Full wwPDB X-ray Structure Validation Report (i)

Dec 19, 2023 – 01:12 PM EST

PDB ID	:	3MMA
Title	:	Dissimilatory sulfite reductase phosphate complex
Authors	:	Parey, K.; Warkentin, E.; Kroneck, P.M.H.; Ermler, U.
Deposited on	:	2010-04-19
Resolution	:	2.30 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 (i) 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 (i)) were used in the production of this report:

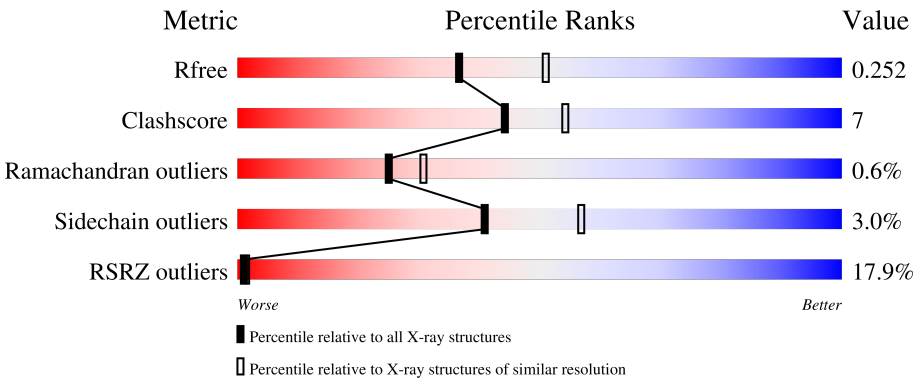
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	7% 86% 13%
1	D	418	31% 85% 14% •
2	B	366	5% 86% 12% ••
2	E	366	28% 79% 18% ••

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	PO4	A	590	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12960 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.

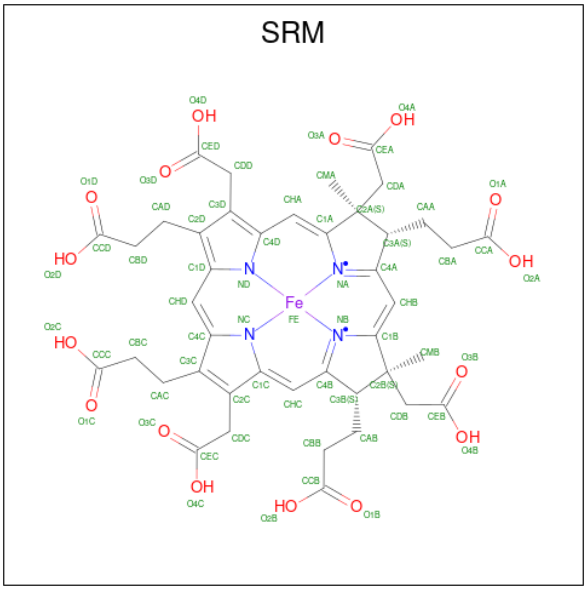
- Molecule 1 is a protein called Sulfite reductase, dissimilatory-type subunit alpha.

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

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

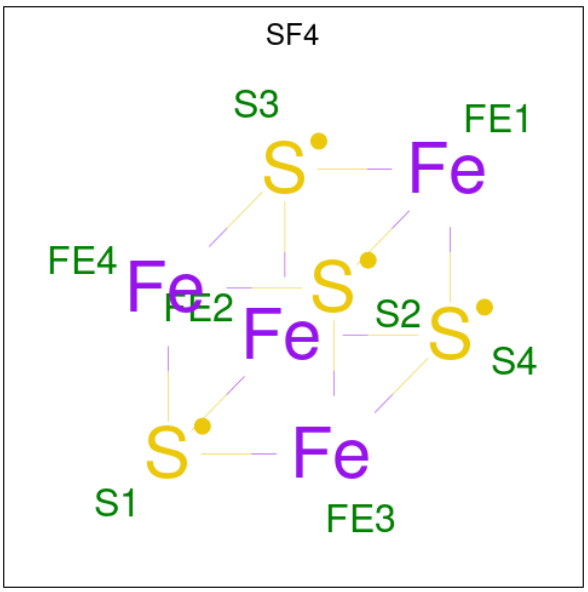
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	363	2901	1862	491	526	22	0	0	0
2	E	363	2901	1862	491	526	22	0	0	0

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



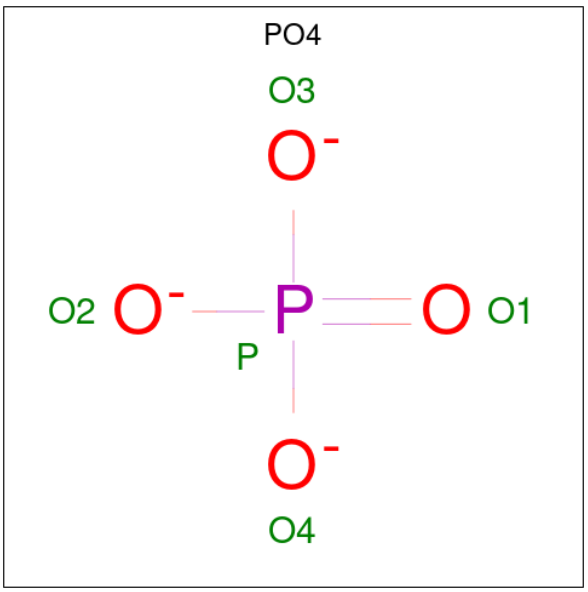
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
3	A	1	63	42	1	4	16	0	0
3	B	1	63	42	1	4	16	0	0
3	D	1	63	42	1	4	16	0	0
3	E	1	63	42	1	4	16	0	0

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 6 is water.

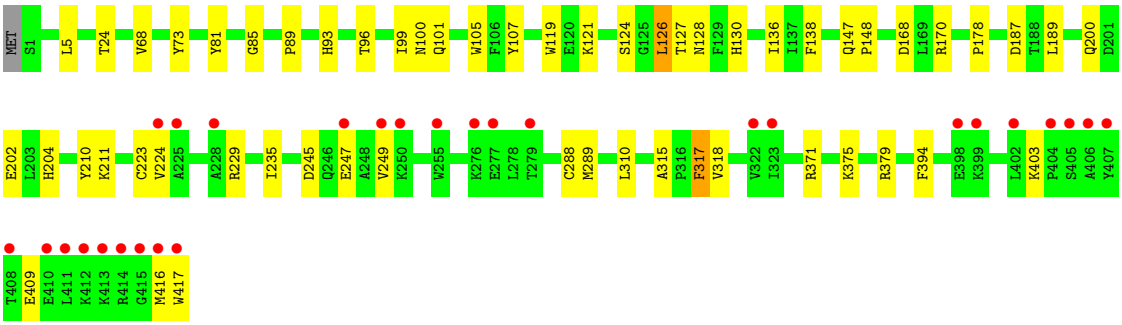
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	78	78	78	0	0
			Total	O		
6	B	84	84	84	0	0
			Total	O		
6	D	11	11	11	0	0
			Total	O		
6	E	6	6	6	0	0

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.

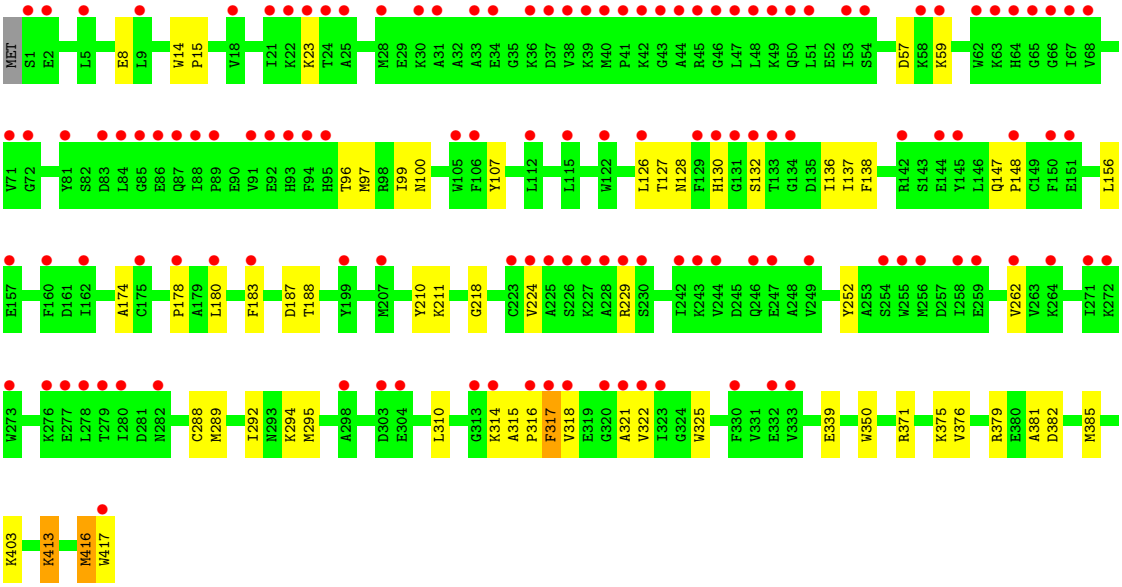
• Molecule 1: Sulfite reductase, dissimilatory-type subunit alpha

Chain A:



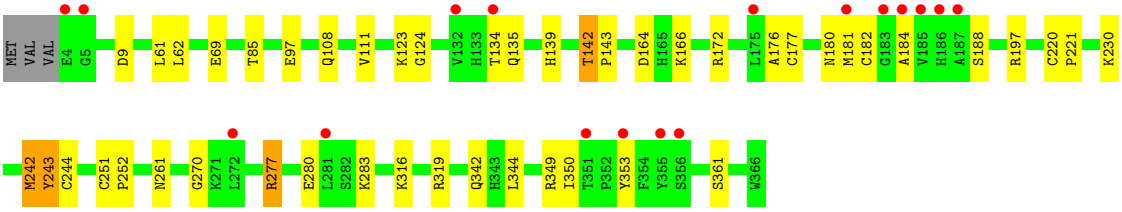
• Molecule 1: Sulfite reductase, dissimilatory-type subunit alpha

Chain D:



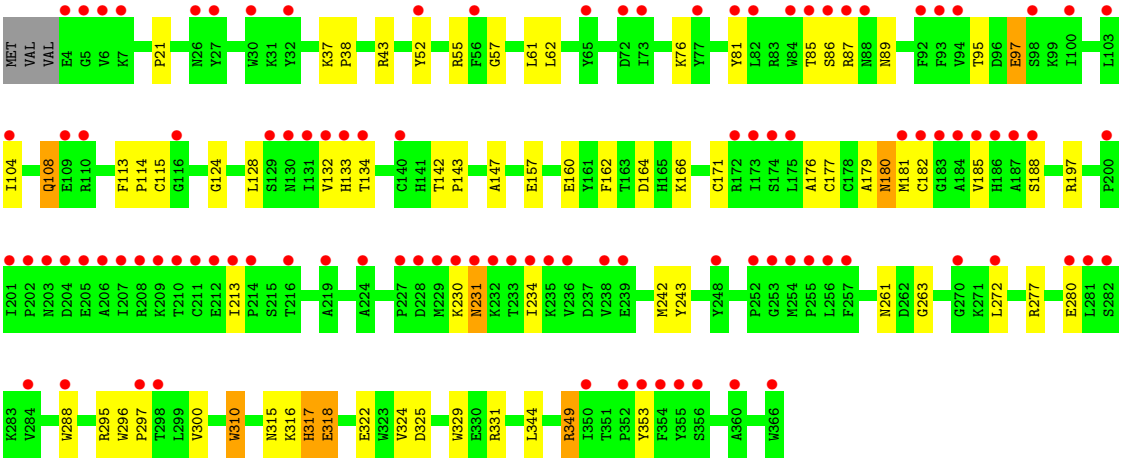
• Molecule 2: Sulfite reductase, dissimilatory-type subunit beta

Chain B:



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

Chain E:



4 Data and refinement statistics (i)

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)	48.34 – 2.30 48.33 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.34-2.30) 98.8 (48.33-2.30)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	4.81 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0046	Depositor
R, R_{free}	0.192 , 0.236 0.213 , 0.252	Depositor DCC
R_{free} test set	3930 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	34.8	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12960	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, SF4, SRM

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	0.55	1/3416 (0.0%)	0.63	0/4610
1	D	0.42	1/3416 (0.0%)	0.53	0/4610
2	B	0.54	0/2984	0.65	1/4058 (0.0%)
2	E	0.40	0/2984	0.55	0/4058
All	All	0.48	2/12800 (0.0%)	0.59	1/17336 (0.0%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	223	CYS	CB-SG	8.13	1.96	1.82
1	D	23	LYS	CD-CE	5.95	1.66	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	277	ARG	NE-CZ-NH1	5.13	122.87	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	317	PHE	Peptide

5.2 Too-close contacts (i)

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	45	0
1	D	3329	0	3276	44	0
2	B	2901	0	2837	37	0
2	E	2901	0	2838	53	0
3	A	63	0	34	12	0
3	B	63	0	34	6	0
3	D	63	0	34	6	0
3	E	63	0	34	11	0
4	A	16	0	0	0	0
4	B	16	0	0	0	0
4	D	16	0	0	1	0
4	E	16	0	0	2	0
5	A	5	0	0	2	0
6	A	78	0	0	1	0
6	B	84	0	0	1	0
6	D	11	0	0	2	0
6	E	6	0	0	0	0
All	All	12960	0	12363	167	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 (167) 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:E:570:SRM:HDD2	3:E:570:SRM:HBD2	1.33	1.07
1:A:403:LYS:H	2:E:261:ASN:HD21	1.07	0.97
2:E:230:LYS:HB2	2:E:231:ASN:HB2	1.48	0.95
1:D:317:PHE:HD2	2:E:180:ASN:HB3	1.35	0.88
2:E:177:CYS:HB2	4:E:585:SF4:S3	2.14	0.88
2:E:157:GLU:HG3	2:E:300:VAL:HG11	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:570:SRM:HDD2	3:E:570:SRM:CBD	2.03	0.88
2:B:261:ASN:HD21	1:D:403:LYS:H	1.21	0.87
1:D:128:ASN:HB2	1:D:137:ILE:HB	1.59	0.84
1:D:317:PHE:CD2	2:E:180:ASN:HB3	2.14	0.83
2:E:55:ARG:HH22	3:E:570:SRM:HBA2	1.45	0.80
2:E:230:LYS:CB	2:E:231:ASN:HB2	2.12	0.79
2:E:157:GLU:HG3	2:E:300:VAL:CG1	2.14	0.78
2:E:197:ARG:HH21	2:E:261:ASN:HD22	1.32	0.77
2:E:52:TYR:CE1	2:E:97:GLU:HB3	2.18	0.77
2:E:230:LYS:HB2	2:E:231:ASN:CB	2.14	0.77
2:E:134:THR:HG21	2:E:182:CYS:HB2	1.65	0.77
2:B:124:GLY:HA3	2:B:316:LYS:HD3	1.67	0.75
1:A:107:TYR:OH	1:A:130:HIS:HE1	1.70	0.74
1:A:317:PHE:CD2	2:B:180:ASN:HB3	2.22	0.74
2:E:85:THR:HB	3:E:570:SRM:HAB2	1.69	0.73
1:A:229:ARG:HD3	2:B:184:ALA:HB2	1.69	0.72
1:D:178:PRO:HG3	1:D:187:ASP:HA	1.72	0.69
1:A:317:PHE:HD2	2:B:180:ASN:HB3	1.60	0.67
1:A:379:ARG:HH11	1:A:379:ARG:HG3	1.60	0.66
1:D:379:ARG:HG3	1:D:379:ARG:HH11	1.61	0.65
2:E:86:SER:OG	3:E:570:SRM:HAB1	1.96	0.65
2:B:69:GLU:HG2	6:B:381:HOH:O	1.96	0.65
2:E:124:GLY:HA3	2:E:316:LYS:HD2	1.79	0.64
1:D:147:GLN:HB3	1:D:148:PRO:HD3	1.79	0.64
1:D:218:GLY:HA3	4:D:575:SF4:S2	2.39	0.64
1:A:96:THR:HG23	2:B:139:HIS:CE1	2.33	0.63
1:A:128:ASN:ND2	2:B:135:GLN:HE22	1.97	0.63
1:D:107:TYR:OH	1:D:130:HIS:HE1	1.83	0.61
2:E:230:LYS:CA	2:E:231:ASN:HB2	2.31	0.61
1:A:416:MET:O	1:A:417:TRP:HB2	2.00	0.60
2:B:261:ASN:HD21	1:D:403:LYS:N	1.94	0.60
1:A:403:LYS:N	2:E:261:ASN:HD21	1.90	0.60
2:E:57:GLY:HA2	2:E:89:ASN:ND2	2.17	0.60
1:D:99:ILE:HB	1:D:136:ILE:HB	1.83	0.60
1:A:128:ASN:HD21	2:B:135:GLN:HE22	1.49	0.59
1:D:132:SER:N	3:D:580:SRM:HBB1	2.17	0.59
1:A:394:PHE:HE2	2:E:179:ALA:HB1	1.68	0.59
2:B:350:ILE:O	2:E:349:ARG:NH2	2.28	0.59
2:E:272:LEU:HB2	3:E:570:SRM:CCC	2.33	0.59
1:A:315:ALA:HB3	3:A:580:SRM:HBD1	1.84	0.58
1:A:371:ARG:O	1:A:375:LYS:HD3	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:570:SRM:HBA1	3:E:570:SRM:CHB	2.31	0.56
3:D:580:SRM:HMB1	3:D:580:SRM:HBB2	1.87	0.56
1:D:211:LYS:NZ	3:D:580:SRM:HAD1	2.21	0.55
1:D:317:PHE:HE2	2:E:180:ASN:HD22	1.54	0.55
1:A:119:TRP:CH2	1:A:138:PHE:HB3	2.41	0.55
2:E:37:LYS:HB2	2:E:38:PRO:CD	2.36	0.55
2:B:197:ARG:HH21	2:B:261:ASN:HD22	1.55	0.55
1:A:168:ASP:OD1	1:A:170:ARG:HD3	2.06	0.55
2:B:277:ARG:NH2	2:B:280:GLU:OE1	2.38	0.55
3:A:580:SRM:CBB	3:A:580:SRM:CMB	2.85	0.55
1:A:107:TYR:OH	1:A:130:HIS:CE1	2.58	0.54
3:A:580:SRM:C4C	2:B:182:CYS:HA	2.36	0.54
1:A:394:PHE:CE2	2:E:179:ALA:HB1	2.41	0.54
2:E:108:GLN:NE2	2:E:113:PHE:O	2.40	0.53
1:A:170:ARG:HH12	5:A:590:PO4:P	2.32	0.53
1:D:15:PRO:HD3	2:E:114:PRO:HD3	1.90	0.53
1:A:99:ILE:HB	1:A:136:ILE:HB	1.89	0.53
1:D:156:LEU:HD12	6:D:428:HOH:O	2.08	0.53
1:A:379:ARG:HH11	1:A:379:ARG:CG	2.21	0.52
1:D:262:VAL:HG22	1:D:294:LYS:HG3	1.90	0.52
1:D:413:LYS:HG2	6:D:420:HOH:O	2.08	0.52
2:E:128:LEU:O	2:E:162:PHE:HA	2.10	0.52
2:E:181:MET:HG2	2:E:185:VAL:HB	1.92	0.52
1:A:211:LYS:NZ	5:A:590:PO4:O1	2.30	0.52
2:E:134:THR:HB	4:E:585:SF4:S4	2.50	0.51
2:E:87:ARG:HG3	3:E:570:SRM:HBB2	1.93	0.51
2:E:133:HIS:HB2	2:E:147:ALA:HB1	1.92	0.51
1:A:229:ARG:HG2	3:A:580:SRM:HCD1	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:HB2	1.93	0.51
2:E:324:VAL:HG11	2:E:329:TRP:CE2	2.45	0.50
2:B:85:THR:HB	3:B:570:SRM:CAB	2.41	0.50
2:B:176:ALA:HB1	2:B:181:MET:HA	1.94	0.50
1:D:180:LEU:O	2:E:43:ARG:HD3	2.12	0.49
1:D:229:ARG:HG2	3:D:580:SRM:HCD1	1.93	0.49
1:A:211:LYS:HZ1	3:A:580:SRM:HAD1	1.77	0.49
2:B:172:ARG:HH21	3:B:570:SRM:C2C	2.25	0.49
3:A:580:SRM:HBA1	3:A:580:SRM:HHB	1.95	0.49
1:D:8:GLU:O	2:E:295:ARG:NH2	2.44	0.49
1:D:379:ARG:HH11	1:D:379:ARG:CG	2.24	0.48
1:A:24:THR:HG21	1:A:126:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:322:GLU:O	2:E:325:ASP:HB2	2.12	0.48
1:D:288:CYS:O	1:D:289:MET:HB2	2.13	0.48
2:E:315:ASN:O	2:E:318:GLU:HB3	2.14	0.48
1:A:245:ASP:OD1	1:A:247:GLU:HG2	2.14	0.48
3:E:570:SRM:CHB	3:E:570:SRM:CBA	2.91	0.48
2:B:353:TYR:HA	2:E:353:TYR:HA	1.96	0.47
2:E:316:LYS:O	2:E:317:HIS:HB2	2.14	0.47
1:D:416:MET:O	1:D:417:TRP:HB3	2.14	0.47
2:E:230:LYS:HB2	2:E:231:ASN:CG	2.34	0.47
1:A:147:GLN:HB3	1:A:148:PRO:HD3	1.95	0.47
2:E:164:ASP:HB3	2:E:166:LYS:HG3	1.96	0.47
1:A:288:CYS:O	1:A:289:MET:HB2	2.14	0.47
1:A:317:PHE:CE2	2:B:180:ASN:HB3	2.49	0.47
1:A:168:ASP:HB2	1:A:202:GLU:O	2.15	0.47
2:B:142:THR:N	2:B:143:PRO:CD	2.77	0.46
2:E:142:THR:N	2:E:143:PRO:HD3	2.30	0.46
1:A:245:ASP:O	1:A:249:VAL:HG23	2.15	0.46
1:D:97:MET:HB2	1:D:138:PHE:HB2	1.96	0.46
2:E:57:GLY:HA2	2:E:89:ASN:HD22	1.80	0.45
1:A:200:GLN:NE2	1:A:204:HIS:NE2	2.65	0.45
1:D:107:TYR:OH	1:D:130:HIS:CE1	2.67	0.45
3:A:580:SRM:HHB	3:A:580:SRM:CBA	2.47	0.45
1:D:315:ALA:HB1	1:D:316:PRO:CD	2.47	0.45
3:A:580:SRM:CEB	2:B:134:THR:HG22	2.46	0.45
1:A:121:LYS:NZ	6:A:477:HOH:O	2.49	0.45
2:E:263:GLY:HA3	2:E:288:TRP:NE1	2.31	0.45
2:B:124:GLY:HA3	2:B:316:LYS:CD	2.44	0.44
1:D:339:GLU:OE2	1:D:379:ARG:NH2	2.50	0.44
1:D:314:LYS:HG2	1:D:322:VAL:HB	1.99	0.44
2:B:85:THR:HB	3:B:570:SRM:HAB1	1.99	0.44
1:D:252:TYR:CE2	1:D:295:MET:HB3	2.53	0.44
1:A:127:THR:O	2:B:61:LEU:HD12	2.17	0.44
1:D:316:PRO:HA	1:D:321:ALA:N	2.32	0.44
2:B:242:MET:SD	2:B:244:CYS:HB3	2.58	0.44
3:B:570:SRM:HDD2	3:B:570:SRM:HBD2	1.99	0.44
2:B:85:THR:HB	3:B:570:SRM:HAB2	1.99	0.44
2:B:69:GLU:OE2	2:B:111:VAL:HG12	2.17	0.43
1:D:57:ASP:HB3	1:D:59:LYS:HG2	1.99	0.43
1:A:379:ARG:CG	1:A:379:ARG:NH1	2.81	0.43
3:A:580:SRM:HBB2	3:A:580:SRM:HMB3	2.00	0.43
1:D:310:LEU:HA	1:D:325:TRP:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:GLN:HE21	2:B:9:ASP:HA	1.83	0.43
2:E:21:PRO:HD3	2:E:81:TYR:CE1	2.55	0.42
1:A:211:LYS:NZ	3:A:580:SRM:HAD1	2.35	0.42
1:D:174:ALA:HB1	1:D:188:THR:HB	2.00	0.42
2:E:176:ALA:HB1	2:E:181:MET:HA	2.01	0.42
2:B:342:GLN:HB3	1:D:381:ALA:HB2	2.02	0.42
1:D:127:THR:O	2:E:61:LEU:HD12	2.20	0.42
2:B:164:ASP:HB3	2:B:166:LYS:HG3	2.01	0.42
2:E:296:TRP:N	2:E:297:PRO:HD3	2.34	0.42
1:A:85:GLY:O	1:A:89:PRO:HA	2.20	0.42
3:A:580:SRM:CMB	3:A:580:SRM:HBB2	2.48	0.42
2:B:188:SER:N	2:B:270:GLY:HA3	2.35	0.42
1:D:132:SER:H	3:D:580:SRM:HBB1	1.83	0.42
1:D:382:ASP:O	1:D:385:MET:HG3	2.20	0.41
2:E:171:CYS:HB2	2:E:310:TRP:CH2	2.55	0.41
3:E:570:SRM:CBD	3:E:570:SRM:CDD	2.86	0.41
1:A:73:TYR:CD1	1:A:204:HIS:HB3	2.55	0.41
1:D:315:ALA:HB3	3:D:580:SRM:HBD1	2.01	0.41
2:B:123:LYS:HA	2:B:123:LYS:HD2	1.92	0.41
2:B:251:CYS:HA	2:B:252:PRO:HD2	1.88	0.41
1:A:124:SER:OG	1:A:126:LEU:HB2	2.21	0.41
1:D:183:PHE:CE1	1:D:292:ILE:HG22	2.56	0.41
1:A:101:GLN:HG3	1:A:105:TRP:CD1	2.55	0.41
3:E:570:SRM:HAC2	3:E:570:SRM:HCD1	1.66	0.41
1:A:235:ILE:HD12	1:A:310:LEU:HD22	2.01	0.41
2:B:242:MET:C	2:B:243:TYR:CG	2.94	0.41
2:B:220:CYS:HA	2:B:221:PRO:HD3	1.91	0.40
2:E:213:ILE:HG23	2:E:234:ILE:HG12	2.03	0.40
2:E:277:ARG:NH2	2:E:280:GLU:OE1	2.50	0.40
1:A:178:PRO:HG3	1:A:187:ASP:HA	2.02	0.40
2:B:319:ARG:HH22	3:B:570:SRM:CCC	2.34	0.40
1:A:119:TRP:CZ3	1:A:138:PHE:HB3	2.56	0.40
3:A:580:SRM:HAD1	3:A:580:SRM:O4D	2.22	0.40
2:E:197:ARG:NH2	2:E:261:ASN:HD22	2.09	0.40
1:A:81:TYR:CE2	1:A:93:HIS:CD2	3.10	0.40
2:B:342:GLN:CD	1:D:371:ARG:HG3	2.42	0.40
1:D:127:THR:HA	1:D:137:ILE:O	2.22	0.40
1:D:350:TRP:CG	1:D:376:VAL:HG21	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%)	402 (97%)	12 (3%)	1 (0%)	47	58
1	D	415/418 (99%)	393 (95%)	21 (5%)	1 (0%)	47	58
2	B	361/366 (99%)	343 (95%)	16 (4%)	2 (1%)	25	31
2	E	361/366 (99%)	331 (92%)	25 (7%)	5 (1%)	11	11
All	All	1552/1568 (99%)	1469 (95%)	74 (5%)	9 (1%)	25	31

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	318	VAL
2	E	317	HIS
1	D	318	VAL
2	E	76	LYS
2	E	231	ASN
2	E	160	GLU
2	B	361	SER
2	E	318	GLU
2	B	142	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	353/354 (100%)	345 (98%)	8 (2%)	50	67
1	D	353/354 (100%)	344 (98%)	9 (2%)	47	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	314/317 (99%)	304 (97%)	10 (3%)	39	54
2	E	314/317 (99%)	301 (96%)	13 (4%)	30	43
All	All	1334/1342 (99%)	1294 (97%)	40 (3%)	41	57

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	68	VAL
1	A	100	ASN
1	A	126	LEU
1	A	189	LEU
1	A	210	TYR
1	A	224	VAL
1	A	409	GLU
2	B	62	LEU
2	B	97	GLU
2	B	108	GLN
2	B	177	CYS
2	B	230	LYS
2	B	242	MET
2	B	243	TYR
2	B	283	LYS
2	B	344	LEU
2	B	349	ARG
1	D	96	THR
1	D	100	ASN
1	D	126	LEU
1	D	210	TYR
1	D	224	VAL
1	D	317	PHE
1	D	375	LYS
1	D	413	LYS
1	D	416	MET
2	E	62	LEU
2	E	95	THR
2	E	97	GLU
2	E	108	GLN
2	E	132	VAL
2	E	180	ASN
2	E	188	SER

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Mol	Chain	Res	Type
2	E	242	MET
2	E	243	TYR
2	E	310	TRP
2	E	331	ARG
2	E	344	LEU
2	E	349	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	128	ASN
1	A	130	HIS
1	A	200	GLN
2	B	89	ASN
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	231	ASN
2	E	261	ASN
2	E	363	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
4	SF4	B	586	2	0,12,12	-	-	-		
5	PO4	A	590	-	4,4,4	1.12	0	6,6,6	0.93	0
4	SF4	D	575	1	0,12,12	-	-	-		
3	SRM	B	570	1	68,70,70	2.22	10 (14%)	81,112,112	3.13	35 (43%)
4	SF4	D	576	1	0,12,12	-	-	-		
4	SF4	E	585	2	0,12,12	-	-	-		
3	SRM	D	580	-	68,70,70	2.01	13 (19%)	81,112,112	2.59	26 (32%)
4	SF4	B	585	2	0,12,12	-	-	-		
3	SRM	A	580	2	68,70,70	1.99	13 (19%)	81,112,112	2.88	33 (40%)
3	SRM	E	570	-	68,70,70	2.27	9 (13%)	81,112,112	3.02	31 (38%)
4	SF4	A	575	1	0,12,12	-	-	-		
4	SF4	A	576	1	0,12,12	-	-	-		
4	SF4	E	586	2	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
4	SF4	B	586	2	-	-	0/6/5/5
4	SF4	D	575	1	-	-	0/6/5/5
3	SRM	B	570	1	1/1/19/23	17/38/126/126	-
4	SF4	D	576	1	-	-	0/6/5/5
4	SF4	E	585	2	-	-	0/6/5/5
3	SRM	D	580	-	1/1/19/23	18/38/126/126	-
4	SF4	B	585	2	-	-	0/6/5/5
3	SRM	A	580	2	2/2/19/23	12/38/126/126	-
3	SRM	E	570	-	1/1/19/23	19/38/126/126	-
4	SF4	A	575	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	A	576	1	-	-	0/6/5/5
4	SF4	E	586	2	-	-	0/6/5/5

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	570	SRM	C4A-NA	-10.26	1.28	1.35
3	E	570	SRM	C4A-NA	-9.82	1.28	1.35
3	E	570	SRM	C3C-C2C	6.85	1.51	1.36
3	B	570	SRM	C3C-C2C	6.63	1.50	1.36
3	D	580	SRM	C3D-C2D	6.53	1.54	1.39
3	A	580	SRM	C3D-C2D	6.44	1.54	1.39
3	D	580	SRM	C3C-C2C	6.18	1.50	1.36
3	E	570	SRM	C3D-C2D	6.00	1.53	1.39
3	E	570	SRM	C4C-NC	-5.86	1.28	1.39
3	A	580	SRM	C3A-C4A	-5.80	1.38	1.51
3	D	580	SRM	C3A-C4A	-5.76	1.38	1.51
3	A	580	SRM	C3C-C2C	5.76	1.49	1.36
3	B	570	SRM	C3D-C2D	5.64	1.52	1.39
3	E	570	SRM	C1C-NC	-5.63	1.28	1.39
3	D	580	SRM	C3B-C4B	-5.62	1.39	1.51
3	A	580	SRM	C3B-C4B	-5.54	1.39	1.51
3	B	570	SRM	C4C-NC	-5.24	1.29	1.39
3	B	570	SRM	C1C-NC	-4.47	1.31	1.39
3	D	580	SRM	FE-NC	3.38	2.08	1.95
3	A	580	SRM	FE-NC	3.38	2.08	1.95
3	A	580	SRM	C4C-NC	-3.21	1.33	1.39
3	D	580	SRM	C4C-NC	-3.09	1.33	1.39
3	E	570	SRM	C4C-C3C	3.09	1.50	1.45
3	B	570	SRM	C1C-C2C	3.06	1.50	1.45
3	E	570	SRM	C1C-C2C	2.98	1.50	1.45
3	A	580	SRM	CHD-C4C	2.96	1.39	1.35
3	D	580	SRM	C1C-C2C	2.92	1.50	1.45
3	D	580	SRM	C4A-NA	-2.88	1.33	1.35
3	A	580	SRM	C1C-NC	-2.87	1.34	1.39
3	B	570	SRM	C2B-C3B	-2.85	1.47	1.55
3	A	580	SRM	C4A-NA	-2.83	1.33	1.35
3	D	580	SRM	C1C-NC	-2.80	1.34	1.39
3	D	580	SRM	C4C-C3C	2.70	1.50	1.45
3	A	580	SRM	FE-NA	2.69	2.11	1.97
3	A	580	SRM	C1C-C2C	2.68	1.50	1.45
3	B	570	SRM	C4C-C3C	2.43	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	580	SRM	FE-NB	2.35	2.10	1.97
3	B	570	SRM	CAD-C2D	2.31	1.55	1.52
3	D	580	SRM	FE-NB	2.29	2.09	1.97
3	D	580	SRM	CHD-C4C	2.26	1.38	1.35
3	D	580	SRM	FE-NA	2.26	2.09	1.97
3	B	570	SRM	C1D-CHD	-2.23	1.34	1.41
3	E	570	SRM	CHA-C1A	2.13	1.39	1.35
3	E	570	SRM	C1B-NB	-2.02	1.29	1.41
3	A	580	SRM	C4C-C3C	2.02	1.48	1.45

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	580	SRM	C2A-C3A-C4A	10.19	113.94	100.90
3	A	580	SRM	CAA-C3A-C4A	9.85	128.56	111.19
3	D	580	SRM	C2A-C3A-C4A	8.96	112.36	100.90
3	E	570	SRM	CAB-C3B-C4B	8.27	125.77	111.19
3	E	570	SRM	C2B-C1B-CHB	-7.64	116.56	123.54
3	E	570	SRM	C2A-C1A-CHA	-7.55	116.64	123.54
3	B	570	SRM	CAB-C3B-C4B	7.18	123.85	111.19
3	B	570	SRM	C2B-C3B-C4B	7.13	110.03	100.90
3	D	580	SRM	CAA-C3A-C4A	7.10	123.71	111.19
3	E	570	SRM	C4C-C3C-C2C	-7.03	98.73	106.86
3	B	570	SRM	CBD-CAD-C2D	7.00	124.57	112.62
3	E	570	SRM	C3C-C4C-NC	6.93	117.07	110.32
3	B	570	SRM	C2B-C1B-CHB	-6.56	117.55	123.54
3	B	570	SRM	CMB-C2B-C3B	6.46	124.01	112.08
3	B	570	SRM	C2A-C1A-CHA	-6.40	117.69	123.54
3	E	570	SRM	CAC-C3C-C2C	-6.40	116.02	129.51
3	B	570	SRM	C3D-CDD-CED	6.35	121.81	114.21
3	A	580	SRM	C2B-C3B-C4B	6.29	108.95	100.90
3	D	580	SRM	CDD-C3D-C2D	-6.13	115.55	126.49
3	D	580	SRM	C2B-C3B-C4B	6.05	108.65	100.90
3	E	570	SRM	C3D-CDD-CED	5.86	121.22	114.21
3	A	580	SRM	C3D-CDD-CED	5.84	121.19	114.21
3	B	570	SRM	C3C-C4C-NC	5.62	115.79	110.32
3	A	580	SRM	CMB-C2B-C3B	5.59	122.42	112.08
3	B	570	SRM	C4C-C3C-C2C	-5.55	100.44	106.86
3	D	580	SRM	C3C-C4C-NC	5.46	115.63	110.32
3	E	570	SRM	C2B-C1B-NB	5.29	119.72	111.21
3	B	570	SRM	CAC-C3C-C2C	-5.24	118.48	129.51
3	B	570	SRM	C4D-CHA-C1A	-5.20	119.83	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	570	SRM	C4D-CHA-C1A	-5.14	119.94	130.12
3	E	570	SRM	CAC-C3C-C4C	-5.09	115.30	124.89
3	D	580	SRM	C1A-NA-C4A	5.03	110.92	105.23
3	A	580	SRM	C3C-C4C-NC	5.01	115.20	110.32
3	E	570	SRM	C2B-C3B-C4B	4.95	107.23	100.90
3	B	570	SRM	CHD-C4C-C3C	-4.86	117.07	124.93
3	D	580	SRM	C2C-C1C-NC	4.81	115.00	110.32
3	E	570	SRM	CDA-C2A-C1A	4.76	122.08	107.12
3	B	570	SRM	CHC-C1C-C2C	-4.75	117.24	124.94
3	B	570	SRM	C2B-C1B-NB	4.74	118.84	111.21
3	A	580	SRM	CAD-C2D-C3D	-4.72	110.02	124.90
3	E	570	SRM	C2C-C1C-NC	4.66	114.86	110.32
3	A	580	SRM	CDD-C3D-C2D	-4.62	118.24	126.49
3	D	580	SRM	C2A-C1A-CHA	4.60	127.74	123.54
3	B	570	SRM	CDA-C2A-C1A	4.55	121.44	107.12
3	E	570	SRM	C3A-C4A-NA	4.46	119.62	110.85
3	B	570	SRM	CHC-C1C-NC	4.45	129.25	124.44
3	B	570	SRM	C3B-C2B-C1B	-4.40	93.37	100.92
3	A	580	SRM	C1A-NA-C4A	4.38	110.19	105.23
3	E	570	SRM	CAB-C3B-C2B	4.37	126.17	114.14
3	A	580	SRM	C4C-C3C-C2C	-4.29	101.90	106.86
3	D	580	SRM	C4C-C3C-C2C	-4.27	101.92	106.86
3	D	580	SRM	CDD-C3D-C4D	-4.25	120.92	127.36
3	D	580	SRM	CHD-C4C-NC	-4.25	119.83	124.43
3	A	580	SRM	CBD-CAD-C2D	4.17	119.74	112.62
3	E	570	SRM	C1C-C2C-C3C	-4.17	102.03	106.86
3	B	570	SRM	CEC-CDC-C2C	-4.12	103.11	113.79
3	B	570	SRM	CBC-CAC-C3C	-4.09	101.28	112.63
3	E	570	SRM	CDD-C3D-C2D	-4.02	119.31	126.49
3	B	570	SRM	C1C-C2C-C3C	-3.99	102.25	106.86
3	D	580	SRM	C1C-C2C-C3C	-3.98	102.26	106.86
3	B	570	SRM	C3A-C4A-NA	3.82	118.35	110.85
3	B	570	SRM	CAB-CBB-CCB	3.78	122.53	112.51
3	A	580	SRM	C2B-C1B-CHB	-3.75	120.12	123.54
3	E	570	SRM	CDD-C3D-C4D	-3.72	121.73	127.36
3	A	580	SRM	CBB-CAB-C3B	3.70	125.40	114.73
3	D	580	SRM	C4D-CHA-C1A	-3.69	122.80	130.12
3	E	570	SRM	C3B-C2B-C1B	-3.65	94.66	100.92
3	D	580	SRM	CMA-C2A-CDA	3.62	116.78	110.80
3	A	580	SRM	C3A-C2A-C1A	-3.55	94.83	100.92
3	D	580	SRM	C3D-CDD-CED	3.54	118.44	114.21
3	D	580	SRM	CBB-CAB-C3B	3.49	124.80	114.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	570	SRM	CHC-C1C-C2C	-3.44	119.37	124.94
3	E	570	SRM	C3A-C4A-CHB	-3.39	116.01	123.32
3	A	580	SRM	CHC-C1C-NC	-3.33	120.83	124.44
3	B	570	SRM	CMA-C2A-CDA	-3.27	105.41	110.80
3	A	580	SRM	CAC-CBC-CCC	-3.23	106.66	113.60
3	A	580	SRM	CDD-C3D-C4D	-3.22	122.48	127.36
3	A	580	SRM	C2C-C1C-NC	3.21	113.44	110.32
3	E	570	SRM	C2A-C1A-NA	3.16	116.29	111.21
3	B	570	SRM	C2C-C1C-NC	3.14	113.38	110.32
3	A	580	SRM	C1C-C2C-C3C	-3.13	103.24	106.86
3	A	580	SRM	CAB-C3B-C4B	-2.97	105.95	111.19
3	A	580	SRM	CBA-CAA-C3A	2.96	123.28	114.73
3	B	570	SRM	C2A-C1A-NA	2.95	115.95	111.21
3	D	580	SRM	C2B-C1B-NB	2.94	115.94	111.21
3	D	580	SRM	C3A-C2A-C1A	-2.91	95.93	100.92
3	A	580	SRM	CMA-C2A-CDA	2.90	115.59	110.80
3	E	570	SRM	CHD-C4C-NC	-2.89	121.31	124.43
3	A	580	SRM	CAB-C3B-C2B	-2.86	106.27	114.14
3	D	580	SRM	CMB-C2B-C3B	2.79	117.23	112.08
3	B	570	SRM	C3A-C4A-CHB	-2.76	117.35	123.32
3	E	570	SRM	C1C-CHC-C4B	-2.76	119.97	126.62
3	A	580	SRM	O2A-CCA-CBA	2.76	122.89	114.03
3	D	580	SRM	CAD-C2D-C3D	-2.71	116.35	124.90
3	B	570	SRM	CAA-CBA-CCA	2.64	119.52	112.51
3	A	580	SRM	C3A-C4A-CHB	2.64	129.03	123.32
3	D	580	SRM	CHC-C1C-NC	-2.59	121.63	124.44
3	B	570	SRM	C1C-CHC-C4B	-2.59	120.38	126.62
3	A	580	SRM	CDA-C2A-C1A	2.58	115.23	107.12
3	D	580	SRM	CDA-C2A-C1A	2.56	115.17	107.12
3	A	580	SRM	C2B-C1B-NB	2.53	115.28	111.21
3	B	570	SRM	O2D-CCD-CBD	2.50	122.07	114.03
3	B	570	SRM	CAA-C3A-C4A	-2.48	106.83	111.19
3	B	570	SRM	C4C-NC-C1C	2.47	107.77	105.35
3	E	570	SRM	C1A-NA-C4A	-2.47	102.44	105.23
3	B	570	SRM	CDB-C2B-C3B	-2.46	101.80	108.39
3	D	580	SRM	C3B-C2B-C1B	-2.45	96.72	100.92
3	B	570	SRM	O4B-CEB-CDB	2.37	121.95	114.35
3	D	580	SRM	CAC-C3C-C4C	2.32	129.28	124.89
3	B	570	SRM	CAB-C3B-C2B	2.30	120.48	114.14
3	A	580	SRM	C3B-C2B-C1B	-2.30	96.97	100.92
3	D	580	SRM	O3D-CED-CDD	-2.27	116.56	123.04
3	B	570	SRM	CHD-C4C-NC	2.27	126.88	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	570	SRM	CAD-C2D-C3D	-2.22	117.90	124.90
3	A	580	SRM	C4D-CHA-C1A	-2.20	125.75	130.12
3	A	580	SRM	O3B-CEB-CDB	-2.19	116.54	122.94
3	E	570	SRM	CDB-C2B-C3B	2.15	114.16	108.39
3	E	570	SRM	CMA-C2A-CDA	-2.13	107.30	110.80
3	A	580	SRM	CAC-C3C-C4C	2.13	128.91	124.89
3	A	580	SRM	O3D-CED-CDD	-2.11	117.01	123.04
3	E	570	SRM	CHD-C4C-C3C	-2.05	121.61	124.93
3	A	580	SRM	O2B-CCB-CBB	2.04	120.59	114.03
3	E	570	SRM	O2A-CCA-CBA	2.03	120.57	114.03
3	D	580	SRM	C2B-C1B-CHB	-2.03	121.69	123.54
3	E	570	SRM	O2D-CCD-CBD	2.00	120.46	114.03

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	580	SRM	C3A
3	A	580	SRM	NC
3	B	570	SRM	NC
3	D	580	SRM	NC
3	E	570	SRM	C3B

All (66) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
3	E	570	SRM	C3B-CAB-CBB-CCB
3	A	580	SRM	C2D-CAD-CBD-CCD
3	E	570	SRM	C2B-C3B-CAB-CBB
3	E	570	SRM	C4D-C3D-CDD-CED
3	D	580	SRM	C2D-CAD-CBD-CCD
3	A	580	SRM	C3B-CAB-CBB-CCB
3	E	570	SRM	C3B-C2B-CDB-CEB
3	B	570	SRM	C2B-CDB-CEB-O3B
3	E	570	SRM	C2B-CDB-CEB-O4B
3	D	580	SRM	C1B-C2B-CDB-CEB
3	E	570	SRM	C3C-CAC-CBC-CCC
3	E	570	SRM	C2B-CDB-CEB-O3B
3	B	570	SRM	C2B-CDB-CEB-O4B
3	E	570	SRM	C3D-C2D-CAD-CBD
3	D	580	SRM	C4A-C3A-CAA-CBA
3	D	580	SRM	C1A-C2A-CDA-CEA
3	B	570	SRM	C3B-CAB-CBB-CCB
3	B	570	SRM	CAA-CBA-CCA-O1A
3	D	580	SRM	CAD-CBD-CCD-O1D
3	D	580	SRM	CAA-CBA-CCA-O1A
3	B	570	SRM	CAA-CBA-CCA-O2A
3	D	580	SRM	CAA-CBA-CCA-O2A
3	D	580	SRM	CAC-CBC-CCC-O2C
3	A	580	SRM	CAB-CBB-CCB-O2B
3	A	580	SRM	CAD-CBD-CCD-O2D
3	D	580	SRM	CAC-CBC-CCC-O1C
3	D	580	SRM	CAB-CBB-CCB-O2B
3	A	580	SRM	CAB-CBB-CCB-O1B
3	D	580	SRM	CAD-CBD-CCD-O2D
3	B	570	SRM	C4D-C3D-CDD-CED
3	D	580	SRM	C4D-C3D-CDD-CED
3	A	580	SRM	CAD-CBD-CCD-O1D
3	A	580	SRM	CAC-CBC-CCC-O2C
3	D	580	SRM	C3D-CDD-CED-O4D
3	A	580	SRM	CAC-CBC-CCC-O1C
3	B	570	SRM	CAC-CBC-CCC-O1C
3	B	570	SRM	CAC-CBC-CCC-O2C
3	D	580	SRM	CAB-CBB-CCB-O1B
3	B	570	SRM	CAD-CBD-CCD-O1D
3	D	580	SRM	C3A-CAA-CBA-CCA
3	E	570	SRM	CAD-CBD-CCD-O2D
3	D	580	SRM	C3D-CDD-CED-O3D

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Mol	Chain	Res	Type	Atoms
3	B	570	SRM	CAD-CBD-CCD-O2D
3	E	570	SRM	CAD-CBD-CCD-O1D
3	E	570	SRM	CAA-CBA-CCA-O2A
3	A	580	SRM	CAA-CBA-CCA-O2A
3	E	570	SRM	CAA-CBA-CCA-O1A
3	B	570	SRM	C3A-CAA-CBA-CCA
3	E	570	SRM	CAC-CBC-CCC-O1C

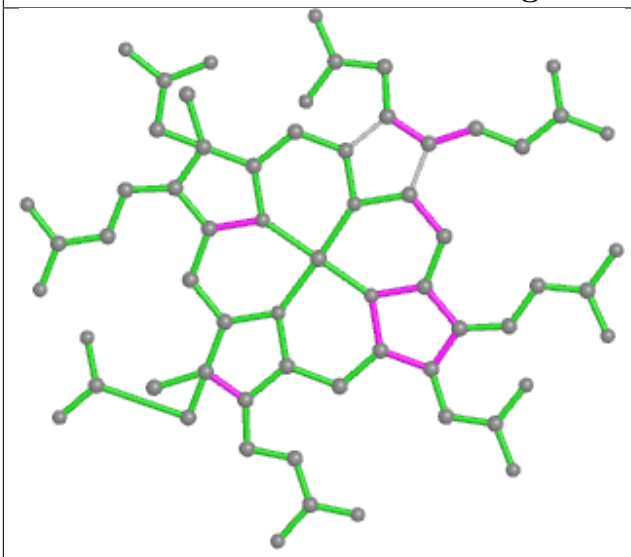
There are no ring outliers.

7 monomers are involved in 40 short contacts:

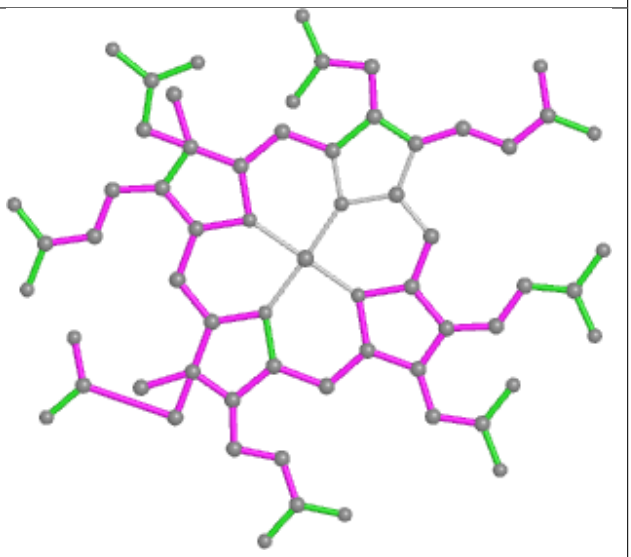
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	590	PO4	2	0
4	D	575	SF4	1	0
3	B	570	SRM	6	0
4	E	585	SF4	2	0
3	D	580	SRM	6	0
3	A	580	SRM	12	0
3	E	570	SRM	11	0

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.

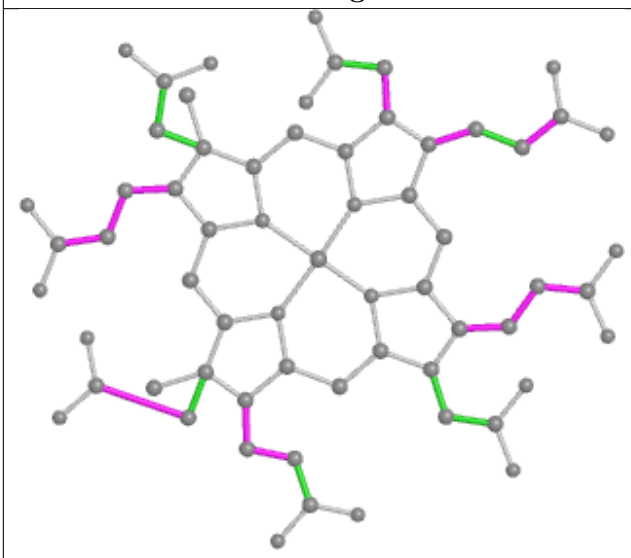
Ligand SRM B 570



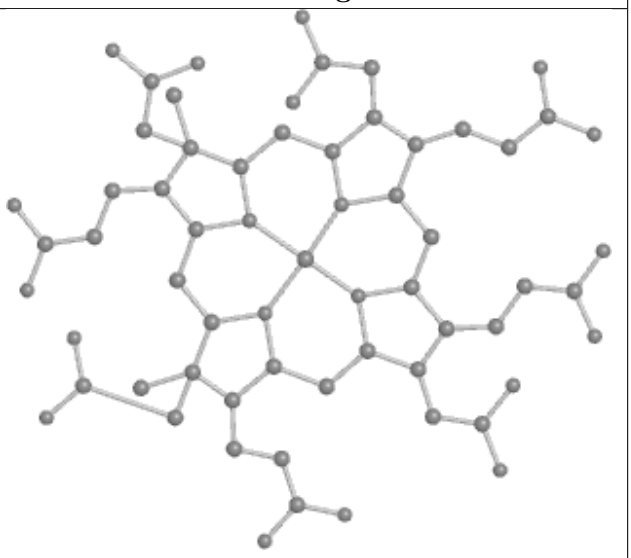
Bond lengths



Bond angles

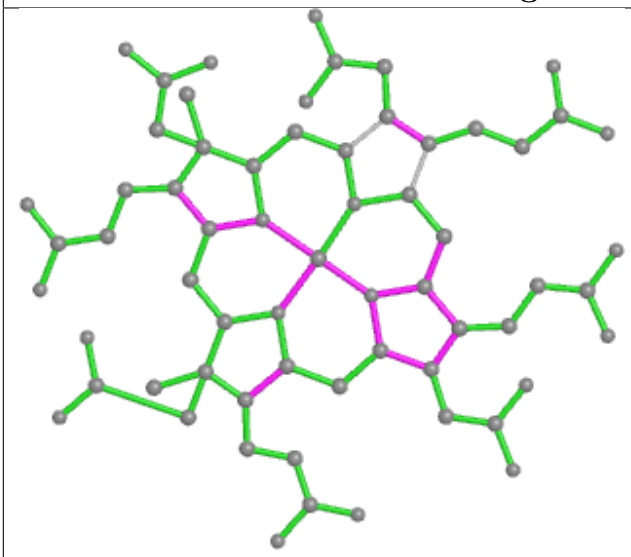


Torsions

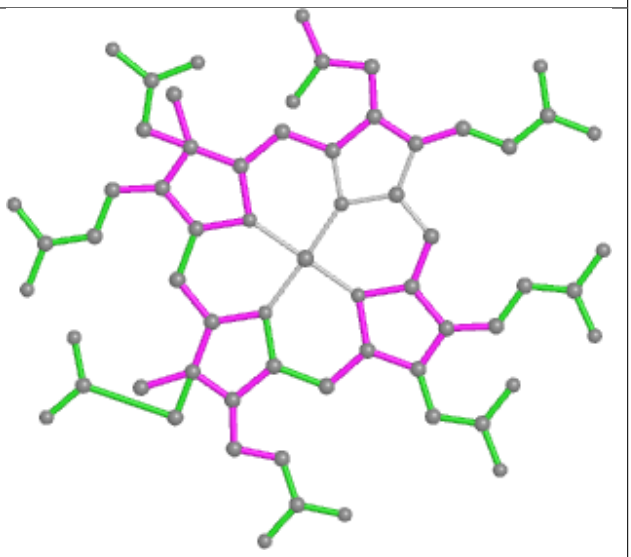


Rings

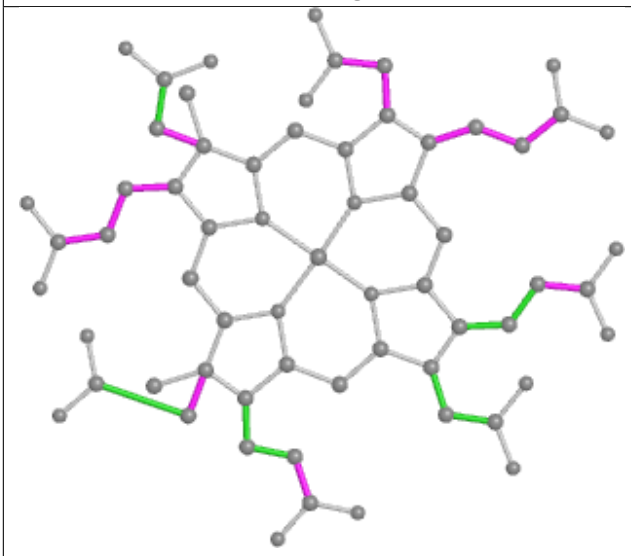
Ligand SRM D 580



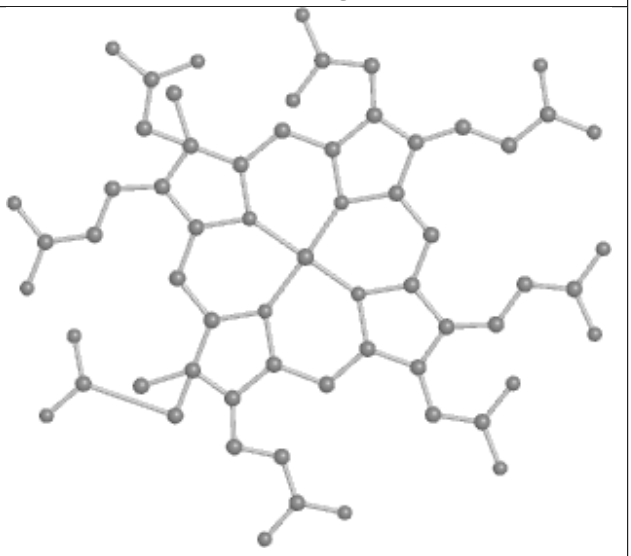
Bond lengths



Bond angles

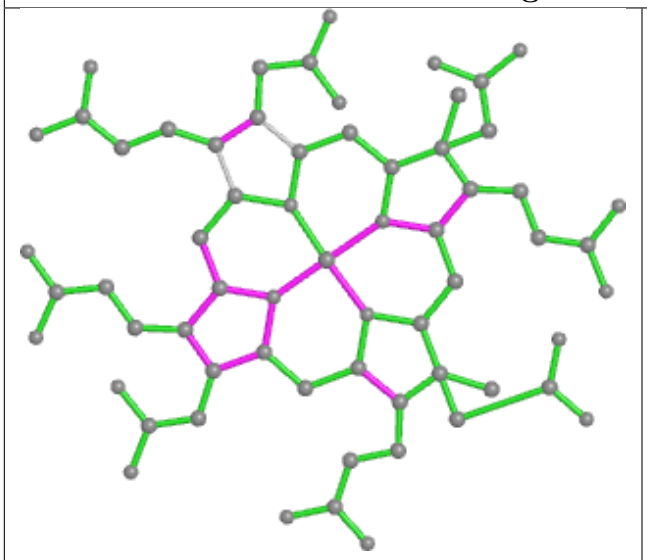


Torsions

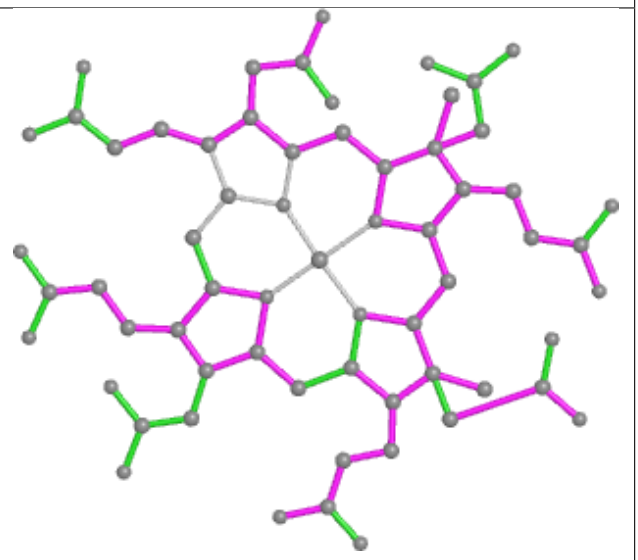


Rings

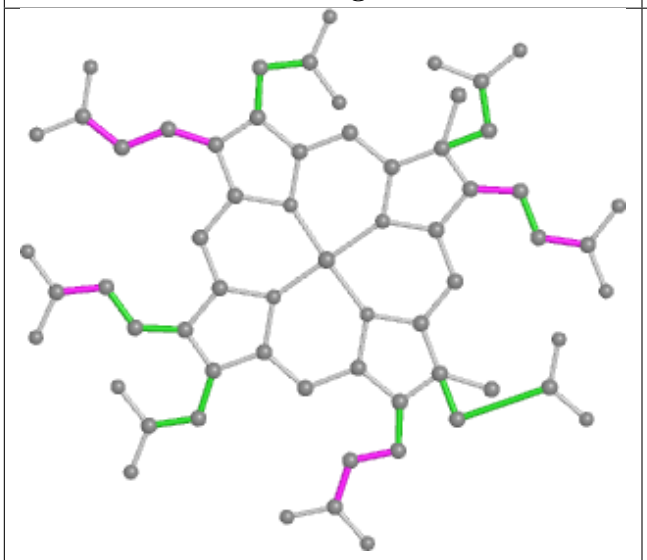
Ligand SRM A 580



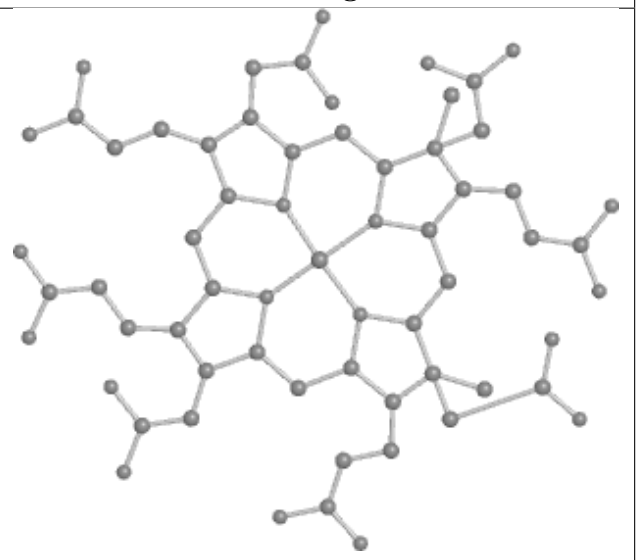
Bond lengths



Bond angles

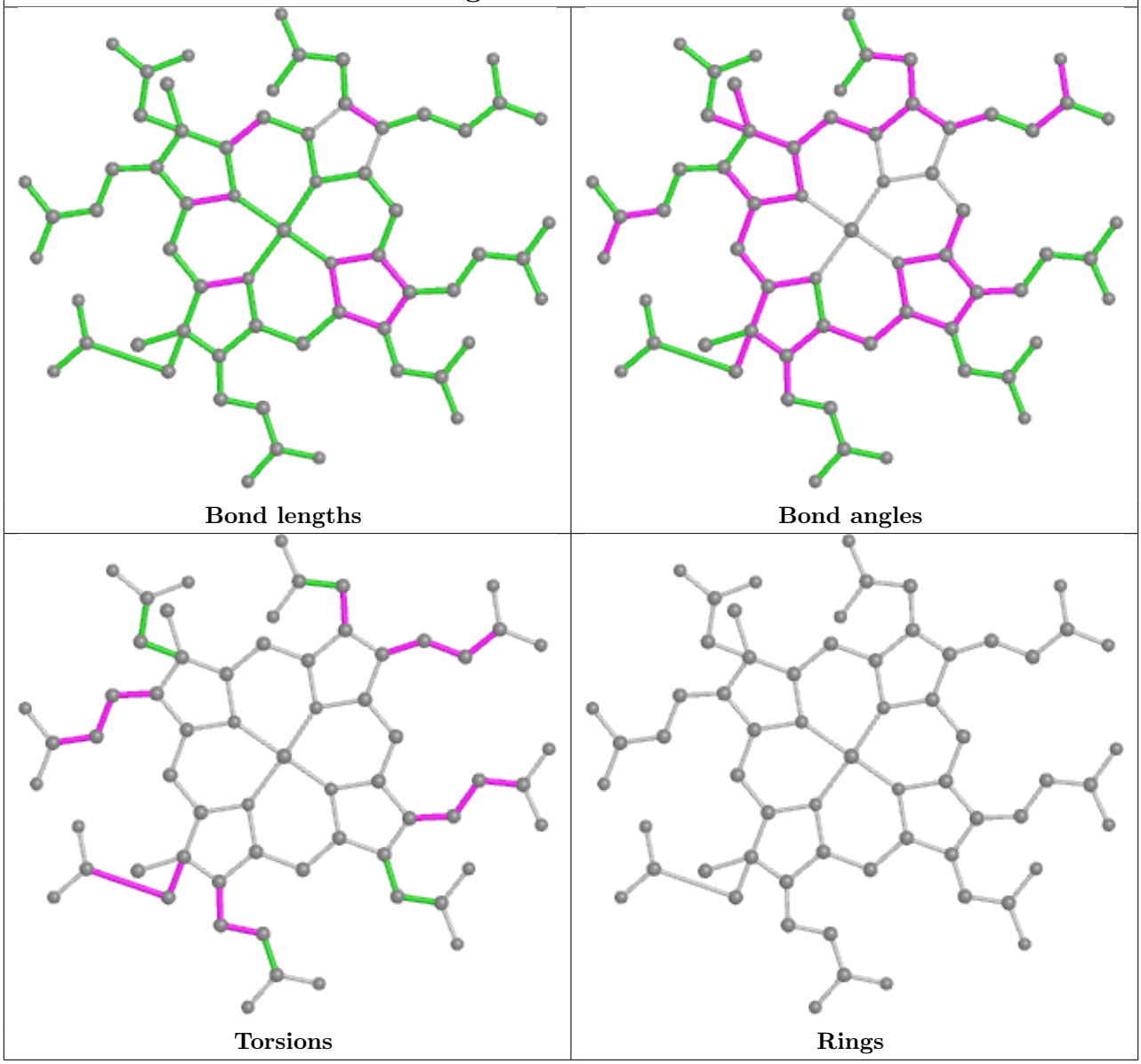


Torsions



Rings

Ligand SRM E 570



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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.38	28 (6%)	17	23	12, 19, 35, 78	0
1	D	417/418 (99%)	1.48	130 (31%)	0	0	13, 23, 36, 54	0
2	B	363/366 (99%)	0.34	17 (4%)	31	38	11, 18, 28, 63	0
2	E	363/366 (99%)	1.54	104 (28%)	0	0	6, 20, 53, 78	0
All	All	1560/1568 (99%)	0.94	279 (17%)	1	1	6, 20, 42, 78	0

All (279) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	67	ILE	8.7
2	E	6	VAL	8.3
2	E	4	GLU	8.1
2	E	207	ILE	7.8
2	E	229	MET	7.4
1	A	417	TRP	7.4
1	D	1	SER	7.3
1	D	72	GLY	6.7
2	E	184	ALA	6.5
1	D	47	LEU	6.4
2	E	232	LYS	6.3
2	E	183	GLY	6.2
2	E	233	THR	6.0
2	E	234	ILE	5.9
2	E	210	THR	5.9
1	D	273	TRP	5.7
1	D	81	TYR	5.5
2	E	5	GLY	5.5
2	E	205	GLU	5.4
1	D	88	ILE	5.4
1	D	417	TRP	5.3

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Mol	Chain	Res	Type	RSRZ
2	E	209	LYS	5.3
2	E	185	VAL	5.2
2	E	186	HIS	5.2
2	E	7	LYS	5.2
1	D	43	GLY	5.1
2	E	202	PRO	5.0
1	D	229	ARG	4.9
2	E	188	SER	4.7
1	D	33	ALA	4.5
1	D	46	GLY	4.5
1	D	86	GLU	4.5
2	E	187	ALA	4.4
1	A	407	TYR	4.4
2	E	77	TYR	4.4
1	D	22	LYS	4.3
2	E	211	CYS	4.3
2	E	116	GLY	4.3
1	D	40	MET	4.3
1	D	207	MET	4.3
2	E	181	MET	4.3
1	A	415	GLY	4.3
1	A	250	LYS	4.2
1	A	416	MET	4.2
1	D	132	SER	4.2
1	D	276	LYS	4.2
1	A	411	LEU	4.2
1	D	106	PHE	4.2
1	D	45	ARG	4.1
1	A	406	ALA	4.1
2	E	132	VAL	4.1
1	D	24	THR	4.1
2	E	85	THR	4.1
2	E	182	CYS	4.1
1	D	228	ALA	4.0
1	D	38	VAL	4.0
2	E	27	TYR	4.0
2	E	230	LYS	4.0
1	D	89	PRO	3.9
2	E	92	PHE	3.9
1	D	131	GLY	3.9
2	E	201	ILE	3.9
2	E	200	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	332	GLU	3.8
2	E	86	SER	3.8
1	D	320	GLY	3.8
2	E	206	ALA	3.8
1	D	313	GLY	3.8
2	E	231	ASN	3.8
1	D	93	HIS	3.7
1	D	83	ASP	3.7
1	D	223	CYS	3.7
2	E	281	LEU	3.7
1	D	242	ILE	3.7
1	D	64	HIS	3.7
2	E	208	ARG	3.7
2	E	227	PRO	3.7
2	E	174	SER	3.6
2	E	82	LEU	3.6
2	E	213	ILE	3.6
1	D	94	PHE	3.5
2	B	187	ALA	3.5
2	E	254	MET	3.4
1	D	277	GLU	3.4
1	D	48	LEU	3.4
1	D	105	TRP	3.4
2	E	255	PRO	3.4
1	D	323	ILE	3.4
1	D	278	LEU	3.4
1	D	160	PHE	3.3
1	A	414	ARG	3.3
1	D	2	GLU	3.3
2	E	109	GLU	3.3
2	E	355	TYR	3.3
1	D	258	ILE	3.3
1	D	318	VAL	3.3
2	E	87	ARG	3.3
1	D	87	GLN	3.3
2	E	219	ALA	3.2
1	D	85	GLY	3.2
2	E	257	PHE	3.2
1	D	225	ALA	3.2
1	A	276	LYS	3.2
1	D	30	LYS	3.2
2	B	183	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	244	VAL	3.2
1	D	133	THR	3.2
1	D	157	GLU	3.2
1	D	115	LEU	3.2
2	E	52	TYR	3.1
1	D	130	HIS	3.1
2	E	204	ASP	3.1
2	B	5	GLY	3.1
1	A	413	LYS	3.1
1	D	84	LEU	3.0
2	E	26	ASN	3.0
1	D	150	PHE	3.0
2	E	252	PRO	3.0
1	D	5	LEU	3.0
2	E	84	TRP	3.0
2	E	248	TYR	3.0
1	D	31	ALA	3.0
1	D	92	GLU	3.0
1	D	134	GLY	3.0
1	D	62	TRP	3.0
2	E	73	ILE	2.9
1	D	256	MET	2.9
1	D	122	TRP	2.9
1	A	225	ALA	2.9
1	D	41	PRO	2.9
1	D	316	PRO	2.9
2	E	175	LEU	2.9
1	D	91	VAL	2.9
1	A	412	LYS	2.8
1	D	34	GLU	2.8
1	D	68	VAL	2.8
2	E	30	TRP	2.8
2	E	173	ILE	2.8
2	E	235	LYS	2.8
2	E	282	SER	2.8
1	D	18	VAL	2.8
1	D	49	LYS	2.8
2	E	94	VAL	2.8
1	D	280	ILE	2.8
2	E	32	TYR	2.8
2	E	110	ARG	2.8
1	D	25	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	42	LYS	2.8
1	D	151	GLU	2.8
2	E	203	ASN	2.7
2	E	134	THR	2.7
1	A	323	ILE	2.7
2	B	184	ALA	2.7
1	D	65	GLY	2.7
2	B	356	SER	2.7
2	E	238	VAL	2.7
2	E	253	GLY	2.7
1	D	199	TYR	2.7
2	B	272	LEU	2.7
1	D	272	LYS	2.7
1	D	71	VAL	2.7
2	E	133	HIS	2.6
2	E	103	LEU	2.6
1	A	255	TRP	2.6
2	E	65	TYR	2.6
2	E	256	LEU	2.6
1	D	255	TRP	2.6
1	D	148	PRO	2.6
1	D	249	VAL	2.6
2	E	56	PHE	2.6
2	E	236	VAL	2.6
1	D	59	LYS	2.6
1	D	227	LYS	2.6
1	D	53	ILE	2.6
2	E	298	THR	2.5
1	D	66	GLY	2.5
1	A	398	GLU	2.5
1	D	317	PHE	2.5
2	E	284	VAL	2.5
1	D	36	LYS	2.5
1	D	44	ALA	2.5
1	A	402	LEU	2.5
1	D	243	LYS	2.5
2	B	355	TYR	2.5
2	E	88	ASN	2.5
2	E	131	ILE	2.5
2	E	272	LEU	2.5
2	E	297	PRO	2.4
1	D	175	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	230	SER	2.4
2	B	175	LEU	2.4
2	E	360	ALA	2.4
1	D	321	ALA	2.4
1	D	129	PHE	2.4
2	E	353	TYR	2.4
1	D	162	ILE	2.4
1	D	262	VAL	2.4
2	B	281	LEU	2.4
1	D	28	MET	2.4
2	B	186	HIS	2.4
1	D	178	PRO	2.4
1	A	224	VAL	2.4
1	A	408	THR	2.4
2	E	93	PHE	2.4
1	D	314	LYS	2.4
2	E	100	ILE	2.4
2	E	366	TRP	2.4
2	B	185	VAL	2.4
1	D	254	SER	2.4
2	E	98	SER	2.4
2	B	181	MET	2.3
1	D	63	LYS	2.3
2	E	214	PRO	2.3
2	E	104	ILE	2.3
1	D	9	LEU	2.3
1	D	298	ALA	2.3
1	A	322	VAL	2.3
1	A	399	LYS	2.3
1	A	279	THR	2.3
1	D	279	THR	2.3
2	E	356	SER	2.3
1	D	304	GLU	2.3
2	E	280	GLU	2.3
1	D	333	VAL	2.3
2	E	130	ASN	2.3
1	D	51	LEU	2.2
1	D	37	ASP	2.2
2	E	216	THR	2.2
2	E	72	ASP	2.2
1	D	21	ILE	2.2
1	A	277	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	144	GLU	2.2
1	D	183	PHE	2.2
1	D	126	LEU	2.2
2	B	353	TYR	2.2
2	E	352	PRO	2.2
1	D	226	SER	2.2
1	D	259	GLU	2.2
2	B	4	GLU	2.2
2	E	228	ASP	2.2
2	E	140	CYS	2.2
2	E	212	GLU	2.2
2	B	351	THR	2.2
1	D	145	TYR	2.2
2	E	81	TYR	2.2
1	A	249	VAL	2.2
1	D	224	VAL	2.2
2	E	354	PHE	2.2
1	D	112	LEU	2.2
1	A	410	GLU	2.2
1	A	404	PRO	2.2
1	D	54	SER	2.2
2	E	129	SER	2.2
1	A	228	ALA	2.1
1	D	264	LYS	2.1
2	E	288	TRP	2.1
2	E	350	ILE	2.1
1	D	180	LEU	2.1
1	D	39	LYS	2.1
1	D	322	VAL	2.1
1	D	95	HIS	2.1
1	D	330	PHE	2.1
1	D	271	ILE	2.1
1	D	58	LYS	2.1
1	D	50	GLN	2.1
2	B	134	THR	2.1
1	D	247	GLU	2.1
1	D	23	LYS	2.1
1	D	246	GLN	2.0
2	E	239	GLU	2.0
1	D	303	ASP	2.0
1	D	142	ARG	2.0
1	D	282	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
2	E	270	GLY	2.0
2	B	132	VAL	2.0
1	A	247	GLU	2.0
1	A	405	SER	2.0
2	E	172	ARG	2.0
2	E	224	ALA	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 monosaccharides in this entry.

6.4 Ligands (i)

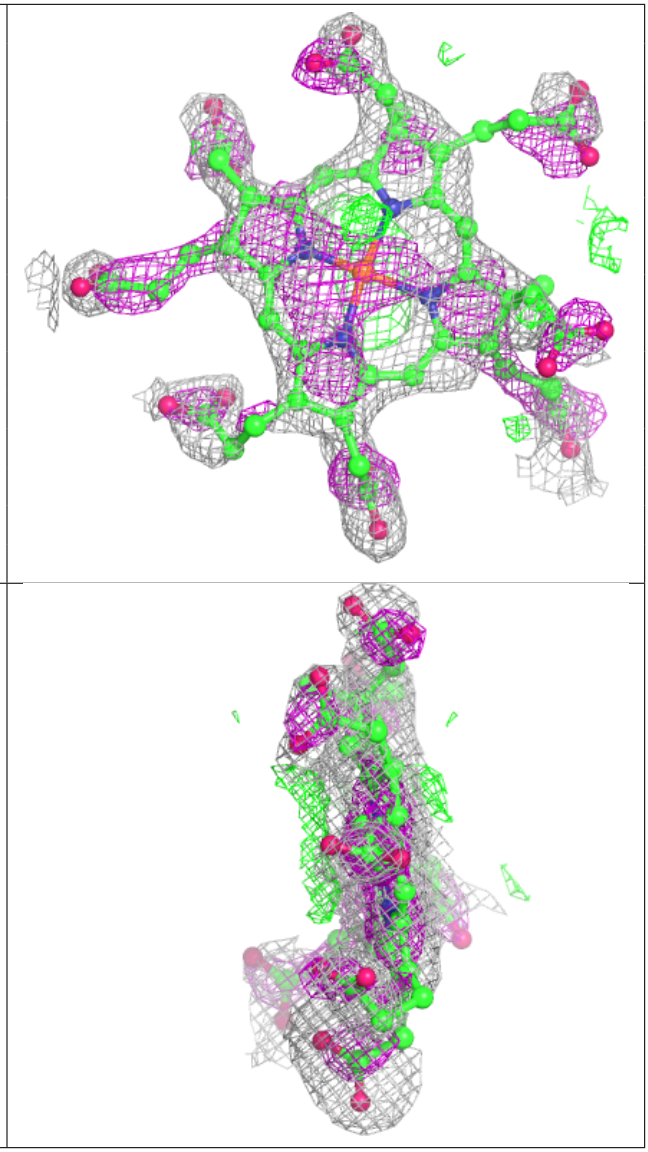
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.85	0.28	40,55,58,60	0
3	SRM	E	570	63/63	0.88	0.25	16,20,24,28	0
4	SF4	D	575	8/8	0.92	0.13	14,15,16,16	0
4	SF4	D	576	8/8	0.92	0.10	17,20,21,22	0
4	SF4	E	585	8/8	0.93	0.17	70,74,77,78	0
4	SF4	A	576	8/8	0.95	0.06	13,14,15,16	0
3	SRM	A	580	63/63	0.95	0.15	23,27,36,40	0
3	SRM	B	570	63/63	0.96	0.14	13,16,20,23	0
4	SF4	E	586	8/8	0.96	0.12	35,38,39,43	0
5	PO4	A	590	5/5	0.97	0.14	59,59,61,63	0
4	SF4	B	586	8/8	0.98	0.06	15,17,18,19	0
4	SF4	A	575	8/8	0.98	0.10	14,16,18,20	0
4	SF4	B	585	8/8	0.98	0.06	21,24,28,29	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.

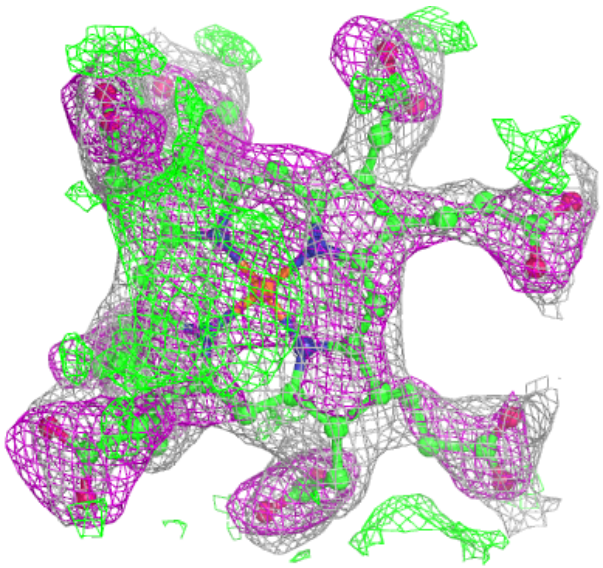
Electron density around SRM D 580:

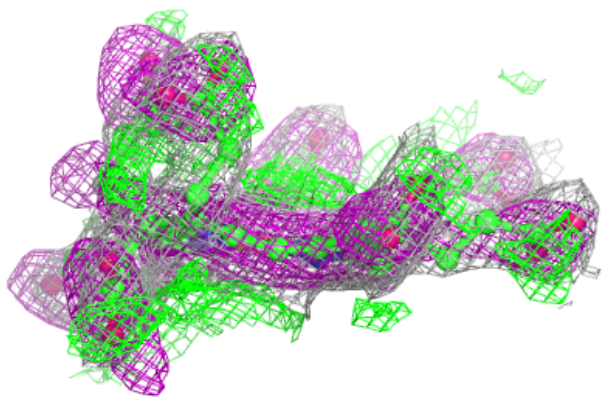
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

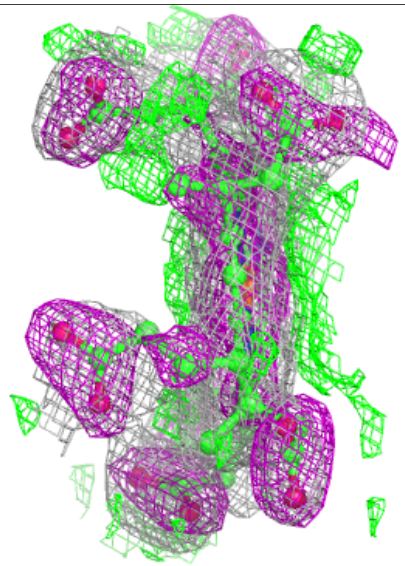


Electron density around SRM E 570:

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

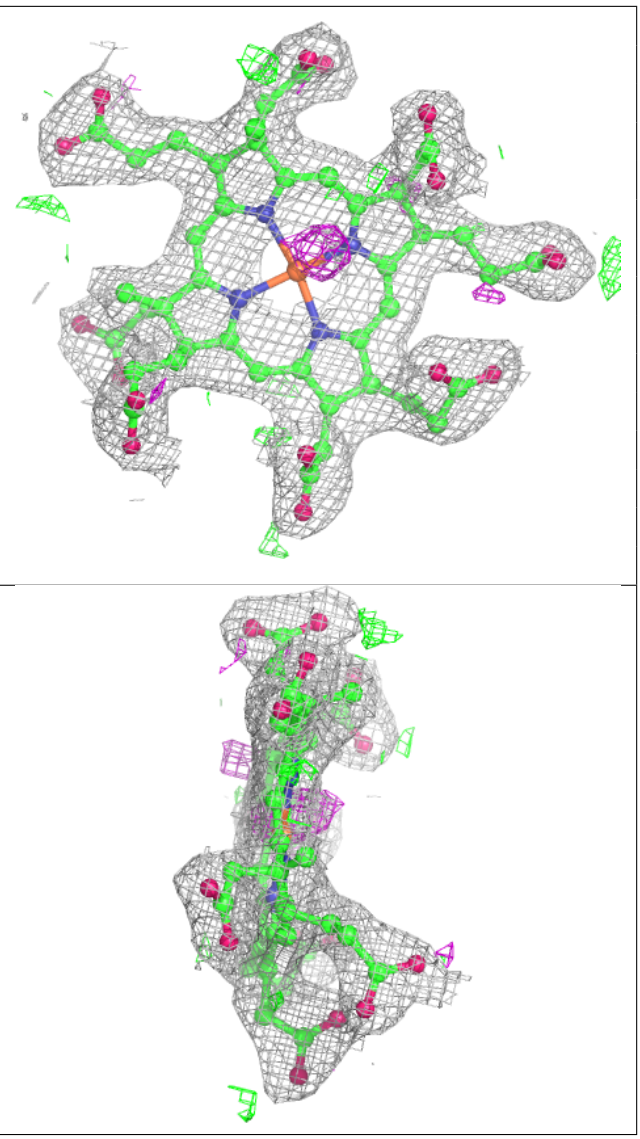






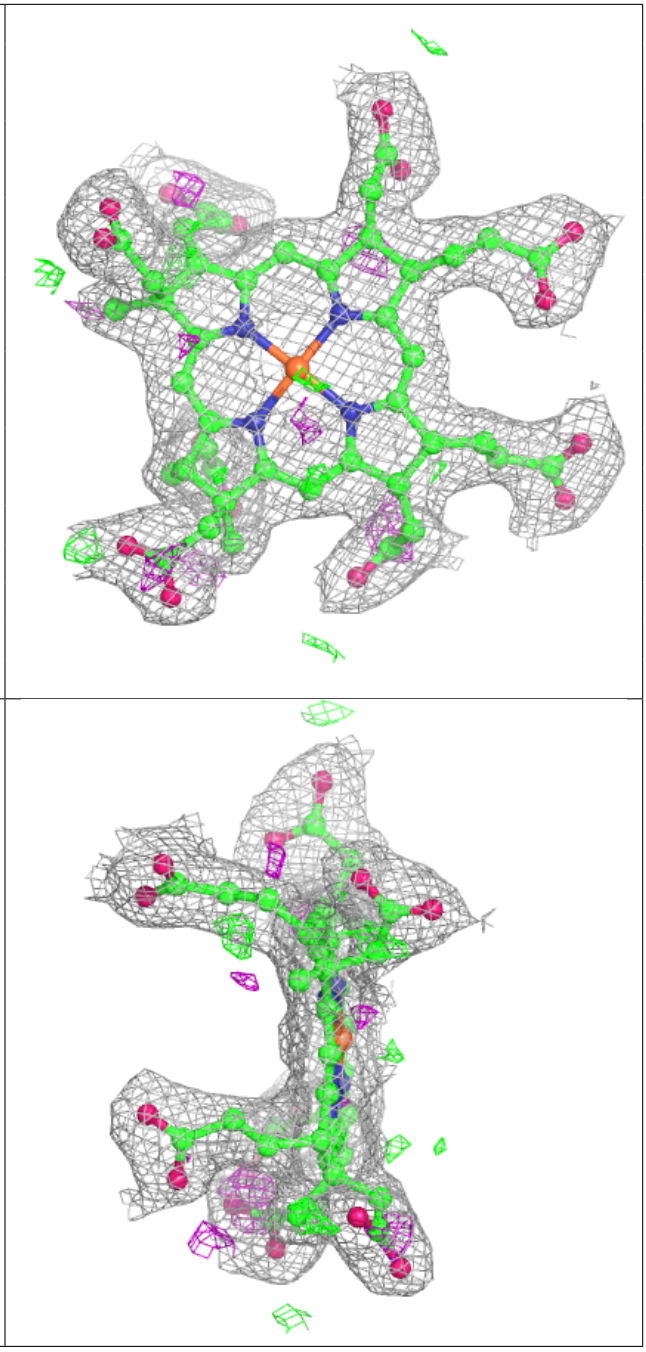
Electron density around SRM A 580:

$2mF_o$-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 (i)

There are no such residues in this entry.