



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 12:38 pm BST

PDB ID : 3MM8
Title : Dissimilatory sulfite reductase nitrate complex
Authors : Parey, K.; Warkentin, E.; Kroneck, P.M.H.; Ermler, U.
Deposited on : 2010-04-19
Resolution : 2.28 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

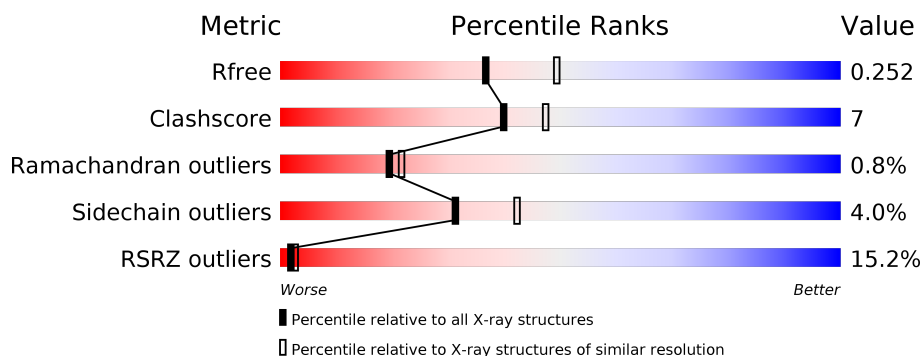
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	418	<div> <div>5%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>
1	D	418	<div> <div>26%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
2	B	366	<div> <div>%</div> <div>82%</div> <div>16%</div> <div>..</div> </div>
2	E	366	<div> <div>28%</div> <div>75%</div> <div>21%</div> <div>...</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SF4	D	576	-	-	X	-
4	SF4	E	585	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12915 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.

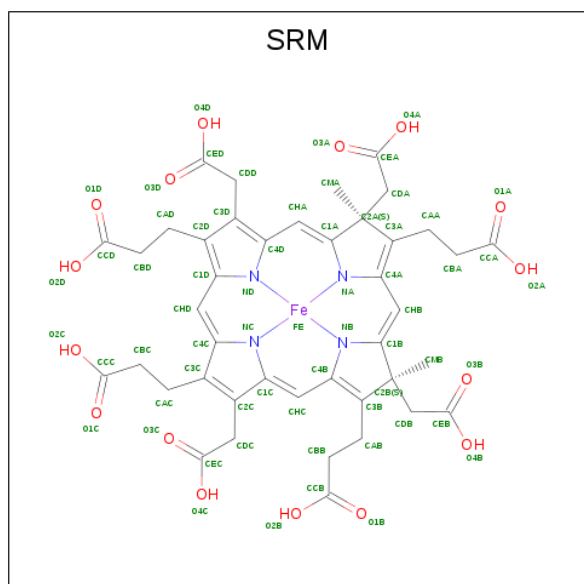
- Molecule 1 is a protein called Sulfite reductase, dissimilatory-type subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3329	2134	557	612	26			
1	D	417	Total	C	N	O	S	0	0	0
			3329	2134	557	612	26			

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

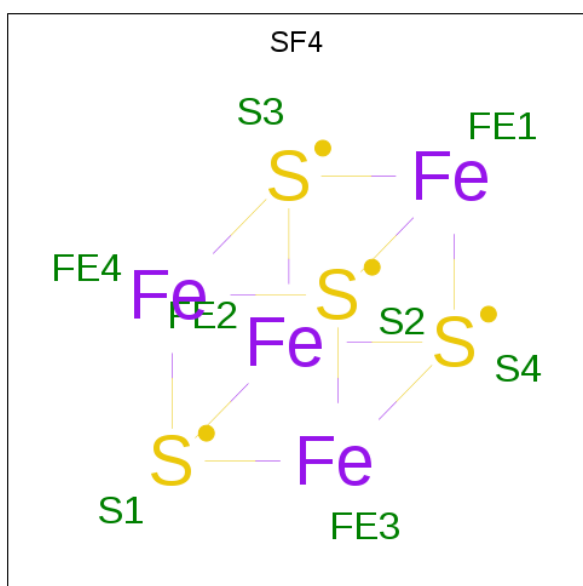
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	363	Total	C	N	O	S	0	0	0
			2900	1862	491	525	22			
2	E	363	Total	C	N	O	S	0	0	0
			2900	1862	491	525	22			

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



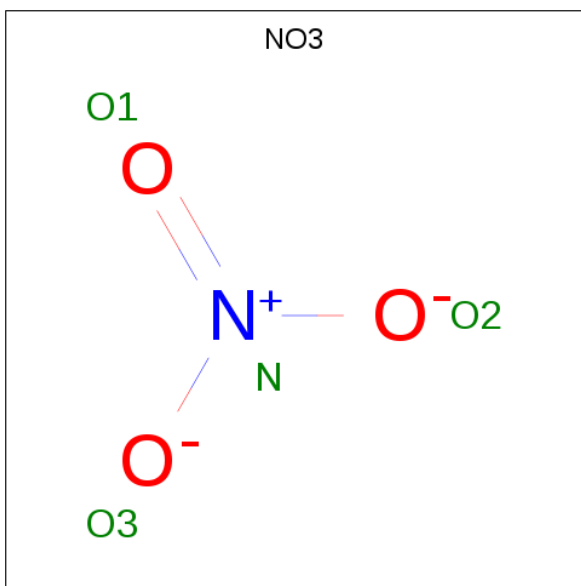
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	
			63	42	1	4	16	
3	B	1	Total	C	Fe	N	O	
			63	42	1	4	16	
3	D	1	Total	C	Fe	N	O	
			63	42	1	4	16	
3	E	1	Total	C	Fe	N	O	
			63	42	1	4	16	

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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 NITRATE ION (three-letter code: NO3) (formula: NO₃).



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

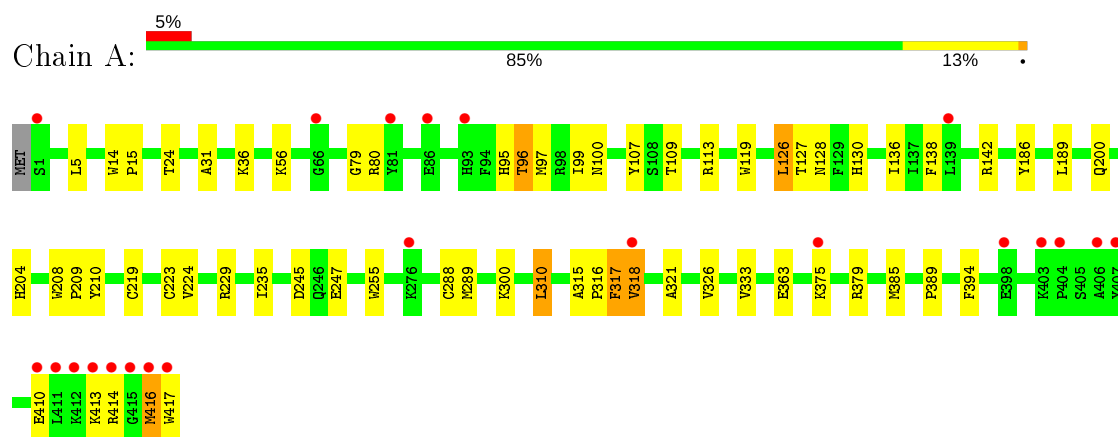
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	64	Total	O	0	0
			64	64		
6	B	62	Total	O	0	0
			62	62		
6	D	10	Total	O	0	0
			10	10		
6	E	1	Total	O	0	0
			1	1		

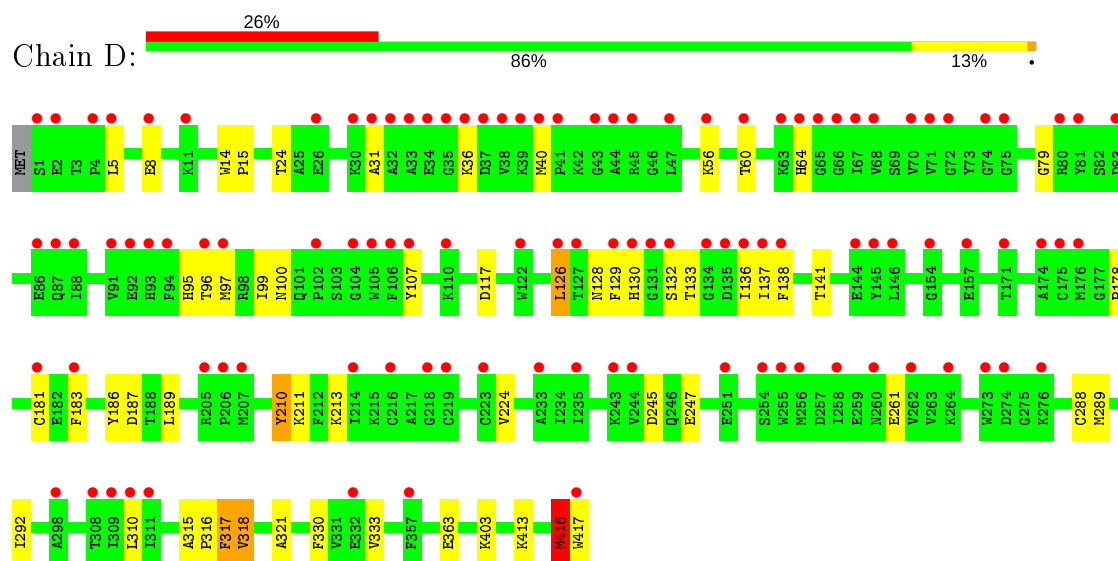
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

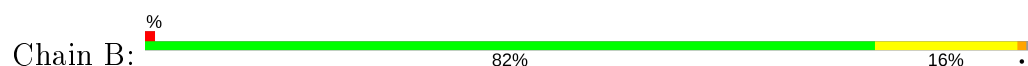
- Molecule 1: Sulfite reductase, dissimilatory-type subunit alpha

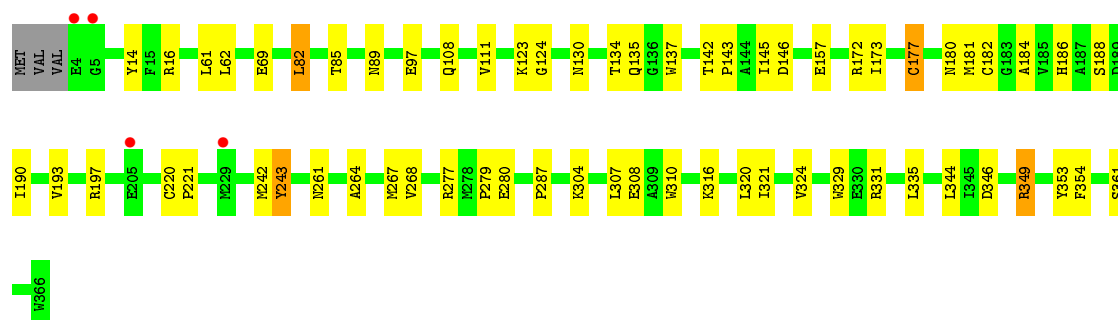


- Molecule 1: Sulfite reductase, dissimilatory-type subunit alpha

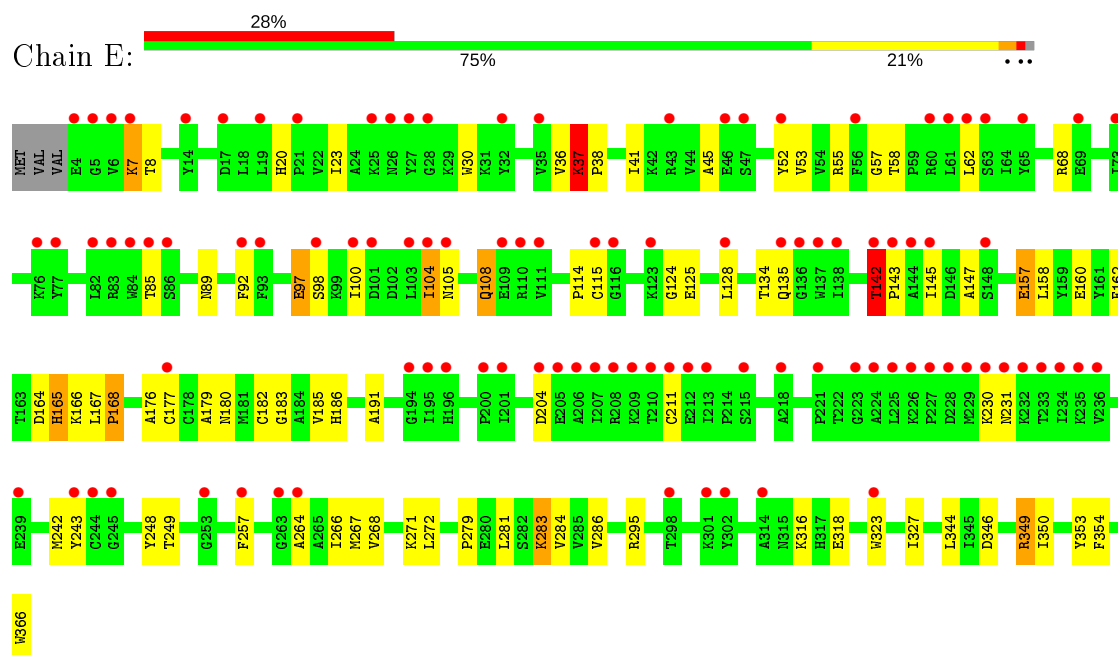


- Molecule 2: Sulfite reductase, dissimilatory-type subunit beta





- 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)	30.00 – 2.28 29.59 – 2.28	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-2.28) 96.6 (29.59-2.28)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0046	Depositor
R, R_{free}	0.198 , 0.231 0.223 , 0.252	Depositor DCC
R_{free} test set	3947 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12915	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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: SF4, SRM, NO3

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	1/3416 (0.0%)	0.60	0/4610
1	D	0.39	0/3416	0.53	0/4610
2	B	0.63	1/2983 (0.0%)	0.68	0/4058
2	E	0.46	1/2983 (0.0%)	0.59	0/4058
All	All	0.50	3/12798 (0.0%)	0.60	0/17336

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
2	E	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	308	GLU	C-N	6.26	1.48	1.34
1	A	223	CYS	CB-SG	5.22	1.91	1.82
2	E	37	LYS	CE-NZ	5.20	1.62	1.49

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	317	PHE	Peptide
1	D	317	PHE	Peptide
2	E	165	HIS	Mainchain

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	3329	0	3276	43	0
1	D	3329	0	3276	46	0
2	B	2900	0	2836	52	0
2	E	2900	0	2838	62	0
3	A	63	0	34	4	0
3	B	63	0	34	7	0
3	D	63	0	34	15	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	3	0
4	E	16	0	0	2	0
5	A	4	0	0	0	0
6	A	64	0	0	3	0
6	B	62	0	0	0	0
6	D	10	0	0	3	0
6	E	1	0	0	0	0
All	All	12915	0	12362	184	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 7.

All (184) 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)
3:D:580:SRM:HMB3	2:E:182:CYS:HA	1.27	1.16
2:E:230:LYS:HB2	2:E:231:ASN:HB2	1.07	1.07
3:E:570:SRM:HBD2	3:E:570:SRM:HDD2	1.35	1.04
2:E:230:LYS:CB	2:E:231:ASN:HB2	1.93	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:LYS:HZ2	3:D:580:SRM:HDB2	1.33	0.92
2:E:230:LYS:HB2	2:E:231:ASN:CB	1.97	0.90
3:B:570:SRM:HDD2	3:B:570:SRM:HBD2	1.53	0.90
2:B:134:THR:OG1	2:B:177:CYS:SG	2.37	0.83
2:E:134:THR:HG21	2:E:182:CYS:HB2	1.60	0.82
2:B:261:ASN:HD21	1:D:403:LYS:H	1.30	0.78
2:E:85:THR:HB	3:E:570:SRM:HAB2	1.66	0.77
2:E:124:GLY:HA3	2:E:316:LYS:HD2	1.65	0.77
2:B:197:ARG:HH21	2:B:261:ASN:HD22	1.32	0.76
1:D:213:LYS:NZ	3:D:580:SRM:HDB2	2.01	0.76
1:D:213:LYS:HZ2	3:D:580:SRM:CDB	1.98	0.74
1:A:317:PHE:CD2	2:B:180:ASN:HB3	2.22	0.74
1:D:213:LYS:NZ	3:D:580:SRM:CDB	2.51	0.73
2:B:349:ARG:NH2	2:E:350:ILE:O	2.23	0.72
1:A:128:ASN:ND2	2:B:135:GLN:HE22	1.88	0.72
1:A:107:TYR:OH	1:A:130:HIS:HE1	1.74	0.71
1:D:64:HIS:NE2	2:E:248:TYR:O	2.22	0.71
3:A:580:SRM:HHB	3:A:580:SRM:HBA1	1.72	0.70
4:D:576:SF4:S4	6:D:423:HOH:O	2.48	0.70
2:E:7:LYS:HE2	2:E:8:THR:H	1.57	0.69
1:D:178:PRO:HG3	1:D:187:ASP:HA	1.74	0.69
2:B:85:THR:HB	3:B:570:SRM:HAB2	1.72	0.69
2:E:104:ILE:HG23	2:E:115:CYS:HB2	1.74	0.68
1:A:255:TRP:HZ3	2:B:123:LYS:HD3	1.59	0.68
1:D:60:THR:HG22	2:E:257:PHE:CE1	2.28	0.68
1:A:229:ARG:HG3	2:B:184:ALA:HB2	1.77	0.67
2:B:85:THR:HB	3:B:570:SRM:CAB	2.24	0.66
1:A:317:PHE:HD2	2:B:180:ASN:HB3	1.58	0.66
2:B:82:LEU:HD23	2:B:82:LEU:N	2.10	0.66
1:A:96:THR:HG21	6:A:426:HOH:O	1.94	0.66
2:E:37:LYS:HB2	2:E:38:PRO:CD	2.26	0.65
1:D:107:TYR:OH	1:D:130:HIS:HE1	1.80	0.65
4:D:576:SF4:S2	6:D:423:HOH:O	2.55	0.64
2:E:55:ARG:HH22	3:E:570:SRM:HBA2	1.62	0.64
2:E:52:TYR:CE1	2:E:97:GLU:HG2	2.35	0.62
1:A:394:PHE:CE2	2:E:179:ALA:HB1	2.35	0.62
1:D:60:THR:HG22	2:E:257:PHE:HE1	1.64	0.60
3:A:580:SRM:HAD1	2:B:180:ASN:HB2	1.84	0.60
2:B:157:GLU:OE2	2:B:304:LYS:NZ	2.35	0.59
2:E:281:LEU:O	2:E:283:LYS:HE2	2.03	0.59
1:D:213:LYS:NZ	3:D:580:SRM:HDB1	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ASN:HD21	2:B:135:GLN:HE22	1.50	0.58
2:B:277:ARG:NH2	2:B:280:GLU:OE1	2.36	0.58
3:D:580:SRM:HAB1	2:E:183:GLY:H	1.68	0.56
1:D:183:PHE:CE1	1:D:292:ILE:HG22	2.40	0.56
2:E:142:THR:N	2:E:143:PRO:HD3	2.21	0.56
1:D:210:TYR:OH	3:D:580:SRM:HDA1	2.05	0.56
3:E:570:SRM:HBD2	3:E:570:SRM:CDD	2.24	0.56
2:B:197:ARG:NH2	2:B:261:ASN:HD22	2.02	0.55
1:A:255:TRP:CZ3	2:B:123:LYS:HD3	2.41	0.55
2:E:37:LYS:HB2	2:E:38:PRO:HD3	1.89	0.55
1:A:394:PHE:HE2	2:E:179:ALA:HB1	1.70	0.54
2:B:277:ARG:NH1	2:B:321:ILE:HG13	2.23	0.54
1:A:14:TRP:CD2	1:A:15:PRO:HD2	2.42	0.54
2:B:137:TRP:CE3	2:B:146:ASP:HB2	2.42	0.54
2:E:134:THR:CG2	2:E:182:CYS:HB2	2.34	0.53
1:D:183:PHE:HD2	4:D:575:SF4:S4	2.31	0.53
2:B:69:GLU:OE2	2:B:111:VAL:HG12	2.07	0.53
2:E:145:ILE:HG21	2:E:264:ALA:HB2	1.91	0.53
2:B:279:PRO:HD2	2:B:361:SER:HB2	1.91	0.52
2:E:272:LEU:HB2	3:E:570:SRM:CCC	2.39	0.52
1:D:417:TRP:HB3	6:D:421:HOH:O	2.09	0.52
2:B:124:GLY:HA3	2:B:316:LYS:CD	2.40	0.52
1:D:213:LYS:HZ3	3:D:580:SRM:HDB1	1.75	0.52
2:B:261:ASN:HD21	1:D:403:LYS:N	2.03	0.51
1:A:300:LYS:HG2	6:A:434:HOH:O	2.11	0.51
2:B:124:GLY:HA3	2:B:316:LYS:HD2	1.92	0.51
1:D:14:TRP:CD2	1:D:15:PRO:HD2	2.45	0.51
2:E:104:ILE:HG23	2:E:115:CYS:CB	2.41	0.51
2:E:157:GLU:O	2:E:158:LEU:HD23	2.09	0.51
1:A:416:MET:O	1:A:417:TRP:CB	2.58	0.50
2:E:267:MET:HG2	2:E:284:VAL:HG22	1.93	0.50
1:A:235:ILE:HD12	1:A:310:LEU:HD22	1.93	0.50
2:B:181:MET:SD	2:B:186:HIS:HB3	2.51	0.50
2:B:145:ILE:HG21	2:B:264:ALA:HB2	1.92	0.50
1:D:132:SER:H	3:D:580:SRM:CDC	2.25	0.49
2:B:82:LEU:HD23	2:B:82:LEU:H	1.75	0.49
1:D:245:ASP:OD1	1:D:247:GLU:HG2	2.12	0.49
1:A:389:PRO:HB2	2:E:283:LYS:HB3	1.94	0.49
1:D:416:MET:O	1:D:417:TRP:CB	2.59	0.49
1:A:186:TYR:CD1	1:A:333:VAL:HG11	2.48	0.49
1:A:24:THR:HG21	1:A:126:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:LEU:CD2	2:B:82:LEU:N	2.75	0.49
2:B:197:ARG:HA	2:B:243:TYR:CD2	2.47	0.48
1:A:288:CYS:O	1:A:289:MET:HB2	2.13	0.48
1:A:245:ASP:OD1	1:A:247:GLU:HG2	2.13	0.47
1:D:181:CYS:SG	1:D:183:PHE:HB2	2.54	0.47
2:E:185:VAL:HG13	2:E:191:ALA:HB1	1.96	0.47
2:E:177:CYS:HB2	4:E:585:SF4:S3	2.55	0.47
1:D:317:PHE:CD2	2:E:180:ASN:ND2	2.82	0.47
2:E:142:THR:N	2:E:143:PRO:CD	2.78	0.47
2:E:30:TRP:HA	2:E:45:ALA:HA	1.96	0.47
1:D:315:ALA:HB1	1:D:316:PRO:HD2	1.96	0.47
1:D:416:MET:O	1:D:417:TRP:HB3	2.15	0.47
1:A:80:ARG:NH2	3:A:580:SRM:O2A	2.43	0.47
1:A:315:ALA:HB1	1:A:316:PRO:HD2	1.97	0.47
2:B:346:ASP:HB3	2:E:354:PHE:HB2	1.96	0.47
3:A:580:SRM:HHB	3:A:580:SRM:CBA	2.41	0.46
1:A:318:VAL:HB	1:A:363:GLU:OE2	2.16	0.46
1:D:97:MET:HB2	1:D:138:PHE:HB2	1.96	0.46
1:D:99:ILE:HB	1:D:136:ILE:HB	1.97	0.46
2:E:128:LEU:O	2:E:162:PHE:HA	2.16	0.46
1:A:109:THR:O	1:A:113:ARG:HG3	2.15	0.46
1:A:379:ARG:HG2	1:A:379:ARG:HH11	1.81	0.46
1:A:416:MET:O	1:A:417:TRP:HB3	2.16	0.46
1:D:211:LYS:NZ	3:D:580:SRM:HDA2	2.31	0.46
1:A:200:GLN:NE2	1:A:204:HIS:NE2	2.64	0.46
1:D:24:THR:HG21	1:D:126:LEU:HD13	1.97	0.46
2:E:230:LYS:CA	2:E:231:ASN:HB2	2.44	0.46
2:B:142:THR:N	2:B:143:PRO:CD	2.79	0.46
2:E:176:ALA:HB2	2:E:185:VAL:HG21	1.98	0.46
3:B:570:SRM:HDD2	3:B:570:SRM:CBD	2.34	0.46
2:B:354:PHE:HB2	2:E:346:ASP:HB3	1.97	0.45
1:D:288:CYS:O	1:D:289:MET:HB2	2.16	0.45
1:A:31:ALA:HB1	1:A:36:LYS:HD2	1.98	0.45
2:E:20:HIS:HB3	2:E:23:ILE:HD12	1.99	0.45
1:D:40:MET:SD	1:D:141:THR:HA	2.56	0.45
2:B:134:THR:HG21	2:B:182:CYS:HB2	1.98	0.45
1:D:8:GLU:O	2:E:295:ARG:NH2	2.39	0.45
1:D:318:VAL:HB	1:D:363:GLU:OE2	2.17	0.45
2:E:323:TRP:CE2	2:E:327:ILE:HD13	2.52	0.45
2:B:85:THR:HB	3:B:570:SRM:HAB1	1.97	0.45
1:D:186:TYR:CD1	1:D:333:VAL:HG11	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:108:GLN:HE22	2:E:114:PRO:HA	1.82	0.44
2:E:125:GLU:C	2:E:165:HIS:HB3	2.37	0.44
2:B:354:PHE:HE2	2:E:349:ARG:HG2	1.82	0.44
1:A:229:ARG:CG	2:B:184:ALA:HB2	2.46	0.44
1:A:79:GLY:HA2	1:A:95:HIS:ND1	2.33	0.44
1:A:208:TRP:HB3	1:A:209:PRO:CD	2.47	0.44
2:B:123:LYS:HD2	2:B:123:LYS:HA	1.82	0.44
1:A:316:PRO:HA	1:A:321:ALA:N	2.32	0.44
1:A:127:THR:O	2:B:61:LEU:HD12	2.18	0.43
2:B:307:LEU:HD12	2:B:310:TRP:CE3	2.53	0.43
3:D:580:SRM:HAD1	3:D:580:SRM:HDD1	1.85	0.43
2:B:193:VAL:HG21	2:B:267:MET:SD	2.59	0.43
2:E:271:LYS:HB3	2:E:279:PRO:HA	2.01	0.43
1:A:99:ILE:HB	1:A:136:ILE:HB	1.99	0.43
2:B:268:VAL:HG13	2:B:320:LEU:HD22	2.00	0.43
1:D:128:ASN:HB2	1:D:137:ILE:HB	2.00	0.43
1:A:375:LYS:N	1:A:375:LYS:HD2	2.34	0.43
1:A:416:MET:H	1:A:416:MET:HG2	1.73	0.43
1:A:97:MET:HB2	1:A:138:PHE:HB2	2.01	0.43
2:B:172:ARG:HH21	3:B:570:SRM:C2C	2.31	0.43
3:E:570:SRM:HAC2	3:E:570:SRM:HCD1	1.75	0.43
2:E:85:THR:HB	3:E:570:SRM:CAB	2.43	0.43
2:B:324:VAL:HG11	2:B:329:TRP:CE2	2.53	0.43
1:D:117:ASP:OD1	2:E:68:ARG:NH2	2.52	0.43
1:D:64:HIS:HE1	2:E:249:THR:O	2.02	0.42
2:B:220:CYS:HA	2:B:221:PRO:HD3	1.83	0.42
3:B:570:SRM:HCD1	3:B:570:SRM:HAC2	1.82	0.42
1:D:31:ALA:HB1	1:D:36:LYS:HD2	2.01	0.42
1:A:119:TRP:CH2	1:A:138:PHE:HB3	2.55	0.42
2:E:167:LEU:HA	2:E:168:PRO:HD2	1.45	0.42
2:B:331:ARG:NH2	2:E:366:TRP:O	2.52	0.42
1:A:326:VAL:HB	1:A:385:MET:HA	2.01	0.42
1:D:133:THR:HA	3:D:580:SRM:O2B	2.20	0.42
2:B:320:LEU:O	2:B:320:LEU:HD23	2.20	0.42
2:B:353:TYR:HA	2:E:353:TYR:HA	2.01	0.42
3:D:580:SRM:CEA	3:D:580:SRM:HHA	2.49	0.42
1:D:316:PRO:HA	1:D:321:ALA:N	2.35	0.41
2:E:134:THR:HB	4:E:585:SF4:S4	2.60	0.41
2:B:173:ILE:HA	2:B:190:ILE:O	2.21	0.41
1:D:129:PHE:HB2	2:E:62:LEU:HD22	2.03	0.41
2:E:53:VAL:HA	2:E:92:PHE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:SER:H	3:D:580:SRM:HCD1	1.86	0.41
1:D:128:ASN:HD21	2:E:135:GLN:HE22	1.69	0.41
1:A:410:GLU:O	1:A:414:ARG:HG2	2.21	0.41
1:D:79:GLY:HA2	1:D:95:HIS:ND1	2.36	0.41
3:E:570:SRM:HHA	3:E:570:SRM:HMA2	1.79	0.41
2:E:57:GLY:HA2	2:E:89:ASN:ND2	2.36	0.41
1:A:128:ASN:O	1:A:130:HIS:HA	2.20	0.41
2:B:89:ASN:HD21	2:B:130:ASN:HB2	1.86	0.41
1:A:142:ARG:NH1	6:A:466:HOH:O	2.48	0.40
2:B:287:PRO:HG3	2:B:344:LEU:HD13	2.03	0.40
2:E:266:ILE:HB	2:E:286:VAL:HB	2.03	0.40
1:A:394:PHE:HE2	2:E:179:ALA:CB	2.33	0.40
1:D:261:GLU:OE2	2:E:316:LYS:HE3	2.21	0.40
2:E:108:GLN:NE2	2:E:114:PRO:HA	2.37	0.40
1:D:330:PHE:HB2	2:E:366:TRP:CH2	2.56	0.40
2:B:14:TYR:CE2	2:B:16:ARG:HB2	2.57	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	415/418 (99%)	401 (97%)	12 (3%)	2 (0%)	29	34
1	D	415/418 (99%)	403 (97%)	10 (2%)	2 (0%)	29	34
2	B	361/366 (99%)	346 (96%)	15 (4%)	0	100	100
2	E	361/366 (99%)	321 (89%)	32 (9%)	8 (2%)	6	4
All	All	1552/1568 (99%)	1471 (95%)	69 (4%)	12 (1%)	19	22

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	318	VAL
1	D	318	VAL
2	E	168	PRO
2	E	211	CYS
2	E	37	LYS
2	E	147	ALA
2	E	166	LYS
1	A	416	MET
1	D	416	MET
2	E	318	GLU
2	E	142	THR
2	E	36	VAL

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%)	342 (97%)	11 (3%)	40	53
1	D	353/354 (100%)	342 (97%)	11 (3%)	40	53
2	B	314/317 (99%)	304 (97%)	10 (3%)	39	52
2	E	314/317 (99%)	293 (93%)	21 (7%)	16	19
All	All	1334/1342 (99%)	1281 (96%)	53 (4%)	31	42

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	56	LYS
1	A	96	THR
1	A	100	ASN
1	A	126	LEU
1	A	189	LEU
1	A	210	TYR
1	A	219	CYS
1	A	224	VAL
1	A	310	LEU

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Mol	Chain	Res	Type
1	A	413	LYS
2	B	62	LEU
2	B	82	LEU
2	B	97	GLU
2	B	108	GLN
2	B	177	CYS
2	B	188	SER
2	B	242	MET
2	B	243	TYR
2	B	335	LEU
2	B	349	ARG
1	D	5	LEU
1	D	56	LYS
1	D	96	THR
1	D	100	ASN
1	D	126	LEU
1	D	189	LEU
1	D	210	TYR
1	D	224	VAL
1	D	310	LEU
1	D	413	LYS
1	D	416	MET
2	E	7	LYS
2	E	41	ILE
2	E	58	THR
2	E	97	GLU
2	E	98	SER
2	E	100	ILE
2	E	104	ILE
2	E	105	ASN
2	E	108	GLN
2	E	142	THR
2	E	157	GLU
2	E	160	GLU
2	E	164	ASP
2	E	186	HIS
2	E	204	ASP
2	E	242	MET
2	E	243	TYR
2	E	268	VAL
2	E	283	LYS
2	E	344	LEU

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Mol	Chain	Res	Type
2	E	349	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	100	ASN
1	A	128	ASN
1	A	130	HIS
1	A	200	GLN
2	B	89	ASN
2	B	108	GLN
2	B	261	ASN
1	D	93	HIS
1	D	100	ASN
1	D	130	HIS
1	D	200	GLN
2	E	89	ASN
2	E	108	GLN
2	E	135	GLN
2	E	180	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

13 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	$\# Z > 2$
3	SRM	A	580	5	34,70,70	2.15	9 (26%)	38,112,112	3.71	18 (47%)
3	SRM	B	570	1	34,70,70	2.24	11 (32%)	38,112,112	3.99	22 (57%)
5	NO3	A	590	3	1,3,3	3.44	1 (100%)	0,3,3	0.00	-
4	SF4	E	585	2	0,12,12	0.00	-	-		
4	SF4	B	585	2	0,12,12	0.00	-	-		
3	SRM	E	570	-	34,70,70	2.35	11 (32%)	38,112,112	3.81	19 (50%)
4	SF4	A	576	1	0,12,12	0.00	-	-		
3	SRM	D	580	-	34,70,70	2.07	8 (23%)	38,112,112	3.25	18 (47%)
4	SF4	A	575	1	0,12,12	0.00	-	-		
4	SF4	B	586	2	0,12,12	0.00	-	-		
4	SF4	D	576	1,6	0,12,12	0.00	-	-		
4	SF4	E	586	2	0,12,12	0.00	-	-		
4	SF4	D	575	1	0,12,12	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SRM	A	580	5	-	9/22/126/126	-
3	SRM	B	570	1	-	9/22/126/126	-
4	SF4	E	586	2	-	-	0/6/5/5
4	SF4	E	585	2	-	-	0/6/5/5
4	SF4	B	585	2	-	-	0/6/5/5
4	SF4	A	576	1	-	-	0/6/5/5
3	SRM	D	580	-	-	9/22/126/126	-
4	SF4	A	575	1	-	-	0/6/5/5
4	SF4	B	586	2	-	-	0/6/5/5
4	SF4	D	576	1,6	-	-	0/6/5/5
3	SRM	E	570	-	-	10/22/126/126	-
4	SF4	D	575	1	-	-	0/6/5/5

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	580	SRM	C3D-C2D	6.97	1.55	1.39
3	D	580	SRM	C3D-C2D	6.42	1.54	1.39
3	E	570	SRM	C3D-C2D	6.28	1.53	1.39
3	B	570	SRM	C3D-C2D	5.91	1.52	1.39
3	E	570	SRM	C4A-NA	-5.84	1.28	1.39
3	B	570	SRM	C4A-NA	-5.63	1.28	1.39
3	E	570	SRM	C3C-C2C	4.47	1.50	1.37
3	B	570	SRM	C1B-NB	-4.45	1.30	1.37
3	E	570	SRM	C1B-NB	-4.44	1.30	1.37
3	D	580	SRM	C3C-C2C	4.23	1.50	1.37
3	B	570	SRM	C3C-C2C	4.13	1.49	1.37
3	A	580	SRM	C3C-C2C	3.93	1.49	1.37
3	E	570	SRM	C1C-C2C	3.86	1.51	1.42
3	A	580	SRM	C4A-NA	-3.80	1.32	1.39
3	A	580	SRM	C1C-C2C	3.69	1.50	1.42
3	B	570	SRM	C1C-C2C	3.66	1.50	1.42
3	A	580	SRM	FE-NA	3.65	2.10	1.95
3	A	580	SRM	FE-NB	3.61	2.09	1.95
3	E	570	SRM	C4C-C3C	3.55	1.50	1.42
5	A	590	NO3	O1-N	3.44	1.39	1.24
3	D	580	SRM	C1C-C2C	3.36	1.50	1.42
3	D	580	SRM	FE-NA	3.33	2.08	1.95
3	B	570	SRM	C4C-C3C	3.29	1.50	1.42
3	D	580	SRM	C4C-C3C	3.01	1.49	1.42
3	D	580	SRM	FE-NB	3.01	2.07	1.95
3	D	580	SRM	C4A-NA	-2.93	1.34	1.39
3	A	580	SRM	C4C-C3C	2.90	1.49	1.42
3	A	580	SRM	CAD-C2D	2.64	1.55	1.52
3	E	570	SRM	C4B-NB	-2.60	1.34	1.39
3	D	580	SRM	C4B-NB	-2.55	1.34	1.39
3	E	570	SRM	CHA-C1A	2.42	1.39	1.36
3	B	570	SRM	C1A-NA	-2.38	1.33	1.37
3	B	570	SRM	CDA-C2A	-2.36	1.52	1.56
3	E	570	SRM	CAD-C2D	2.34	1.55	1.52
3	B	570	SRM	C1D-CHD	-2.33	1.34	1.41
3	B	570	SRM	C4B-NB	-2.23	1.35	1.39
3	A	580	SRM	C4B-NB	-2.11	1.35	1.39
3	B	570	SRM	CAA-C3A	2.11	1.55	1.51
3	E	570	SRM	C1D-CHD	-2.10	1.35	1.41
3	E	570	SRM	CHC-C4B	-2.08	1.34	1.39

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	580	SRM	CAB-C3B-C2B	-14.86	106.72	123.52
3	B	570	SRM	CAA-C3A-C2A	-13.09	108.73	123.52
3	E	570	SRM	CAA-C3A-C2A	-11.70	110.29	123.52
3	D	580	SRM	C4A-NA-C1A	10.32	112.15	106.28
3	D	580	SRM	CDD-C3D-C4D	-8.17	114.98	127.36
3	E	570	SRM	C3A-C4A-NA	7.72	118.75	110.14
3	A	580	SRM	C4A-NA-C1A	7.58	110.59	106.28
3	E	570	SRM	C4A-NA-C1A	-7.07	102.26	106.28
3	B	570	SRM	C3A-C4A-NA	7.00	117.95	110.14
3	B	570	SRM	CBC-CAC-C3C	-6.57	100.38	112.48
3	D	580	SRM	CAB-C3B-C2B	-6.55	116.12	123.52
3	B	570	SRM	CEC-CDC-C2C	-6.36	103.57	115.96
3	A	580	SRM	CBD-CAD-C2D	6.03	123.61	112.49
3	A	580	SRM	CAA-C3A-C2A	-5.88	116.87	123.52
3	B	570	SRM	CBD-CAD-C2D	5.68	122.96	112.49
3	B	570	SRM	C4A-NA-C1A	-5.45	103.18	106.28
3	E	570	SRM	C4D-CHA-C1A	-5.37	119.48	130.12
3	B	570	SRM	C2B-CDB-CEB	5.36	123.14	115.29
3	B	570	SRM	CAB-CBB-CCB	5.31	121.58	112.67
3	E	570	SRM	CEC-CDC-C2C	-5.24	105.76	115.96
3	E	570	SRM	CDC-C2C-C1C	-5.22	119.52	127.39
3	E	570	SRM	CDC-C2C-C3C	-5.04	117.49	126.49
3	E	570	SRM	CBD-CAD-C2D	4.98	121.67	112.49
3	B	570	SRM	C4D-CHA-C1A	-4.92	120.38	130.12
3	A	580	SRM	CBB-CAB-C3B	4.81	124.70	113.40
3	E	570	SRM	CBC-CAC-C3C	-4.80	103.64	112.48
3	A	580	SRM	CBA-CAA-C3A	4.56	124.12	113.40
3	B	570	SRM	CDC-C2C-C3C	-4.55	118.36	126.49
3	D	580	SRM	CEC-CDC-C2C	-4.49	107.21	115.96
3	B	570	SRM	C3B-C2B-C1B	-4.46	93.64	101.20
3	A	580	SRM	CMA-C2A-CDA	4.41	116.17	109.96
3	D	580	SRM	CAA-C3A-C2A	-4.28	118.68	123.52
3	D	580	SRM	CDD-C3D-C2D	-4.21	118.97	126.49
3	E	570	SRM	C2B-CDB-CEB	4.19	121.43	115.29
3	E	570	SRM	C3B-C2B-C1B	-4.15	94.16	101.20
3	B	570	SRM	CMA-C2A-CDA	-4.15	104.12	109.96
3	B	570	SRM	CAA-CBA-CCA	4.06	119.49	112.67
3	E	570	SRM	CAB-CBB-CCB	3.94	119.28	112.67
3	D	580	SRM	C3A-C4A-NA	-3.84	105.85	110.14
3	E	570	SRM	CDD-C3D-C2D	-3.81	119.69	126.49
3	E	570	SRM	CAA-CBA-CCA	3.76	118.97	112.67
3	E	570	SRM	CHB-C4A-C3A	-3.76	117.13	125.36
3	A	580	SRM	C3A-C2A-C1A	-3.71	94.91	101.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	580	SRM	C4B-NB-C1B	-3.61	104.23	106.28
3	D	580	SRM	C4B-NB-C1B	3.57	108.31	106.28
3	B	570	SRM	CED-CDD-C3D	3.57	122.91	115.96
3	B	570	SRM	CHB-C4A-C3A	-3.52	117.64	125.36
3	D	580	SRM	C3A-C2A-C1A	-3.39	95.45	101.20
3	D	580	SRM	C3B-C2B-C1B	-3.37	95.49	101.20
3	A	580	SRM	CDD-C3D-C2D	-3.32	120.56	126.49
3	D	580	SRM	CAD-C2D-C3D	-3.29	114.54	124.90
3	E	570	SRM	CDD-C3D-C4D	-3.28	122.39	127.36
3	D	580	SRM	CBA-CAA-C3A	3.22	120.97	113.40
3	D	580	SRM	CBB-CAB-C3B	3.04	120.56	113.40
3	A	580	SRM	CAD-CBD-CCD	-3.00	107.63	112.67
3	B	570	SRM	CDD-C3D-C2D	-2.98	121.16	126.49
3	D	580	SRM	CED-CDD-C3D	-2.94	110.24	115.96
3	A	580	SRM	C3B-C4B-NB	2.80	113.26	110.14
3	E	570	SRM	CAD-CBD-CCD	-2.78	108.00	112.67
3	A	580	SRM	CBC-CAC-C3C	2.78	117.60	112.48
3	A	580	SRM	C3B-C2B-C1B	-2.69	96.64	101.20
3	B	570	SRM	CAB-C3B-C2B	-2.49	120.71	123.52
3	D	580	SRM	C4D-CHA-C1A	-2.45	125.26	130.12
3	B	570	SRM	CAD-CBD-CCD	-2.37	108.70	112.67
3	D	580	SRM	CBD-CAD-C2D	2.35	116.81	112.49
3	E	570	SRM	CED-CDD-C3D	2.34	120.52	115.96
3	A	580	SRM	C3A-C4A-NA	-2.25	107.63	110.14
3	D	580	SRM	CHB-C1B-NB	-2.24	120.92	124.20
3	A	580	SRM	CDC-C2C-C1C	2.23	130.76	127.39
3	B	570	SRM	C2A-CDA-CEA	2.23	118.55	115.29
3	A	580	SRM	C2A-CDA-CEA	2.22	118.55	115.29
3	B	570	SRM	CDC-C2C-C1C	-2.20	124.07	127.39
3	B	570	SRM	CHC-C4B-NB	2.15	127.82	123.84
3	A	580	SRM	CED-CDD-C3D	2.15	120.14	115.96
3	E	570	SRM	CAC-C3C-C2C	-2.13	118.18	124.90
3	D	580	SRM	CMB-C2B-CDB	2.08	112.90	109.96
3	B	570	SRM	CDD-C3D-C4D	-2.01	124.32	127.36

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	580	SRM	C4A-C3A-CAA-CBA
3	A	580	SRM	C3D-C2D-CAD-CBD
3	B	570	SRM	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
3	B	570	SRM	C3D-C2D-CAD-CBD
3	E	570	SRM	C4B-C3B-CAB-CBB
3	E	570	SRM	C3B-CAB-CBB-CCB
3	E	570	SRM	C4C-C3C-CAC-CBC
3	E	570	SRM	C3D-C2D-CAD-CBD
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	C4B-C3B-CAB-CBB
3	D	580	SRM	C3C-CAC-CBC-CCC
3	D	580	SRM	C1D-C2D-CAD-CBD
3	D	580	SRM	C2D-CAD-CBD-CCD
3	A	580	SRM	C4B-C3B-CAB-CBB
3	B	570	SRM	C4A-C3A-CAA-CBA
3	B	570	SRM	C4B-C3B-CAB-CBB
3	E	570	SRM	C4A-C3A-CAA-CBA
3	B	570	SRM	C3B-CAB-CBB-CCB
3	E	570	SRM	C3A-CAA-CBA-CCA
3	E	570	SRM	C4D-C3D-CDD-CED
3	A	580	SRM	C3B-CAB-CBB-CCB
3	B	570	SRM	C3A-CAA-CBA-CCA
3	B	570	SRM	C4D-C3D-CDD-CED
3	A	580	SRM	C1A-C2A-CDA-CEA
3	D	580	SRM	C4A-C3A-CAA-CBA
3	A	580	SRM	CMA-C2A-CDA-CEA
3	B	570	SRM	CMA-C2A-CDA-CEA
3	E	570	SRM	CMA-C2A-CDA-CEA
3	A	580	SRM	C3A-CAA-CBA-CCA
3	E	570	SRM	C1B-C2B-CDB-CEB
3	A	580	SRM	CMB-C2B-CDB-CEB
3	B	570	SRM	CMB-C2B-CDB-CEB
3	E	570	SRM	CMB-C2B-CDB-CEB
3	D	580	SRM	CMA-C2A-CDA-CEA
3	A	580	SRM	C4D-C3D-CDD-CED

There are no ring outliers.

7 monomers are involved in 39 short contacts:

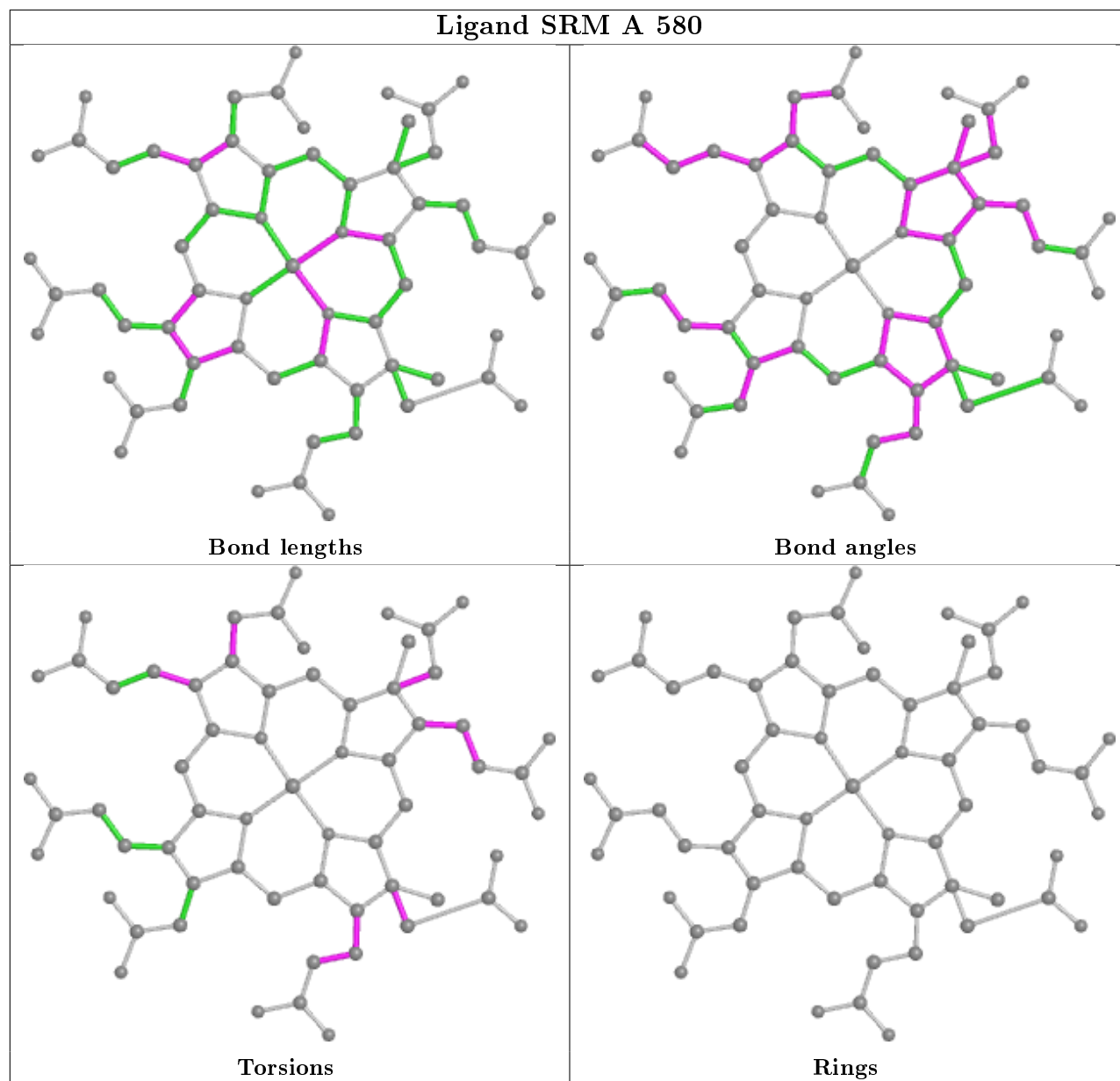
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	580	SRM	4	0
3	B	570	SRM	7	0
4	E	585	SF4	2	0

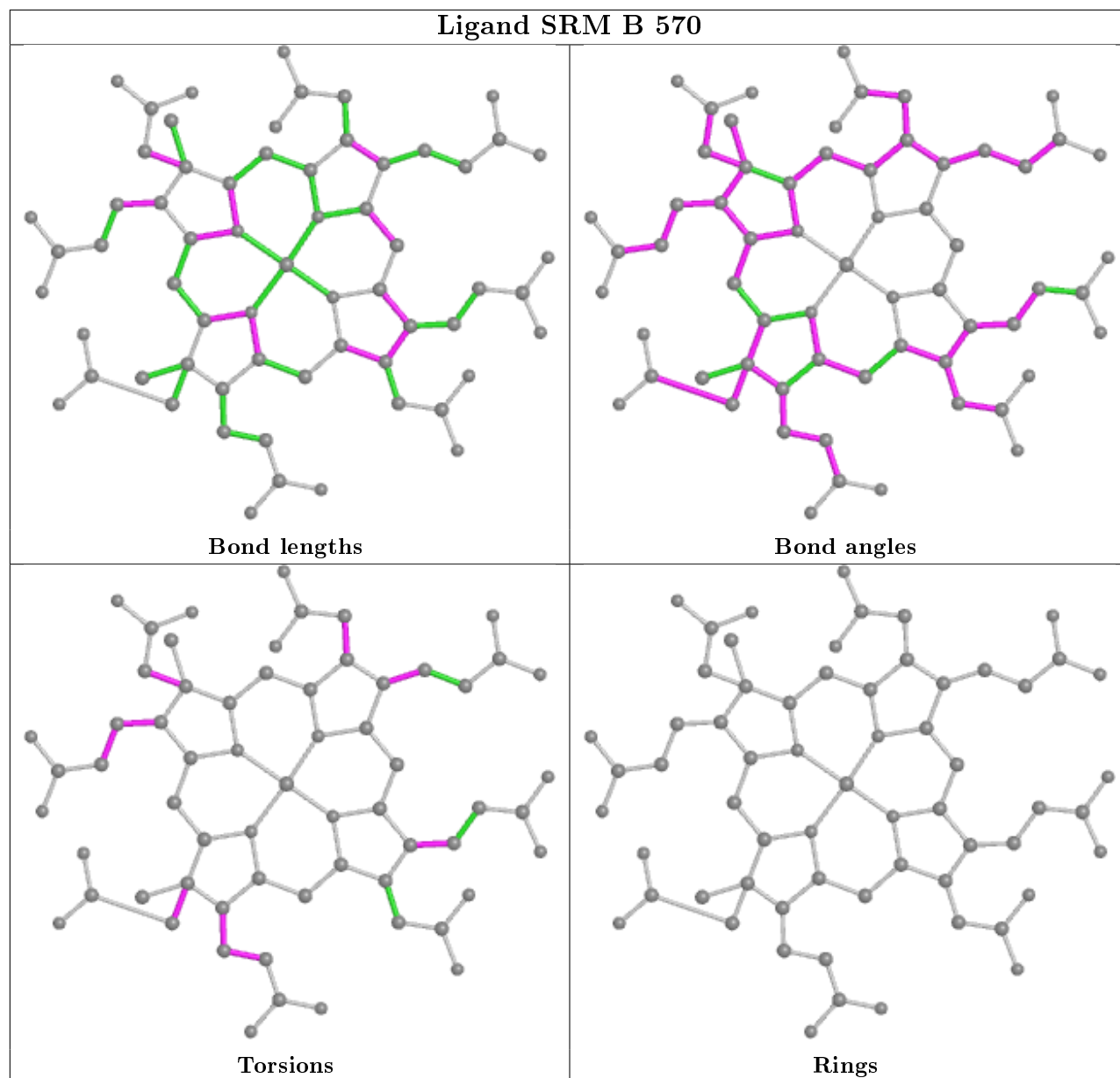
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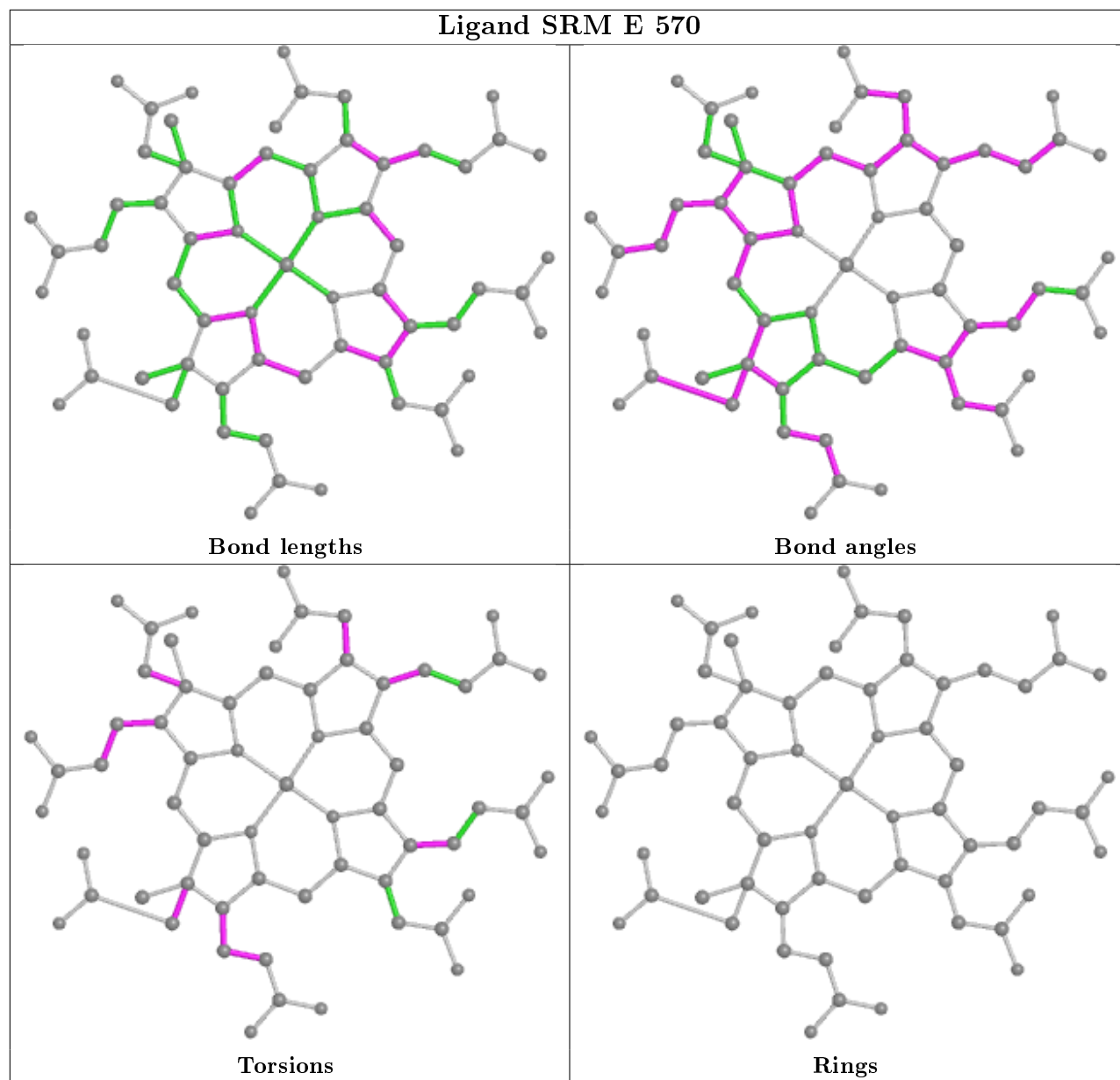
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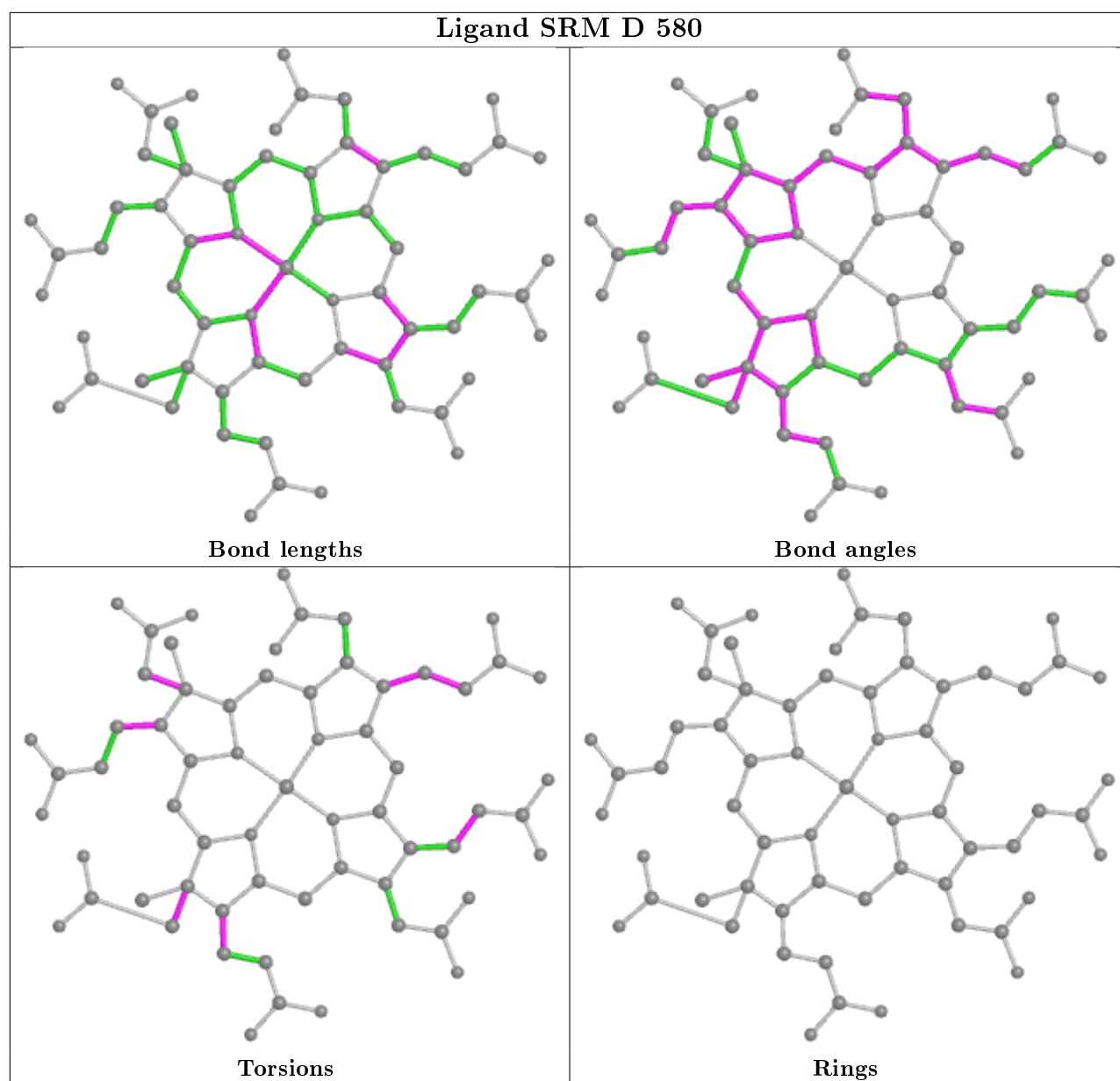
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	570	SRM	8	0
3	D	580	SRM	15	0
4	D	576	SF4	2	0
4	D	575	SF4	1	0

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 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%)	0.27	22 (5%) 26 31	12, 23, 42, 87	0
1	D	417/418 (99%)	1.39	108 (25%) 0 0	12, 28, 46, 71	0
2	B	363/366 (99%)	-0.06	4 (1%) 80 84	10, 19, 30, 66	0
2	E	363/366 (99%)	1.35	103 (28%) 0 0	2, 21, 59, 88	0
All	All	1560/1568 (99%)	0.75	237 (15%) 2 3	2, 22, 48, 88	0

All (237) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	417	TRP	10.6
1	D	67	ILE	8.9
2	E	5	GLY	8.1
1	D	33	ALA	7.8
2	E	229	MET	7.6
2	E	4	GLU	7.2
1	D	1	SER	7.0
2	E	207	ILE	6.9
1	D	207	MET	6.9
2	E	234	ILE	6.7
1	D	129	PHE	6.1
1	D	105	TRP	6.1
2	E	227	PRO	5.8
1	D	223	CYS	5.7
1	D	88	ILE	5.7
2	E	232	LYS	5.6
2	E	230	LYS	5.6
1	A	415	GLY	5.6
1	D	102	PRO	5.6
1	D	127	THR	5.5
1	D	219	CYS	5.5

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Mol	Chain	Res	Type	RSRZ
1	D	244	VAL	5.3
1	D	36	LYS	5.3
2	E	209	LYS	5.3
1	D	134	GLY	5.3
2	E	205	GLU	5.2
1	A	413	LYS	5.2
2	E	77	TYR	5.1
1	D	5	LEU	5.1
1	D	132	SER	5.0
1	D	74	GLY	5.0
1	D	154	GLY	4.9
2	E	233	THR	4.8
1	D	65	GLY	4.7
1	D	417	TRP	4.7
1	A	416	MET	4.6
1	D	2	GLU	4.6
1	D	93	HIS	4.6
2	E	6	VAL	4.6
2	E	104	ILE	4.6
1	D	175	CYS	4.6
2	E	244	CYS	4.6
1	D	30	LYS	4.5
1	D	72	GLY	4.5
1	D	157	GLU	4.5
2	E	76	LYS	4.5
2	E	226	LYS	4.4
1	A	406	ALA	4.3
1	D	81	TYR	4.3
1	A	414	ARG	4.2
2	B	4	GLU	4.2
1	D	31	ALA	4.2
1	D	86	GLU	4.2
2	E	145	ILE	4.1
2	E	7	LYS	4.1
1	D	91	VAL	4.0
2	E	25	LYS	3.9
1	D	126	LEU	3.9
2	B	5	GLY	3.9
2	E	100	ILE	3.9
1	D	332	GLU	3.8
1	D	47	LEU	3.8
1	D	40	MET	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	68	VAL	3.7
1	D	45	ARG	3.6
1	D	137	ILE	3.6
1	D	106	PHE	3.6
1	D	64	HIS	3.6
1	D	273	TRP	3.5
1	D	63	LYS	3.5
2	E	84	TRP	3.5
2	E	101	ASP	3.5
2	E	14	TYR	3.5
1	D	130	HIS	3.5
1	D	136	ILE	3.5
2	E	116	GLY	3.4
2	E	211	CYS	3.4
1	D	235	ILE	3.4
2	E	239	GLU	3.4
1	D	171	THR	3.4
2	E	231	ASN	3.4
2	E	177	CYS	3.4
1	D	41	PRO	3.3
1	A	407	TYR	3.3
1	D	309	ILE	3.3
2	E	135	GLN	3.3
2	E	253	GLY	3.3
2	E	98	SER	3.3
2	E	110	ARG	3.3
1	D	83	ASP	3.2
2	E	46	GLU	3.2
2	E	73	ILE	3.2
2	E	27	TYR	3.2
2	E	103	LEU	3.2
2	E	195	ILE	3.2
1	D	38	VAL	3.2
1	D	243	LYS	3.2
1	D	138	PHE	3.1
1	D	255	TRP	3.1
1	A	86	GLU	3.1
1	D	298	ALA	3.1
2	E	142	THR	3.1
2	E	228	ASP	3.1
1	D	254	SER	3.1
2	E	86	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	43	GLY	3.1
1	D	107	TYR	3.0
1	A	412	LYS	3.0
1	D	104	GLY	3.0
2	E	85	THR	3.0
1	D	256	MET	2.9
2	B	229	MET	2.9
2	E	62	LEU	2.9
2	E	243	TYR	2.9
2	E	128	LEU	2.9
2	E	215	SER	2.9
1	D	97	MET	2.9
2	E	235	LYS	2.9
2	E	314	ALA	2.9
2	E	56	PHE	2.9
1	D	260	ASN	2.9
1	D	66	GLY	2.8
2	E	245	GLY	2.8
1	D	218	GLY	2.8
1	D	258	ILE	2.8
2	E	236	VAL	2.8
1	D	176	MET	2.8
1	D	96	THR	2.8
1	D	94	PHE	2.8
2	E	26	ASN	2.8
1	D	32	ALA	2.7
2	E	208	ARG	2.8
1	A	411	LEU	2.7
2	E	213	ILE	2.7
2	E	144	ALA	2.7
2	E	17	ASP	2.7
1	D	146	LEU	2.7
2	E	201	ILE	2.7
1	D	8	GLU	2.7
2	E	196	HIS	2.7
1	A	1	SER	2.7
2	E	111	VAL	2.7
1	D	131	GLY	2.7
2	E	83	ARG	2.6
1	A	403	LYS	2.6
1	D	92	GLU	2.6
2	E	210	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	357	PHE	2.6
2	E	32	TYR	2.6
1	D	71	VAL	2.6
2	E	21	PRO	2.6
2	E	263	GLY	2.6
1	D	70	VAL	2.5
2	E	302	TYR	2.5
2	E	143	PRO	2.5
2	E	223	GLY	2.5
2	E	137	TRP	2.5
1	A	404	PRO	2.4
2	E	52	TYR	2.4
1	D	4	PRO	2.4
2	E	115	CYS	2.4
1	D	44	ALA	2.4
2	E	35	VAL	2.4
2	E	60	ARG	2.4
1	D	87	GLN	2.4
1	D	37	ASP	2.4
1	D	122	TRP	2.4
1	D	144	GLU	2.4
2	E	224	ALA	2.4
2	E	257	PHE	2.4
2	E	61	LEU	2.3
1	D	276	LYS	2.3
2	E	301	LYS	2.3
1	A	318	VAL	2.3
1	D	35	GLY	2.3
2	E	264	ALA	2.3
1	D	205	ARG	2.3
2	E	148	SER	2.3
2	E	123	LYS	2.3
1	D	214	ILE	2.3
1	D	310	LEU	2.3
2	E	136	GLY	2.3
1	A	93	HIS	2.3
1	D	216	CYS	2.3
1	A	81	TYR	2.2
1	D	174	ALA	2.2
1	D	308	THR	2.2
1	D	110	LYS	2.2
1	D	251	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	28	GLY	2.2
2	E	194	GLY	2.2
2	E	218	ALA	2.2
2	E	298	THR	2.2
1	D	274	ASP	2.2
1	A	276	LYS	2.2
2	E	82	LEU	2.2
2	E	200	PRO	2.2
1	D	262	VAL	2.2
2	E	19	LEU	2.2
1	D	26	GLU	2.2
2	E	212	GLU	2.2
1	D	135	ASP	2.2
1	D	56	LYS	2.1
1	D	145	TYR	2.1
1	D	34	GLU	2.1
2	E	105	ASN	2.1
1	A	398	GLU	2.1
2	E	93	PHE	2.1
1	A	139	LEU	2.1
1	D	206	PRO	2.1
2	B	205	GLU	2.1
1	D	183	PHE	2.1
1	D	233	ALA	2.1
1	D	80	ARG	2.1
2	E	221	PRO	2.1
1	D	60	THR	2.1
2	E	138	ILE	2.1
2	E	69	GLU	2.1
1	A	375	LYS	2.1
1	D	11	LYS	2.1
1	A	66	GLY	2.1
2	E	47	SER	2.1
2	E	63	SER	2.1
2	E	43	ARG	2.0
1	D	264	LYS	2.0
1	D	75	GLY	2.0
2	E	323	TRP	2.0
1	D	39	LYS	2.0
2	E	225	LEU	2.0
2	E	206	ALA	2.0
2	E	92	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
2	E	65	TYR	2.0
1	D	181	CYS	2.0
1	A	410	GLU	2.0
1	D	311	ILE	2.0
2	E	109	GLU	2.0
2	E	204	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

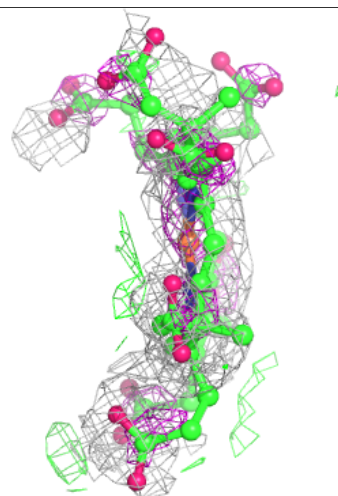
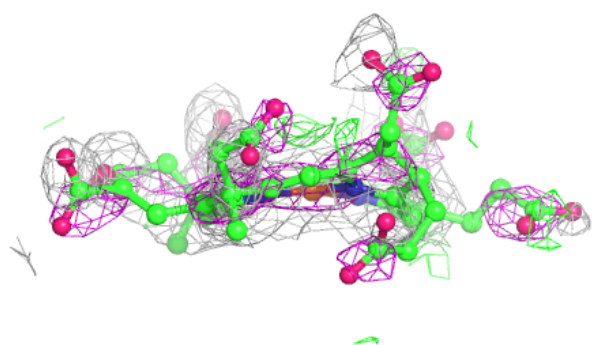
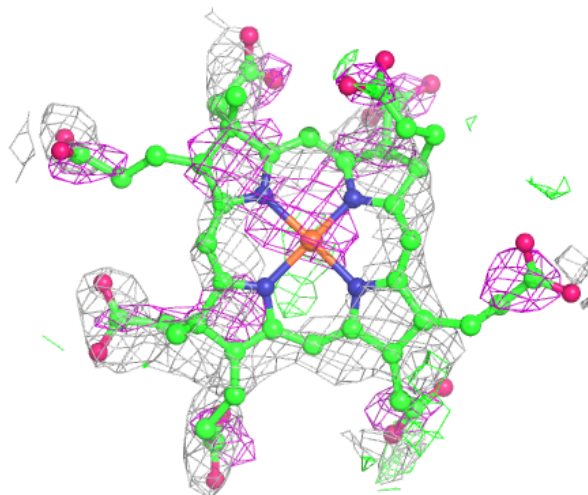
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SRM	D	580	63/63	0.80	0.33	51,71,81,83	0
3	SRM	E	570	63/63	0.89	0.29	15,21,26,30	0
4	SF4	E	585	8/8	0.90	0.14	97,104,107,112	0
4	SF4	D	576	8/8	0.93	0.10	14,16,17,18	0
4	SF4	E	586	8/8	0.95	0.10	38,40,44,46	0
5	NO3	A	590	4/4	0.95	0.21	39,39,43,45	0
4	SF4	D	575	8/8	0.95	0.11	15,17,17,18	0
3	SRM	A	580	63/63	0.96	0.12	22,30,40,48	0
3	SRM	B	570	63/63	0.96	0.14	16,18,24,30	0
4	SF4	A	576	8/8	0.96	0.06	11,11,14,14	0
4	SF4	B	585	8/8	0.97	0.05	21,24,26,28	0
4	SF4	B	586	8/8	0.98	0.04	16,17,20,21	0
4	SF4	A	575	8/8	0.98	0.11	15,19,23,23	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.

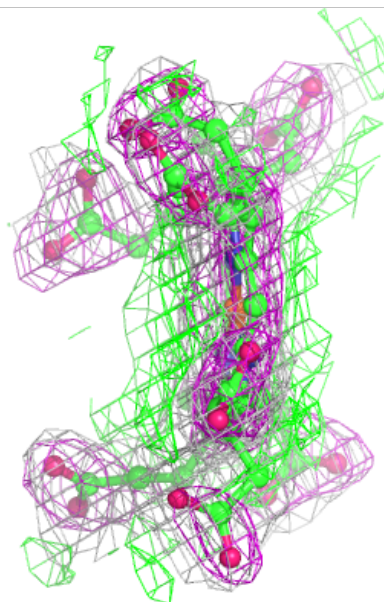
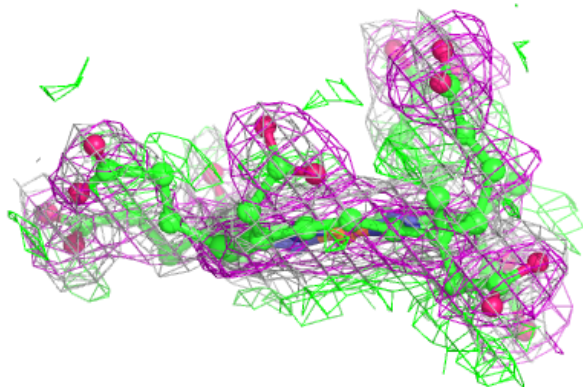
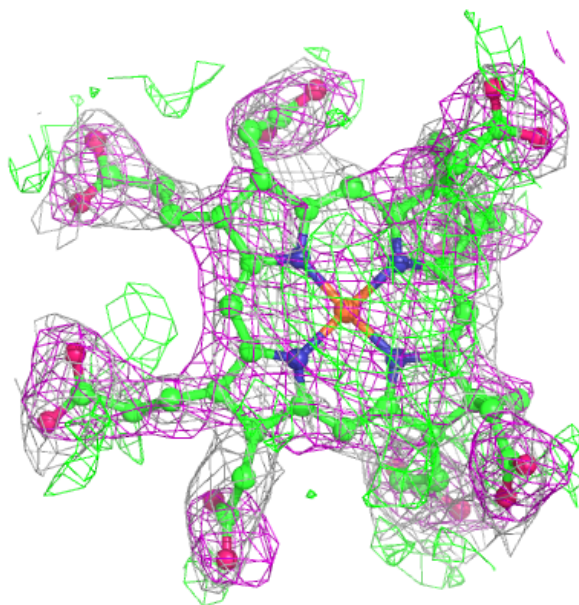
Electron density around SRM D 580:

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



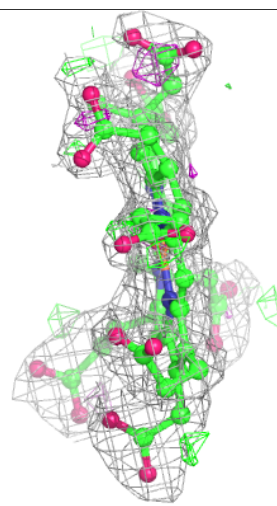
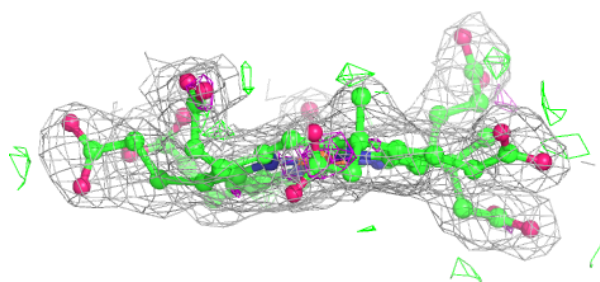
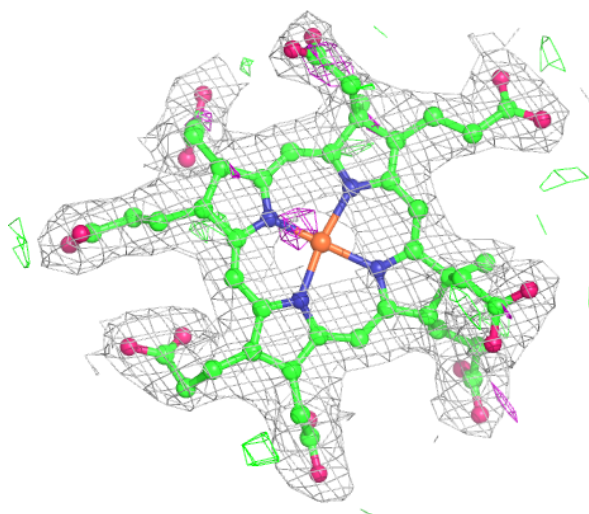
Electron density around SRM E 570:

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



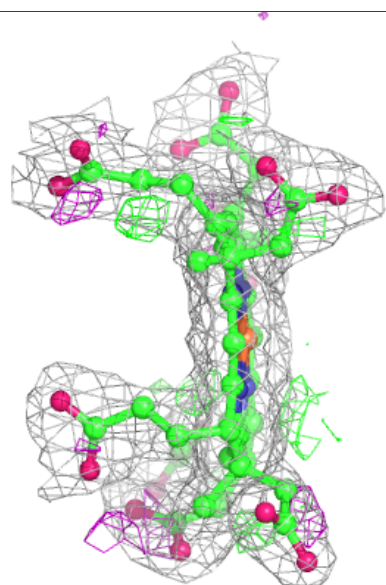
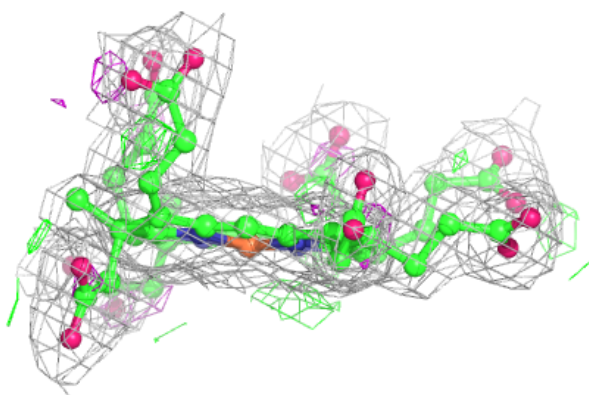
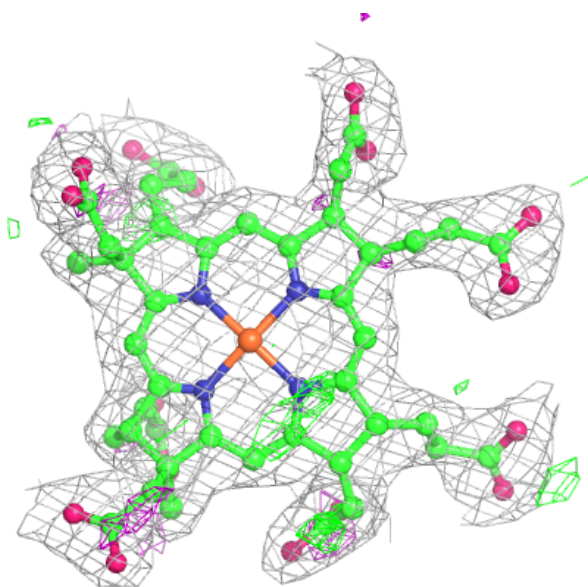
Electron density around SRM A 580:

$2mF_o-DF_c$ (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:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.