



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:06 AM UTC

PDB ID : 2V4J / pdb_00002v4j
Title : THE CRYSTAL STRUCTURE OF *Desulfovibrio vulgaris* DISSIMILATORY SULFITE REDUCTASE BOUND TO DsrC PROVIDES NOVEL INSIGHTS INTO THE MECHANISM OF SULFATE RESPIRATION
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Deposited on : 2008-09-22
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtrriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

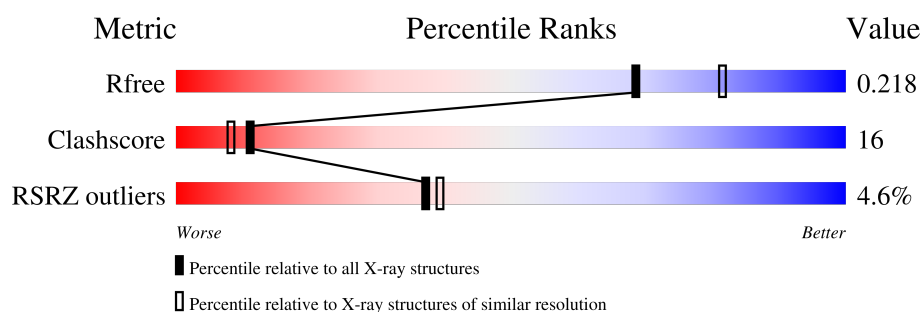
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	437	73% 25% .
1	D	437	8% 71% 27% .
2	B	381	78% 20% .
2	E	381	10% 73% 26% .
3	C	105	67% 30% ..
3	F	105	4% 65% 32% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SH0	A	503	X	-	-	-
5	SH0	D	503	X	-	-	-
6	SRM	B	503	X	-	-	-
6	SRM	E	503	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15816 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called SULFITE REDUCTASE, DISSIMILATORY-TYPE SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3443	2180	592	648	23			
1	D	436	Total	C	N	O	S	0	0	0
			3443	2180	592	648	23			

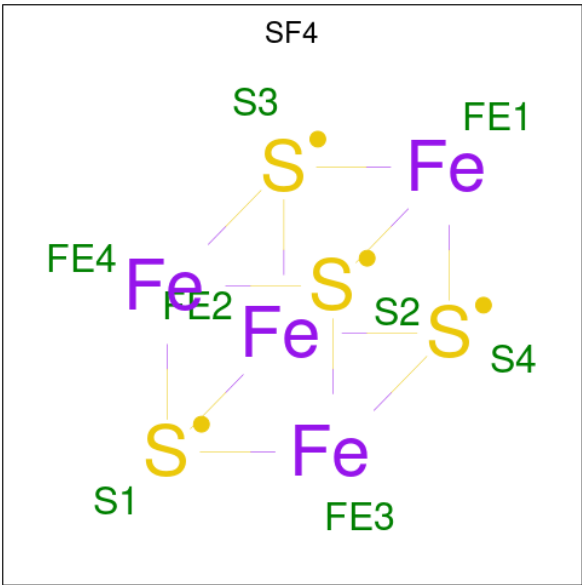
- Molecule 2 is a protein called SULFITE REDUCTASE, DISSIMILATORY-TYPE SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	380	Total	C	N	O	S	0	0	0
			2975	1897	513	539	26			
2	E	380	Total	C	N	O	S	0	0	0
			2975	1897	513	539	26			

- Molecule 3 is a protein called SULFITE REDUCTASE, DISSIMILATORY-TYPE SUBUNIT GAMMA.

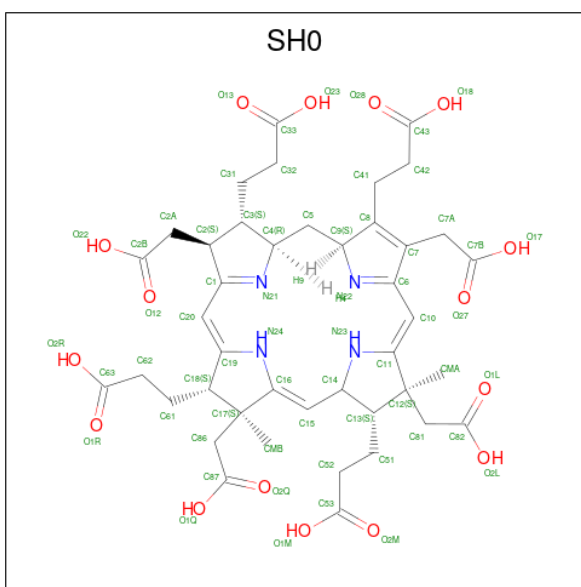
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	103	Total	C	N	O	S	0	0	0
			821	532	129	155	5			
3	F	103	Total	C	N	O	S	0	0	0
			821	532	129	155	5			

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



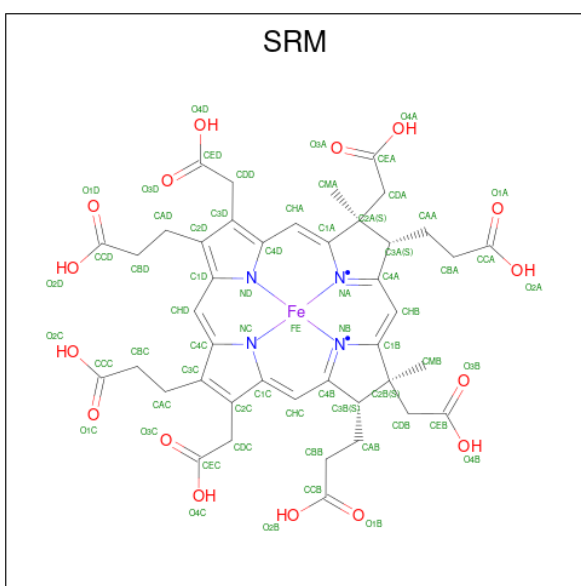
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	D	1	Total	Fe	S	0	0
			8	4	4		
4	D	1	Total	Fe	S	0	0
			8	4	4		
4	E	1	Total	Fe	S	0	0
			8	4	4		
4	E	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is 3,3',3'',3'''-[(1R,2S,3S,4S,7S,8S,11S,12S,13S,16S,19S)-3,8,13,17-tetrakis(carboxylatomethyl)-8,13-dimethyl-1,2,3,4,7,8,11,12,13,16,19,20,22,24-tetradecahydroporphyrin-2,7,12,18-tetrayl]tetrapropanoate (CCD ID: SH0) (formula: C₄₂H₅₂N₄O₁₆).



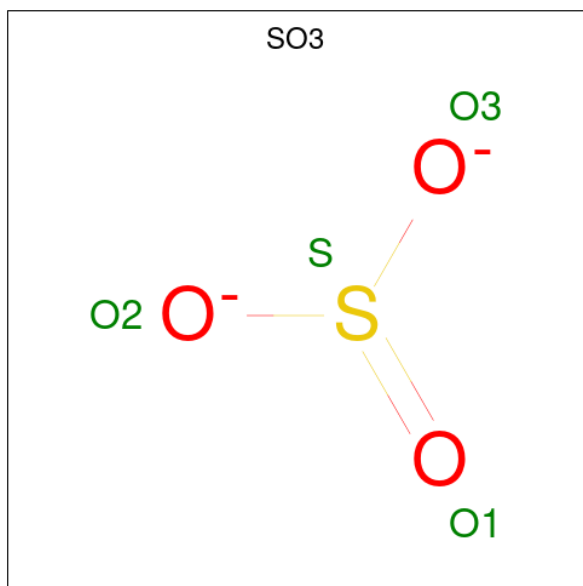
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 62	C 42	N 4	O 16	0	0
5	D	1	Total 62	C 42	N 4	O 16	0	0

- Molecule 6 is SIROHEME (CCD ID: SRM) (formula: $\text{C}_{42}\text{H}_{44}\text{FeN}_4\text{O}_{16}$).



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

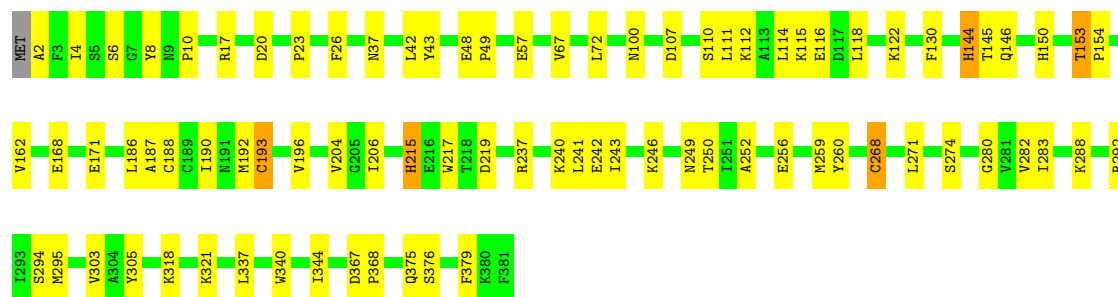
- Molecule 7 is SULFITE ION (CCD ID: SO3) (formula: O_3S).



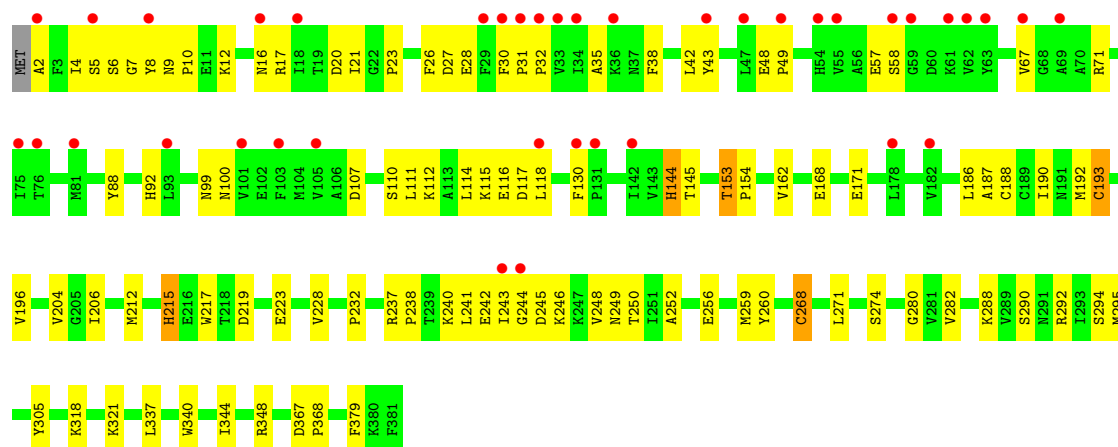
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	S	0	0
			4	3	1		
7	E	1	Total	O	S	0	0
			4	3	1		

- Molecule 8 is water.

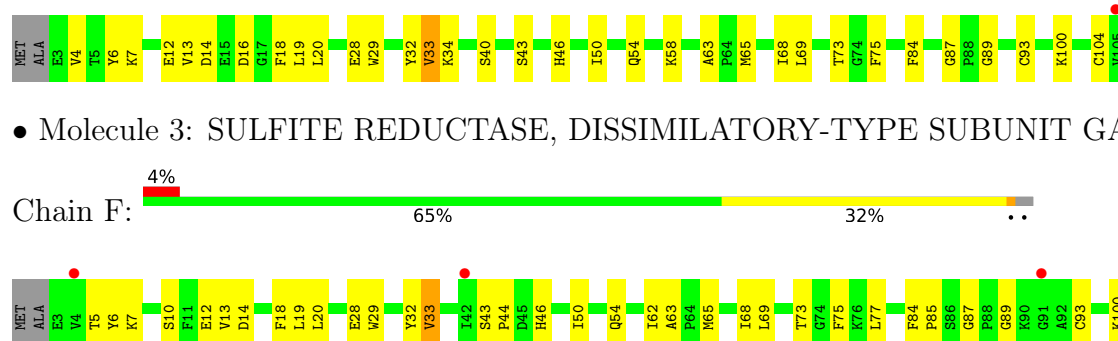
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	312	Total	O	0	0
			312	312		
8	B	274	Total	O	0	0
			274	274		
8	C	58	Total	O	0	0
			58	58		
8	D	181	Total	O	0	0
			181	181		
8	E	164	Total	O	0	0
			164	164		
8	F	27	Total	O	0	0
			27	27		



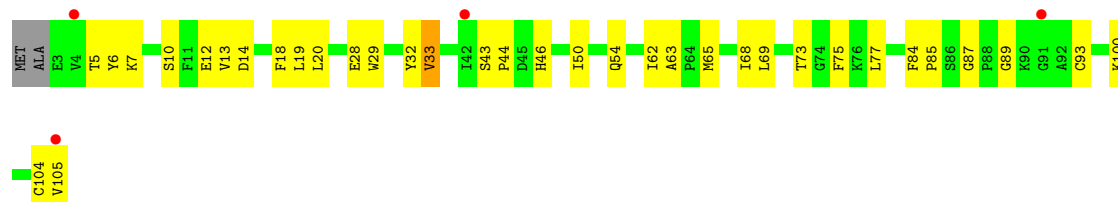
• Molecule 2: SULFITE REDUCTASE, DISSIMILATORY-TYPE SUBUNIT BETA



• Molecule 3: SULFITE REDUCTASE, DISSIMILATORY-TYPE SUBUNIT GAMMA



• Molecule 3: SULFITE REDUCTASE, DISSIMILATORY-TYPE SUBUNIT GAMMA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.41Å 118.90Å 132.24Å 90.00° 104.13° 90.00°	Depositor
Resolution (Å)	128.04 – 2.10 128.04 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.9 (128.04-2.10) 98.1 (128.04-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.10Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, R_{free}	0.190 , 0.219 (Not available) , 0.218	Depositor DCC
R_{free} test set	5616 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15816	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO3, SF4, SRM, SH0

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	0.44	0/3534	0.91	12/4783 (0.3%)
1	D	0.39	0/3534	0.92	15/4783 (0.3%)
2	B	0.47	0/3055	0.91	9/4141 (0.2%)
2	E	0.41	0/3055	0.90	9/4141 (0.2%)
3	C	0.35	0/843	0.90	7/1136 (0.6%)
3	F	0.32	0/843	0.90	7/1136 (0.6%)
All	All	0.42	0/14864	0.91	59/20120 (0.3%)

There are no bond length outliers.

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	87	GLN	CA-C-N	9.98	130.25	119.28
1	D	87	GLN	C-N-CA	9.98	130.25	119.28
1	A	87	GLN	CA-C-N	9.78	130.04	119.28
1	A	87	GLN	C-N-CA	9.78	130.04	119.28
2	E	153	THR	CA-C-N	-9.61	111.00	120.52
2	E	153	THR	C-N-CA	-9.61	111.00	120.52
2	B	153	THR	CA-C-N	-9.32	111.29	120.52
2	B	153	THR	C-N-CA	-9.32	111.29	120.52
1	D	420	VAL	N-CA-C	8.52	117.44	107.73
3	F	84	PHE	CA-C-N	7.52	127.89	119.32
3	F	84	PHE	C-N-CA	7.52	127.89	119.32
3	C	84	PHE	CA-C-N	7.41	127.76	119.32
3	C	84	PHE	C-N-CA	7.41	127.76	119.32
1	A	139	ILE	N-CA-C	-6.99	99.70	109.21
1	D	139	ILE	N-CA-C	-6.67	100.14	109.21
3	C	63	ALA	CA-C-N	-6.54	113.20	120.14
3	C	63	ALA	C-N-CA	-6.54	113.20	120.14
2	B	268	CYS	CA-C-N	6.45	126.14	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	268	CYS	C-N-CA	6.45	126.14	119.56
2	E	268	CYS	CA-C-N	6.44	126.13	119.56
2	E	268	CYS	C-N-CA	6.44	126.13	119.56
1	D	413	ILE	N-CA-C	6.43	117.38	108.89
3	F	87	GLY	CA-C-N	6.40	125.98	119.19
3	F	87	GLY	C-N-CA	6.40	125.98	119.19
1	D	337	ASP	N-CA-C	6.39	120.69	113.02
1	A	91	PHE	CA-C-N	6.36	126.28	119.28
1	A	91	PHE	C-N-CA	6.36	126.28	119.28
1	D	91	PHE	CA-C-N	6.36	126.28	119.28
1	D	91	PHE	C-N-CA	6.36	126.28	119.28
3	F	63	ALA	CA-C-N	-6.20	113.59	119.85
3	F	63	ALA	C-N-CA	-6.20	113.59	119.85
1	A	142	LEU	N-CA-C	6.16	118.83	108.23
3	C	87	GLY	CA-C-N	6.15	125.71	119.19
3	C	87	GLY	C-N-CA	6.15	125.71	119.19
1	A	413	ILE	N-CA-C	6.15	117.00	108.89
1	A	337	ASP	N-CA-C	6.09	120.33	113.02
1	D	142	LEU	N-CA-C	5.90	119.07	107.98
2	B	193	CYS	N-CA-C	-5.88	101.71	110.23
1	A	405	LYS	N-CA-C	-5.85	105.24	112.90
2	E	26	PHE	N-CA-C	5.67	118.19	111.33
1	A	313	MET	CA-C-N	5.66	125.33	119.56
1	A	313	MET	C-N-CA	5.66	125.33	119.56
1	D	313	MET	CA-C-N	5.65	125.32	119.56
1	D	313	MET	C-N-CA	5.65	125.32	119.56
1	D	420	VAL	CA-C-N	5.62	126.87	119.84
1	D	420	VAL	C-N-CA	5.62	126.87	119.84
2	B	26	PHE	N-CA-C	5.60	118.11	111.33
1	D	177	CYS	N-CA-C	-5.58	103.33	110.53
2	B	100	ASN	N-CA-C	-5.47	102.36	110.46
2	E	100	ASN	N-CA-C	-5.44	102.41	110.46
2	E	193	CYS	N-CA-C	-5.42	102.36	110.23
3	C	33	VAL	N-CA-C	5.42	116.91	111.00
2	B	144	HIS	N-CA-C	5.38	116.44	108.86
1	D	405	LYS	N-CA-C	-5.32	105.53	112.23
3	F	33	VAL	N-CA-C	5.29	116.77	111.00
2	E	144	HIS	N-CA-C	5.14	116.10	108.86
2	B	215	HIS	N-CA-C	5.09	117.49	111.33
1	A	177	CYS	N-CA-C	-5.03	104.04	110.53
2	E	215	HIS	N-CA-C	5.01	117.39	111.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3443	0	3310	121	0
1	D	3443	0	3310	122	0
2	B	2975	0	2923	76	0
2	E	2975	0	2923	123	0
3	C	821	0	804	36	0
3	F	821	0	804	37	0
4	A	16	0	0	1	0
4	B	16	0	0	0	0
4	D	16	0	0	1	0
4	E	16	0	0	0	0
5	A	62	0	41	4	0
5	D	62	0	41	6	0
6	B	63	0	33	8	0
6	E	63	0	33	8	0
7	B	4	0	0	0	0
7	E	4	0	0	0	0
8	A	312	0	0	19	0
8	B	274	0	0	4	0
8	C	58	0	0	3	0
8	D	181	0	0	18	0
8	E	164	0	0	36	0
8	F	27	0	0	3	0
All	All	15816	0	14222	476	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 16.

All (476) 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:6:SER:CA	8:E:2003:HOH:O	1.81	1.28
1:A:400:VAL:HG13	1:A:402:GLN:HE21	1.04	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ASP:CA	8:A:2200:HOH:O	1.87	1.17
2:E:35:ALA:HB2	8:E:2012:HOH:O	1.00	1.17
1:A:275:ASP:CB	8:A:2197:HOH:O	1.93	1.16
1:A:275:ASP:HB2	8:A:2197:HOH:O	1.46	1.16
1:D:163:ASP:CA	8:D:2047:HOH:O	1.93	1.14
1:D:400:VAL:HG13	1:D:402:GLN:HE21	1.03	1.14
2:E:27:ASP:C	8:E:2008:HOH:O	1.92	1.12
2:E:28:GLU:N	8:E:2008:HOH:O	1.81	1.12
2:E:35:ALA:HB3	8:E:2010:HOH:O	1.51	1.10
1:D:98:HIS:HE1	1:D:146:THR:HG22	1.12	1.09
1:D:276:ILE:O	8:D:2092:HOH:O	1.60	1.09
2:E:35:ALA:HB1	8:E:2013:HOH:O	1.53	1.09
1:A:98:HIS:HE1	1:A:146:THR:HG22	1.11	1.08
1:D:157:THR:O	8:D:2041:HOH:O	1.71	1.08
1:A:274:PHE:C	8:A:2200:HOH:O	1.97	1.06
1:D:163:ASP:N	8:D:2047:HOH:O	1.84	1.06
2:E:6:SER:C	8:E:2003:HOH:O	1.89	1.01
1:D:39:ASP:HB3	2:E:4:ILE:HD11	1.47	0.95
1:D:276:ILE:C	8:D:2092:HOH:O	1.77	0.94
2:E:32:PRO:HA	8:E:2010:HOH:O	1.67	0.94
1:A:98:HIS:CE1	1:A:146:THR:HG22	2.04	0.92
2:E:38:PHE:CD1	8:E:2011:HOH:O	2.24	0.91
2:E:92:HIS:CE1	8:E:2036:HOH:O	2.24	0.91
2:E:38:PHE:HD1	8:E:2011:HOH:O	1.54	0.89
2:E:92:HIS:HE1	8:E:2036:HOH:O	1.55	0.89
1:D:98:HIS:CE1	1:D:146:THR:HG22	2.05	0.88
1:D:400:VAL:HG13	1:D:402:GLN:NE2	1.88	0.88
2:E:71:ARG:NH1	8:E:2023:HOH:O	2.04	0.88
1:A:275:ASP:N	8:A:2200:HOH:O	1.91	0.88
2:E:35:ALA:CB	8:E:2012:HOH:O	1.67	0.88
1:D:245:LYS:HG2	8:D:2077:HOH:O	1.74	0.87
2:E:35:ALA:CA	8:E:2012:HOH:O	2.02	0.87
8:D:2047:HOH:O	2:E:21:ILE:CG1	2.23	0.87
1:A:400:VAL:HG13	1:A:402:GLN:NE2	1.88	0.86
2:E:192:MET:HG2	2:E:196:VAL:CG2	2.05	0.86
2:E:32:PRO:O	8:E:2010:HOH:O	1.93	0.86
2:B:192:MET:HG2	2:B:196:VAL:CG2	2.05	0.85
1:A:274:PHE:O	8:A:2200:HOH:O	1.91	0.85
1:A:275:ASP:OD2	8:A:2197:HOH:O	1.94	0.84
8:D:2047:HOH:O	2:E:21:ILE:HG13	1.78	0.83
2:E:6:SER:HA	8:E:2003:HOH:O	1.56	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:42:LEU:HD21	2:E:57:GLU:HG2	1.61	0.82
1:D:46:CYS:HB3	1:D:47:PRO:HD3	1.62	0.82
1:A:131:ASN:HB2	1:A:140:VAL:HB	1.61	0.81
2:E:28:GLU:HA	8:E:2008:HOH:O	1.79	0.81
2:E:28:GLU:CA	8:E:2008:HOH:O	2.25	0.80
1:D:131:ASN:HB2	1:D:140:VAL:HB	1.62	0.80
1:A:275:ASP:HA	8:A:2200:HOH:O	1.63	0.79
1:D:400:VAL:H	1:D:403:HIS:HD2	1.29	0.79
2:B:42:LEU:HD21	2:B:57:GLU:HG2	1.63	0.79
1:D:181:SER:HB3	1:D:191:GLN:HE22	1.48	0.78
2:B:204:VAL:CG1	2:B:282:VAL:HG22	2.12	0.78
1:D:163:ASP:CB	8:D:2047:HOH:O	2.26	0.78
2:E:204:VAL:CG1	2:E:282:VAL:HG22	2.13	0.78
1:D:327:ILE:HB	1:D:346:VAL:HG13	1.64	0.78
1:A:181:SER:HB3	1:A:191:GLN:HE22	1.49	0.78
1:A:400:VAL:H	1:A:403:HIS:HD2	1.32	0.78
2:B:288:LYS:HE2	2:B:294:SER:OG	1.84	0.77
1:D:246:ILE:O	8:D:2078:HOH:O	2.01	0.77
1:A:327:ILE:HB	1:A:346:VAL:HG13	1.65	0.77
1:A:46:CYS:HB3	1:A:47:PRO:HD3	1.64	0.77
1:D:308:HIS:HD2	2:E:292:ARG:HE	1.31	0.77
2:E:32:PRO:C	8:E:2010:HOH:O	2.28	0.77
2:E:5:SER:O	8:E:2003:HOH:O	2.02	0.76
3:C:73:THR:CG2	3:C:75:PHE:H	1.99	0.76
1:D:247:ASP:OD2	1:D:249:GLU:HG3	1.86	0.76
2:B:204:VAL:HG12	2:B:282:VAL:HG22	1.68	0.76
2:E:30:PHE:HB3	8:E:2012:HOH:O	1.86	0.76
2:E:288:LYS:HE2	2:E:294:SER:OG	1.85	0.76
3:F:73:THR:CG2	3:F:75:PHE:H	1.98	0.76
1:A:247:ASP:OD2	1:A:249:GLU:HG3	1.87	0.75
1:A:83:ARG:H	1:A:98:HIS:HD2	1.35	0.73
1:D:39:ASP:HB3	2:E:4:ILE:CD1	2.18	0.73
1:D:83:ARG:H	1:D:98:HIS:HD2	1.36	0.73
2:B:111:LEU:O	2:B:115:LYS:HG3	1.88	0.73
2:E:111:LEU:O	2:E:115:LYS:HG3	1.88	0.73
2:E:192:MET:HG2	2:E:196:VAL:HG21	1.71	0.72
2:E:204:VAL:HG12	2:E:282:VAL:HG22	1.71	0.72
8:B:2160:HOH:O	1:D:426:ARG:HD3	1.89	0.72
2:E:35:ALA:N	8:E:2012:HOH:O	2.13	0.72
2:B:192:MET:HG2	2:B:196:VAL:HG23	1.72	0.72
2:E:154:PRO:HB3	2:E:188:CYS:HB2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:ALA:O	1:D:116:ARG:HG3	1.90	0.71
1:A:146:THR:HG21	8:A:2069:HOH:O	1.89	0.71
2:B:154:PRO:HB3	2:B:188:CYS:HB2	1.73	0.71
2:B:192:MET:HG2	2:B:196:VAL:HG21	1.71	0.71
2:E:32:PRO:CA	8:E:2010:HOH:O	2.33	0.71
3:C:43:SER:H	3:C:46:HIS:HD2	1.39	0.70
3:C:43:SER:H	3:C:46:HIS:CD2	2.09	0.70
3:F:44:PRO:HD2	8:F:2012:HOH:O	1.92	0.70
2:E:192:MET:HG2	2:E:196:VAL:HG23	1.73	0.70
3:F:73:THR:HG22	3:F:75:PHE:H	1.56	0.69
3:C:73:THR:HG22	3:C:75:PHE:H	1.57	0.69
1:A:275:ASP:CB	8:A:2200:HOH:O	2.29	0.69
3:F:43:SER:H	3:F:46:HIS:CD2	2.10	0.69
1:A:202:GLN:HE21	2:B:20:ASP:HA	1.58	0.69
1:D:202:GLN:HE21	2:E:20:ASP:HA	1.58	0.68
2:E:5:SER:C	8:E:2003:HOH:O	2.32	0.68
1:A:39:ASP:OD1	2:B:2:ALA:HB3	1.93	0.68
1:A:268:GLY:O	8:A:2194:HOH:O	2.11	0.67
1:A:2:ALA:N	1:A:45:ASP:OD1	2.28	0.67
3:F:73:THR:HG23	3:F:75:PHE:CD2	2.30	0.67
1:A:39:ASP:HB3	2:B:4:ILE:HD11	1.77	0.67
3:C:12:GLU:HG2	8:C:2001:HOH:O	1.94	0.67
1:D:162:THR:C	8:D:2047:HOH:O	2.29	0.67
1:A:305:ARG:NH2	2:E:379:PHE:O	2.27	0.67
3:C:73:THR:HG23	3:C:75:PHE:CD2	2.30	0.67
3:C:19:LEU:HD22	3:C:29:TRP:CE2	2.30	0.66
3:F:19:LEU:HD22	3:F:29:TRP:CE2	2.29	0.66
1:A:308:HIS:HD2	2:B:292:ARG:HE	1.42	0.66
1:D:2:ALA:N	1:D:45:ASP:OD1	2.28	0.66
1:D:400:VAL:H	1:D:403:HIS:CD2	2.12	0.66
3:F:43:SER:H	3:F:46:HIS:HD2	1.41	0.66
1:D:152:ILE:HG22	1:D:156:LEU:HD22	1.77	0.66
2:E:9:ASN:ND2	2:E:12:LYS:HG3	2.11	0.66
1:A:152:ILE:HG22	1:A:156:LEU:HD22	1.77	0.66
1:D:245:LYS:HE2	8:D:2077:HOH:O	1.96	0.66
2:B:193:CYS:HA	6:B:503:SRM:C4C	2.26	0.65
3:F:73:THR:CG2	3:F:75:PHE:HB2	2.26	0.65
1:A:87:GLN:NE2	1:A:90:LYS:HE3	2.11	0.65
1:A:249:GLU:HB3	8:A:2183:HOH:O	1.95	0.65
1:A:269:ARG:HG2	1:A:270:ASP:N	2.11	0.65
2:E:168:GLU:HG3	2:E:321:LYS:HD2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:69:LEU:O	3:C:73:THR:HB	1.96	0.65
1:A:400:VAL:CG1	1:A:402:GLN:HE21	1.96	0.64
3:C:73:THR:CG2	3:C:75:PHE:HB2	2.27	0.64
3:F:69:LEU:O	3:F:73:THR:HB	1.95	0.64
2:E:280:GLY:HA3	2:E:305:TYR:CE1	2.32	0.64
2:E:256:GLU:CD	2:E:256:GLU:H	2.05	0.64
2:B:171:GLU:H	2:B:171:GLU:CD	2.06	0.64
2:B:256:GLU:CD	2:B:256:GLU:H	2.06	0.64
1:D:39:ASP:OD1	2:E:2:ALA:HB1	1.98	0.64
1:D:87:GLN:NE2	1:D:90:LYS:HE3	2.13	0.64
2:B:168:GLU:HG3	2:B:321:LYS:HD2	1.80	0.63
2:E:193:CYS:HA	6:E:503:SRM:C4C	2.27	0.63
1:A:275:ASP:HB2	8:A:2200:HOH:O	1.92	0.63
2:E:27:ASP:OD1	8:E:2008:HOH:O	2.15	0.63
1:D:244:ILE:H	1:D:300:ASN:HD21	1.47	0.63
1:A:400:VAL:H	1:A:403:HIS:CD2	2.16	0.62
2:B:379:PHE:O	1:D:305:ARG:NH2	2.32	0.62
1:A:244:ILE:H	1:A:300:ASN:HD21	1.47	0.62
1:D:400:VAL:CG1	1:D:402:GLN:HG2	2.30	0.61
1:D:269:ARG:HG2	1:D:270:ASP:N	2.14	0.61
1:A:400:VAL:CG1	1:A:402:GLN:HG2	2.30	0.61
2:B:280:GLY:HA3	2:B:305:TYR:CE1	2.35	0.61
1:D:220:ALA:HB3	4:D:501:SF4:S1	2.41	0.61
2:E:171:GLU:CD	2:E:171:GLU:H	2.08	0.60
5:A:503:SH0:H52	5:A:503:SH0:HMAB	1.83	0.60
1:D:146:THR:HA	1:D:149:LEU:HD22	1.83	0.60
2:B:375:GLN:NE2	8:B:2271:HOH:O	2.35	0.60
1:D:178:LEU:HD13	5:D:503:SH0:H86A	1.84	0.60
1:D:313:MET:HE3	1:D:317:LEU:HD11	1.84	0.60
2:E:114:LEU:HD22	2:E:118:LEU:CD1	2.32	0.59
1:D:163:ASP:HA	8:D:2047:HOH:O	1.78	0.59
1:A:146:THR:HA	1:A:149:LEU:HD22	1.85	0.59
2:E:241:LEU:HD23	2:E:243:ILE:HD11	1.83	0.59
2:B:114:LEU:HD22	2:B:118:LEU:CD1	2.32	0.59
1:D:46:CYS:CB	1:D:47:PRO:HD3	2.33	0.59
1:D:219:ASP:OD1	1:D:226:VAL:HG23	2.03	0.59
2:B:241:LEU:HD23	2:B:243:ILE:HD11	1.85	0.58
2:E:31:PRO:HB3	8:E:2035:HOH:O	2.02	0.58
1:A:219:ASP:OD1	1:A:226:VAL:HG23	2.03	0.58
1:D:308:HIS:CD2	2:E:292:ARG:HE	2.18	0.58
1:D:39:ASP:CB	2:E:4:ILE:HD11	2.26	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:LEU:O	1:D:403:HIS:HE1	1.87	0.57
1:A:313:MET:HE3	1:A:317:LEU:HD11	1.86	0.57
2:B:242:GLU:C	2:B:243:ILE:HG13	2.28	0.57
5:D:503:SHO:H52	5:D:503:SHO:HMAB	1.87	0.57
1:A:184:GLU:HG2	2:B:43:TYR:HA	1.85	0.57
1:A:345:LEU:O	1:A:403:HIS:HE1	1.87	0.57
1:D:427:ASP:OD2	1:D:429:THR:OG1	2.22	0.57
3:C:16:ASP:OD2	3:C:100:LYS:NZ	2.30	0.57
3:F:13:VAL:HG21	3:F:29:TRP:HH2	1.70	0.57
1:A:46:CYS:CB	1:A:47:PRO:HD3	2.35	0.56
1:D:184:GLU:HG2	2:E:43:TYR:HA	1.86	0.56
1:A:178:LEU:HD13	5:A:503:SHO:H86A	1.87	0.56
8:D:2047:HOH:O	2:E:21:ILE:HD11	2.05	0.56
1:A:96:HIS:CE1	1:A:146:THR:HG23	2.41	0.56
2:E:242:GLU:C	2:E:243:ILE:HG13	2.29	0.56
3:F:73:THR:HG23	3:F:75:PHE:H	1.70	0.56
1:D:96:HIS:CE1	1:D:146:THR:HG23	2.41	0.56
1:A:30:TYR:OH	1:A:36:LYS:HE3	2.06	0.55
1:A:220:ALA:HB3	4:A:501:SF4:S1	2.46	0.55
3:C:73:THR:HG23	3:C:75:PHE:H	1.71	0.55
1:D:336:LEU:HD12	2:E:232:PRO:HG3	1.89	0.55
1:D:245:LYS:HE3	1:D:321:ASP:OD2	2.06	0.55
1:D:333:ALA:HB1	1:D:334:PRO:HD2	1.88	0.55
2:E:112:LYS:O	2:E:116:GLU:HG3	2.07	0.54
3:C:13:VAL:HG13	3:C:14:ASP:N	2.22	0.54
2:E:206:ILE:HG12	2:E:282:VAL:HG13	1.88	0.54
1:A:49:ASP:O	1:A:53:VAL:HG23	2.08	0.54
1:D:400:VAL:CG1	1:D:402:GLN:HE21	1.96	0.54
3:F:73:THR:HG21	3:F:75:PHE:HB2	1.89	0.54
3:F:13:VAL:HG13	3:F:14:ASP:N	2.23	0.54
1:D:244:ILE:H	1:D:300:ASN:ND2	2.05	0.53
1:D:49:ASP:O	1:D:53:VAL:HG23	2.08	0.53
2:E:67:VAL:HG11	2:E:130:PHE:HB3	1.89	0.53
3:C:13:VAL:HG21	3:C:29:TRP:HH2	1.73	0.53
1:D:110:TYR:OH	1:D:133:HIS:HE1	1.92	0.53
1:A:108:LYS:NZ	1:A:175:GLU:OE2	2.41	0.53
2:B:206:ILE:HG12	2:B:282:VAL:HG13	1.91	0.53
1:D:30:TYR:OH	1:D:36:LYS:HE3	2.08	0.53
2:E:186:LEU:HD13	2:E:187:ALA:N	2.23	0.53
1:A:244:ILE:H	1:A:300:ASN:ND2	2.06	0.53
1:A:73:VAL:HG13	2:B:17:ARG:HH21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:TYR:OH	1:A:133:HIS:HE1	1.91	0.52
3:C:73:THR:HG21	3:C:75:PHE:HB2	1.89	0.52
1:D:318:HIS:HE1	2:E:42:LEU:O	1.92	0.52
1:A:150:GLU:OE1	2:B:17:ARG:NH2	2.29	0.52
1:A:306:CYS:O	1:A:307:MET:HB2	2.09	0.52
3:F:89:GLY:O	3:F:93:CYS:HB2	2.09	0.52
1:A:245:LYS:HE3	1:A:321:ASP:OD2	2.09	0.52
2:E:243:ILE:N	2:E:246:LYS:O	2.36	0.52
1:A:318:HIS:HE1	2:B:42:LEU:O	1.92	0.52
2:B:154:PRO:CB	2:B:188:CYS:HB2	2.39	0.52
1:D:264:GLY:HA2	8:D:2084:HOH:O	2.09	0.52
2:E:8:TYR:O	2:E:10:PRO:HD3	2.09	0.52
1:D:354:PRO:O	1:D:359:LYS:HE3	2.10	0.52
1:A:70:ILE:HG13	3:C:100:LYS:CG	2.39	0.52
1:A:404:VAL:HG13	1:A:406:GLU:N	2.25	0.52
2:B:112:LYS:O	2:B:116:GLU:HG3	2.10	0.52
2:E:154:PRO:CB	2:E:188:CYS:HB2	2.39	0.52
2:B:8:TYR:O	2:B:10:PRO:HD3	2.10	0.51
1:D:404:VAL:HG13	1:D:406:GLU:N	2.25	0.51
2:E:30:PHE:CB	8:E:2012:HOH:O	2.49	0.51
1:D:209:ALA:HB2	3:F:77:LEU:CD2	2.40	0.51
1:A:184:GLU:HG2	2:B:43:TYR:CA	2.41	0.51
1:A:318:HIS:HD2	8:A:2226:HOH:O	1.93	0.51
3:C:89:GLY:O	3:C:93:CYS:HB2	2.10	0.51
3:F:50:ILE:O	3:F:54:GLN:HG3	2.10	0.51
1:D:259:PHE:CD2	1:D:315:ARG:HD3	2.46	0.51
2:E:219:ASP:HB2	2:E:249:ASN:O	2.11	0.50
1:A:64:HIS:HD2	1:A:86:ASP:OD2	1.94	0.50
3:C:50:ILE:O	3:C:54:GLN:HG3	2.11	0.50
1:A:36:LYS:HB2	8:A:2031:HOH:O	2.12	0.50
2:B:186:LEU:HD13	2:B:187:ALA:N	2.26	0.50
1:A:354:PRO:O	1:A:359:LYS:HE3	2.11	0.50
1:A:437:ARG:HH11	2:E:217:TRP:CD1	2.30	0.50
1:A:402:GLN:NE2	1:A:402:GLN:H	2.10	0.50
2:B:219:ASP:HB2	2:B:249:ASN:O	2.11	0.50
2:E:215:HIS:HD2	2:E:250:THR:OG1	1.94	0.50
3:C:4:VAL:HG11	3:C:32:TYR:CZ	2.47	0.50
3:F:6:TYR:CG	3:F:32:TYR:HB2	2.47	0.50
1:A:404:VAL:HG13	1:A:406:GLU:O	2.12	0.50
2:B:215:HIS:HD2	2:B:250:THR:OG1	1.95	0.50
1:D:306:CYS:O	1:D:307:MET:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ALA:HB1	1:A:334:PRO:HD2	1.93	0.49
1:D:184:GLU:HG2	2:E:43:TYR:CA	2.41	0.49
1:D:150:GLU:OE1	2:E:17:ARG:NH2	2.28	0.49
1:A:99:THR:HG23	1:A:140:VAL:HG13	1.95	0.49
2:B:67:VAL:HG11	2:B:130:PHE:HB3	1.93	0.49
3:C:6:TYR:CG	3:C:32:TYR:HB2	2.48	0.49
1:D:53:VAL:HG22	1:D:91:PHE:CG	2.47	0.49
1:D:70:ILE:HG13	3:F:100:LYS:CG	2.43	0.49
1:D:64:HIS:HD2	1:D:86:ASP:OD2	1.96	0.49
1:D:99:THR:HG23	1:D:140:VAL:HG13	1.95	0.49
2:E:204:VAL:HG13	2:E:282:VAL:HG22	1.91	0.49
2:E:223:GLU:HB3	3:F:62:ILE:HG22	1.95	0.49
6:E:503:SRM:HMA1	6:E:503:SRM:O3A	2.13	0.49
1:D:269:ARG:HD2	1:D:271:TRP:CE2	2.48	0.48
3:F:12:GLU:HB3	3:F:20:LEU:HD23	1.94	0.48
1:D:163:ASP:HB2	8:D:2047:HOH:O	2.03	0.48
1:A:83:ARG:H	1:A:98:HIS:CD2	2.24	0.48
1:D:116:ARG:NE	8:E:2030:HOH:O	2.46	0.48
6:B:503:SRM:HMA2	3:C:104:CYS:HB3	1.95	0.48
1:A:53:VAL:HG22	1:A:91:PHE:CG	2.49	0.48
1:A:247:ASP:O	1:A:251:VAL:HG12	2.14	0.48
1:A:259:PHE:CD2	1:A:315:ARG:HD3	2.49	0.48
1:D:247:ASP:HB3	1:D:250:ALA:HB3	1.95	0.48
1:D:404:VAL:HG13	1:D:406:GLU:O	2.13	0.48
2:B:204:VAL:HG13	2:B:282:VAL:HG22	1.94	0.48
3:F:29:TRP:CE2	3:F:33:VAL:HG21	2.49	0.48
1:D:181:SER:HB3	1:D:191:GLN:NE2	2.25	0.47
3:C:7:LYS:HD2	3:C:28:GLU:OE1	2.15	0.47
1:D:116:ARG:NH2	8:E:2030:HOH:O	2.48	0.47
1:A:426:ARG:HG3	2:E:212:MET:CG	2.44	0.47
3:C:12:GLU:HB3	3:C:20:LEU:HD23	1.96	0.47
1:A:251:VAL:O	1:A:255:VAL:HG23	2.13	0.47
2:B:217:TRP:CD1	1:D:437:ARG:HH11	2.32	0.47
1:D:96:HIS:CE1	1:D:146:THR:CG2	2.96	0.47
1:A:96:HIS:CE1	1:A:146:THR:CG2	2.98	0.47
1:A:269:ARG:HD2	1:A:271:TRP:CE2	2.49	0.47
2:B:153:THR:N	2:B:154:PRO:CD	2.78	0.47
1:D:131:ASN:HB2	1:D:140:VAL:CB	2.39	0.47
2:E:153:THR:N	2:E:154:PRO:CD	2.78	0.47
2:E:243:ILE:O	2:E:246:LYS:HB3	2.15	0.47
1:D:402:GLN:NE2	1:D:402:GLN:H	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:29:TRP:CZ2	3:F:33:VAL:HG21	2.49	0.47
1:A:17:TRP:CD2	1:A:18:PRO:HD2	2.50	0.47
1:A:125:ARG:HE	1:A:155:GLU:CD	2.23	0.47
1:A:308:HIS:CD2	2:B:292:ARG:HE	2.29	0.47
3:C:13:VAL:CG1	3:C:14:ASP:N	2.78	0.47
2:E:240:LYS:HE3	2:E:249:ASN:OD1	2.15	0.47
2:E:42:LEU:HD21	2:E:57:GLU:CG	2.40	0.47
3:C:29:TRP:CE2	3:C:33:VAL:HG21	2.50	0.46
5:D:503:SH0:O13	2:E:290:SER:HB3	2.15	0.46
3:F:5:THR:HG22	3:F:10:SER:OG	2.15	0.46
6:B:503:SRM:HMA2	3:C:104:CYS:CB	2.46	0.46
1:D:125:ARG:HE	1:D:155:GLU:CD	2.23	0.46
2:B:243:ILE:O	2:B:246:LYS:HB3	2.14	0.46
1:D:155:GLU:HG3	2:E:6:SER:HB2	1.98	0.46
2:E:337:LEU:O	2:E:337:LEU:HD23	2.15	0.46
1:A:400:VAL:N	1:A:403:HIS:HD2	2.06	0.46
2:E:321:LYS:HB3	8:E:2120:HOH:O	2.16	0.46
1:A:279:GLU:O	1:A:308:HIS:HE1	1.99	0.46
2:B:340:TRP:O	2:B:344:ILE:HG12	2.16	0.46
1:D:17:TRP:CD2	1:D:18:PRO:HD2	2.50	0.46
2:E:107:ASP:OD2	2:E:110:SER:OG	2.29	0.46
2:E:340:TRP:O	2:E:344:ILE:HG12	2.15	0.46
2:B:240:LYS:HE3	2:B:249:ASN:OD1	2.16	0.46
1:D:251:VAL:O	1:D:255:VAL:HG23	2.15	0.46
2:B:337:LEU:HD23	2:B:337:LEU:O	2.16	0.46
1:D:247:ASP:O	1:D:251:VAL:HG12	2.16	0.46
1:D:87:GLN:HE22	1:D:90:LYS:NZ	2.14	0.46
3:C:7:LYS:HD3	8:C:2002:HOH:O	2.16	0.46
3:C:73:THR:CG2	3:C:75:PHE:CD2	2.99	0.46
3:C:29:TRP:CZ2	3:C:33:VAL:HG21	2.50	0.45
3:F:7:LYS:HD2	3:F:28:GLU:OE1	2.16	0.45
3:C:58:LYS:NZ	8:C:2029:HOH:O	2.49	0.45
3:F:105:VAL:HG22	3:F:105:VAL:O	2.16	0.45
1:A:87:GLN:HE22	1:A:90:LYS:NZ	2.14	0.45
5:A:503:SH0:HMAB	5:A:503:SH0:C52	2.45	0.45
2:B:107:ASP:OD2	2:B:110:SER:OG	2.30	0.45
1:D:215:LYS:NZ	6:E:503:SRM:O3C	2.34	0.45
2:B:37:ASN:ND2	8:B:2039:HOH:O	2.36	0.45
2:E:115:LYS:HE2	2:E:115:LYS:HB3	1.60	0.45
6:E:503:SRM:CDA	3:F:104:CYS:SG	3.04	0.45
8:D:2047:HOH:O	2:E:21:ILE:CD1	2.53	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:13:VAL:CG1	3:F:14:ASP:N	2.79	0.45
1:A:39:ASP:HB3	2:B:4:ILE:CD1	2.45	0.45
1:D:371:GLU:HG2	8:D:2127:HOH:O	2.17	0.45
1:D:437:ARG:HE	1:D:437:ARG:HB2	1.47	0.45
1:A:42:VAL:HG22	8:A:2102:HOH:O	2.16	0.45
1:A:155:GLU:HG3	2:B:6:SER:HB2	1.98	0.45
1:A:240:TRP:CZ2	1:A:305:ARG:HG2	2.51	0.45
2:B:190:ILE:C	2:B:190:ILE:HD12	2.42	0.45
1:D:308:HIS:HD2	2:E:292:ARG:NE	2.06	0.45
3:F:68:ILE:HD12	8:F:2016:HOH:O	2.15	0.45
1:A:232:SER:O	1:A:331:ALA:HB3	2.17	0.45
2:B:243:ILE:N	2:B:246:LYS:O	2.36	0.45
6:B:503:SRM:CDA	3:C:104:CYS:SG	3.05	0.45
6:B:503:SRM:HMA1	6:B:503:SRM:O3A	2.15	0.45
1:A:103:ALA:HB1	2:B:23:PRO:HB3	1.98	0.45
1:A:247:ASP:HB3	1:A:250:ALA:HB3	1.98	0.45
2:E:318:LYS:N	2:E:318:LYS:HD3	2.32	0.45
1:D:279:GLU:O	1:D:308:HIS:HE1	2.00	0.44
6:E:503:SRM:HMA2	3:F:104:CYS:CB	2.47	0.44
1:A:239:THR:HB	8:A:2234:HOH:O	2.17	0.44
1:A:249:GLU:HG2	8:A:2178:HOH:O	2.17	0.44
2:B:122:LYS:HE2	8:B:2102:HOH:O	2.17	0.44
6:B:503:SRM:CBB	6:B:503:SRM:CMB	2.96	0.44
1:D:225:CYS:HA	5:D:503:SH0:C1	2.47	0.44
2:E:30:PHE:CD2	8:E:2011:HOH:O	2.70	0.44
3:F:13:VAL:HG21	3:F:29:TRP:CH2	2.49	0.44
1:A:426:ARG:HG3	2:E:212:MET:HG3	1.99	0.44
3:C:65:MET:HE3	3:C:68:ILE:CD1	2.48	0.44
1:D:430:GLU:O	1:D:433:LYS:HB2	2.17	0.44
2:B:237:ARG:HG2	2:B:252:ALA:HB3	1.99	0.44
3:F:65:MET:HE3	3:F:68:ILE:CD1	2.47	0.44
1:D:240:TRP:CZ2	1:D:305:ARG:HG2	2.53	0.44
3:F:73:THR:CG2	3:F:75:PHE:CD2	2.99	0.44
2:E:228:VAL:HG21	2:E:238:PRO:HD3	1.99	0.44
2:E:246:LYS:HE2	2:E:248:VAL:HG12	1.99	0.44
2:B:274:SER:O	1:D:426:ARG:NH2	2.51	0.44
1:D:96:HIS:HB2	1:D:145:GLN:HG2	1.99	0.44
2:E:237:ARG:HG2	2:E:252:ALA:HB3	1.99	0.44
6:E:503:SRM:CBB	6:E:503:SRM:CMB	2.96	0.44
2:B:318:LYS:HD3	2:B:318:LYS:N	2.32	0.44
1:D:404:VAL:HG13	1:D:406:GLU:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:367:ASP:N	2:E:368:PRO:CD	2.81	0.44
1:A:404:VAL:HG13	1:A:406:GLU:H	1.83	0.43
2:B:114:LEU:HD22	2:B:118:LEU:HD12	1.98	0.43
2:B:115:LYS:HB3	2:B:115:LYS:HE2	1.63	0.43
1:D:259:PHE:CE2	1:D:315:ARG:HD3	2.53	0.43
1:A:430:GLU:O	1:A:433:LYS:HB2	2.17	0.43
1:D:73:VAL:HG13	2:E:17:ARG:HH21	1.83	0.43
6:E:503:SRM:HMA2	3:F:104:CYS:HB3	2.00	0.43
1:A:434:ARG:HG3	1:A:435:HIS:CD2	2.54	0.43
1:D:404:VAL:HG13	1:D:406:GLU:C	2.44	0.43
2:E:144:HIS:CG	2:E:162:VAL:HG21	2.53	0.43
2:E:168:GLU:CG	2:E:321:LYS:HD2	2.48	0.43
1:A:87:GLN:NE2	1:A:90:LYS:CE	2.81	0.43
1:A:437:ARG:NH1	2:E:217:TRP:CD1	2.87	0.43
2:B:114:LEU:HD22	2:B:118:LEU:HD11	2.01	0.43
2:E:114:LEU:HD22	2:E:118:LEU:HD12	1.99	0.43
1:D:83:ARG:H	1:D:98:HIS:CD2	2.24	0.43
2:E:7:GLY:N	8:E:2003:HOH:O	2.32	0.43
2:E:145:THR:HG21	2:E:193:CYS:HB2	2.01	0.43
1:D:232:SER:O	1:D:331:ALA:HB3	2.19	0.43
1:D:283:ARG:HD2	1:D:283:ARG:HA	1.83	0.43
2:E:190:ILE:HD12	2:E:190:ILE:C	2.44	0.43
1:A:404:VAL:HG13	1:A:406:GLU:C	2.44	0.43
3:F:85:PRO:HD2	8:F:2022:HOH:O	2.19	0.43
1:D:86:ASP:OD2	1:D:87:GLN:HG3	2.18	0.42
1:D:313:MET:HE3	1:D:317:LEU:CD1	2.47	0.42
2:E:268:CYS:SG	2:E:271:LEU:HD22	2.58	0.42
2:B:42:LEU:HD21	2:B:57:GLU:CG	2.41	0.42
3:C:34:LYS:HE3	3:C:40:SER:O	2.19	0.42
2:B:168:GLU:CG	2:B:321:LYS:HD2	2.48	0.42
2:B:268:CYS:SG	2:B:271:LEU:HD22	2.59	0.42
3:C:13:VAL:HG21	3:C:29:TRP:CH2	2.52	0.42
1:D:333:ALA:HB1	1:D:334:PRO:CD	2.50	0.42
1:D:420:VAL:HA	1:D:421:PRO:HD3	1.74	0.42
2:B:204:VAL:HG12	2:B:282:VAL:CG2	2.44	0.42
2:E:88:TYR:HA	8:E:2033:HOH:O	2.19	0.42
1:A:76:TYR:CD2	1:A:206:HIS:HB3	2.55	0.42
1:A:86:ASP:OD2	1:A:87:GLN:HG3	2.18	0.42
1:D:133:HIS:H	2:E:99:ASN:ND2	2.17	0.42
1:D:434:ARG:HG3	1:D:435:HIS:CD2	2.55	0.42
2:E:48:GLU:HB2	2:E:49:PRO:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:244:GLY:O	2:E:245:ASP:HB3	2.20	0.42
2:E:268:CYS:HB3	2:E:271:LEU:HD22	2.02	0.42
1:A:335:ILE:HA	1:A:336:LEU:HA	1.70	0.42
2:B:268:CYS:HB3	2:B:271:LEU:HD22	2.02	0.42
1:A:402:GLN:NE2	8:A:2286:HOH:O	2.53	0.42
1:D:57:SER:O	1:D:61:GLY:N	2.53	0.42
1:D:76:TYR:CD2	1:D:206:HIS:HB3	2.55	0.42
1:A:426:ARG:NH2	2:E:274:SER:O	2.53	0.42
2:B:367:ASP:N	2:B:368:PRO:CD	2.82	0.42
2:E:58:SER:CB	8:E:2021:HOH:O	0.78	0.42
2:B:144:HIS:CG	2:B:162:VAL:HG21	2.55	0.41
3:C:13:VAL:HG22	3:C:18:PHE:C	2.45	0.41
1:D:103:ALA:HB1	2:E:23:PRO:HB3	2.01	0.41
1:D:158:HIS:CE1	2:E:16:ASN:O	2.73	0.41
2:E:88:TYR:OH	2:E:117:ASP:OD2	2.37	0.41
2:E:114:LEU:HD22	2:E:118:LEU:HD11	2.00	0.41
1:D:46:CYS:HB3	1:D:47:PRO:CD	2.43	0.41
2:E:348:ARG:HE	2:E:348:ARG:HA	1.85	0.41
1:A:130:THR:O	2:B:72:LEU:HD12	2.21	0.41
1:A:313:MET:HE3	1:A:317:LEU:CD1	2.49	0.41
1:D:260:LYS:HA	1:D:261:PRO:HD3	1.88	0.41
2:E:9:ASN:HD21	2:E:12:LYS:HG3	1.85	0.41
2:E:58:SER:HB2	8:E:2021:HOH:O	0.48	0.41
1:A:96:HIS:HB2	1:A:145:GLN:HG2	2.01	0.41
1:A:131:ASN:HB2	1:A:140:VAL:CB	2.39	0.41
1:A:353:GLU:HG3	1:A:354:PRO:N	2.33	0.41
2:B:145:THR:HG21	2:B:193:CYS:HB2	2.01	0.41
2:E:204:VAL:HG12	2:E:282:VAL:CG2	2.46	0.41
1:A:405:LYS:HE3	2:B:295:MET:SD	2.60	0.41
1:A:97:PHE:CE1	1:A:143:GLY:HA3	2.56	0.41
1:A:146:THR:N	1:A:147:PRO:CD	2.83	0.41
1:D:146:THR:N	1:D:147:PRO:CD	2.83	0.41
5:D:503:SH0:H20	5:D:503:SH0:H62	2.03	0.41
6:E:503:SRM:CDD	3:F:104:CYS:SG	3.09	0.41
1:A:41:GLN:HB2	1:A:125:ARG:HA	2.03	0.41
2:B:376:SER:HB3	2:E:295:MET:HE2	2.02	0.41
1:A:215:LYS:NZ	6:B:503:SRM:O3C	2.42	0.41
2:B:337:LEU:HD23	2:B:337:LEU:C	2.46	0.41
1:D:41:GLN:HB2	1:D:125:ARG:HA	2.02	0.41
1:A:241:LYS:HB2	1:A:241:LYS:HE2	1.77	0.41
1:A:260:LYS:HA	1:A:261:PRO:HD3	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:259:MET:C	2:B:260:TYR:CG	2.98	0.41
1:D:97:PHE:CE1	1:D:143:GLY:HA3	2.55	0.41
1:D:182:ARG:O	1:D:182:ARG:HG2	2.21	0.41
5:D:503:SHO:C11	5:D:503:SHO:C52	2.99	0.41
1:A:437:ARG:HE	1:A:437:ARG:HB2	1.45	0.41
2:B:283:ILE:HB	2:B:303:VAL:HB	2.03	0.41
1:D:335:ILE:HA	1:D:336:LEU:HA	1.67	0.41
2:E:186:LEU:CD1	2:E:186:LEU:C	2.94	0.41
2:E:337:LEU:HD23	2:E:337:LEU:C	2.46	0.41
5:A:503:SHO:C52	5:A:503:SHO:C11	2.99	0.40
2:E:259:MET:C	2:E:260:TYR:CG	2.98	0.40
1:A:70:ILE:HG13	3:C:100:LYS:HG3	2.03	0.40
1:A:259:PHE:CE2	1:A:315:ARG:HD3	2.56	0.40
2:B:146:GLN:HE21	2:B:150:HIS:HB3	1.86	0.40
1:A:184:GLU:HG2	2:B:43:TYR:N	2.35	0.40
2:B:186:LEU:CD1	2:B:186:LEU:C	2.95	0.40
3:F:13:VAL:HG22	3:F:18:PHE:C	2.45	0.40
1:A:53:VAL:HG21	1:A:94:VAL:HG21	2.03	0.40
6:B:503:SRM:CDD	3:C:104:CYS:SG	3.10	0.40
1:D:353:GLU:HG3	1:D:354:PRO:N	2.33	0.40
1:A:60:GLU:OE2	1:A:64:HIS:CE1	2.74	0.40
2:B:48:GLU:HB2	2:B:49:PRO:HD2	2.03	0.40
3:F:73:THR:CG2	3:F:75:PHE:CB	2.98	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SF4	A	501	1	0,12,12	-	-	-		
4	SF4	E	501	2	0,12,12	-	-	-		
7	SO3	B	504	6	1,3,3	0.11	0	0,3,3	-	-
6	SRM	B	503	3,7,2	68,70,70	2.32	16 (23%)	86,112,112	1.84	17 (19%)
5	SH0	A	503	-	58,66,66	2.65	10 (17%)	63,98,98	1.96	15 (23%)
4	SF4	B	502	2	0,12,12	-	-	-		
7	SO3	E	504	6	1,3,3	0.12	0	0,3,3	-	-
4	SF4	B	501	2	0,12,12	-	-	-		
4	SF4	D	501	1	0,12,12	-	-	-		
4	SF4	D	502	1	0,12,12	-	-	-		
5	SH0	D	503	-	58,66,66	2.62	10 (17%)	63,98,98	2.05	16 (25%)
4	SF4	A	502	1	0,12,12	-	-	-		
6	SRM	E	503	3,7,2	68,70,70	2.35	17 (25%)	86,112,112	1.84	16 (18%)
4	SF4	E	502	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	A	501	1	-	-	0/6/5/5
4	SF4	E	501	2	-	-	0/6/5/5
6	SRM	B	503	3,7,2	1/1/19/23	15/38/126/126	-
4	SF4	B	502	2	-	-	0/6/5/5
4	SF4	B	501	2	-	-	0/6/5/5
5	SH0	D	503	-	1/1/24/29	22/52/126/126	0/4/5/5
4	SF4	D	501	1	-	-	0/6/5/5
4	SF4	D	502	1	-	-	0/6/5/5
4	SF4	E	502	2	-	-	0/6/5/5
4	SF4	A	502	1	-	-	0/6/5/5
6	SRM	E	503	3,7,2	1/1/19/23	15/38/126/126	-
5	SH0	A	503	-	1/1/24/29	23/52/126/126	0/4/5/5

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	503	SH0	C8-C7	12.08	1.48	1.33
5	A	503	SH0	C8-C7	12.04	1.48	1.33
6	E	503	SRM	C4A-NA	-10.24	1.27	1.35
6	B	503	SRM	C4A-NA	-9.70	1.28	1.35
5	D	503	SH0	C4-N21	-8.37	1.35	1.48
5	A	503	SH0	C4-N21	-8.23	1.36	1.48
5	A	503	SH0	C9-N22	-7.71	1.35	1.47
5	D	503	SH0	C9-N22	-7.53	1.35	1.47
6	E	503	SRM	C3C-C2C	5.84	1.48	1.36
6	B	503	SRM	C3C-C2C	5.75	1.48	1.36
6	B	503	SRM	CHC-C1C	5.35	1.48	1.38
5	A	503	SH0	C13-C14	-5.34	1.50	1.54
6	B	503	SRM	CHD-C4C	5.32	1.48	1.38
6	E	503	SRM	CHD-C4C	5.08	1.48	1.38
6	E	503	SRM	CHC-C1C	5.01	1.48	1.38
6	B	503	SRM	FE-NC	4.86	2.11	1.95
6	E	503	SRM	FE-NC	4.73	2.10	1.95
5	D	503	SH0	C13-C14	-4.51	1.50	1.54
6	B	503	SRM	CHA-C4D	4.39	1.49	1.39
6	E	503	SRM	CHA-C4D	4.34	1.49	1.39
6	E	503	SRM	FE-ND	4.33	2.09	1.95
6	B	503	SRM	FE-ND	4.14	2.08	1.95
6	E	503	SRM	CHD-C1D	4.07	1.48	1.39
6	B	503	SRM	CHD-C1D	4.05	1.48	1.39
5	D	503	SH0	C10-C6	4.04	1.49	1.40
5	A	503	SH0	C10-C6	3.98	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	503	SH0	C20-C1	3.79	1.49	1.40
5	A	503	SH0	C20-C1	3.67	1.49	1.40
6	E	503	SRM	C4D-ND	-3.07	1.33	1.39
5	A	503	SH0	C16-N24	-3.02	1.33	1.38
6	E	503	SRM	C4D-C3D	2.90	1.50	1.44
6	B	503	SRM	C4D-ND	-2.87	1.34	1.39
5	D	503	SH0	C16-N24	-2.85	1.33	1.38
5	A	503	SH0	C2-C3	-2.68	1.48	1.54
5	D	503	SH0	C6-C7	2.65	1.49	1.45
6	B	503	SRM	C4D-C3D	2.65	1.49	1.44
6	E	503	SRM	CHB-C4A	2.63	1.46	1.39
6	B	503	SRM	C1C-C2C	2.62	1.49	1.45
6	B	503	SRM	CHB-C4A	2.53	1.46	1.39
5	D	503	SH0	C2-C3	-2.50	1.48	1.54
6	B	503	SRM	C4C-C3C	2.48	1.49	1.45
6	B	503	SRM	C1D-ND	-2.47	1.35	1.39
6	E	503	SRM	C1C-C2C	2.41	1.49	1.45
6	E	503	SRM	C1D-ND	-2.38	1.35	1.39
5	A	503	SH0	C6-C7	2.37	1.49	1.45
6	E	503	SRM	C1C-NC	-2.35	1.35	1.39
6	E	503	SRM	C1D-C2D	2.28	1.49	1.44
6	E	503	SRM	C4C-C3C	2.22	1.49	1.45
6	E	503	SRM	C4C-NC	-2.21	1.35	1.39
6	B	503	SRM	C4C-NC	-2.20	1.35	1.39
6	B	503	SRM	C1C-NC	-2.18	1.35	1.39
5	A	503	SH0	C19-N24	-2.17	1.33	1.37
5	D	503	SH0	C19-N24	-2.10	1.33	1.37

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	503	SH0	C20-C1-N21	-6.45	112.06	124.73
5	A	503	SH0	C20-C1-N21	-5.70	113.55	124.73
5	D	503	SH0	C10-C6-N22	-5.66	114.69	125.77
6	E	503	SRM	CHC-C1C-NC	-5.61	118.34	124.45
5	A	503	SH0	C10-C6-N22	-5.61	114.81	125.77
6	B	503	SRM	CHC-C1C-NC	-5.39	118.59	124.45
5	D	503	SH0	C31-C3-C4	5.32	126.28	113.92
5	A	503	SH0	C31-C3-C4	5.15	125.89	113.92
6	B	503	SRM	C3C-C4C-NC	5.02	115.17	110.32
6	E	503	SRM	C3C-C4C-NC	4.74	114.90	110.32
6	E	503	SRM	C2C-C1C-NC	4.51	114.67	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	503	SRM	C2C-C1C-NC	4.49	114.66	110.32
6	B	503	SRM	C4D-C3D-C2D	-4.15	102.46	106.81
6	E	503	SRM	CHA-C4D-ND	-4.11	116.42	123.86
5	D	503	SH0	C10-C6-C7	-4.06	116.25	124.57
6	B	503	SRM	CHA-C4D-ND	-4.01	116.60	123.86
6	B	503	SRM	C4C-C3C-C2C	-3.96	102.41	106.84
5	A	503	SH0	C10-C6-C7	-3.96	116.46	124.57
6	E	503	SRM	C4D-C3D-C2D	-3.93	102.69	106.81
6	E	503	SRM	C1C-C2C-C3C	-3.90	102.47	106.84
5	D	503	SH0	C32-C31-C3	-3.84	107.90	115.53
5	A	503	SH0	C32-C31-C3	-3.81	107.96	115.53
6	E	503	SRM	C4C-C3C-C2C	-3.78	102.61	106.84
6	E	503	SRM	C1D-C2D-C3D	-3.78	102.85	106.81
6	B	503	SRM	C1C-C2C-C3C	-3.75	102.64	106.84
6	B	503	SRM	C4A-CHB-C1B	-3.58	120.58	125.84
6	E	503	SRM	C4A-CHB-C1B	-3.50	120.70	125.84
5	D	503	SH0	C2A-C2-C3	3.47	126.10	116.34
6	E	503	SRM	C2D-C1D-ND	3.41	113.93	110.15
6	E	503	SRM	C3D-C4D-ND	3.25	113.76	110.15
6	B	503	SRM	CHD-C4C-NC	-3.24	120.93	124.45
6	B	503	SRM	C1D-C2D-C3D	-3.22	103.44	106.81
6	E	503	SRM	CDA-C2A-C1A	3.19	116.99	107.11
6	B	503	SRM	CDA-C2A-C1A	3.08	116.64	107.11
5	A	503	SH0	C2A-C2-C3	3.07	124.97	116.34
6	B	503	SRM	C3D-C4D-ND	3.06	113.54	110.15
6	B	503	SRM	C2D-C1D-ND	3.01	113.49	110.15
6	E	503	SRM	CHD-C4C-NC	-2.92	121.28	124.45
5	D	503	SH0	C86-C17-C18	2.81	115.79	108.37
5	D	503	SH0	C41-C8-C9	2.76	128.46	122.12
5	A	503	SH0	C86-C17-C18	2.67	115.41	108.37
5	A	503	SH0	C42-C41-C8	-2.67	109.35	114.61
5	A	503	SH0	C41-C8-C9	2.59	128.07	122.12
6	E	503	SRM	C1A-NA-C4A	2.56	108.51	105.34
5	A	503	SH0	C61-C18-C17	-2.48	107.36	114.19
5	D	503	SH0	C61-C18-C19	-2.40	105.96	110.84
5	D	503	SH0	C42-C41-C8	-2.39	109.90	114.61
5	D	503	SH0	C2-C1-C20	-2.37	117.72	121.95
6	B	503	SRM	C1A-NA-C4A	2.37	108.26	105.34
6	B	503	SRM	C3A-C4A-NA	2.31	115.33	110.83
5	D	503	SH0	C19-C20-C1	-2.31	123.82	126.41
5	D	503	SH0	C61-C18-C17	-2.26	107.98	114.19
5	A	503	SH0	C12-C11-C10	-2.18	123.43	126.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	503	SRM	CMA-C2A-CDA	2.17	114.42	110.74
5	A	503	SH0	C61-C18-C19	-2.17	106.43	110.84
5	A	503	SH0	C19-N24-C16	-2.12	108.55	111.44
5	D	503	SH0	C17-C16-N24	2.11	111.52	108.58
5	A	503	SH0	C17-C16-N24	2.08	111.48	108.58
6	E	503	SRM	C3A-C4A-NA	2.07	114.87	110.83
5	D	503	SH0	O18-C43-C42	2.03	120.40	114.00
6	E	503	SRM	CMA-C2A-CDA	2.02	114.16	110.74
5	D	503	SH0	C7-C6-N22	-2.01	107.20	110.39
6	B	503	SRM	O3D-CED-CDD	-2.00	116.40	122.11
5	A	503	SH0	O2Q-C87-C86	-2.00	117.28	122.95

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	503	SH0	C14
5	D	503	SH0	C14
6	B	503	SRM	NC
6	E	503	SRM	NC

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	503	SH0	N21-C1-C20-C19
5	A	503	SH0	C1-C2-C2A-C2B
5	A	503	SH0	C42-C41-C8-C7
5	A	503	SH0	C18-C19-C20-C1
5	A	503	SH0	N24-C19-C20-C1
5	D	503	SH0	N21-C1-C20-C19
5	D	503	SH0	C1-C2-C2A-C2B
5	D	503	SH0	C18-C19-C20-C1
5	D	503	SH0	N24-C19-C20-C1
6	B	503	SRM	C1A-C2A-CDA-CEA
6	B	503	SRM	CMA-C2A-CDA-CEA
6	B	503	SRM	C3A-C2A-CDA-CEA
6	E	503	SRM	C1A-C2A-CDA-CEA
6	E	503	SRM	CMA-C2A-CDA-CEA
6	E	503	SRM	C3A-C2A-CDA-CEA
5	A	503	SH0	C11-C10-C6-N22
5	D	503	SH0	C11-C10-C6-N22
6	B	503	SRM	C3B-CAB-CBB-CCB
6	E	503	SRM	C3B-CAB-CBB-CCB

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Mol	Chain	Res	Type	Atoms
5	D	503	SH0	C6-C10-C11-N23
5	A	503	SH0	C6-C10-C11-N23
5	D	503	SH0	C4-C5-C9-C8
5	A	503	SH0	C2-C3-C31-C32
5	D	503	SH0	C2-C3-C31-C32
5	D	503	SH0	C17-C86-C87-O1Q
5	A	503	SH0	C14-C13-C51-C52
5	D	503	SH0	C42-C41-C8-C7
5	D	503	SH0	C14-C13-C51-C52
5	A	503	SH0	C17-C86-C87-O2Q
5	D	503	SH0	C17-C86-C87-O2Q
5	A	503	SH0	C3-C2-C2A-C2B
5	A	503	SH0	C2-C2A-C2B-O12
5	A	503	SH0	C2-C2A-C2B-O22
5	D	503	SH0	C2-C2A-C2B-O22
5	A	503	SH0	C17-C86-C87-O1Q
6	E	503	SRM	CAB-CBB-CCB-O1B
5	A	503	SH0	C4-C5-C9-C8
6	B	503	SRM	C4A-C3A-CAA-CBA
6	E	503	SRM	CAC-CBC-CCC-O2C
6	B	503	SRM	CAC-CBC-CCC-O2C
6	E	503	SRM	CAC-CBC-CCC-O1C
5	D	503	SH0	C61-C62-C63-O2R
5	D	503	SH0	C2-C2A-C2B-O12
6	E	503	SRM	C4A-C3A-CAA-CBA
5	A	503	SH0	C31-C32-C33-O13
5	A	503	SH0	C31-C32-C33-O23
6	B	503	SRM	CAA-CBA-CCA-O1A
5	D	503	SH0	C61-C62-C63-O1R
6	B	503	SRM	CAB-CBB-CCB-O1B
6	B	503	SRM	CAC-CBC-CCC-O1C
6	E	503	SRM	CAA-CBA-CCA-O1A
6	E	503	SRM	CAB-CBB-CCB-O2B
5	A	503	SH0	C41-C42-C43-O28
6	B	503	SRM	CAA-CBA-CCA-O2A
6	E	503	SRM	CAA-CBA-CCA-O2A
6	B	503	SRM	CAB-CBB-CCB-O2B
6	B	503	SRM	C3D-CDD-CED-O3D
6	E	503	SRM	C3D-CDD-CED-O3D
6	B	503	SRM	CAD-CBD-CCD-O2D
5	A	503	SH0	C61-C62-C63-O2R
5	D	503	SH0	C41-C42-C43-O28

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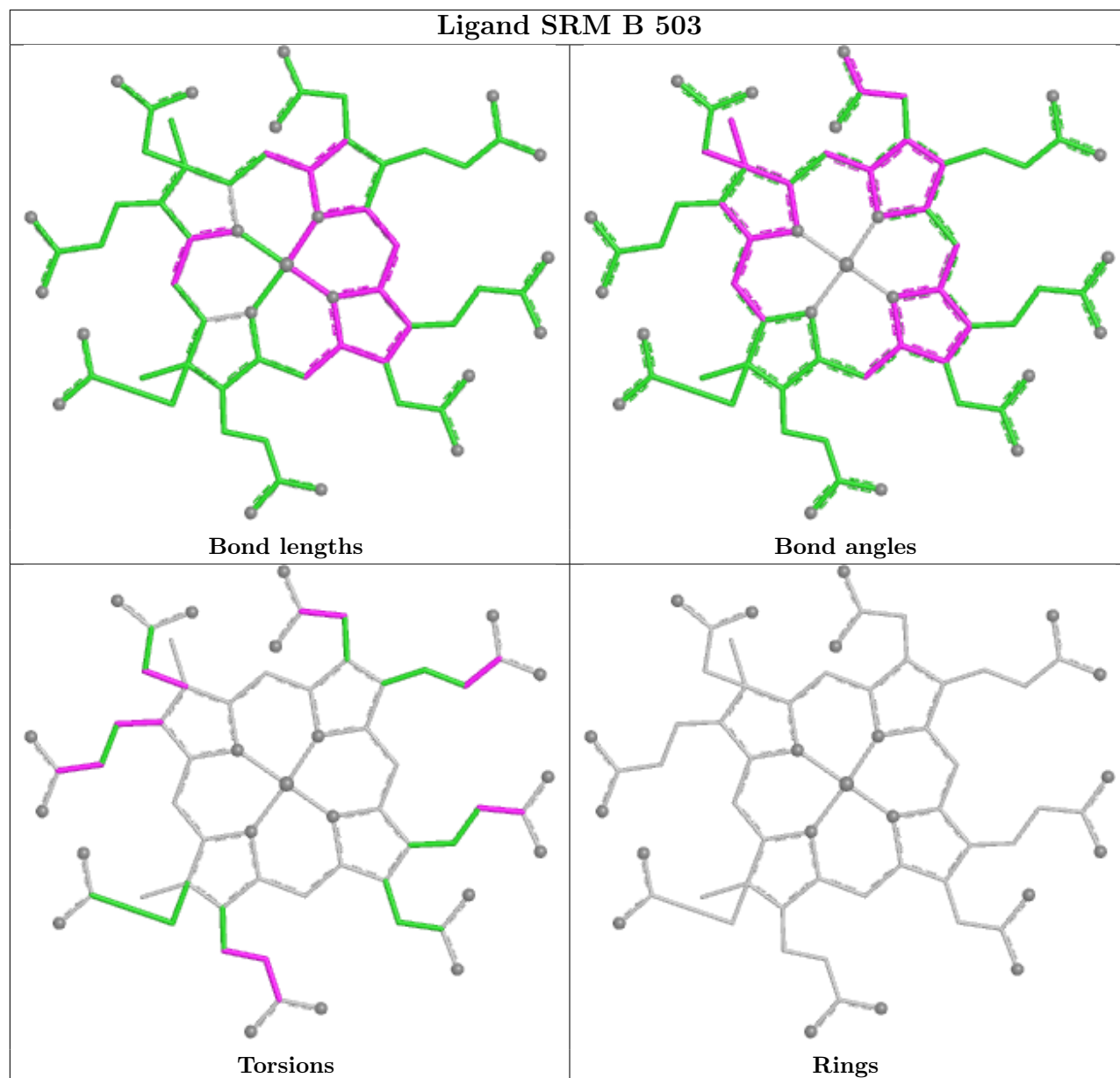
Mol	Chain	Res	Type	Atoms
5	A	503	SH0	C61-C62-C63-O1R
5	D	503	SH0	C31-C32-C33-O23
5	A	503	SH0	C19-C18-C61-C62
5	A	503	SH0	C41-C42-C43-O18
6	B	503	SRM	CAD-CBD-CCD-O1D
5	A	503	SH0	C12-C13-C51-C52
5	D	503	SH0	C12-C13-C51-C52
5	D	503	SH0	C31-C32-C33-O13
6	B	503	SRM	C3D-CDD-CED-O4D
6	E	503	SRM	C3D-CDD-CED-O4D
5	D	503	SH0	C41-C42-C43-O18
6	E	503	SRM	CAD-CBD-CCD-O2D
5	D	503	SH0	C19-C18-C61-C62
6	E	503	SRM	CAD-CBD-CCD-O1D

There are no ring outliers.

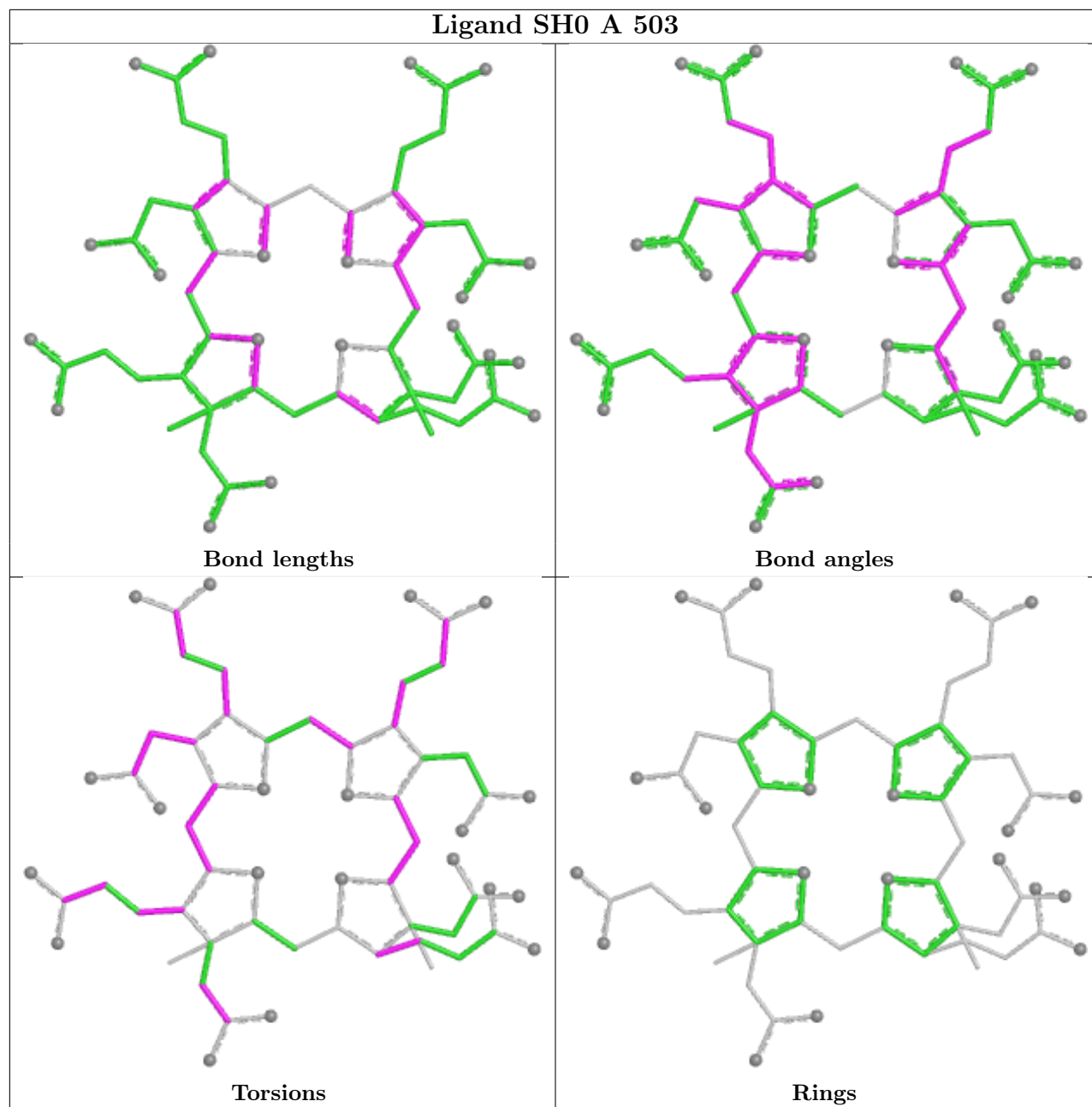
6 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	SF4	1	0
6	B	503	SRM	8	0
5	A	503	SH0	4	0
4	D	501	SF4	1	0
5	D	503	SH0	6	0
6	E	503	SRM	8	0

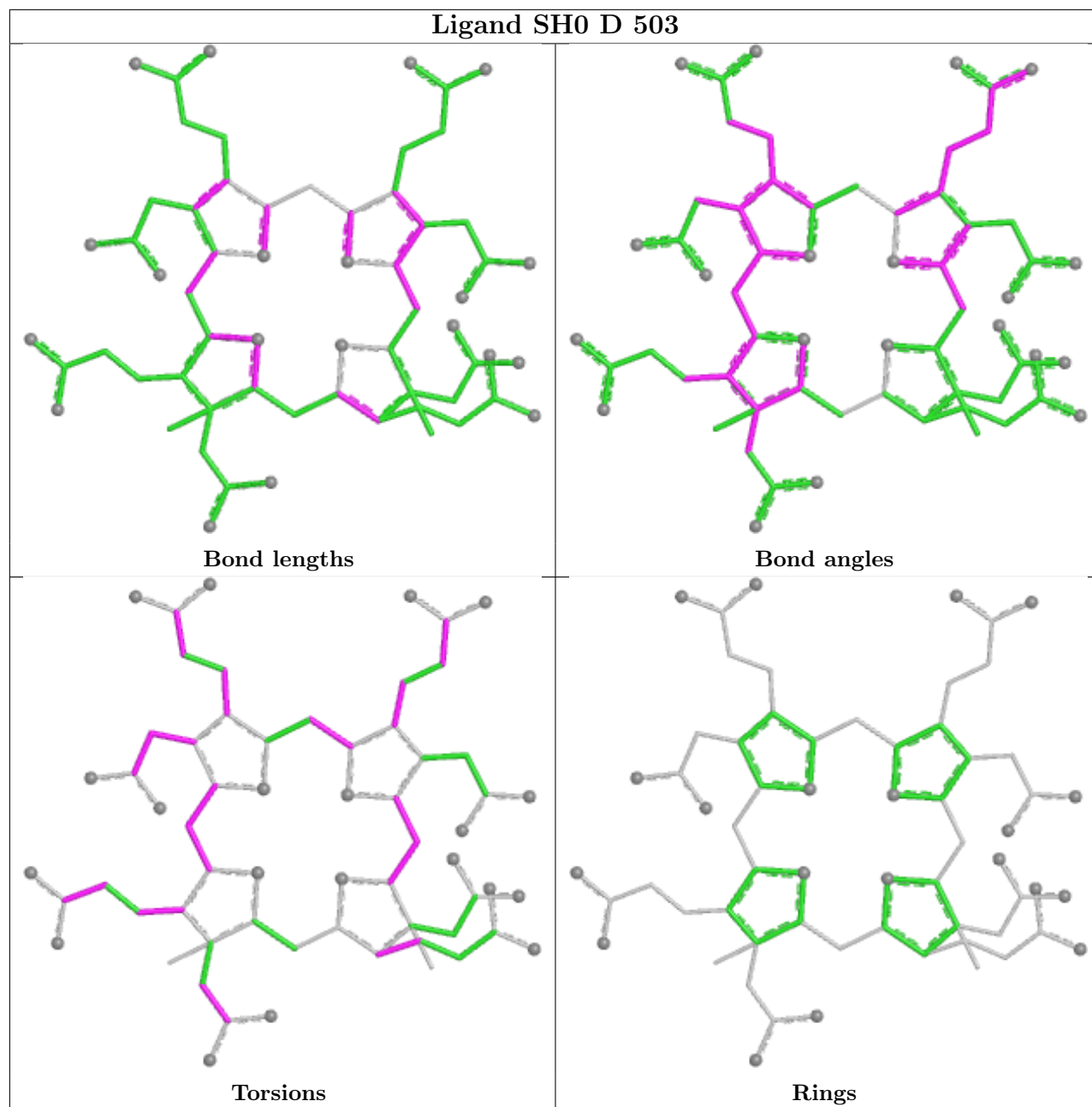
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

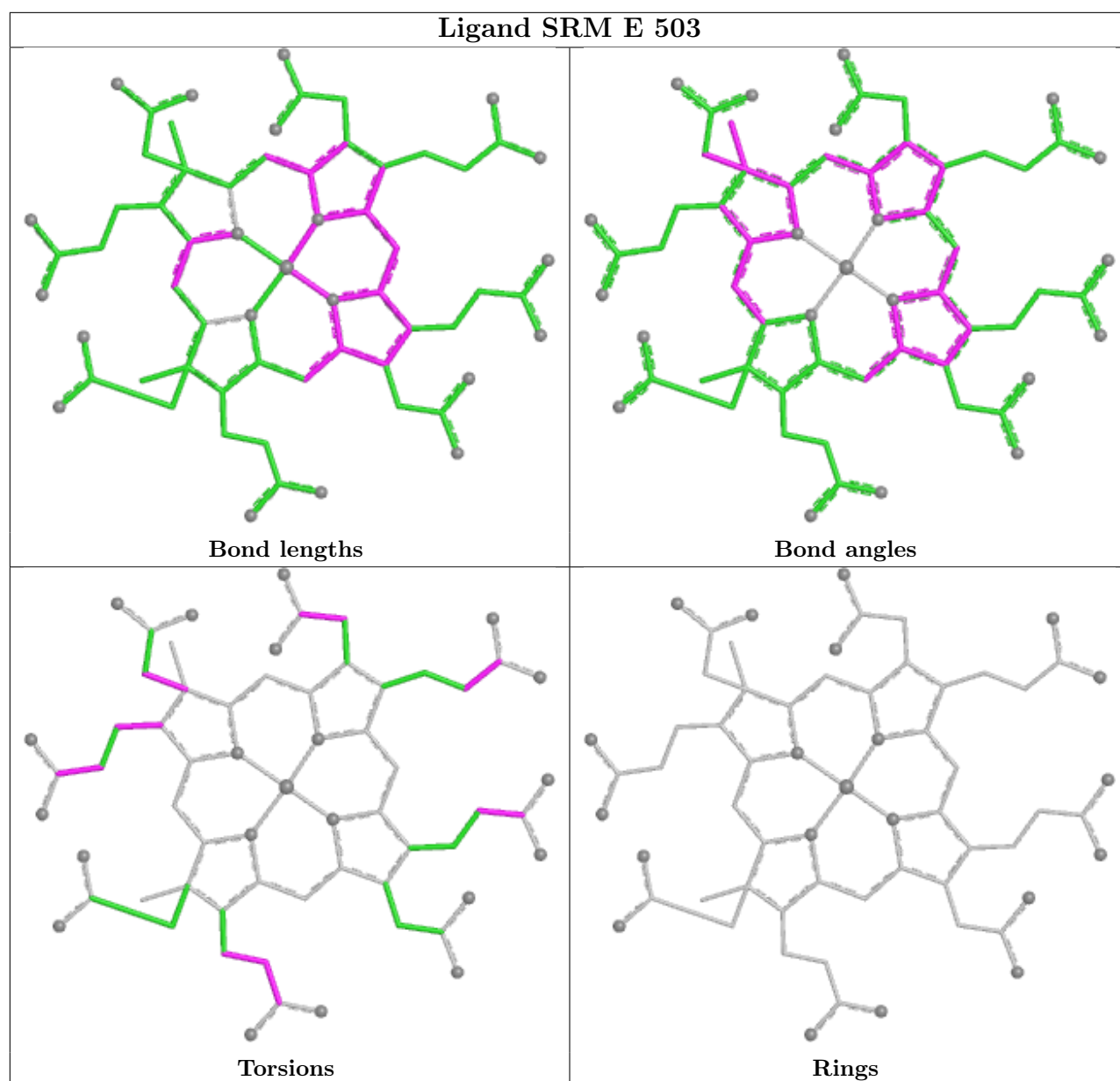


Ligand SH0 A 503



Ligand SH0 D 503





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	436/437 (99%)	-0.22	4 (0%) 81 83	21, 32, 56, 78	0
1	D	436/437 (99%)	0.87	37 (8%) 16 17	26, 50, 67, 79	0
2	B	380/381 (99%)	-0.24	0 100 100	21, 31, 53, 88	0
2	E	380/381 (99%)	0.82	39 (10%) 12 12	22, 47, 74, 100	0
3	C	103/105 (98%)	0.20	1 (0%) 79 81	32, 44, 63, 78	0
3	F	103/105 (98%)	0.83	4 (3%) 43 45	45, 59, 76, 82	0
All	All	1838/1846 (99%)	0.33	85 (4%) 37 39	21, 41, 68, 100	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	128	GLY	3.5
2	E	33	VAL	3.4
2	E	130	PHE	3.4
1	D	32	ALA	3.3
2	E	8	TYR	3.3
1	D	160	LEU	3.3
1	D	154	PHE	3.3
2	E	75	ILE	3.2
2	E	105	VAL	3.1
1	D	162	THR	3.1
1	D	38	LEU	3.0
1	D	164	LEU	2.9
2	E	93	LEU	2.9
2	E	18	ILE	2.9
2	E	16	ASN	2.9
1	D	115	LEU	2.9
1	D	178	LEU	2.9
1	A	2	ALA	2.9
1	D	309	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
2	E	81	MET	2.8
1	D	126	GLY	2.8
1	D	2	ALA	2.8
2	E	243	ILE	2.8
2	E	59	GLY	2.8
2	E	142	ILE	2.7
1	D	259	PHE	2.7
1	D	24	ILE	2.7
2	E	118	LEU	2.7
3	F	105	VAL	2.6
2	E	2	ALA	2.6
2	E	49	PRO	2.6
1	D	53	VAL	2.5
1	D	157	THR	2.5
2	E	32	PRO	2.5
1	D	118	LEU	2.5
1	D	40	TYR	2.5
2	E	30	PHE	2.5
1	D	94	VAL	2.5
2	E	31	PRO	2.5
1	D	129	LEU	2.5
1	D	316	ALA	2.4
1	D	143	GLY	2.4
2	E	47	LEU	2.4
2	E	34	ILE	2.4
3	F	42	ILE	2.4
1	D	159	ASN	2.3
1	D	97	PHE	2.3
2	E	36	LYS	2.3
2	E	55	VAL	2.3
2	E	131	PRO	2.3
2	E	103	PHE	2.3
1	D	17	TRP	2.3
1	D	110	TYR	2.3
2	E	67	VAL	2.3
3	C	105	VAL	2.3
2	E	29	PHE	2.2
2	E	76	THR	2.2
1	D	39	ASP	2.2
1	D	142	LEU	2.2
2	E	62	VAL	2.2
1	D	35	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	101	VAL	2.2
2	E	5	SER	2.2
2	E	43	TYR	2.2
1	D	122	TRP	2.2
1	A	420	VAL	2.1
2	E	69	ALA	2.1
2	E	61	LYS	2.1
1	D	114	TYR	2.1
1	D	246	ILE	2.1
2	E	244	GLY	2.1
1	D	28	ALA	2.1
2	E	54	HIS	2.1
1	A	424	TRP	2.1
2	E	58	SER	2.1
1	A	431	TYR	2.1
1	D	254	TYR	2.1
3	F	4	VAL	2.1
1	D	124	LEU	2.0
1	D	244	ILE	2.0
2	E	182	VAL	2.0
2	E	178	LEU	2.0
1	D	119	CYS	2.0
3	F	91	GLY	2.0
2	E	63	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

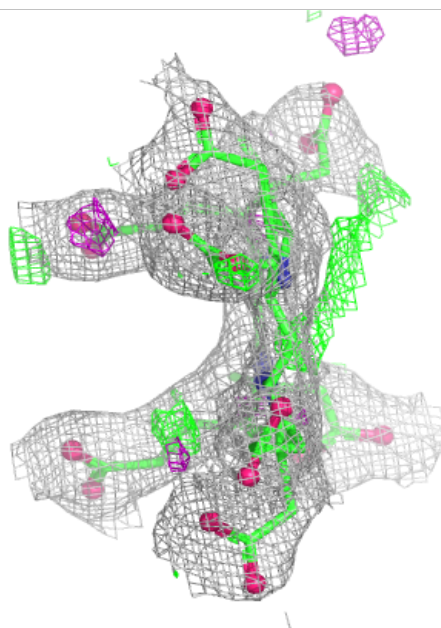
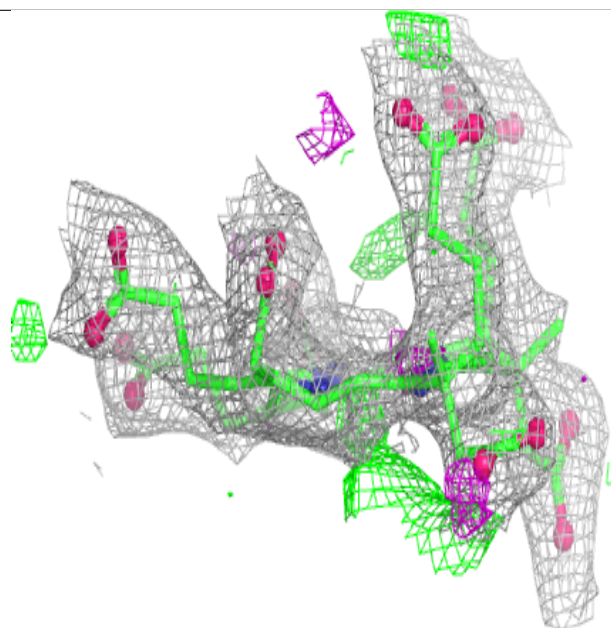
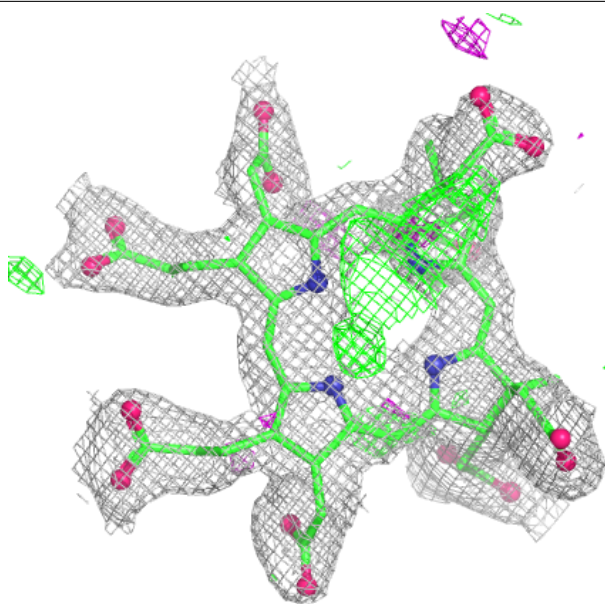
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SH0	D	503	62/62	0.86	0.12	39,47,52,58	0
6	SRM	E	503	63/63	0.92	0.10	35,47,55,60	0
7	SO3	E	504	4/4	0.92	0.10	76,76,76,77	0
5	SH0	A	503	62/62	0.95	0.06	19,24,28,34	0
4	SF4	D	501	8/8	0.96	0.07	38,41,44,46	0
6	SRM	B	503	63/63	0.96	0.07	25,29,35,43	0
7	SO3	B	504	4/4	0.97	0.11	47,47,47,48	0
4	SF4	D	502	8/8	0.97	0.07	38,41,42,46	0
4	SF4	A	501	8/8	0.98	0.07	23,26,26,27	0
4	SF4	E	501	8/8	0.98	0.04	41,42,45,49	0
4	SF4	B	502	8/8	0.99	0.04	25,28,29,30	0
4	SF4	E	502	8/8	0.99	0.03	35,37,39,41	0
4	SF4	A	502	8/8	0.99	0.06	29,30,34,35	0
4	SF4	B	501	8/8	0.99	0.03	28,30,32,37	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.

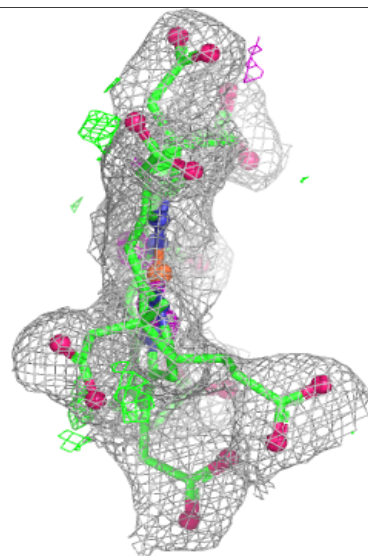
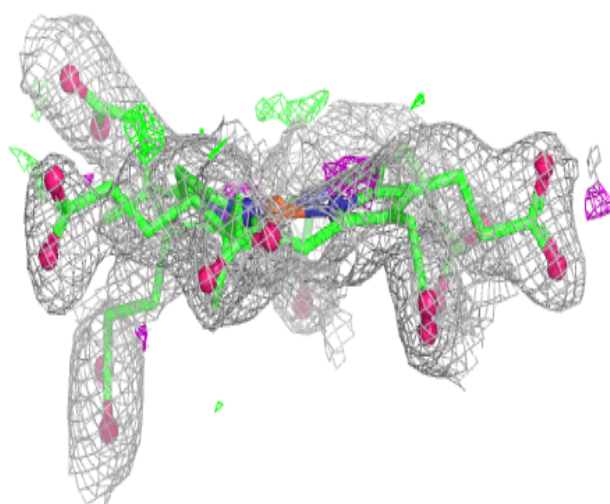
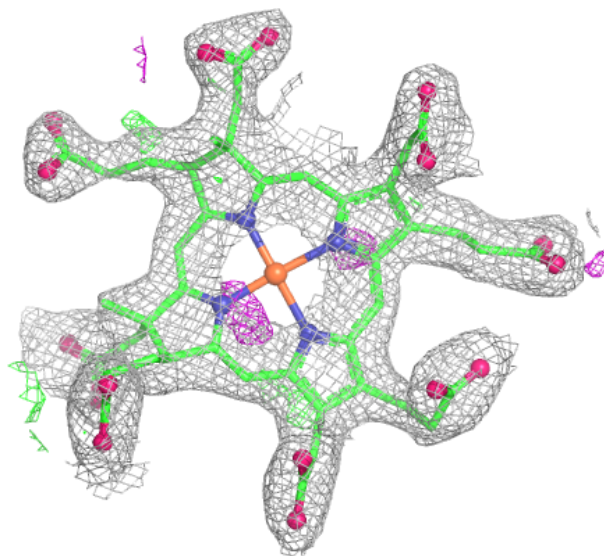
Electron density around SH0 D 503:

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



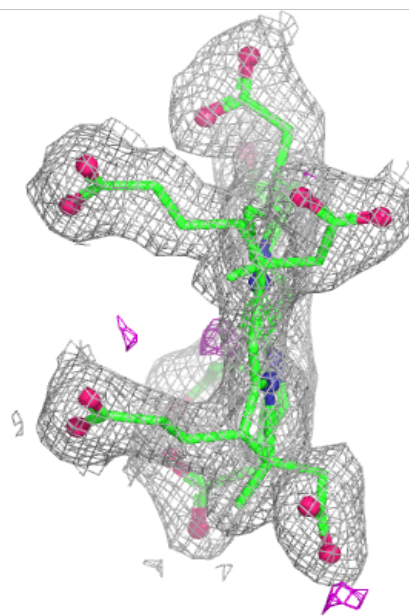
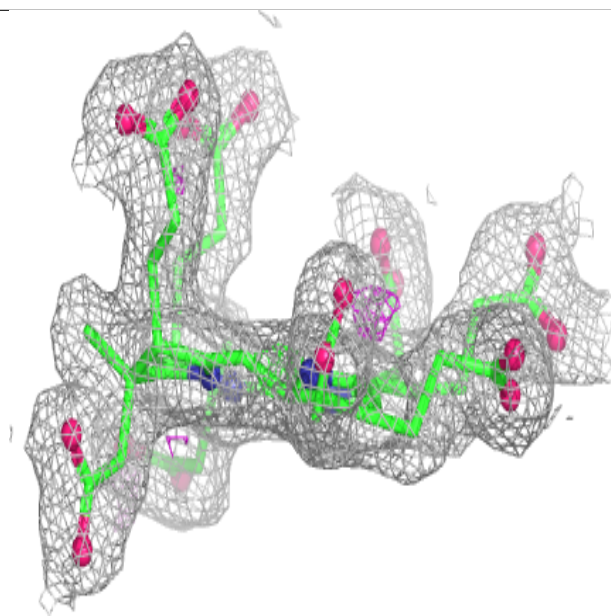
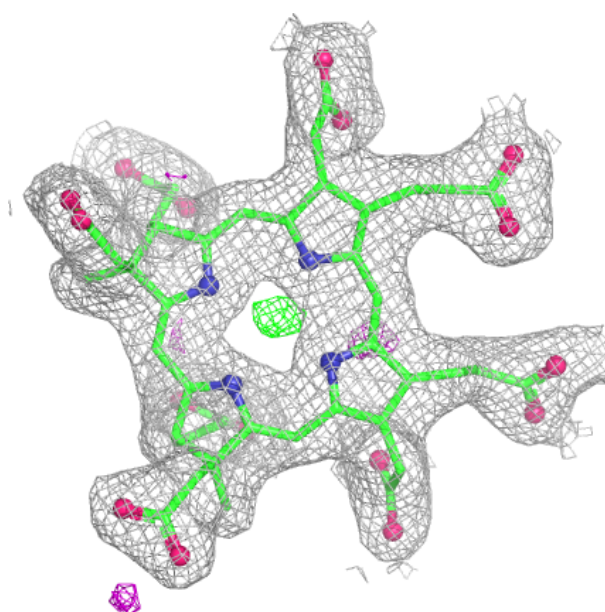
Electron density around SRM E 503:

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



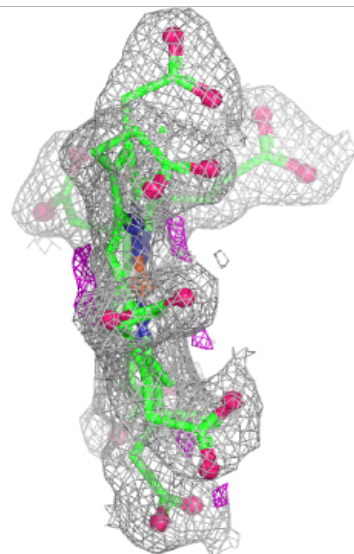
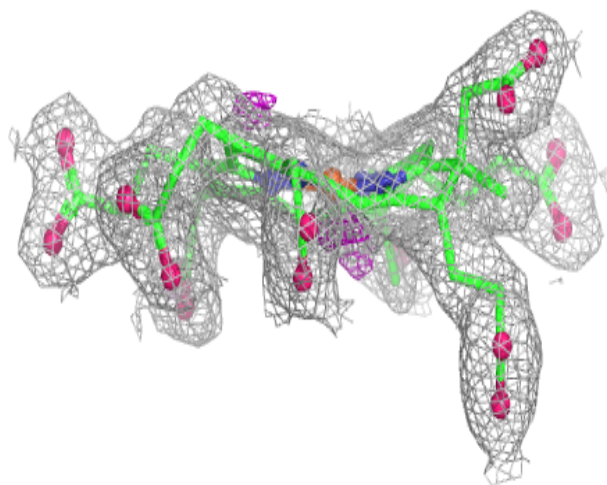
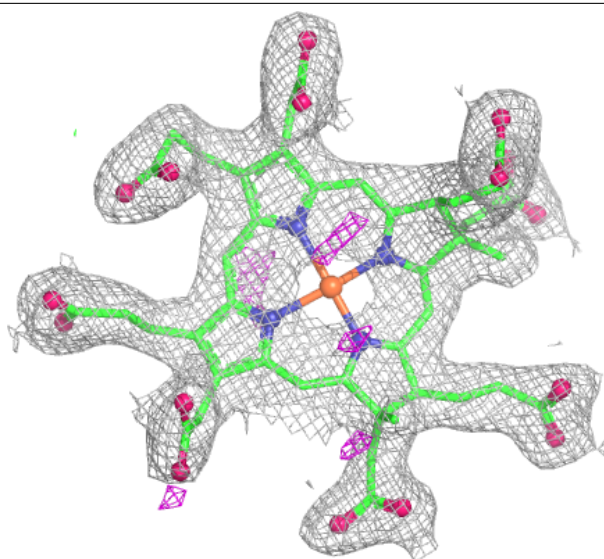
Electron density around SH0 A 503:

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



Electron density around SRM B 503:

$2mF_o-DF_c$ (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.