-CAD-C2D	5.13	121.37	112.62
3	B	570	SRM	CAB-C3B-C4B	4.83	119.71	111.19
3	E	570	SRM	C2B-C1B-NB	4.77	118.87	111.21
3	D	580	SRM	C3C-C4C-NC	4.72	114.91	110.32
3	A	580	SRM	CDD-C3D-C2D	-4.66	118.16	126.49
3	D	580	SRM	C2C-C1C-NC	4.65	114.85	110.32
3	D	580	SRM	CBB-CAB-C3B	4.61	128.04	114.73
3	B	570	SRM	C4D-CHA-C1A	-4.45	121.31	130.12
3	D	580	SRM	CMB-C2B-C3B	4.36	120.13	112.08
3	B	570	SRM	CHC-C1C-C2C	-4.23	118.08	124.94
3	D	580	SRM	C1C-C2C-C3C	-4.18	102.03	106.86
3	E	570	SRM	C3A-C4A-NA	4.15	119.00	110.85
3	E	570	SRM	C3B-C2B-C1B	-4.11	93.86	100.92
3	E	570	SRM	CHD-C4C-C3C	-4.06	118.37	124.93
3	A	580	SRM	CAB-C3B-C2B	-4.01	103.10	114.14
3	E	570	SRM	CBB-CAB-C3B	-3.98	103.24	114.73
3	A	580	SRM	C1A-NA-C4A	3.95	109.70	105.23
3	E	570	SRM	CDA-C2A-C1A	3.94	119.52	107.12
3	A	580	SRM	CBD-CAD-C2D	3.88	119.25	112.62
3	E	570	SRM	CBC-CAC-C3C	-3.86	101.89	112.63
3	E	570	SRM	CHC-C1C-C2C	-3.86	118.68	124.94
3	E	570	SRM	CAB-CBB-CCB	3.84	122.71	112.51
3	A	580	SRM	CAC-CBC-CCC	-3.80	105.43	113.60
3	E	570	SRM	C1C-C2C-C3C	-3.74	102.54	106.86
3	D	580	SRM	C4C-C3C-C2C	-3.73	102.54	106.86
3	D	580	SRM	CDD-C3D-C2D	-3.71	119.86	126.49
3	B	570	SRM	C2A-C1A-NA	3.71	117.18	111.21
3	E	570	SRM	CMB-C2B-C3B	3.68	118.88	112.08
3	D	580	SRM	C4D-CHA-C1A	-3.66	122.86	130.12
3	D	580	SRM	CDD-C3D-C4D	-3.58	121.93	127.36
3	E	570	SRM	CAB-C3B-C2B	3.56	123.95	114.14
3	E	570	SRM	CDD-C3D-C4D	-3.53	122.00	127.36
3	B	570	SRM	C3A-C4A-NA	3.50	117.74	110.85
3	A	580	SRM	CMA-C2A-CDA	3.48	116.54	110.80
3	D	580	SRM	C3A-C2A-C1A	-3.46	94.98	100.92
3	D	580	SRM	CDA-C2A-C1A	3.46	117.99	107.12
3	A	580	SRM	CDA-C2A-C1A	3.45	117.95	107.12
3	B	570	SRM	C2C-C1C-NC	3.40	113.63	110.32
3	B	570	SRM	C2B-C1B-NB	3.40	116.67	111.21
3	D	580	SRM	CHD-C4C-NC	-3.35	120.80	124.43
3	B	570	SRM	CHC-C1C-NC	3.35	128.06	124.44
3	E	570	SRM	C3A-C4A-CHB	-3.33	116.12	123.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	570	SRM	CHC-C1C-NC	3.31	128.02	124.44
3	A	580	SRM	C3D-CDD-CED	3.18	118.01	114.21
3	A	580	SRM	C4C-C3C-C2C	-3.11	103.26	106.86
3	B	570	SRM	O2D-CCD-CBD	3.11	124.02	114.03
3	B	570	SRM	C1A-NA-C4A	-3.08	101.75	105.23
3	E	570	SRM	CEC-CDC-C2C	-3.08	105.81	113.79
3	B	570	SRM	O1D-CCD-CBD	-3.07	113.22	123.08
3	A	580	SRM	C4D-CHA-C1A	-3.07	124.04	130.12
3	D	580	SRM	CMA-C2A-CDA	3.05	115.84	110.80
3	D	580	SRM	CHC-C1C-NC	-3.02	121.17	124.44
3	A	580	SRM	CAB-C3B-C4B	-3.02	105.87	111.19
3	E	570	SRM	CMA-C2A-CDA	-3.01	105.84	110.80
3	A	580	SRM	CAC-C3C-C4C	2.99	130.52	124.89
3	E	570	SRM	C2C-C1C-NC	2.97	113.21	110.32
3	B	570	SRM	C3B-C4B-NB	-2.89	105.17	110.85
3	D	580	SRM	C3A-C4A-CHB	2.77	129.31	123.32
3	D	580	SRM	C2B-C1B-NB	2.74	115.62	111.21
3	A	580	SRM	CDA-C2A-C3A	2.72	115.67	108.39
3	E	570	SRM	C2A-C1A-NA	2.68	115.53	111.21
3	B	570	SRM	C1C-CHC-C4B	-2.68	120.16	126.62
3	B	570	SRM	O4B-CEB-CDB	2.65	122.85	114.35
3	A	580	SRM	C4A-CHB-C1B	-2.65	121.98	125.88
3	A	580	SRM	CMB-C2B-CDB	-2.64	106.46	110.80
3	A	580	SRM	O4A-CEA-O3A	-2.63	116.74	123.30
3	A	580	SRM	CAD-CBD-CCD	-2.60	106.48	113.76
3	B	570	SRM	C1C-C2C-C3C	-2.59	103.86	106.86
3	B	570	SRM	CDB-C2B-C3B	-2.58	101.47	108.39
3	A	580	SRM	CDD-C3D-C4D	2.54	131.21	127.36
3	A	580	SRM	C1C-C2C-C3C	-2.52	103.94	106.86
3	E	570	SRM	O4B-CEB-CDB	2.51	122.40	114.35
3	D	580	SRM	C2A-C1A-CHA	2.51	125.83	123.54
3	B	570	SRM	O4B-CEB-O3B	-2.49	117.10	123.30
3	B	570	SRM	CBB-CAB-C3B	2.48	121.89	114.73
3	A	580	SRM	C2B-C1B-NB	2.47	115.18	111.21
3	E	570	SRM	CAA-CBA-CCA	2.45	119.01	112.51
3	A	580	SRM	C3B-C2B-C1B	-2.45	96.72	100.92
3	A	580	SRM	O2B-CCB-CBB	2.44	121.86	114.03
3	D	580	SRM	CAB-C3B-C2B	-2.37	107.61	114.14
3	B	570	SRM	CMB-C2B-C1B	2.37	121.40	109.57
3	E	570	SRM	O2C-CCC-CBC	2.36	121.61	114.03
3	E	570	SRM	O4C-CEC-CDC	2.36	122.07	114.54
3	B	570	SRM	CEC-CDC-C2C	-2.36	107.68	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	570	SRM	O1C-CCC-CBC	-2.35	115.54	123.08
3	B	570	SRM	CHD-C4C-NC	2.33	126.95	124.43
3	B	570	SRM	O2C-CCC-CBC	2.32	121.49	114.03
3	E	570	SRM	O2D-CCD-CBD	2.32	121.49	114.03
3	E	570	SRM	C4C-NC-C1C	2.30	107.60	105.35
3	A	580	SRM	CHD-C4C-C3C	-2.26	121.28	124.93
3	A	580	SRM	C3A-C2A-C1A	-2.16	97.22	100.92
3	B	570	SRM	C4B-NB-C1B	2.14	107.65	105.23
3	A	580	SRM	O3B-CEB-CDB	-2.13	116.72	122.94
3	D	580	SRM	C3B-C2B-C1B	-2.08	97.35	100.92
3	B	570	SRM	CMA-C2A-CDA	-2.08	107.38	110.80
3	E	570	SRM	CMB-C2B-C1B	2.05	119.84	109.57
3	B	570	SRM	CAC-C3C-C2C	-2.05	125.18	129.51
3	A	580	SRM	O2A-CCA-O1A	-2.01	118.28	123.30

All (4) 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
3	E	570	SRM	NC

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	580	SRM	C2A-C3A-CAA-CBA
3	A	580	SRM	C1D-C2D-CAD-CBD
3	B	570	SRM	C3D-C2D-CAD-CBD
3	D	580	SRM	C1D-C2D-CAD-CBD
3	E	570	SRM	C4A-C3A-CAA-CBA
3	E	570	SRM	C1D-C2D-CAD-CBD
3	E	570	SRM	C3D-C2D-CAD-CBD
3	E	570	SRM	C4C-C3C-CAC-CBC
3	E	570	SRM	C3A-CAA-CBA-CCA
3	E	570	SRM	C2D-CAD-CBD-CCD
3	B	570	SRM	C4A-C3A-CAA-CBA
3	D	580	SRM	C2A-C3A-CAA-CBA
3	A	580	SRM	C3B-CAB-CBB-CCB
3	B	570	SRM	C2B-CDB-CEB-O3B
3	A	580	SRM	C4A-C3A-CAA-CBA
3	B	570	SRM	C2B-CDB-CEB-O4B

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Mol	Chain	Res	Type	Atoms
3	E	570	SRM	C2B-CDB-CEB-O3B
3	E	570	SRM	C2B-CDB-CEB-O4B
3	E	570	SRM	C3C-CAC-CBC-CCC
3	D	580	SRM	C3D-CDD-CED-O3D
3	D	580	SRM	C3D-CDD-CED-O4D
3	B	570	SRM	C3B-C2B-CDB-CEB
3	B	570	SRM	CAA-CBA-CCA-O2A
3	B	570	SRM	CAC-CBC-CCC-O1C
3	B	570	SRM	CAA-CBA-CCA-O1A
3	D	580	SRM	CAC-CBC-CCC-O2C
3	A	580	SRM	CAA-CBA-CCA-O1A
3	D	580	SRM	CAA-CBA-CCA-O1A
3	D	580	SRM	CAB-CBB-CCB-O1B
3	D	580	SRM	CAB-CBB-CCB-O2B
3	D	580	SRM	CAC-CBC-CCC-O1C
3	A	580	SRM	CAA-CBA-CCA-O2A
3	D	580	SRM	CAA-CBA-CCA-O2A
3	D	580	SRM	C1A-C2A-CDA-CEA
3	B	570	SRM	C3C-CAC-CBC-CCC
3	B	570	SRM	CAC-CBC-CCC-O2C
3	A	580	SRM	CAC-CBC-CCC-O2C
3	B	570	SRM	CAB-CBB-CCB-O2B
3	B	570	SRM	CAB-CBB-CCB-O1B
3	A	580	SRM	CAB-CBB-CCB-O2B
3	E	570	SRM	CAC-CBC-CCC-O1C
3	A	580	SRM	CAC-CBC-CCC-O1C
3	D	580	SRM	C4D-C3D-CDD-CED
3	E	570	SRM	CAD-CBD-CCD-O2D
3	A	580	SRM	CAB-CBB-CCB-O1B
3	E	570	SRM	CAC-CBC-CCC-O2C
3	E	570	SRM	CAD-CBD-CCD-O1D
3	B	570	SRM	CAD-CBD-CCD-O2D
3	B	570	SRM	CAD-CBD-CCD-O1D
3	E	570	SRM	CAA-CBA-CCA-O1A

There are no ring outliers.
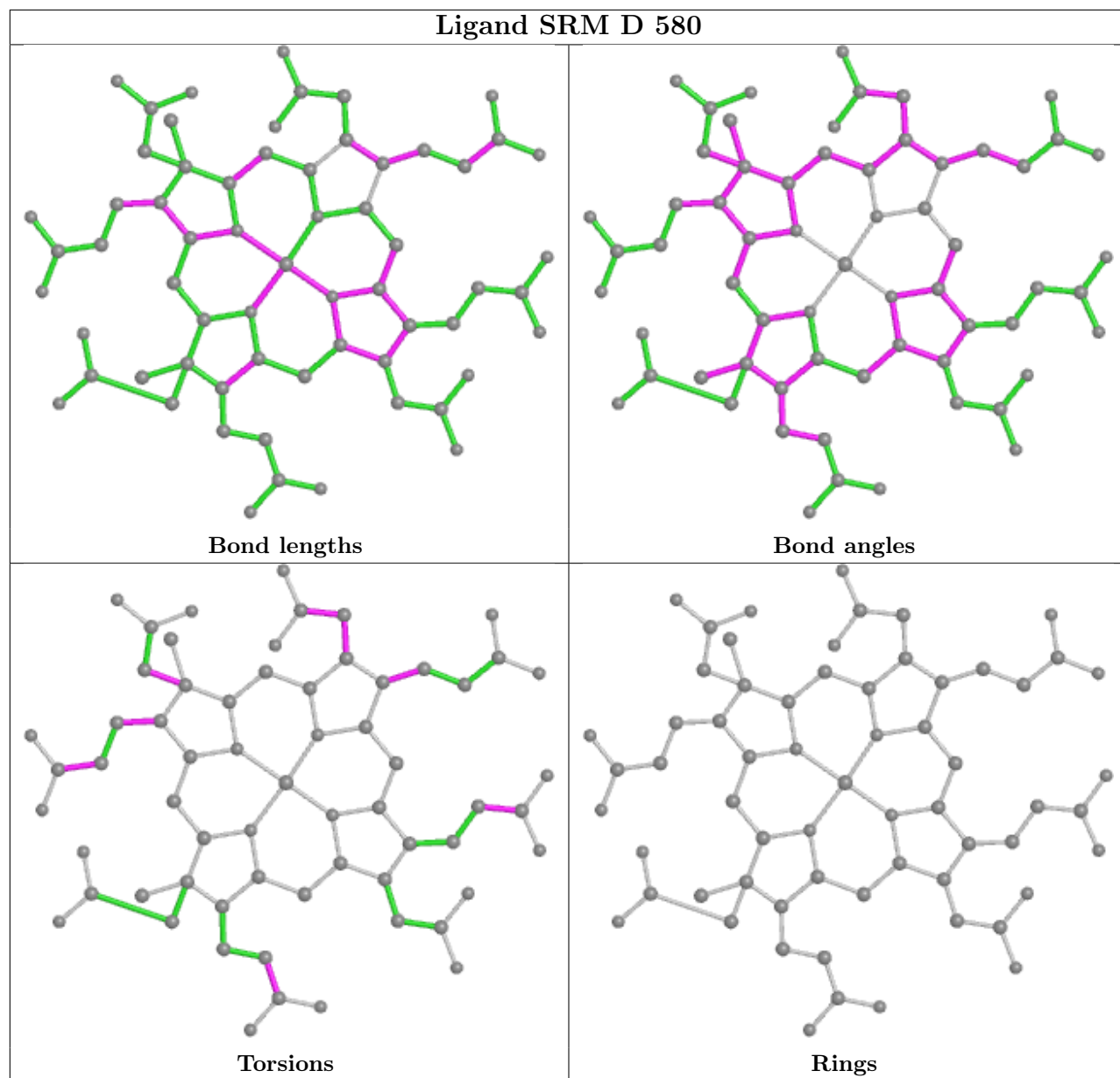
10 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	592	CYN	1	0
5	A	590	CYN	1	0
3	D	580	SRM	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	570	SRM	5	0
3	B	570	SRM	1	0
4	E	585	SF4	2	0
3	A	580	SRM	10	0
4	D	576	SF4	1	0
5	A	591	CYN	4	0
4	D	575	SF4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand SRM D 580

Bond lengths

Bond angles

Torsions

Rings

Ligand SRM E 570

Bond lengths

Bond angles

Torsions

Rings

Ligand SRM B 570

Bond lengths

Bond angles

Torsions

Rings

Ligand SRM A 580

Bond lengths

Bond angles

Torsions

Rings
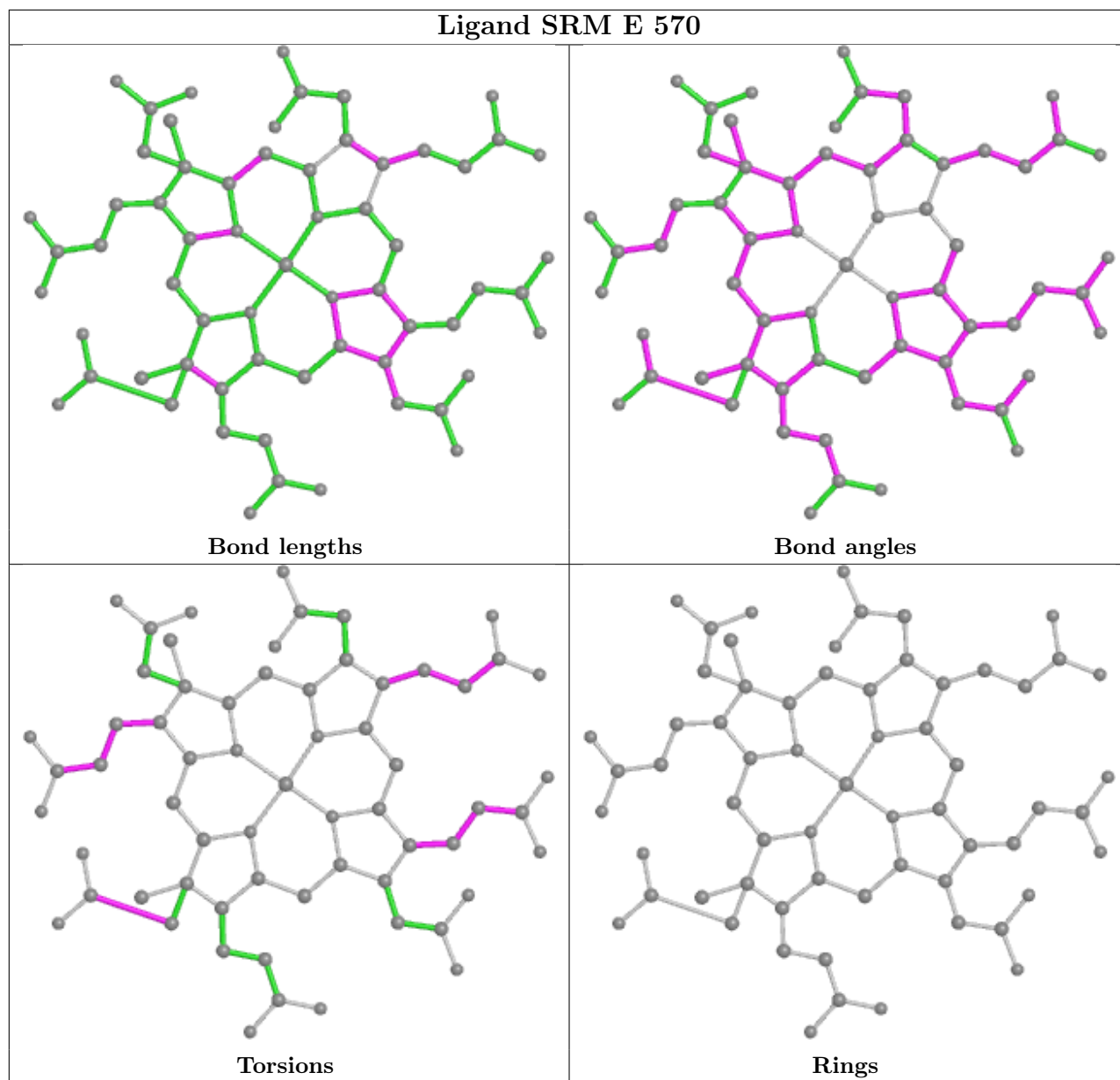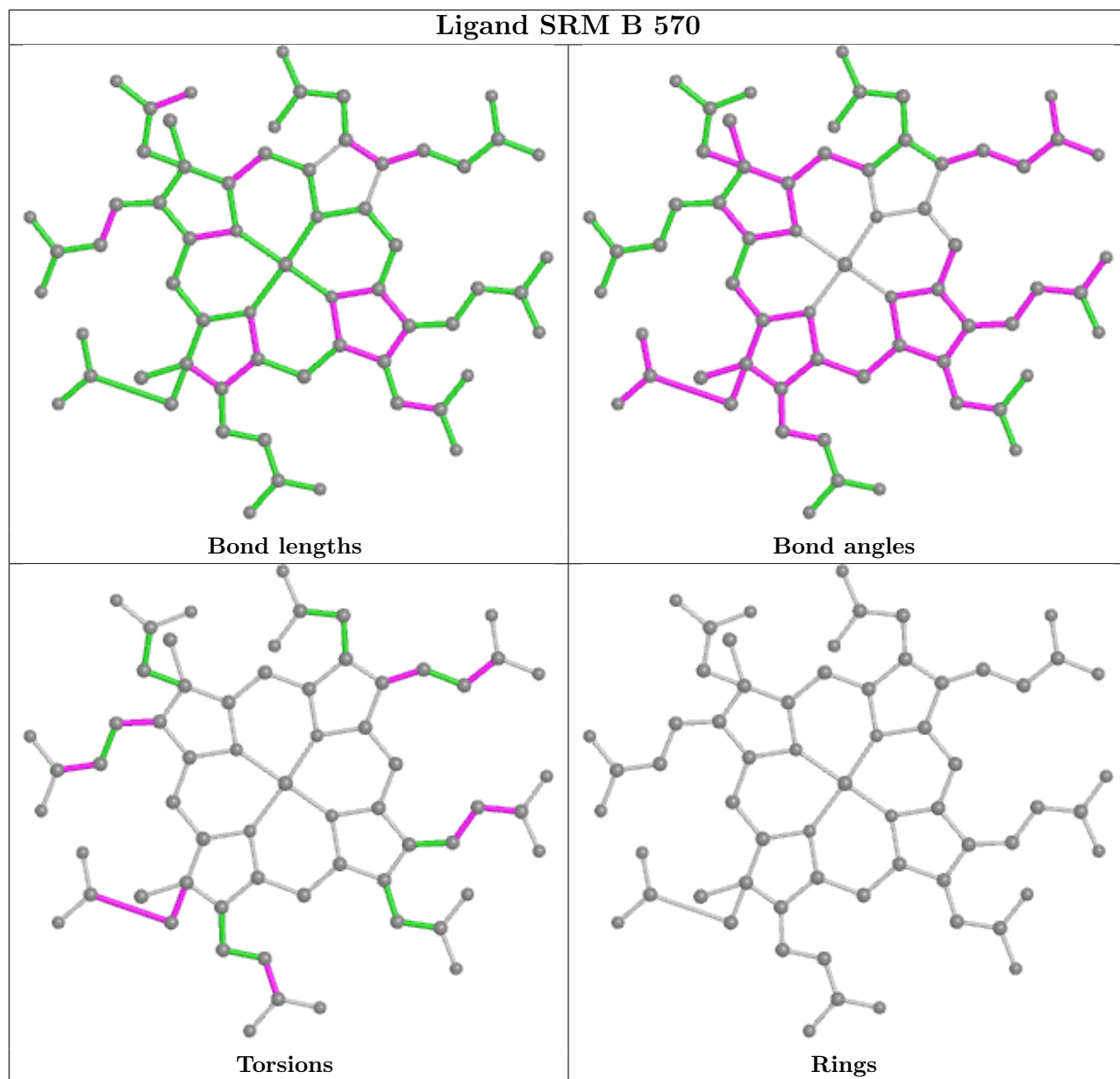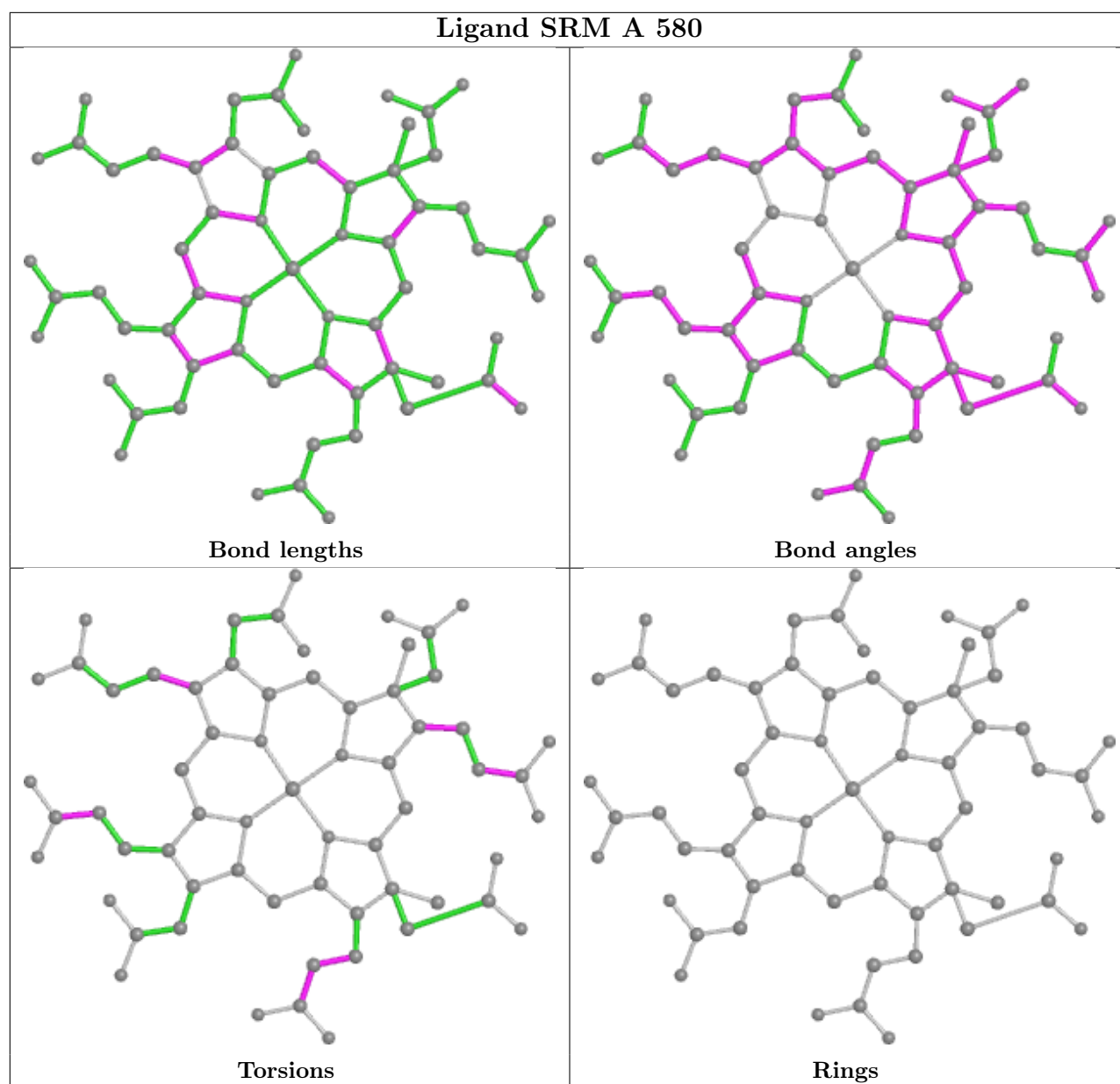
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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(Å²)	Q<0.9
1	A	417/418 (99%)	-0.02	17 (4%)	37	40	18, 31, 64, 112	0
1	D	417/418 (99%)	0.61	46 (11%)	5	6	22, 66, 111, 138	0
2	B	363/366 (99%)	-0.12	6 (1%)	70	72	18, 28, 43, 114	0
2	E	363/366 (99%)	0.75	51 (14%)	2	2	28, 69, 106, 148	0
All	All	1560/1568 (99%)	0.30	120 (7%)	13	15	18, 45, 99, 148	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	4	GLU	9.7
1	A	417	TRP	7.8
1	D	1	SER	7.8
2	B	4	GLU	6.3
2	E	232	LYS	6.0
2	E	229	MET	5.6
2	E	185	VAL	5.2
2	E	186	HIS	4.8
2	E	184	ALA	4.7
2	E	281	LEU	4.5
1	D	43	GLY	4.3
2	B	5	GLY	4.3
2	E	205	GLU	4.2
1	A	415	GLY	4.2
2	E	207	ILE	4.2
1	D	33	ALA	4.2
2	E	209	LYS	4.1
1	A	406	ALA	4.0
1	A	276	LYS	3.9
2	E	230	LYS	3.9
1	A	413	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	228	ALA	3.7
1	D	67	ILE	3.7
1	D	229	ARG	3.7
2	E	201	ILE	3.7
1	D	81	TYR	3.6
2	E	77	TYR	3.5
1	D	68	VAL	3.5
1	D	276	LYS	3.4
1	D	5	LEU	3.4
1	D	30	LYS	3.3
1	D	85	GLY	3.3
2	E	6	VAL	3.2
1	A	412	LYS	3.2
1	A	416	MET	3.2
2	E	188	SER	3.1
1	D	36	LYS	3.1
2	E	100	ILE	3.1
1	A	414	ARG	3.0
2	B	185	VAL	3.0
1	D	323	ILE	3.0
2	E	234	ILE	3.0
1	A	278	LEU	3.0
2	E	210	THR	3.0
2	E	187	ALA	3.0
1	D	86	GLU	2.9
1	D	247	GLU	2.9
1	A	411	LEU	2.8
2	E	355	TYR	2.8
1	D	38	VAL	2.8
2	E	181	MET	2.8
2	E	206	ALA	2.8
1	D	72	GLY	2.8
2	E	233	THR	2.7
2	E	211	CYS	2.7
1	D	2	GLU	2.7
1	A	407	TYR	2.7
2	E	183	GLY	2.7
2	E	208	ARG	2.7
2	E	204	ASP	2.6
2	E	202	PRO	2.6
2	E	102	ASP	2.6
1	D	321	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	273	TRP	2.6
1	D	273	TRP	2.6
2	E	212	GLU	2.6
1	D	134	GLY	2.6
2	E	213	ILE	2.6
1	D	59	LYS	2.6
2	E	182	CYS	2.6
2	E	72	ASP	2.5
2	E	96	ASP	2.5
1	D	320	GLY	2.5
1	D	132	SER	2.5
1	D	71	VAL	2.4
1	A	405	SER	2.4
1	D	279	THR	2.4
1	A	402	LEU	2.4
2	B	272	LEU	2.3
2	E	235	LYS	2.3
1	D	133	THR	2.3
2	B	355	TYR	2.3
1	D	244	VAL	2.3
1	A	410	GLU	2.3
1	D	122	TRP	2.3
2	E	64	ILE	2.3
2	E	26	ASN	2.3
1	D	123	GLY	2.2
2	E	108	GLN	2.2
1	D	254	SER	2.2
1	D	65	GLY	2.2
2	B	353	TYR	2.2
2	E	109	GLU	2.2
1	A	274	ASP	2.2
2	E	105	ASN	2.2
1	D	274	ASP	2.2
2	E	22	VAL	2.2
2	E	94	VAL	2.2
1	D	92	GLU	2.2
1	D	21	ILE	2.2
2	E	103	LEU	2.2
1	D	315	ALA	2.2
1	D	144	GLU	2.2
2	E	5	GLY	2.1
2	E	270	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	32	ALA	2.1
1	D	73	TYR	2.1
2	E	76	LYS	2.1
1	D	225	ALA	2.1
1	D	48	LEU	2.1
1	A	409	GLU	2.1
1	D	278	LEU	2.1
2	E	227	PRO	2.1
2	E	272	LEU	2.1
2	E	354	PHE	2.0
2	E	99	LYS	2.0
1	D	313	GLY	2.0
1	D	257	ASP	2.0
1	D	230	SER	2.0
2	E	56	PHE	2.0

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($\mathring{A}^2$)	Q<0.9
4	SF4	E	585	8/8	0.92	0.05	41,44,50,54	0
5	CYN	D	592	2/2	0.93	0.29	41,41,41,52	0
3	SRM	D	580	63/63	0.94	0.12	40,59,84,98	0
3	SRM	E	570	63/63	0.94	0.12	33,45,56,63	0
4	SF4	D	575	8/8	0.96	0.07	38,42,46,46	0
5	CYN	A	590	2/2	0.97	0.22	18,18,18,27	0
3	SRM	A	580	63/63	0.97	0.12	16,24,37,49	0
4	SF4	A	576	8/8	0.98	0.06	26,28,30,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
4	SF4	E	586	8/8	0.98	0.03	44,46,49,50	0
3	SRM	B	570	63/63	0.98	0.11	14,20,27,30	0
5	CYN	A	591	2/2	0.98	0.08	22,22,22,23	0
4	SF4	D	576	8/8	0.98	0.04	38,42,44,49	0
4	SF4	B	585	8/8	0.99	0.09	18,22,23,25	0
4	SF4	B	586	8/8	0.99	0.09	20,23,24,24	0
4	SF4	A	575	8/8	0.99	0.10	22,22,24,28	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.
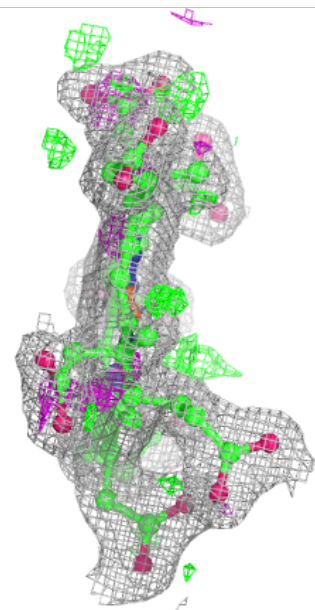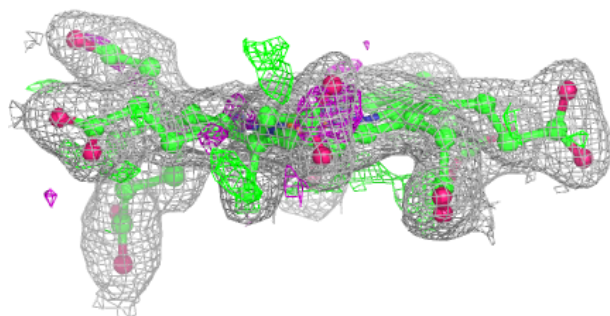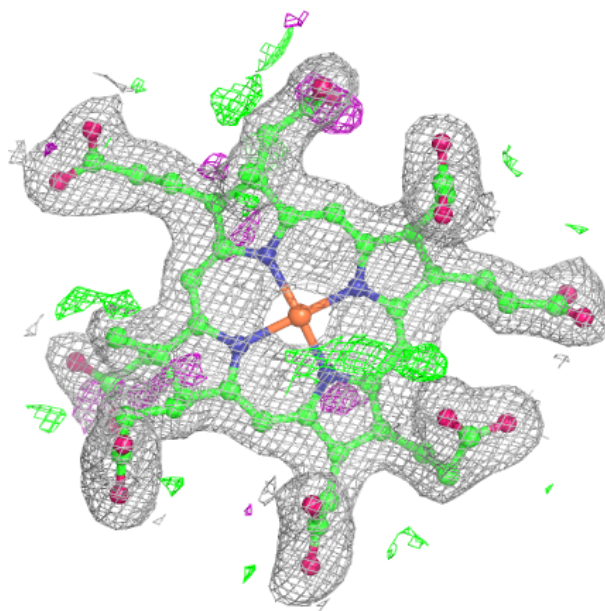
Electron density around SRM D 580:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
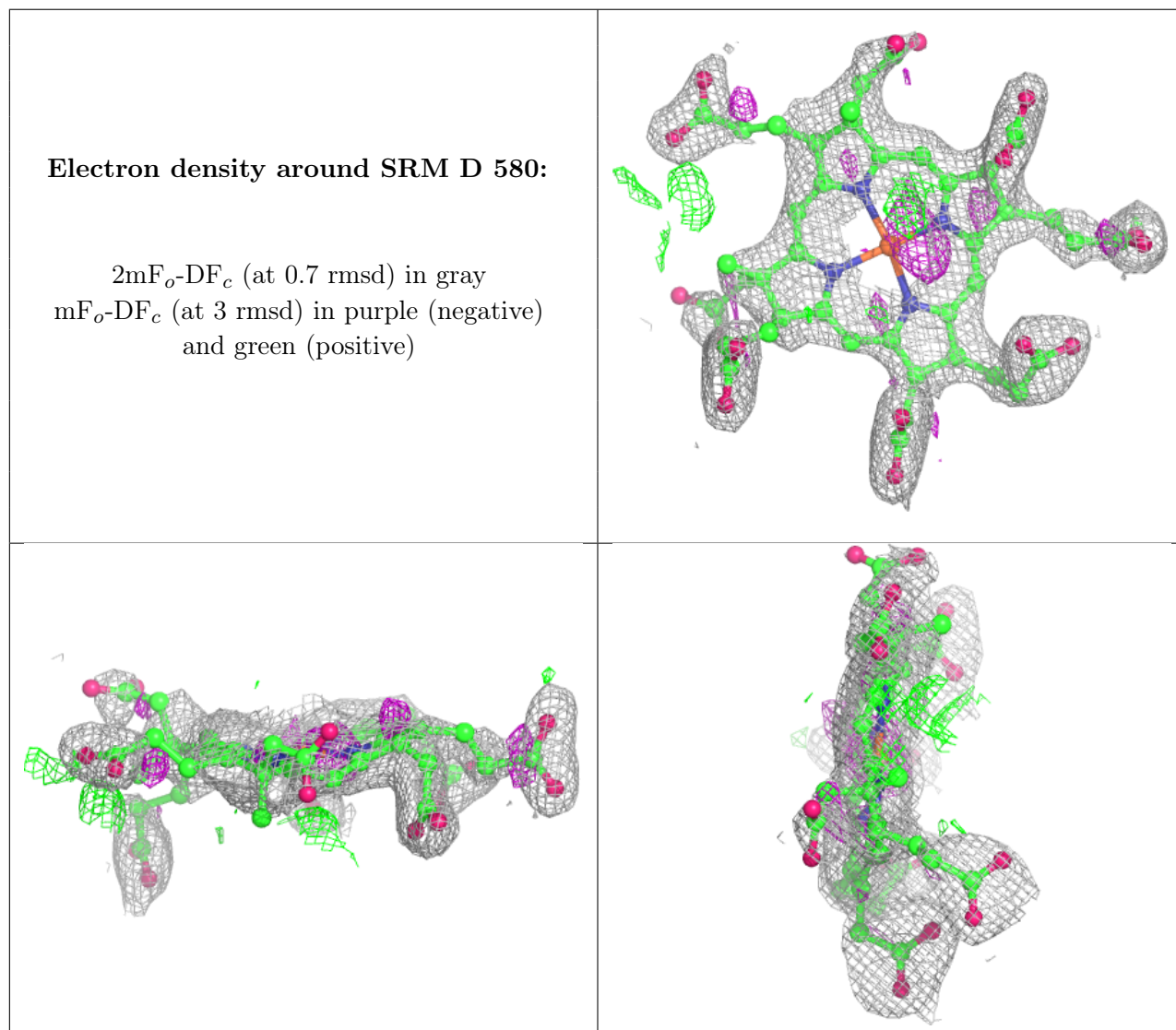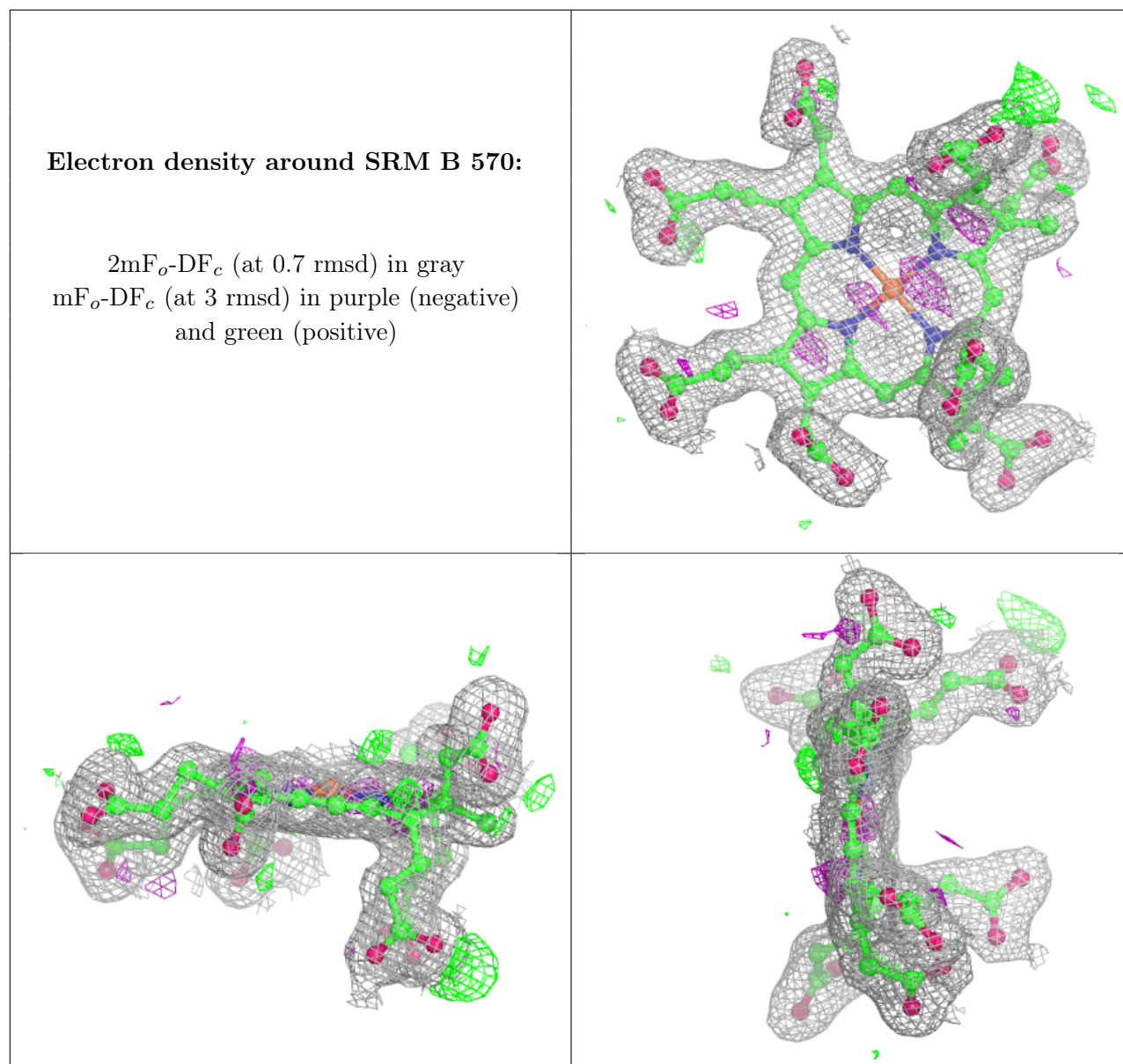
Electron density around SRM E 570:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
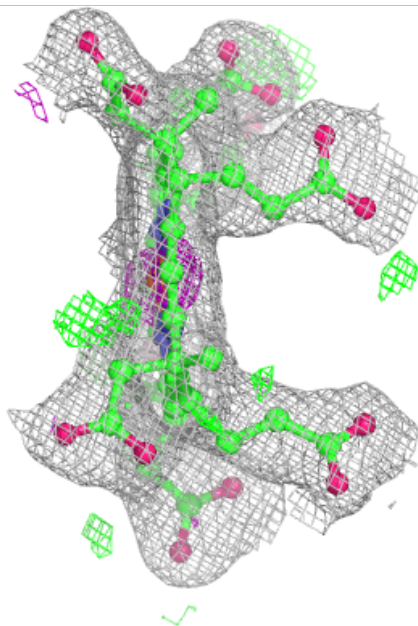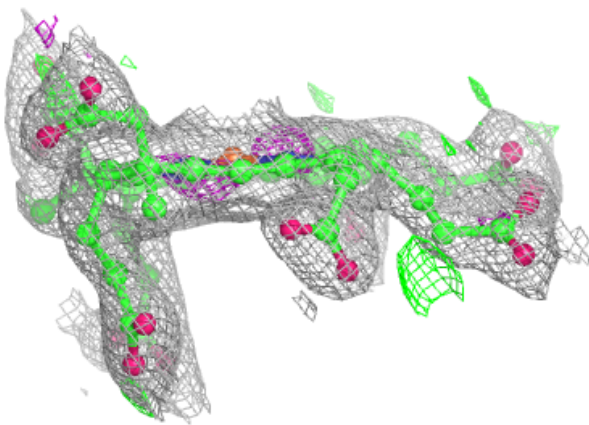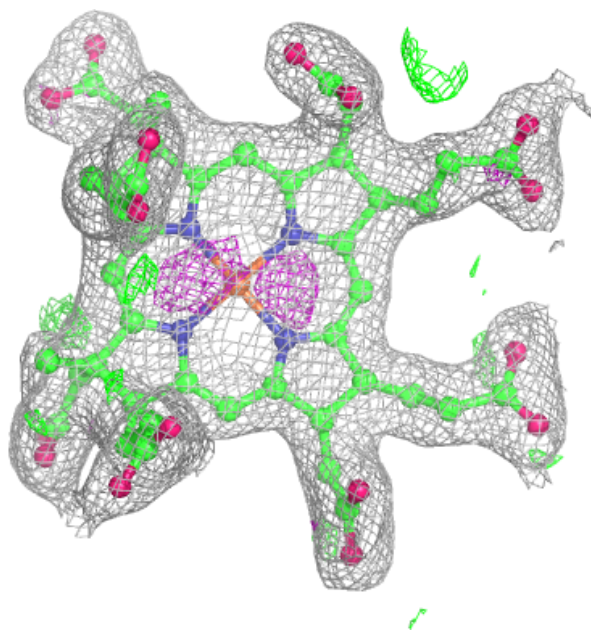
Electron density around SRM A 580:

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

Electron density around SRM B 570:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.