Full wwPDB X-ray Structure Validation Report (i)

Dec 19, 2023 – 12:11 PM EST

PDB ID	:	3MMC
Title	:	Structure of the dissimilatory sulfite reductase from Archaeoglobus fulgidus
Authors	:	Schiffer, A.; Parey, K.; Warkentin, E.; Diederichs, K.; Huber, H.; Stetter, K.O.; Kroneck, P.M.H.; Ermler, U.
Deposited on	:	2010-04-19
Resolution	:	2.04 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:

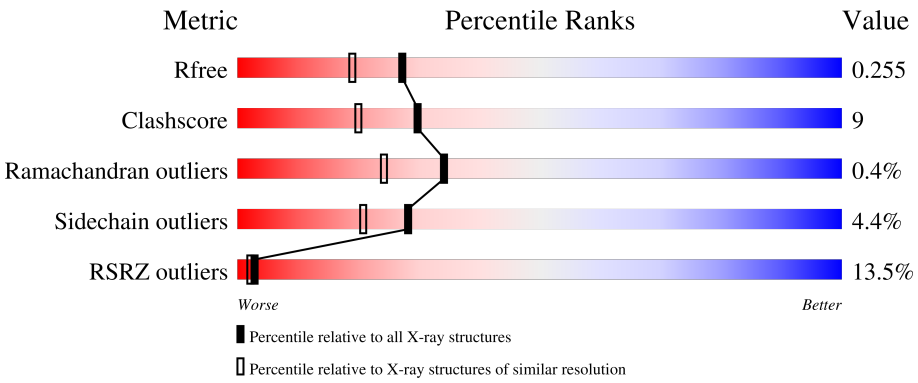
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.04 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	3%, 82%, 16%, •
1	D	418	25%, 83%, 15%, •
2	B	366	%, 83%, 14%, • •
2	E	366	25%, 76%, 21%, • •

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	D	575	-	-	X	-
4	SF4	E	585	-	-	X	-
5	GOL	A	590	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13324 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.

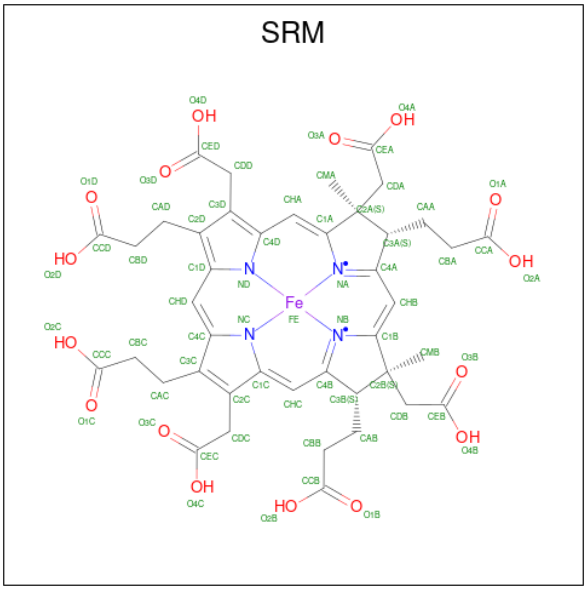
- Molecule 1 is a protein called Sulfite reductase, dissimilatory-type subunit alpha.

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.

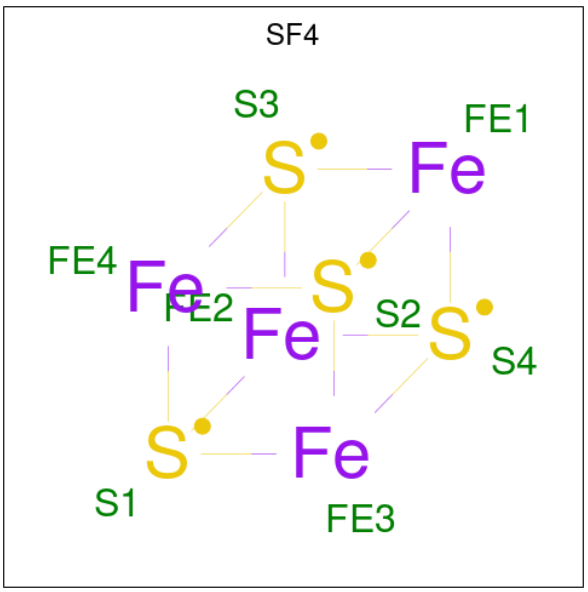
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	363	2901	1862	491	526	22	0	0	0
2	E	363	2901	1862	491	526	22	0	0	0

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



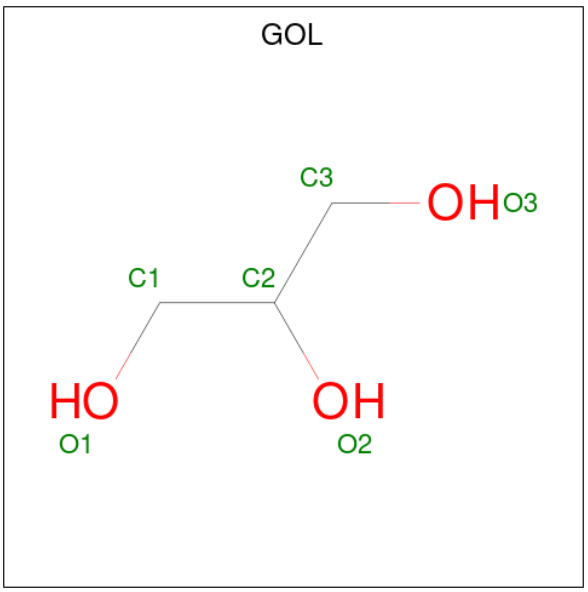
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
3	A	1	63	42	1	4	16	0	0
3	B	1	63	42	1	4	16	0	0
3	D	1	63	42	1	4	16	0	0
3	E	1	63	42	1	4	16	0	0

- 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 GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	6	3	3	0	0

- Molecule 6 is water.

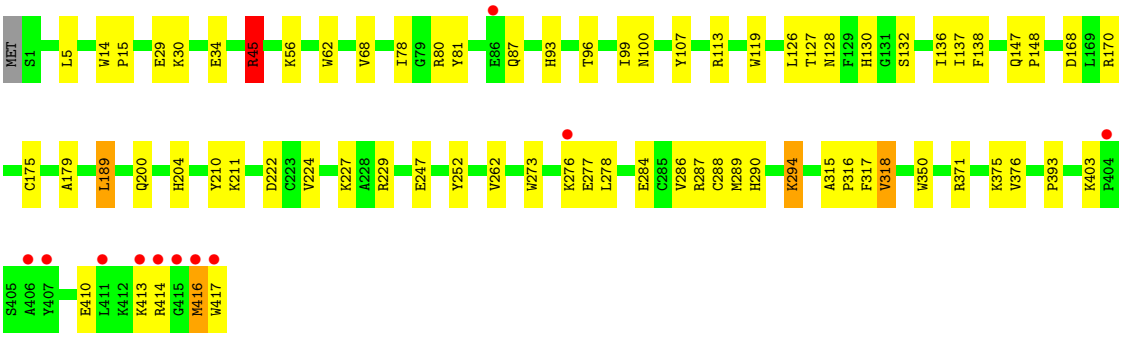
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	220	220	220	0	0
			Total	O		
6	B	265	265	265	0	0
			Total	O		
6	D	39	39	39	0	0
			Total	O		
6	E	18	18	18	0	0

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.

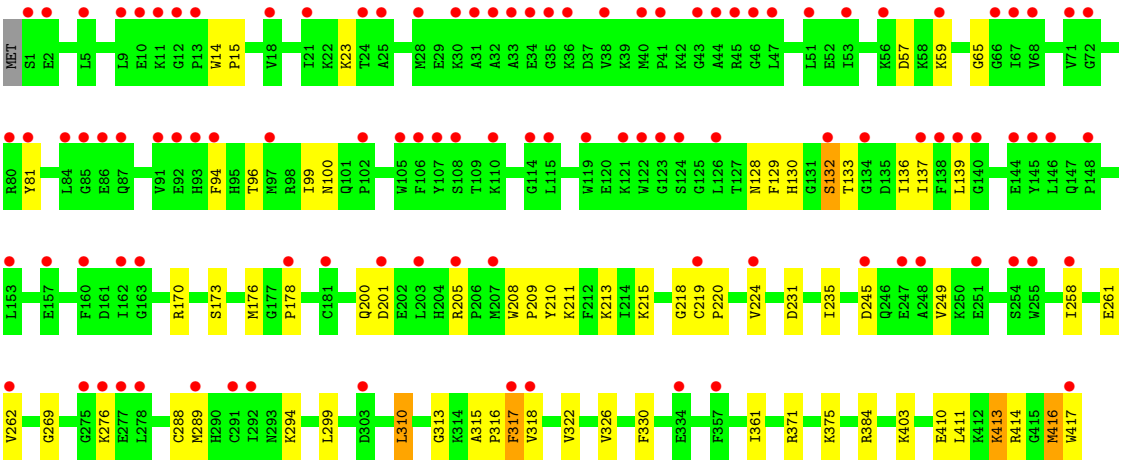
• Molecule 1: Sulfite reductase, dissimilatory-type subunit alpha

Chain A:



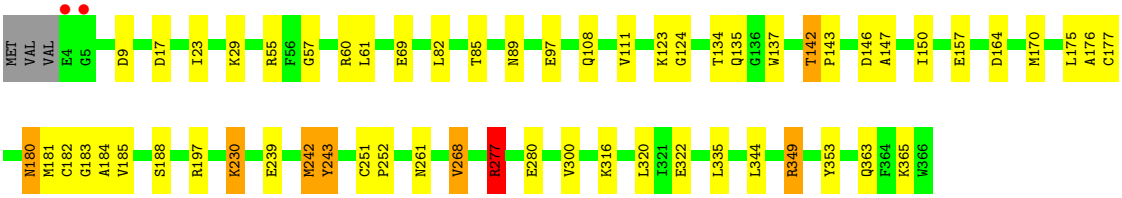
• Molecule 1: Sulfite reductase, dissimilatory-type subunit alpha

Chain D:



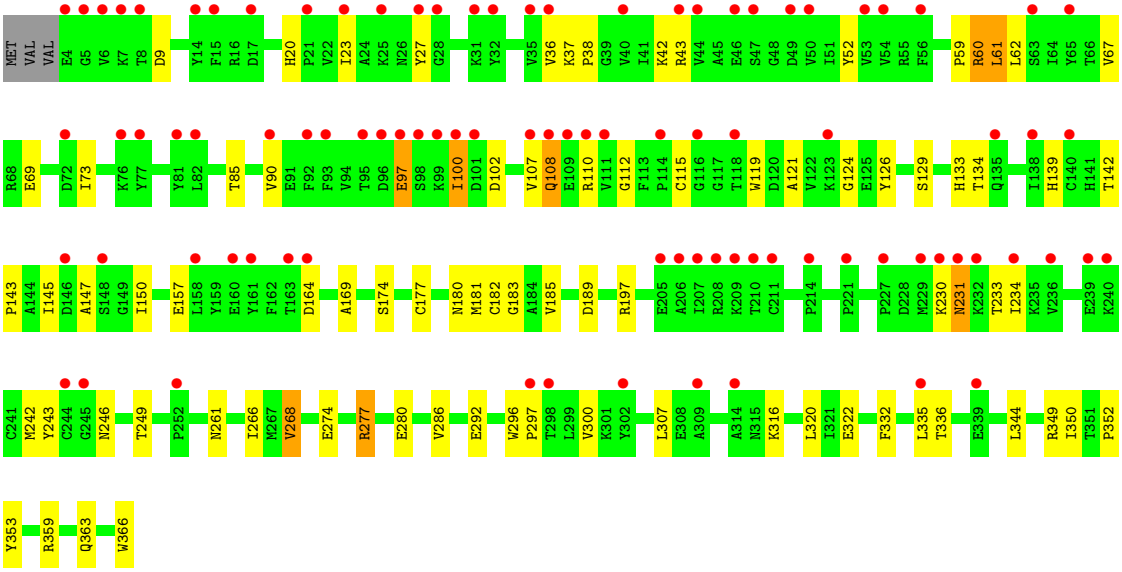
• Molecule 2: Sulfite reductase, dissimilatory-type subunit beta

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	94.91Å 69.26Å 147.21Å 90.00° 107.00° 90.00°	Depositor
Resolution (Å)	20.11 – 2.04 20.07 – 2.04	Depositor EDS
% Data completeness (in resolution range)	97.9 (20.11-2.04) 97.9 (20.07-2.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	3.14 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.6.0046	Depositor
R, R_{free}	0.186 , 0.223 0.227 , 0.255	Depositor DCC
R_{free} test set	5740 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	23.6	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13324	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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: SF4, SRM, GOL

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	0.80	1/3416 (0.0%)	0.78	4/4610 (0.1%)
1	D	0.51	1/3416 (0.0%)	0.60	0/4610
2	B	0.85	0/2984	0.83	6/4058 (0.1%)
2	E	0.52	1/2984 (0.0%)	0.65	0/4058
All	All	0.69	3/12800 (0.0%)	0.72	10/17336 (0.1%)

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
2	B	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	23	LYS	CD-CE	7.93	1.71	1.51
2	E	115	CYS	CB-SG	6.95	1.94	1.82
1	A	175	CYS	CB-SG	-5.71	1.72	1.81

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	277	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	A	45	ARG	NE-CZ-NH2	-6.41	117.09	120.30
2	B	277	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	189	LEU	CB-CG-CD1	6.07	121.31	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	55	ARG	NE-CZ-NH1	6.04	123.32	120.30
2	B	55	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	A	318	VAL	N-CA-C	5.86	126.83	111.00
1	A	287	ARG	NE-CZ-NH2	-5.37	117.62	120.30
2	B	164	ASP	CB-CG-OD2	5.33	123.10	118.30
2	B	17	ASP	CB-CG-OD1	5.04	122.83	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	317	PHE	Peptide
2	B	180	ASN	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	57	0
1	D	3329	0	3276	57	0
2	B	2901	0	2838	62	0
2	E	2901	0	2838	78	0
3	A	63	0	34	7	0
3	B	63	0	34	2	0
3	D	63	0	34	16	0
3	E	63	0	34	13	0
4	A	16	0	0	0	0
4	B	16	0	0	1	0
4	D	16	0	0	2	0
4	E	16	0	0	3	0
5	A	6	0	8	8	0
6	A	220	0	0	2	0
6	B	265	0	0	16	0
6	D	39	0	0	5	0
6	E	18	0	0	2	0
All	All	13324	0	12372	236	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 9.

All (236) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:134:THR:HG21	2:E:182:CYS:HB2	1.39	1.00
3:D:580:SRM:HMB3	2:E:182:CYS:HA	1.50	0.93
2:E:177:CYS:HB2	4:E:585:SF4:S3	2.09	0.92
2:B:134:THR:CG2	6:B:4370:HOH:O	2.17	0.92
2:B:69:GLU:HG2	6:B:4358:HOH:O	1.70	0.92
2:E:90:VAL:HG23	6:E:4492:HOH:O	1.70	0.90
3:E:570:SRM:HDD1	3:E:570:SRM:HBD1	1.51	0.89
1:A:403:LYS:H	2:E:261:ASN:HD21	1.20	0.89
4:D:575:SF4:S4	6:E:4464:HOH:O	2.32	0.86
1:D:128:ASN:HB2	1:D:137:ILE:HB	1.58	0.85
2:E:134:THR:CG2	2:E:182:CYS:HB2	2.05	0.85
2:B:124:GLY:HA3	2:B:316:LYS:HD2	1.60	0.83
1:A:170:ARG:HH22	5:A:590:GOL:H11	1.42	0.83
2:B:183:GLY:N	6:B:4408:HOH:O	2.14	0.81
2:B:60:ARG:HB2	6:B:4420:HOH:O	1.81	0.80
2:E:134:THR:HB	4:E:585:SF4:S4	2.22	0.79
2:E:124:GLY:HA3	2:E:316:LYS:HD2	1.65	0.79
2:B:185:VAL:CG2	6:B:4392:HOH:O	2.30	0.79
2:B:134:THR:HG21	6:B:4370:HOH:O	1.82	0.79
1:D:316:PRO:HG2	2:E:181:MET:HE3	1.67	0.77
2:B:182:CYS:C	6:B:4408:HOH:O	2.24	0.76
3:D:580:SRM:HAB2	2:E:183:GLY:H	1.46	0.76
2:E:52:TYR:CE1	2:E:97:GLU:HB3	2.20	0.76
1:A:211:LYS:HZ3	5:A:590:GOL:H32	1.51	0.75
2:B:261:ASN:HD21	1:D:403:LYS:H	1.32	0.75
1:A:211:LYS:NZ	5:A:590:GOL:H32	2.02	0.73
1:D:316:PRO:HG2	2:E:181:MET:CE	2.19	0.72
2:E:230:LYS:CB	2:E:231:ASN:HB2	2.19	0.72
1:A:371:ARG:O	1:A:375:LYS:HD3	1.90	0.72
3:A:580:SRM:HBA1	3:A:580:SRM:HHB	1.71	0.71
1:A:128:ASN:HD21	2:B:135:GLN:HE22	1.36	0.70
1:A:128:ASN:ND2	2:B:135:GLN:HE22	1.89	0.70
1:A:316:PRO:HG2	2:B:181:MET:HE3	1.72	0.70
1:A:286:VAL:HG23	2:B:363:GLN:HG2	1.74	0.69
2:E:42:LYS:HG3	2:E:52:TYR:CE2	2.28	0.69
1:D:211:LYS:HZ3	3:D:580:SRM:HDA2	1.59	0.67
1:D:176:MET:CE	3:E:570:SRM:HBA2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:ASP:C	6:B:4376:HOH:O	2.32	0.66
1:D:132:SER:HB2	3:D:580:SRM:HBB2	1.76	0.66
1:A:211:LYS:HZ3	5:A:590:GOL:C3	2.08	0.66
2:E:85:THR:HB	3:E:570:SRM:HAB2	1.77	0.66
1:D:14:TRP:CD2	1:D:15:PRO:HD2	2.31	0.65
2:E:230:LYS:HB2	2:E:231:ASN:ND2	2.12	0.64
2:E:119:TRP:HE1	3:E:570:SRM:HDD2	1.63	0.64
2:B:185:VAL:HG21	6:B:4392:HOH:O	1.95	0.64
1:D:211:LYS:NZ	3:D:580:SRM:HDA2	2.12	0.63
2:E:197:ARG:HH21	2:E:261:ASN:HD22	1.43	0.63
1:A:316:PRO:HG2	2:B:181:MET:CE	2.27	0.63
1:A:14:TRP:CD2	1:A:15:PRO:HD2	2.35	0.62
1:D:288:CYS:O	1:D:289:MET:HB2	1.97	0.62
2:E:157:GLU:HG3	2:E:300:VAL:HG11	1.82	0.62
2:E:230:LYS:CA	2:E:231:ASN:HB2	2.29	0.62
1:A:107:TYR:OH	1:A:130:HIS:HE1	1.83	0.61
1:A:262:VAL:HG22	1:A:294:LYS:HG2	1.82	0.61
1:D:261:GLU:HB3	1:D:294:LYS:HE2	1.81	0.61
2:E:266:ILE:HB	2:E:286:VAL:HB	1.84	0.60
1:A:375:LYS:HD2	1:A:375:LYS:N	2.17	0.59
1:A:229:ARG:CD	2:B:184:ALA:HB2	2.32	0.59
1:A:170:ARG:HH12	5:A:590:GOL:H31	1.68	0.58
2:E:292:GLU:HB2	2:E:296:TRP:HA	1.85	0.58
1:A:170:ARG:HH12	5:A:590:GOL:C3	2.16	0.58
2:E:230:LYS:HB2	2:E:231:ASN:HB2	1.86	0.57
1:A:315:ALA:HB1	1:A:316:PRO:HD2	1.87	0.57
2:B:85:THR:HB	3:B:570:SRM:HAB1	1.87	0.56
2:B:147:ALA:HB2	2:B:177:CYS:SG	2.45	0.56
2:B:177:CYS:HB2	4:B:585:SF4:S3	2.46	0.56
2:B:261:ASN:HD21	1:D:403:LYS:N	2.04	0.56
1:D:200:GLN:HE21	2:E:9:ASP:HA	1.70	0.56
3:A:580:SRM:CMB	3:A:580:SRM:CBB	2.84	0.56
2:E:43:ARG:NH2	3:E:570:SRM:O4A	2.32	0.55
1:D:213:LYS:HZ1	3:D:580:SRM:HDB2	1.70	0.55
3:E:570:SRM:CBA	3:E:570:SRM:HHB	2.36	0.55
1:A:119:TRP:CH2	1:A:138:PHE:HB3	2.42	0.55
1:A:276:LYS:HG2	1:A:277:GLU:HG2	1.89	0.55
1:D:258:ILE:HA	1:D:262:VAL:HG23	1.89	0.55
2:B:175:LEU:HD23	2:B:175:LEU:C	2.28	0.54
1:D:57:ASP:HB3	1:D:59:LYS:HG2	1.89	0.54
1:A:286:VAL:CG2	2:B:363:GLN:HG2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:SER:HB2	3:D:580:SRM:CBB	2.38	0.53
1:D:213:LYS:NZ	3:D:580:SRM:HDB2	2.23	0.53
3:E:570:SRM:O4D	3:E:570:SRM:HHA	2.08	0.53
2:E:20:HIS:HB3	2:E:23:ILE:HD12	1.90	0.53
1:D:14:TRP:CG	1:D:15:PRO:HD2	2.44	0.53
1:A:29:GLU:OE2	1:A:45:ARG:HD2	2.09	0.53
1:A:127:THR:O	2:B:61:LEU:HD12	2.08	0.53
2:E:230:LYS:HB2	2:E:231:ASN:CB	2.39	0.53
2:B:57:GLY:HA2	2:B:89:ASN:ND2	2.23	0.53
1:D:262:VAL:HG22	1:D:294:LYS:HG2	1.90	0.53
1:A:30:LYS:O	1:A:34:GLU:HG3	2.09	0.52
2:B:134:THR:HG21	2:B:182:CYS:HB2	1.92	0.52
2:B:146:ASP:O	2:B:150:ILE:HD12	2.10	0.52
1:A:229:ARG:HD3	2:B:184:ALA:HB2	1.92	0.51
2:B:268:VAL:HG13	2:B:320:LEU:CD2	2.40	0.51
1:D:416:MET:O	1:D:417:TRP:HB3	2.09	0.51
1:D:178:PRO:HG2	2:E:27:TYR:CZ	2.46	0.51
2:B:277:ARG:NH2	2:B:280:GLU:OE1	2.40	0.51
1:D:245:ASP:O	1:D:249:VAL:HG23	2.11	0.51
3:A:580:SRM:HBB2	3:A:580:SRM:HMB3	1.91	0.51
2:B:184:ALA:HB3	6:B:4380:HOH:O	2.10	0.50
2:B:349:ARG:NH2	2:E:350:ILE:O	2.44	0.50
1:D:170:ARG:HG3	1:D:213:LYS:HE2	1.94	0.50
1:D:235:ILE:HD12	1:D:310:LEU:HD22	1.93	0.50
2:B:137:TRP:CE3	2:B:146:ASP:HB2	2.46	0.50
1:A:416:MET:O	1:A:417:TRP:HB3	2.12	0.50
1:D:99:ILE:HB	1:D:136:ILE:HB	1.92	0.50
1:D:261:GLU:HB3	1:D:294:LYS:CE	2.42	0.50
1:D:261:GLU:CD	2:E:316:LYS:HE3	2.32	0.49
1:D:317:PHE:CD2	2:E:180:ASN:ND2	2.80	0.49
1:A:403:LYS:N	2:E:261:ASN:HD21	1.98	0.49
2:E:134:THR:CG2	2:E:182:CYS:CB	2.84	0.49
1:A:262:VAL:HG22	1:A:294:LYS:CG	2.42	0.49
2:E:69:GLU:HG2	2:E:110:ARG:HH21	1.78	0.49
2:E:121:ALA:CB	3:E:570:SRM:O3D	2.61	0.49
2:E:268:VAL:HG22	2:E:320:LEU:HD22	1.95	0.49
3:A:580:SRM:C2D	2:B:180:ASN:HB2	2.43	0.49
1:A:62:TRP:HB3	1:A:80:ARG:HD2	1.95	0.49
1:A:410:GLU:O	1:A:414:ARG:HG2	2.13	0.48
2:E:230:LYS:HB2	2:E:231:ASN:HD22	1.79	0.48
2:E:37:LYS:HB2	2:E:38:PRO:CD	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:MET:O	1:A:417:TRP:CB	2.61	0.48
3:D:580:SRM:CAB	2:E:183:GLY:H	2.22	0.48
2:E:277:ARG:HG2	2:E:322:GLU:HG2	1.95	0.48
1:A:99:ILE:HB	1:A:136:ILE:HB	1.94	0.48
2:B:157:GLU:HG3	2:B:300:VAL:HG11	1.95	0.48
2:B:175:LEU:HD23	2:B:176:ALA:N	2.30	0.47
3:E:570:SRM:HDD1	3:E:570:SRM:CBD	2.26	0.47
2:B:134:THR:HG23	6:B:4370:HOH:O	1.97	0.47
2:B:197:ARG:HH21	2:B:261:ASN:HD22	1.63	0.47
1:D:315:ALA:HB1	1:D:316:PRO:CD	2.45	0.47
2:E:145:ILE:HD12	2:E:150:ILE:HD12	1.96	0.47
3:E:570:SRM:HHB	3:E:570:SRM:HBA1	1.95	0.47
2:E:142:THR:N	2:E:143:PRO:HD3	2.29	0.47
1:D:173:SER:OG	1:D:215:LYS:HG2	2.15	0.46
1:D:218:GLY:HA3	4:D:575:SF4:S2	2.54	0.46
1:D:416:MET:O	1:D:417:TRP:CB	2.63	0.46
1:D:213:LYS:NZ	3:D:580:SRM:CDB	2.78	0.46
2:E:296:TRP:N	2:E:297:PRO:HD3	2.30	0.46
2:B:60:ARG:HD3	6:B:4420:HOH:O	2.15	0.46
1:D:129:PHE:HA	1:D:130:HIS:HA	1.73	0.46
3:D:580:SRM:CCD	3:D:580:SRM:HDD1	2.46	0.46
2:E:189:ASP:O	2:E:268:VAL:HA	2.16	0.46
2:E:197:ARG:NH2	2:E:261:ASN:HD22	2.12	0.46
1:D:213:LYS:HZ2	3:D:580:SRM:HDB1	1.81	0.45
1:D:411:LEU:HD13	1:D:417:TRP:HA	1.98	0.45
2:E:108:GLN:H	2:E:108:GLN:HE21	1.64	0.45
2:E:147:ALA:HB2	2:E:177:CYS:SG	2.56	0.45
1:A:130:HIS:HD2	6:B:4031:HOH:O	1.99	0.45
1:A:290:HIS:O	1:A:294:LYS:HB2	2.15	0.45
1:D:317:PHE:HD2	2:E:180:ASN:HD22	1.65	0.45
2:E:73:ILE:HD13	2:E:107:VAL:HG22	1.99	0.45
1:A:119:TRP:CZ3	1:A:138:PHE:HB3	2.52	0.45
2:B:251:CYS:HA	2:B:252:PRO:HD2	1.84	0.45
1:D:176:MET:HE1	3:E:570:SRM:HBA2	1.95	0.45
2:B:349:ARG:HH22	2:E:352:PRO:HD3	1.82	0.45
2:E:142:THR:N	2:E:143:PRO:CD	2.79	0.45
3:E:570:SRM:HCD1	3:E:570:SRM:HAC2	1.78	0.45
1:A:284:GLU:HA	2:B:365:LYS:HD3	1.99	0.45
2:B:29:LYS:HE3	6:B:4374:HOH:O	2.17	0.45
3:D:580:SRM:HAA1	3:D:580:SRM:HDA1	1.71	0.45
1:A:288:CYS:O	1:A:289:MET:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:CYS:CB	6:B:4408:HOH:O	2.64	0.45
1:A:211:LYS:NZ	5:A:590:GOL:C3	2.71	0.44
1:A:81:TYR:CE2	1:A:93:HIS:CD2	3.05	0.44
1:D:201:ASP:OD1	1:D:205:ARG:HD2	2.18	0.44
1:A:222:ASP:OD1	1:A:227:LYS:NZ	2.48	0.44
2:E:126:TYR:CE1	2:E:169:ALA:HA	2.52	0.44
2:B:268:VAL:HG13	2:B:320:LEU:HD22	1.99	0.44
2:E:177:CYS:CB	4:E:585:SF4:S3	2.95	0.44
1:A:393:PRO:HG3	2:E:181:MET:HE2	2.00	0.44
2:B:142:THR:N	2:B:143:PRO:CD	2.81	0.44
6:D:4535:HOH:O	2:E:182:CYS:SG	2.62	0.44
1:A:128:ASN:HB2	1:A:137:ILE:HB	2.00	0.43
2:B:277:ARG:HG2	2:B:322:GLU:HG2	1.99	0.43
1:D:208:TRP:HB3	1:D:209:PRO:CD	2.48	0.43
1:D:219:CYS:HB2	1:D:220:PRO:CD	2.48	0.43
1:D:330:PHE:HB2	2:E:366:TRP:CH2	2.53	0.43
1:D:139:LEU:HD11	2:E:139:HIS:CG	2.54	0.43
1:D:176:MET:HE2	3:E:570:SRM:HBA2	1.99	0.43
1:D:65:GLY:HA3	1:D:81:TYR:CD1	2.53	0.43
2:B:349:ARG:NH2	2:E:352:PRO:HD3	2.34	0.43
1:D:129:PHE:HB2	2:E:62:LEU:HD22	1.99	0.43
2:E:119:TRP:HB2	2:E:126:TYR:CD2	2.53	0.43
1:A:168:ASP:OD1	1:A:170:ARG:HD3	2.19	0.43
2:B:176:ALA:HB1	2:B:181:MET:HA	2.00	0.43
2:B:268:VAL:HG13	2:B:320:LEU:HD21	2.01	0.43
1:A:273:TRP:HB2	1:A:278:LEU:HD12	2.01	0.43
1:D:410:GLU:O	1:D:414:ARG:HG2	2.18	0.43
2:E:62:LEU:HD23	2:E:67:VAL:HG22	2.01	0.43
2:B:82:LEU:N	2:B:82:LEU:HD23	2.34	0.42
1:A:96:THR:HG21	6:A:4356:HOH:O	2.19	0.42
1:A:229:ARG:HD2	2:B:184:ALA:N	2.33	0.42
1:D:310:LEU:HD12	1:D:326:VAL:HA	2.00	0.42
1:A:179:ALA:O	2:B:23:ILE:HG23	2.19	0.42
2:E:174:SER:HB3	2:E:185:VAL:HG22	2.02	0.42
2:E:332:PHE:CE1	2:E:336:THR:HG21	2.55	0.42
1:D:384:ARG:O	2:E:359:ARG:HD2	2.19	0.42
3:A:580:SRM:CMB	3:A:580:SRM:HBB2	2.49	0.42
2:E:277:ARG:NH2	2:E:280:GLU:OE1	2.52	0.42
2:E:60:ARG:HD3	2:E:133:HIS:CE1	2.55	0.42
3:A:580:SRM:O3B	2:B:135:GLN:HG2	2.18	0.42
1:D:128:ASN:OD1	2:E:60:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:ALA:HB3	3:D:580:SRM:HBA1	2.02	0.42
1:D:403:LYS:NZ	6:D:4208:HOH:O	2.52	0.42
2:E:42:LYS:HE2	2:E:42:LYS:HB3	1.86	0.42
2:E:59:PRO:O	2:E:61:LEU:N	2.53	0.42
1:D:269:GLY:HA2	6:D:4331:HOH:O	2.19	0.42
1:A:81:TYR:HE2	1:A:93:HIS:CD2	2.38	0.42
1:D:231:ASP:HB3	1:D:361:ILE:CG2	2.50	0.42
3:D:580:SRM:HMB1	3:D:580:SRM:HAB1	1.85	0.42
2:E:108:GLN:HE21	2:E:108:GLN:N	2.18	0.42
1:A:147:GLN:HB3	1:A:148:PRO:CD	2.50	0.41
1:A:170:ARG:NH1	5:A:590:GOL:H31	2.34	0.41
2:B:353:TYR:HA	2:E:353:TYR:HA	2.02	0.41
2:E:246:ASN:O	2:E:249:THR:HB	2.20	0.41
3:A:580:SRM:HHB	3:A:580:SRM:CBA	2.47	0.41
2:B:242:MET:C	2:B:243:TYR:CG	2.93	0.41
1:A:375:LYS:N	1:A:375:LYS:CD	2.81	0.41
2:B:182:CYS:HB3	6:B:4408:HOH:O	2.21	0.41
2:E:230:LYS:N	2:E:231:ASN:HB2	2.36	0.41
2:B:170:MET:SD	3:B:570:SRM:HBD1	2.60	0.41
1:A:200:GLN:HE21	2:B:9:ASP:HA	1.85	0.41
3:D:580:SRM:CHD	6:D:4535:HOH:O	2.69	0.41
1:A:200:GLN:NE2	1:A:204:HIS:NE2	2.69	0.41
1:A:252:TYR:OH	6:A:4162:HOH:O	2.17	0.41
2:B:69:GLU:OE2	2:B:111:VAL:HG12	2.20	0.41
1:D:413:LYS:HE2	6:D:4364:HOH:O	2.21	0.41
2:E:230:LYS:HB2	2:E:231:ASN:CG	2.41	0.41
1:A:350:TRP:CG	1:A:376:VAL:HG21	2.55	0.41
2:E:100:ILE:H	2:E:100:ILE:HG13	1.61	0.41
1:A:113:ARG:HH11	1:A:113:ARG:HD2	1.77	0.40
2:B:185:VAL:H	2:B:185:VAL:HG23	1.50	0.40
2:B:230:LYS:H	2:B:230:LYS:HG2	1.59	0.40
2:E:108:GLN:HA	2:E:112:GLY:HA2	2.02	0.40
1:D:313:GLY:HA2	1:D:322:VAL:O	2.21	0.40
2:E:233:THR:OG1	2:E:234:ILE:N	2.54	0.40
2:E:274:GLU:OE1	2:E:363:GLN:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	415/418 (99%)	402 (97%)	12 (3%)	1 (0%)	47	39
1	D	415/418 (99%)	395 (95%)	19 (5%)	1 (0%)	47	39
2	B	361/366 (99%)	346 (96%)	14 (4%)	1 (0%)	41	31
2	E	361/366 (99%)	324 (90%)	34 (9%)	3 (1%)	19	10
All	All	1552/1568 (99%)	1467 (94%)	79 (5%)	6 (0%)	34	24

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	318	VAL
2	E	231	ASN
2	E	60	ARG
1	D	318	VAL
2	E	36	VAL
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%)	337 (96%)	16 (4%)	27	20
1	D	353/354 (100%)	338 (96%)	15 (4%)	30	22
2	B	314/317 (99%)	301 (96%)	13 (4%)	30	23
2	E	314/317 (99%)	299 (95%)	15 (5%)	25	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1334/1342 (99%)	1275 (96%)	59 (4%)	28 21

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	45	ARG
1	A	56	LYS
1	A	68	VAL
1	A	78	ILE
1	A	87	GLN
1	A	100	ASN
1	A	126	LEU
1	A	132	SER
1	A	189	LEU
1	A	210	TYR
1	A	224	VAL
1	A	247	GLU
1	A	294	LYS
1	A	413	LYS
1	A	416	MET
2	B	97	GLU
2	B	108	GLN
2	B	123	LYS
2	B	188	SER
2	B	230	LYS
2	B	239	GLU
2	B	242	MET
2	B	243	TYR
2	B	268	VAL
2	B	277	ARG
2	B	335	LEU
2	B	344	LEU
2	B	349	ARG
1	D	94	PHE
1	D	96	THR
1	D	100	ASN
1	D	132	SER
1	D	133	THR
1	D	210	TYR
1	D	224	VAL
1	D	276	LYS

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Mol	Chain	Res	Type
1	D	299	LEU
1	D	310	LEU
1	D	317	PHE
1	D	371	ARG
1	D	375	LYS
1	D	413	LYS
1	D	416	MET
2	E	61	LEU
2	E	97	GLU
2	E	100	ILE
2	E	102	ASP
2	E	108	GLN
2	E	129	SER
2	E	164	ASP
2	E	242	MET
2	E	243	TYR
2	E	268	VAL
2	E	277	ARG
2	E	307	LEU
2	E	335	LEU
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	93	HIS
1	A	128	ASN
1	A	130	HIS
1	A	200	GLN
2	B	89	ASN
2	B	180	ASN
2	B	261	ASN
2	B	313	ASN
2	B	363	GLN
1	D	100	ASN
1	D	200	GLN
2	E	89	ASN
2	E	180	ASN
2	E	231	ASN
2	E	261	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 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	GOL	A	590	-	5,5,5	0.44	0	5,5,5	0.97	0
4	SF4	D	576	1	0,12,12	-	-	-		
4	SF4	B	585	2	0,12,12	-	-	-		
4	SF4	E	585	2,6	0,12,12	-	-	-		
3	SRM	B	570	1	68,70,70	2.03	11 (16%)	81,112,112	3.07	36 (44%)
3	SRM	A	580	2	68,70,70	1.97	17 (25%)	81,112,112	2.84	30 (37%)
4	SF4	A	575	1	0,12,12	-	-	-		
3	SRM	D	580	-	68,70,70	1.99	12 (17%)	81,112,112	2.90	26 (32%)
4	SF4	A	576	1	0,12,12	-	-	-		
4	SF4	E	586	2	0,12,12	-	-	-		
4	SF4	D	575	1	0,12,12	-	-	-		
3	SRM	E	570	1	68,70,70	2.09	10 (14%)	81,112,112	3.04	34 (41%)

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
5	GOL	A	590	-	-	4/4/4/4	-
4	SF4	D	576	1	-	-	0/6/5/5
4	SF4	B	585	2	-	-	0/6/5/5
4	SF4	E	585	2,6	-	-	0/6/5/5
3	SRM	B	570	1	1/1/19/23	13/38/126/126	-
3	SRM	A	580	2	1/1/19/23	11/38/126/126	-
4	SF4	A	575	1	-	-	0/6/5/5
3	SRM	D	580	-	2/2/19/23	20/38/126/126	-
4	SF4	A	576	1	-	-	0/6/5/5
4	SF4	E	586	2	-	-	0/6/5/5
4	SF4	D	575	1	-	-	0/6/5/5
3	SRM	E	570	1	2/2/19/23	20/38/126/126	-

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	570	SRM	C4A-NA	-8.36	1.29	1.35
3	E	570	SRM	C3C-C2C	7.28	1.52	1.36
3	D	580	SRM	C3D-C2D	6.63	1.54	1.39
3	E	570	SRM	C3D-C2D	6.36	1.54	1.39
3	D	580	SRM	C3C-C2C	6.30	1.50	1.36
3	A	580	SRM	C3D-C2D	6.27	1.53	1.39
3	E	570	SRM	C4A-NA	-6.11	1.31	1.35
3	B	570	SRM	C3C-C2C	5.97	1.49	1.36
3	A	580	SRM	C3C-C2C	5.92	1.49	1.36
3	B	570	SRM	C3D-C2D	5.81	1.52	1.39
3	E	570	SRM	C1C-NC	-5.43	1.29	1.39
3	A	580	SRM	C3A-C4A	-5.24	1.40	1.51
3	E	570	SRM	C4C-NC	-5.16	1.29	1.39
3	D	580	SRM	C3B-C4B	-5.14	1.40	1.51
3	D	580	SRM	C3A-C4A	-5.03	1.40	1.51
3	A	580	SRM	C4A-NA	-4.14	1.32	1.35
3	B	570	SRM	C4C-NC	-3.89	1.32	1.39
3	B	570	SRM	C2B-C3B	-3.85	1.44	1.55
3	A	580	SRM	C3B-C4B	-3.58	1.43	1.51
3	E	570	SRM	C1C-C2C	3.46	1.51	1.45
3	A	580	SRM	C1C-C2C	3.45	1.51	1.45
3	E	570	SRM	C4C-C3C	3.43	1.51	1.45
3	D	580	SRM	C1C-NC	-3.31	1.33	1.39
3	D	580	SRM	C4C-NC	-3.25	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	570	SRM	CDC-CEC	3.19	1.56	1.51
3	A	580	SRM	C4C-NC	-3.18	1.33	1.39
3	D	580	SRM	C1C-C2C	3.10	1.50	1.45
3	A	580	SRM	CHD-C4C	3.09	1.39	1.35
3	D	580	SRM	FE-NC	3.07	2.07	1.95
3	B	570	SRM	C1C-NC	-3.02	1.33	1.39
3	B	570	SRM	C1C-C2C	2.90	1.50	1.45
3	B	570	SRM	C4C-C3C	2.84	1.50	1.45
3	A	580	SRM	O3B-CEB	2.55	1.30	1.22
3	A	580	SRM	FE-NA	2.52	2.11	1.97
3	E	570	SRM	CDC-C2C	2.52	1.54	1.51
3	E	570	SRM	CHA-C1A	2.51	1.40	1.35
3	A	580	SRM	FE-NC	2.51	2.05	1.95
3	A	580	SRM	C4C-C3C	2.36	1.49	1.45
3	D	580	SRM	CAB-C3B	-2.36	1.49	1.54
3	E	570	SRM	CAD-C2D	2.30	1.55	1.52
3	B	570	SRM	CHD-C4C	2.25	1.38	1.35
3	A	580	SRM	C4B-NB	2.22	1.36	1.35
3	D	580	SRM	CHD-C4C	2.22	1.38	1.35
3	B	570	SRM	O4C-CEC	-2.21	1.23	1.30
3	D	580	SRM	FE-NA	2.18	2.09	1.97
3	A	580	SRM	C1C-NC	-2.12	1.35	1.39
3	A	580	SRM	CDA-CEA	2.08	1.57	1.50
3	A	580	SRM	CAA-C3A	-2.06	1.49	1.54
3	D	580	SRM	CAD-C2D	2.04	1.55	1.52
3	A	580	SRM	FE-NB	2.01	2.08	1.97

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	570	SRM	C2B-C3B-C4B	11.38	115.47	100.90
3	A	580	SRM	C2A-C3A-C4A	11.13	115.14	100.90
3	E	570	SRM	CDD-C3D-C4D	-10.98	110.71	127.36
3	D	580	SRM	CAA-C3A-C4A	10.00	128.81	111.19
3	D	580	SRM	C2A-C3A-C4A	9.31	112.82	100.90
3	E	570	SRM	C2B-C1B-CHB	-9.23	115.12	123.54
3	D	580	SRM	C2B-C3B-C4B	8.76	112.11	100.90
3	D	580	SRM	CDD-C3D-C4D	-8.35	114.70	127.36
3	E	570	SRM	CAB-C3B-C4B	7.95	125.21	111.19
3	B	570	SRM	CBD-CAD-C2D	7.56	125.53	112.62
3	B	570	SRM	C2B-C1B-CHB	-7.41	116.77	123.54
3	A	580	SRM	CMB-C2B-C3B	7.37	125.70	112.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	580	SRM	CBD-CAD-C2D	7.14	124.81	112.62
3	B	570	SRM	C3B-C2B-C1B	-6.82	89.21	100.92
3	A	580	SRM	C2B-C3B-C4B	6.72	109.51	100.90
3	E	570	SRM	CDD-C3D-C2D	-6.37	115.11	126.49
3	D	580	SRM	C1A-NA-C4A	6.16	112.21	105.23
3	E	570	SRM	C4C-C3C-C2C	-6.16	99.74	106.86
3	B	570	SRM	CMB-C2B-C3B	5.99	123.14	112.08
3	D	580	SRM	CAB-C3B-C4B	5.98	121.73	111.19
3	A	580	SRM	CAA-C3A-C4A	5.91	121.62	111.19
3	E	570	SRM	CAC-C3C-C2C	-5.78	117.33	129.51
3	E	570	SRM	C2B-C3B-C4B	5.73	108.24	100.90
3	B	570	SRM	CBC-CAC-C3C	-5.66	96.90	112.63
3	A	580	SRM	C3A-C2A-C1A	-5.43	91.60	100.92
3	E	570	SRM	C2B-C1B-NB	5.26	119.66	111.21
3	B	570	SRM	C3D-CDD-CED	5.18	120.41	114.21
3	B	570	SRM	C2A-C1A-CHA	-5.08	118.90	123.54
3	E	570	SRM	C3A-C4A-NA	4.84	120.36	110.85
3	D	580	SRM	C3C-C4C-NC	4.83	115.02	110.32
3	E	570	SRM	C4D-CHA-C1A	-4.81	120.60	130.12
3	A	580	SRM	CDA-C2A-C1A	4.79	122.18	107.12
3	D	580	SRM	C4C-C3C-C2C	-4.60	101.53	106.86
3	B	570	SRM	C3C-C4C-NC	4.56	114.76	110.32
3	A	580	SRM	CMB-C2B-CDB	-4.45	103.46	110.80
3	A	580	SRM	C3C-C4C-NC	4.43	114.64	110.32
3	B	570	SRM	C2B-C1B-NB	4.38	118.25	111.21
3	D	580	SRM	CHD-C4C-NC	-4.34	119.73	124.43
3	B	570	SRM	C2A-C1A-NA	4.30	118.13	111.21
3	B	570	SRM	CHD-C4C-C3C	-4.29	118.00	124.93
3	B	570	SRM	C4C-C3C-C2C	-4.29	101.90	106.86
3	A	580	SRM	C4C-C3C-C2C	-4.28	101.91	106.86
3	E	570	SRM	C1C-C2C-C3C	-4.25	101.94	106.86
3	D	580	SRM	CDD-C3D-C2D	-4.21	118.97	126.49
3	D	580	SRM	CHC-C1C-NC	-4.16	119.94	124.44
3	A	580	SRM	CAC-CBC-CCC	-3.94	105.13	113.60
3	E	570	SRM	CAB-C3B-C2B	3.90	124.88	114.14
3	B	570	SRM	CAB-C3B-C4B	3.89	118.05	111.19
3	B	570	SRM	CHC-C1C-C2C	-3.86	118.68	124.94
3	B	570	SRM	C3B-C4B-NB	-3.85	103.28	110.85
3	E	570	SRM	CAC-C3C-C4C	-3.70	117.92	124.89
3	D	580	SRM	CBA-CAA-C3A	3.63	125.22	114.73
3	A	580	SRM	CBB-CAB-C3B	3.63	125.21	114.73
3	E	570	SRM	C3B-C2B-C1B	-3.60	94.73	100.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	580	SRM	C3D-CDD-CED	3.58	118.50	114.21
3	B	570	SRM	CDA-C2A-C1A	3.52	118.17	107.12
3	B	570	SRM	C1C-C2C-C3C	-3.52	102.79	106.86
3	A	580	SRM	C2B-C1B-CHB	-3.50	120.34	123.54
3	A	580	SRM	CAB-C3B-C2B	-3.50	104.51	114.14
3	D	580	SRM	C3D-CDD-CED	-3.44	110.10	114.21
3	E	570	SRM	CAA-CBA-CCA	3.30	121.27	112.51
3	B	570	SRM	C2C-C1C-NC	3.30	113.53	110.32
3	E	570	SRM	C3C-C4C-NC	3.27	113.50	110.32
3	A	580	SRM	CDD-C3D-C2D	-3.21	120.75	126.49
3	E	570	SRM	CAD-C2D-C3D	-3.16	114.94	124.90
3	E	570	SRM	C2A-C3A-C4A	-3.15	96.88	100.90
3	A	580	SRM	C3B-C2B-C1B	-3.11	95.58	100.92
3	B	570	SRM	CHC-C1C-NC	3.09	127.78	124.44
3	A	580	SRM	CAC-C3C-C4C	3.02	130.59	124.89
3	D	580	SRM	C3B-C2B-C1B	-3.00	95.77	100.92
3	D	580	SRM	C4B-NB-C1B	3.00	108.63	105.23
3	E	570	SRM	C4C-NC-C1C	3.00	108.29	105.35
3	D	580	SRM	C1C-C2C-C3C	-3.00	103.39	106.86
3	A	580	SRM	C2B-C1B-NB	2.99	116.03	111.21
3	B	570	SRM	CMA-C2A-CDA	-2.98	105.90	110.80
3	D	580	SRM	C3A-C4A-CHB	2.97	129.74	123.32
3	B	570	SRM	CBB-CAB-C3B	2.97	123.29	114.73
3	B	570	SRM	CAA-CBA-CCA	2.95	120.33	112.51
3	E	570	SRM	C3A-C4A-CHB	-2.95	116.96	123.32
3	A	580	SRM	CAB-C3B-C4B	-2.94	106.01	111.19
3	B	570	SRM	C3A-C4A-NA	2.91	116.56	110.85
3	B	570	SRM	CAA-C3A-C2A	-2.89	106.17	114.14
3	B	570	SRM	CAD-CBD-CCD	-2.77	106.00	113.76
3	B	570	SRM	CAC-C3C-C4C	2.76	130.10	124.89
3	E	570	SRM	C2A-C1A-CHA	-2.75	121.03	123.54
3	A	580	SRM	C2A-C1A-NA	2.75	115.64	111.21
3	D	580	SRM	C3A-C2A-C1A	-2.70	96.28	100.92
3	D	580	SRM	CBD-CAD-C2D	2.68	117.19	112.62
3	D	580	SRM	CAD-C2D-C3D	-2.65	116.56	124.90
3	E	570	SRM	C2A-C1A-NA	2.63	115.44	111.21
3	E	570	SRM	C2C-C1C-NC	2.59	112.84	110.32
3	A	580	SRM	O2B-CCB-CBB	2.55	122.21	114.03
3	E	570	SRM	CHC-C1C-C2C	-2.54	120.82	124.94
3	B	570	SRM	CAC-C3C-C2C	-2.50	124.24	129.51
3	B	570	SRM	CAA-C3A-C4A	-2.46	106.85	111.19
3	A	580	SRM	C1C-C2C-C3C	-2.46	104.01	106.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	570	SRM	C1A-NA-C4A	-2.46	102.45	105.23
3	D	580	SRM	C2C-C1C-NC	2.46	112.71	110.32
3	B	570	SRM	C2A-C3A-C4A	2.45	104.03	100.90
3	E	570	SRM	CBC-CAC-C3C	-2.44	105.84	112.63
3	A	580	SRM	C1A-NA-C4A	2.44	108.00	105.23
3	B	570	SRM	C1C-CHC-C4B	-2.44	120.73	126.62
3	A	580	SRM	CHD-C4C-C3C	-2.40	121.05	124.93
3	D	580	SRM	C3A-C4A-NA	-2.37	106.18	110.85
3	A	580	SRM	CMA-C2A-C3A	-2.33	107.77	112.08
3	B	570	SRM	C3A-C2A-C1A	-2.32	96.93	100.92
3	A	580	SRM	O4A-CEA-O3A	-2.32	117.52	123.30
3	E	570	SRM	O4A-CEA-CDA	2.27	121.63	114.35
3	A	580	SRM	CAD-CBD-CCD	-2.27	107.40	113.76
3	E	570	SRM	C1C-CHC-C4B	-2.26	121.18	126.62
3	A	580	SRM	O3D-CED-CDD	-2.23	116.67	123.04
3	E	570	SRM	CDA-C2A-C3A	2.22	114.34	108.39
3	B	570	SRM	CEC-CDC-C2C	-2.22	108.03	113.79
3	E	570	SRM	C1A-NA-C4A	-2.21	102.73	105.23
3	B	570	SRM	O2A-CCA-CBA	2.15	120.94	114.03
3	D	580	SRM	CBB-CAB-C3B	2.15	120.93	114.73
3	D	580	SRM	C3B-C4B-CHC	2.13	127.92	123.32
3	E	570	SRM	O3D-CED-CDD	-2.11	117.01	123.04
3	E	570	SRM	O1C-CCC-CBC	-2.09	116.35	123.08
3	E	570	SRM	CDB-C2B-C3B	2.08	113.97	108.39
3	A	580	SRM	C4C-NC-C1C	2.07	107.38	105.35
3	E	570	SRM	CMA-C2A-C3A	-2.06	108.28	112.08
3	D	580	SRM	C4D-CHA-C1A	-2.06	126.05	130.12
3	D	580	SRM	C4C-NC-C1C	2.04	107.34	105.35
3	E	570	SRM	O4D-CED-CDD	2.03	121.72	114.02
3	B	570	SRM	CDD-C3D-C4D	-2.00	124.33	127.36

All (6) chirality outliers are listed below:

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

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	570	SRM	C4A-C3A-CAA-CBA
3	D	580	SRM	C1A-C2A-CDA-CEA
3	D	580	SRM	C4A-C3A-CAA-CBA
3	D	580	SRM	C1B-C2B-CDB-CEB
3	D	580	SRM	C1D-C2D-CAD-CBD
3	E	570	SRM	C1B-C2B-CDB-CEB
3	E	570	SRM	C4C-C3C-CAC-CBC
3	E	570	SRM	C1D-C2D-CAD-CBD
5	A	590	GOL	O1-C1-C2-O2
5	A	590	GOL	O1-C1-C2-C3
5	A	590	GOL	C1-C2-C3-O3
3	E	570	SRM	C3B-CAB-CBB-CCB
3	B	570	SRM	C4B-C3B-CAB-CBB
3	D	580	SRM	C3C-CAC-CBC-CCC
3	E	570	SRM	C2B-C3B-CAB-CBB
3	E	570	SRM	CMB-C2B-CDB-CEB
3	E	570	SRM	C3B-C2B-CDB-CEB
3	D	580	SRM	C2D-CAD-CBD-CCD
3	A	580	SRM	C2A-C3A-CAA-CBA
5	A	590	GOL	O2-C2-C3-O3
3	D	580	SRM	CMA-C2A-CDA-CEA
3	D	580	SRM	CMB-C2B-CDB-CEB
3	B	570	SRM	C2B-CDB-CEB-O3B
3	E	570	SRM	C2B-CDB-CEB-O4B
3	E	570	SRM	C2D-C3D-CDD-CED
3	A	580	SRM	C3B-CAB-CBB-CCB
3	B	570	SRM	C2B-CDB-CEB-O4B
3	E	570	SRM	C2B-CDB-CEB-O3B
3	E	570	SRM	C3D-CDD-CED-O4D
3	D	580	SRM	C2C-CDC-CEC-O3C
3	A	580	SRM	C1D-C2D-CAD-CBD
3	E	570	SRM	C3D-CDD-CED-O3D
3	E	570	SRM	C2A-CDA-CEA-O3A
3	A	580	SRM	C2B-C3B-CAB-CBB
3	D	580	SRM	C2C-CDC-CEC-O4C
3	A	580	SRM	CAB-CBB-CCB-O2B
3	A	580	SRM	CAB-CBB-CCB-O1B
3	B	570	SRM	CAA-CBA-CCA-O1A
3	B	570	SRM	CAD-CBD-CCD-O1D
3	D	580	SRM	CAD-CBD-CCD-O1D
3	B	570	SRM	C3C-CAC-CBC-CCC
3	B	570	SRM	CAA-CBA-CCA-O2A
3	B	570	SRM	CAC-CBC-CCC-O1C

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Mol	Chain	Res	Type	Atoms
3	E	570	SRM	CAD-CBD-CCD-O1D
3	D	580	SRM	CAD-CBD-CCD-O2D
3	E	570	SRM	C3A-CAA-CBA-CCA
3	B	570	SRM	CAC-CBC-CCC-O2C
3	E	570	SRM	CAD-CBD-CCD-O2D
3	E	570	SRM	C4A-C3A-CAA-CBA
3	B	570	SRM	CAD-CBD-CCD-O2D
3	D	580	SRM	CAC-CBC-CCC-O1C
3	E	570	SRM	C2A-CDA-CEA-O4A
3	D	580	SRM	CAC-CBC-CCC-O2C
3	D	580	SRM	CAA-CBA-CCA-O1A
3	A	580	SRM	CAC-CBC-CCC-O1C
3	D	580	SRM	CAA-CBA-CCA-O2A
3	E	570	SRM	CAC-CBC-CCC-O1C
3	D	580	SRM	CAB-CBB-CCB-O2B
3	A	580	SRM	CAC-CBC-CCC-O2C
3	B	570	SRM	CAB-CBB-CCB-O1B
3	B	570	SRM	CAB-CBB-CCB-O2B
3	D	580	SRM	CAB-CBB-CCB-O1B
3	A	580	SRM	CAA-CBA-CCA-O1A
3	E	570	SRM	CAC-CBC-CCC-O2C
3	A	580	SRM	C4D-C3D-CDD-CED
3	D	580	SRM	C2B-C3B-CAB-CBB
3	D	580	SRM	C4B-C3B-CAB-CBB
3	A	580	SRM	CAA-CBA-CCA-O2A

There are no ring outliers.

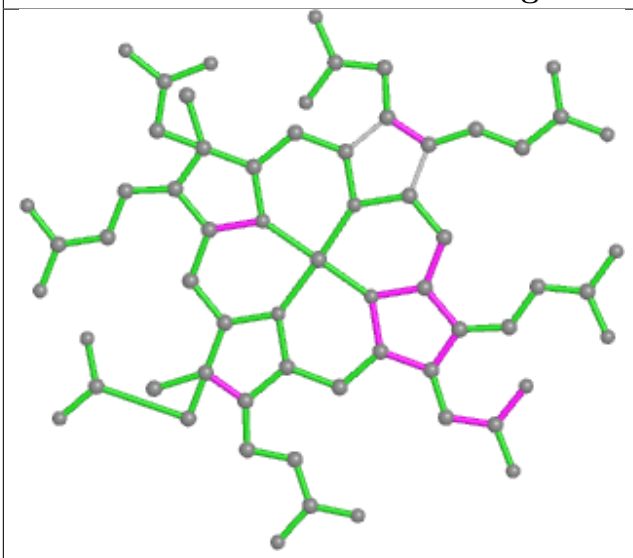
8 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	590	GOL	8	0
4	B	585	SF4	1	0
4	E	585	SF4	3	0
3	B	570	SRM	2	0
3	A	580	SRM	7	0
3	D	580	SRM	16	0
4	D	575	SF4	2	0
3	E	570	SRM	13	0

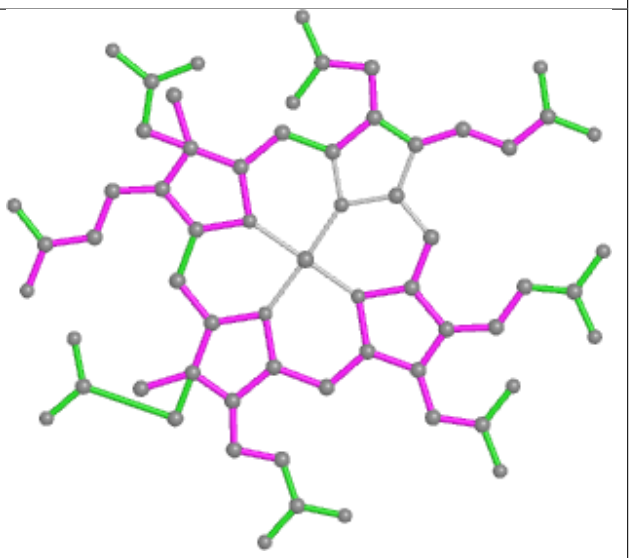
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

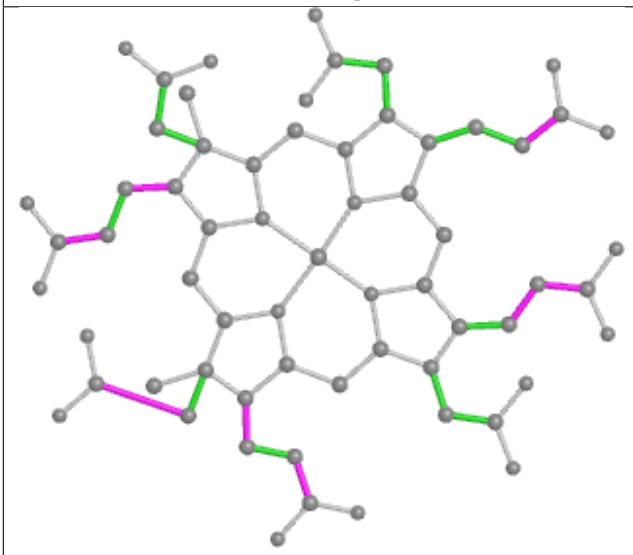
Ligand SRM B 570



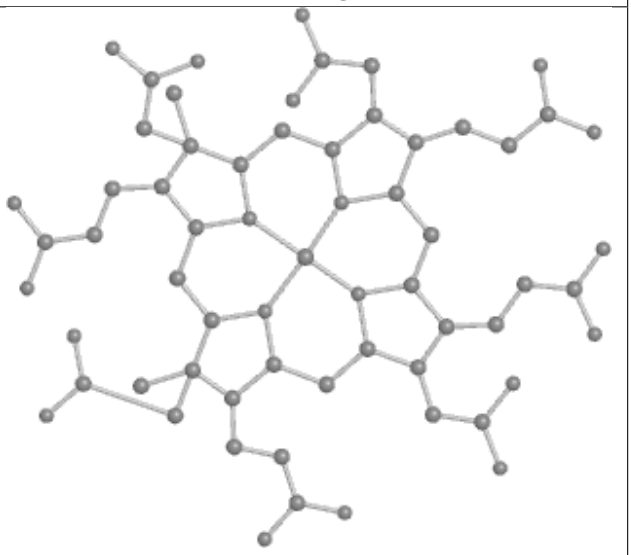
Bond lengths



Bond angles

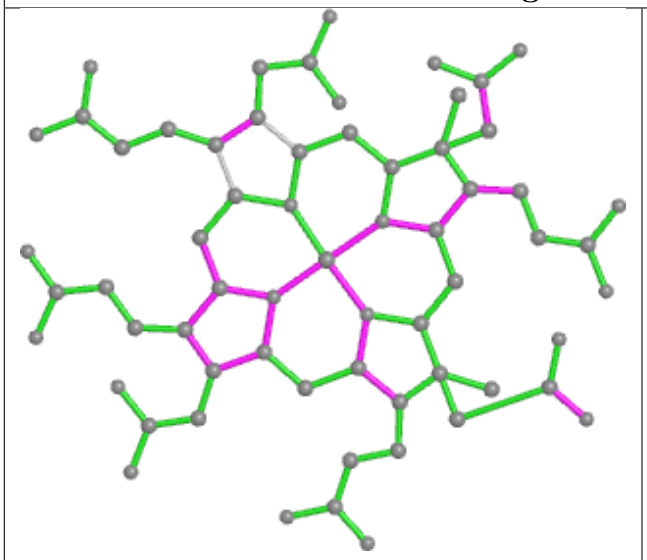


Torsions

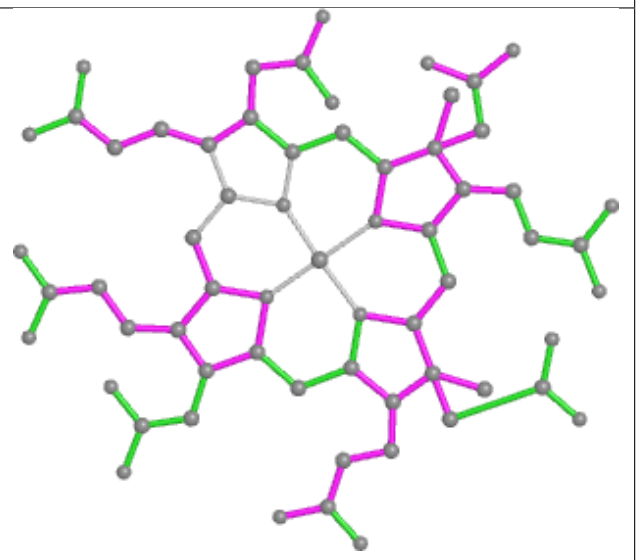


Rings

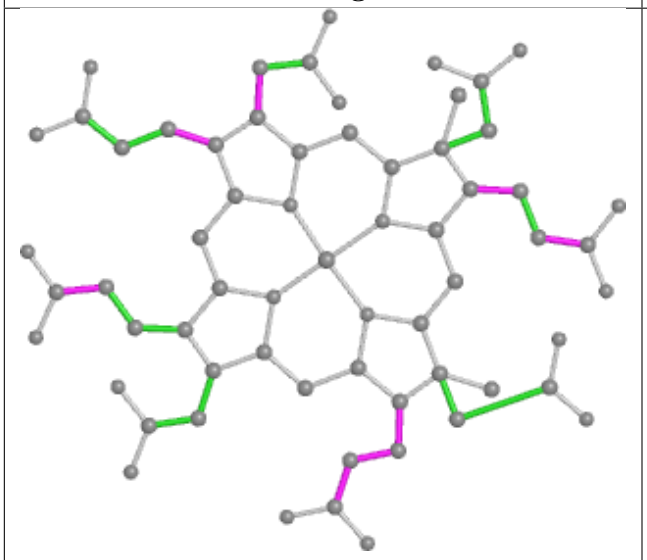
Ligand SRM A 580



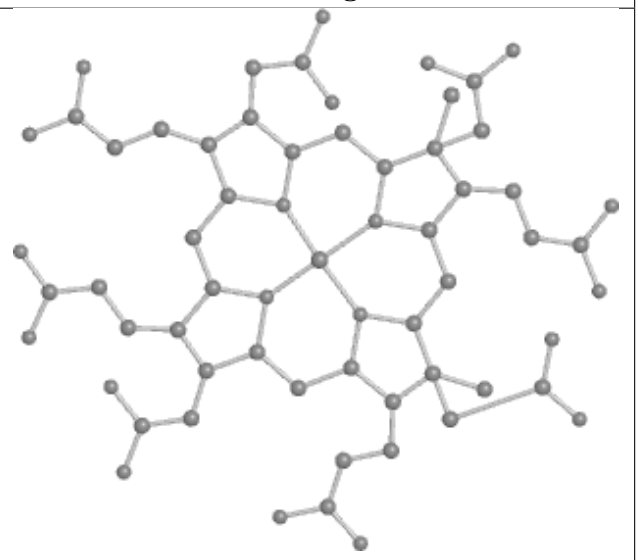
Bond lengths



Bond angles

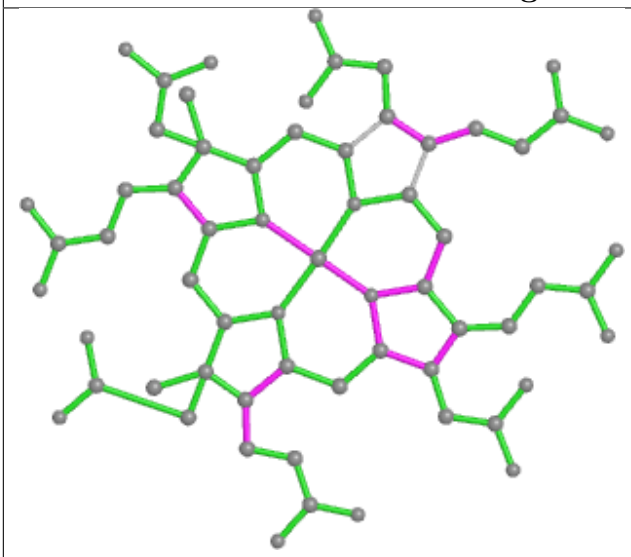


Torsions

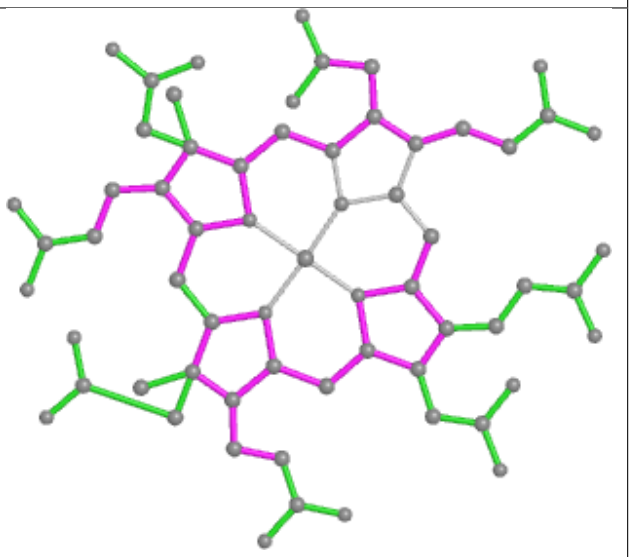


Rings

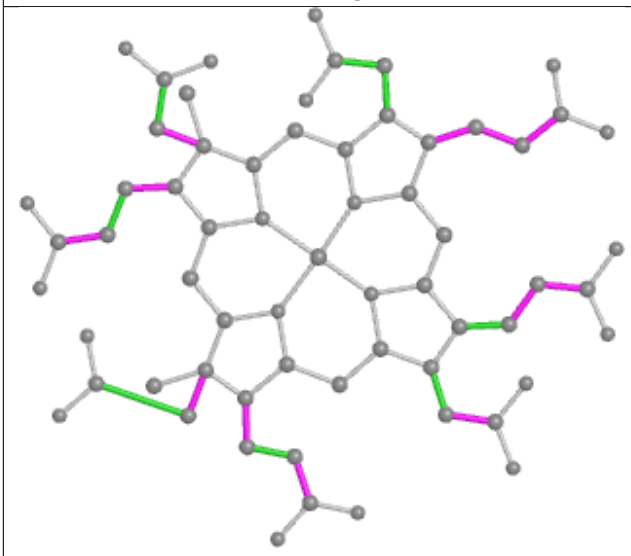
Ligand SRM D 580



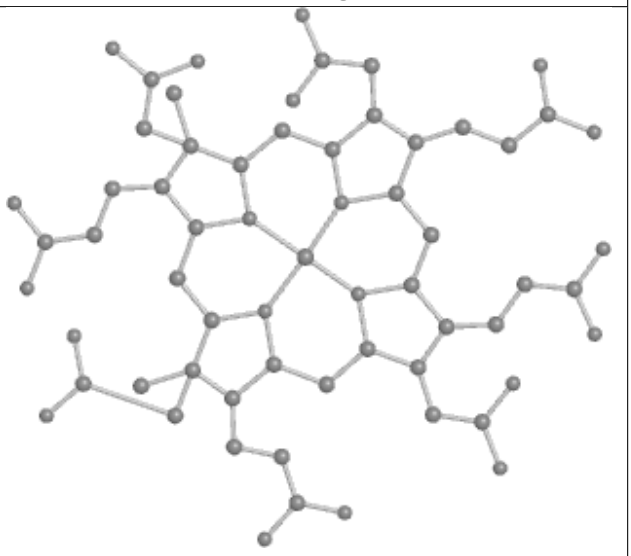
Bond lengths



Bond angles

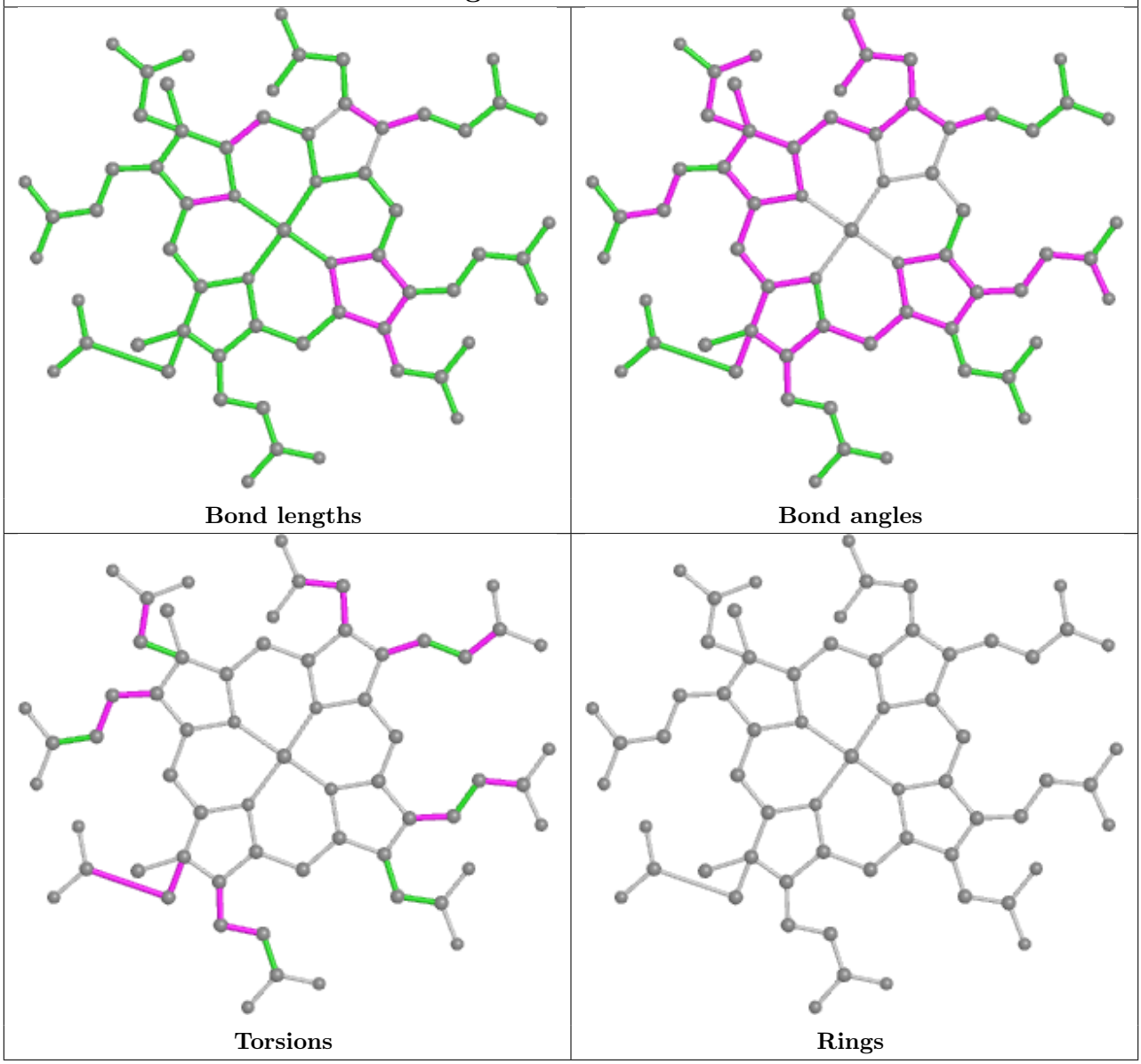


Torsions



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%)	0.03	11 (2%) 56 60	5, 12, 25, 58	0
1	D	417/418 (99%)	1.28	106 (25%) 0 0	4, 13, 25, 41	0
2	B	363/366 (99%)	-0.12	2 (0%) 89 91	5, 11, 19, 57	0
2	E	363/366 (99%)	1.32	91 (25%) 0 0	2, 12, 33, 54	0
All	All	1560/1568 (99%)	0.63	210 (13%) 3 2	2, 12, 26, 58	0

All (210) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	415	GLY	7.3
1	D	132	SER	7.0
1	D	67	ILE	6.8
1	D	71	VAL	6.7
2	E	4	GLU	6.4
2	E	5	GLY	6.2
2	E	6	VAL	5.9
2	E	7	LYS	5.8
1	D	86	GLU	5.8
1	D	33	ALA	5.4
2	E	100	ILE	5.4
1	D	51	LEU	5.4
1	D	157	GLU	5.2
1	A	413	LYS	5.2
2	E	229	MET	5.1
1	D	47	LEU	5.1
1	D	30	LYS	5.0
1	D	94	PHE	5.0
1	D	144	GLU	5.0
2	E	230	LYS	4.9
1	D	255	TRP	4.9

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Mol	Chain	Res	Type	RSRZ
2	E	82	LEU	4.9
2	E	92	PHE	4.9
2	E	93	PHE	4.9
1	D	145	TYR	4.8
1	D	148	PRO	4.8
1	D	122	TRP	4.7
2	E	81	TYR	4.6
2	E	207	ILE	4.6
1	A	406	ALA	4.5
1	D	13	PRO	4.4
2	B	4	GLU	4.3
2	E	116	GLY	4.3
2	E	53	VAL	4.2
1	D	291	CYS	4.2
1	D	247	GLU	4.2
2	E	23	ILE	4.2
2	E	111	VAL	4.2
1	D	276	LYS	4.2
1	D	2	GLU	4.1
2	E	54	VAL	4.1
2	E	232	LYS	4.1
1	D	417	TRP	4.0
1	D	12	GLY	4.0
1	D	110	LYS	4.0
2	E	234	ILE	3.9
1	A	276	LYS	3.9
2	E	109	GLU	3.8
2	E	21	PRO	3.8
1	D	1	SER	3.7
2	E	231	ASN	3.7
1	D	207	MET	3.7
1	A	417	TRP	3.6
2	E	205	GLU	3.6
2	E	46	GLU	3.6
1	D	219	CYS	3.5
2	E	110	ARG	3.5
1	D	68	VAL	3.5
2	E	107	VAL	3.5
1	D	40	MET	3.4
2	E	40	VAL	3.4
2	E	95	THR	3.4
2	E	164	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
2	E	211	CYS	3.4
1	D	36	LYS	3.4
2	E	123	LYS	3.4
1	D	107	TYR	3.4
1	D	357	PHE	3.4
1	D	292	ILE	3.4
2	E	209	LYS	3.3
1	D	251	GLU	3.3
1	A	414	ARG	3.3
1	D	72	GLY	3.3
1	D	126	LEU	3.3
1	D	163	GLY	3.3
2	B	5	GLY	3.3
1	A	411	LEU	3.3
1	D	81	TYR	3.3
1	D	66	GLY	3.3
1	D	102	PRO	3.2
2	E	101	ASP	3.2
2	E	17	ASP	3.2
1	A	404	PRO	3.2
1	D	162	ILE	3.2
1	D	80	ARG	3.2
2	E	49	ASP	3.2
1	D	11	LYS	3.1
2	E	72	ASP	3.1
2	E	35	VAL	3.1
2	E	43	ARG	3.0
1	D	248	ALA	3.0
2	E	32	TYR	3.0
2	E	239	GLU	3.0
2	E	298	THR	2.9
2	E	135	GLN	2.9
2	E	208	ARG	2.9
1	A	86	GLU	2.9
2	E	77	TYR	2.9
1	D	59	LYS	2.9
1	D	53	ILE	2.8
1	D	31	ALA	2.8
2	E	15	PHE	2.8
1	D	115	LEU	2.8
1	D	25	ALA	2.8
2	E	160	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
2	E	28	GLY	2.8
1	D	9	LEU	2.8
1	D	317	PHE	2.7
1	D	84	LEU	2.7
1	D	123	GLY	2.7
2	E	96	ASP	2.7
2	E	56	PHE	2.7
2	E	118	THR	2.7
1	D	178	PRO	2.7
1	D	24	THR	2.7
2	E	8	THR	2.7
1	D	181	CYS	2.7
2	E	99	LYS	2.7
1	D	91	VAL	2.6
2	E	163	THR	2.6
1	D	318	VAL	2.6
2	E	244	CYS	2.6
1	D	138	PHE	2.6
1	D	34	GLU	2.6
2	E	98	SER	2.6
1	D	5	LEU	2.6
1	D	45	ARG	2.6
2	E	14	TYR	2.6
1	D	32	ALA	2.6
1	D	44	ALA	2.6
1	D	21	ILE	2.6
2	E	108	GLN	2.5
2	E	158	LEU	2.5
1	D	18	VAL	2.5
2	E	36	VAL	2.5
1	D	41	PRO	2.5
2	E	25	LYS	2.5
1	D	205	ARG	2.5
1	D	114	GLY	2.5
1	D	160	PHE	2.5
2	E	297	PRO	2.5
1	D	87	GLN	2.5
2	E	245	GLY	2.5
1	D	119	TRP	2.4
2	E	27	TYR	2.4
1	D	258	ILE	2.4
1	A	416	MET	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	221	PRO	2.4
2	E	97	GLU	2.4
1	D	85	GLY	2.4
2	E	50	VAL	2.4
1	D	92	GLU	2.4
2	E	76	LYS	2.4
2	E	236	VAL	2.4
2	E	114	PRO	2.4
1	D	97	MET	2.4
1	D	140	GLY	2.4
2	E	161	TYR	2.4
2	E	339	GLU	2.3
1	D	108	SER	2.3
1	D	124	SER	2.3
2	E	206	ALA	2.3
2	E	302	TYR	2.3
1	D	106	PHE	2.3
1	D	139	LEU	2.3
1	D	303	ASP	2.3
2	E	65	TYR	2.3
2	E	44	VAL	2.3
1	D	254	SER	2.3
1	D	245	ASP	2.3
1	D	277	GLU	2.3
1	D	56	LYS	2.2
2	E	210	THR	2.2
1	D	224	VAL	2.2
1	D	334	GLU	2.2
2	E	63	SER	2.2
1	D	278	LEU	2.2
1	D	201	ASP	2.2
1	D	28	MET	2.2
2	E	309	ALA	2.2
1	D	153	LEU	2.2
1	D	93	HIS	2.2
2	E	335	LEU	2.2
1	D	262	VAL	2.2
1	D	10	GLU	2.2
2	E	148	SER	2.2
2	E	138	ILE	2.1
1	D	105	TRP	2.1
1	D	134	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	227	PRO	2.1
1	D	46	GLY	2.1
2	E	252	PRO	2.1
1	D	121	LYS	2.1
1	D	137	ILE	2.1
1	D	43	GLY	2.1
1	D	289	MET	2.1
2	E	314	ALA	2.1
2	E	90	VAL	2.1
1	A	407	TYR	2.1
2	E	214	PRO	2.1
2	E	31	LYS	2.1
1	D	275	GLY	2.1
2	E	47	SER	2.0
1	D	146	LEU	2.0
2	E	240	LYS	2.0
1	D	35	GLY	2.0
1	D	203	LEU	2.0
2	E	146	ASP	2.0
2	E	140	CYS	2.0
1	D	38	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no 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	0.81	0.42	40,56,68,71	0
3	SRM	E	570	63/63	0.84	0.42	11,15,19,22	0

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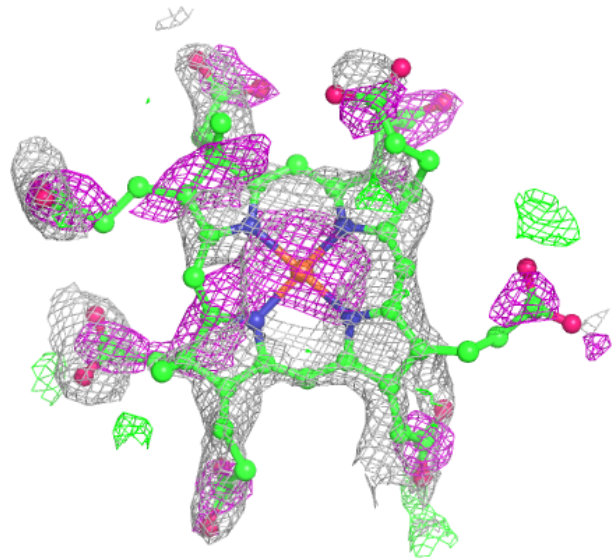
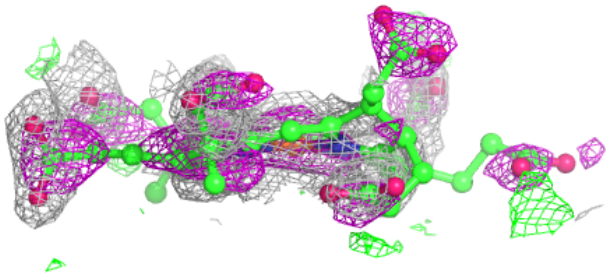
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SF4	E	585	8/8	0.89	0.31	32,34,36,40	0
4	SF4	D	576	8/8	0.92	0.19	7,10,10,10	0
4	SF4	D	575	8/8	0.94	0.26	6,7,7,8	0
5	GOL	A	590	6/6	0.94	0.11	25,30,37,42	0
4	SF4	A	576	8/8	0.95	0.10	4,5,6,6	0
4	SF4	E	586	8/8	0.96	0.16	20,22,24,24	0
3	SRM	A	580	63/63	0.96	0.11	16,23,33,41	0
3	SRM	B	570	63/63	0.97	0.09	6,8,13,16	0
4	SF4	A	575	8/8	0.97	0.05	7,8,10,11	0
4	SF4	B	585	8/8	0.98	0.06	16,19,20,36	0
4	SF4	B	586	8/8	0.99	0.09	19,22,24,25	0

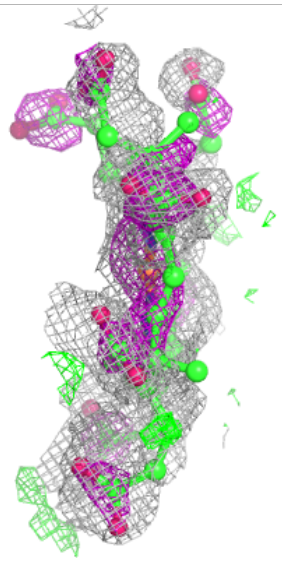
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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)

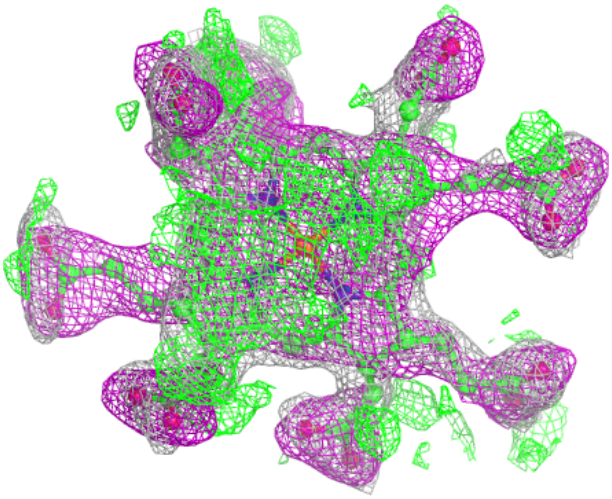


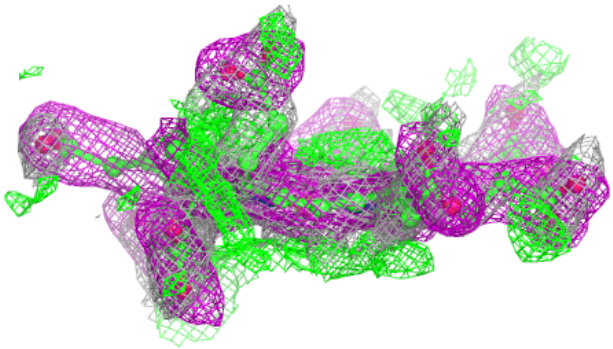


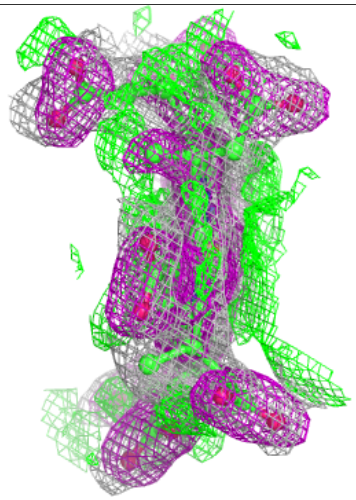


Electron density around SRM E 570:

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

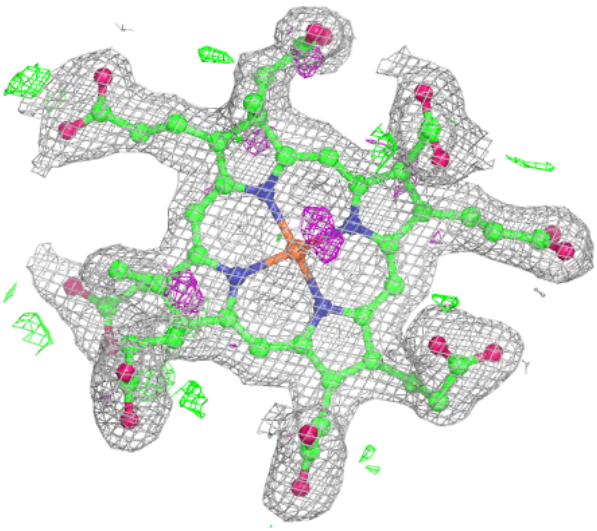


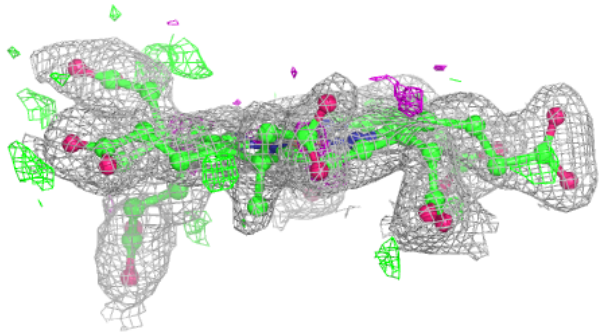




Electron density around SRM A 580:

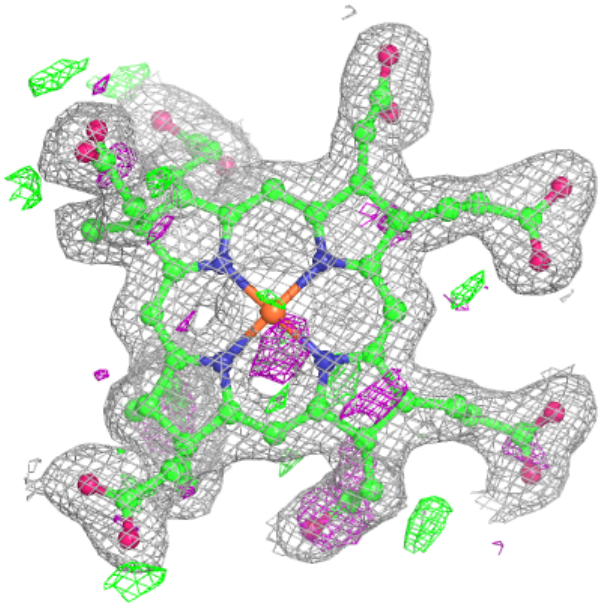
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

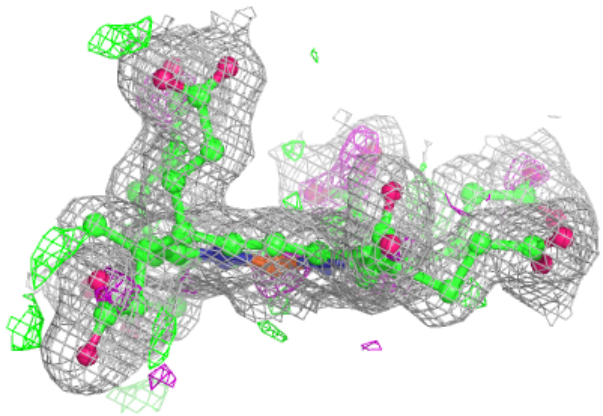


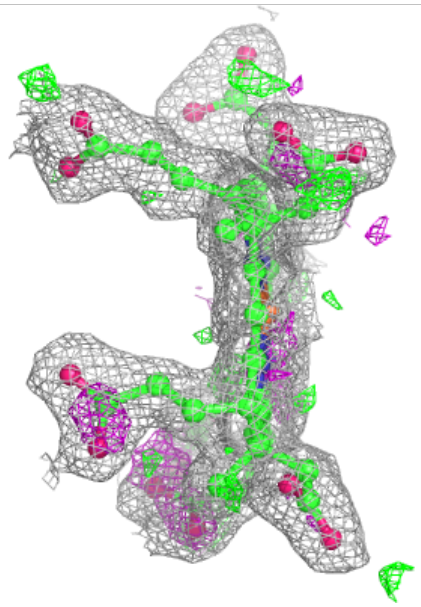


Electron density around SRM B 570:

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.