Full wwPDB X-ray Structure Validation Report (i)

Nov 29, 2023 – 06:42 pm GMT

PDB ID	:	2V4J
Title	:	THE CRYSTAL STRUCTURE OF Desulfovibrio vulgaris DISSIMILATORY SULFITE REDUCTASE BOUND TO DsrC PROVIDES NOVEL INSIGHTS INTO THE MECHANISM OF SULFATE RESPIRATION
Authors	:	Oliveira, T.F.; Vonrhein, C.; Matias, P.M.; Venceslau, S.S.; Pereira, I.A.C.; Archer, M.
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 (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:

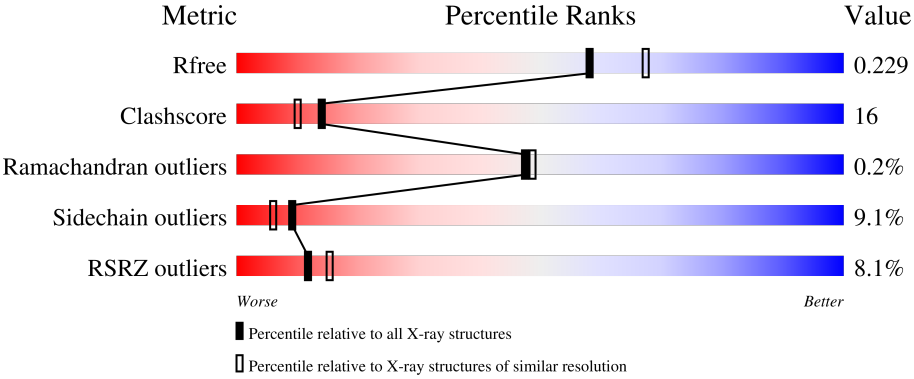
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 <=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	4% 72% 23% •
1	D	437	9% 70% 25% 5%
2	B	381	4% 75% 21% •
2	E	381	14% 70% 25% •
3	C	105	6% 69% 27% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	105	15% 67% 28%

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
5	SH0	A	503	X	-	-	-
5	SH0	D	503	X	-	-	-
6	SRM	B	503	X	-	-	-
6	SRM	E	503	X	-	-	-

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	436	3443	2180	592	648	23	0	0	0
1	D	436	3443	2180	592	648	23	0	0	0

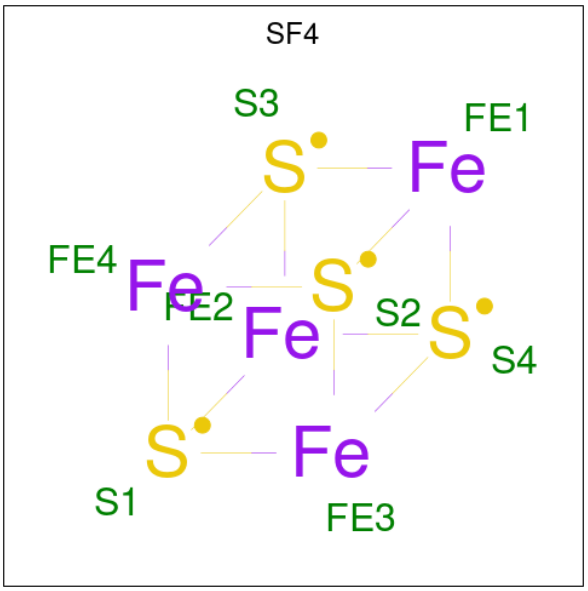
- Molecule 2 is a protein called SULFITE REDUCTASE, DISSIMILATORY-TYPE SUBUNIT BETA.

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

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

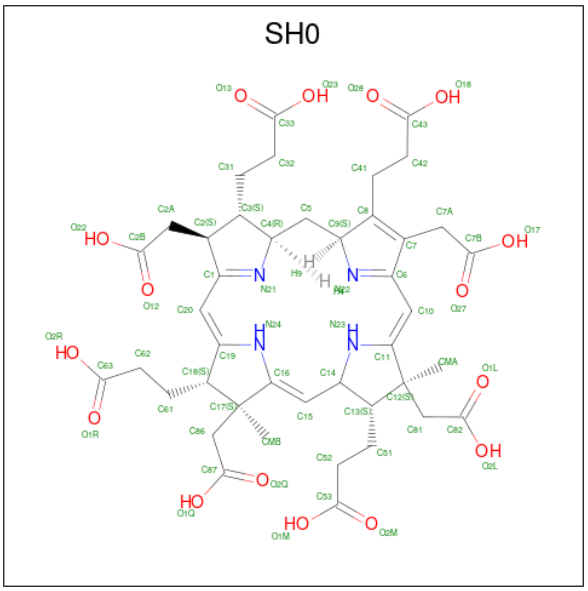
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	103	821	532	129	155	5	0	0	0
3	F	103	821	532	129	155	5	0	0	0

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



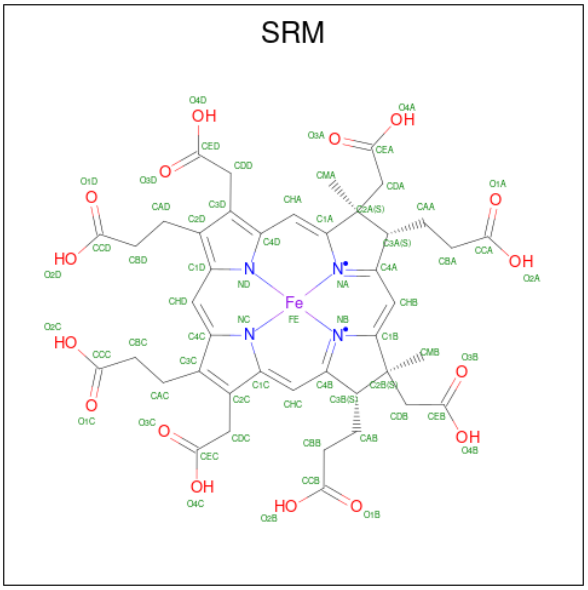
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Fe	S			
4	A	1	8	4	4		0	0
			Total	Fe	S			
4	A	1	8	4	4		0	0
			Total	Fe	S			
4	B	1	8	4	4		0	0
			Total	Fe	S			
4	B	1	8	4	4		0	0
			Total	Fe	S			
4	D	1	8	4	4		0	0
			Total	Fe	S			
4	D	1	8	4	4		0	0
			Total	Fe	S			
4	E	1	8	4	4		0	0
			Total	Fe	S			
4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

- 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 (three-letter code: SH0) (formula: $C_{42}H_{52}N_4O_{16}$).



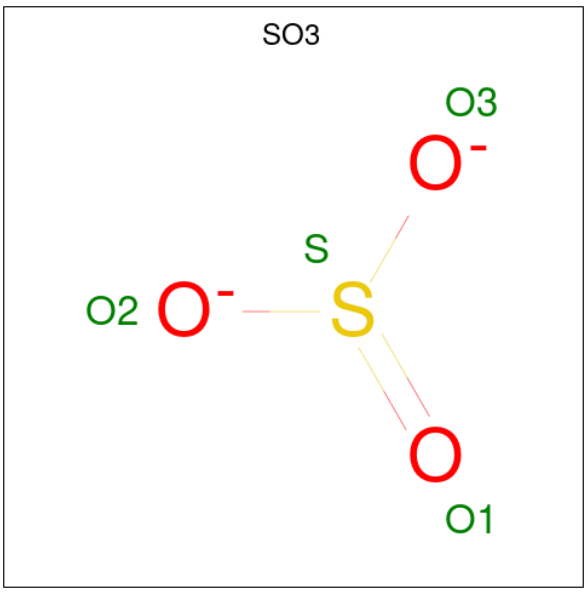
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	62	42	4	16	0	0
5	D	1	62	42	4	16	0	0

- Molecule 6 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		
6	B	1	63	42	1	4	16	0	0
6	E	1	63	42	1	4	16	0	0

- Molecule 7 is SULFITE ION (three-letter code: SO3) (formula: O_3S).



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

- Molecule 8 is water.

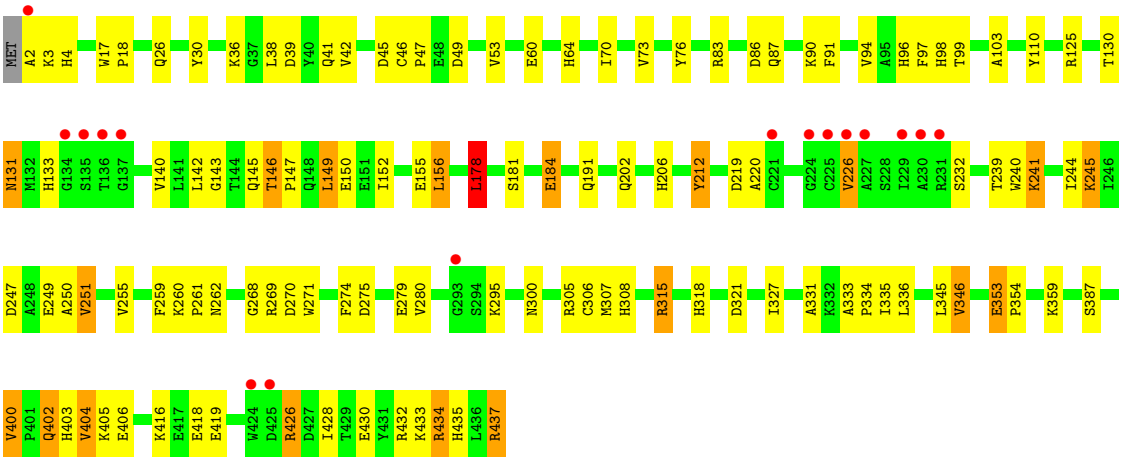
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	312	Total O 312 312	0	0
8	B	274	Total O 274 274	0	0
8	C	58	Total O 58 58	0	0
8	D	181	Total O 181 181	0	0
8	E	164	Total O 164 164	0	0
8	F	27	Total O 27 27	0	0

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.

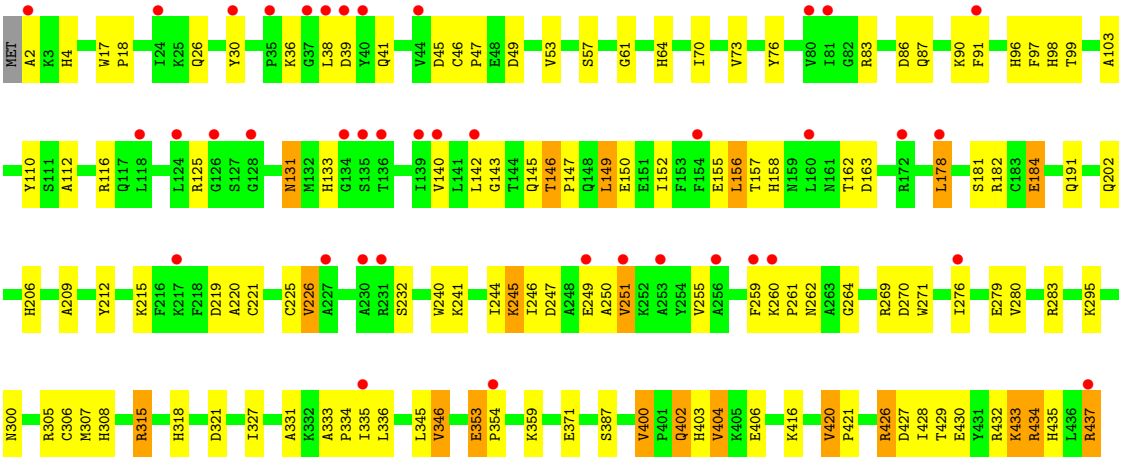
• Molecule 1: SULFITE REDUCTASE, DISSIMILATORY-TYPE SUBUNIT ALPHA

Chain A:



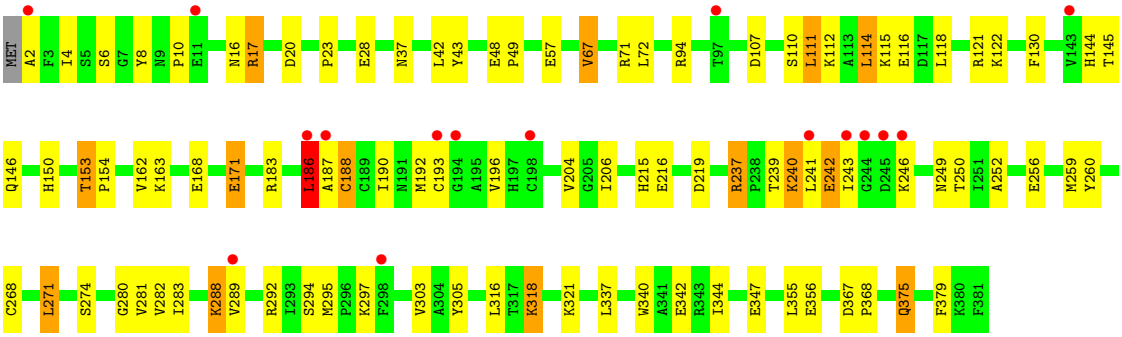
• Molecule 1: SULFITE REDUCTASE, DISSIMILATORY-TYPE SUBUNIT ALPHA

Chain D:



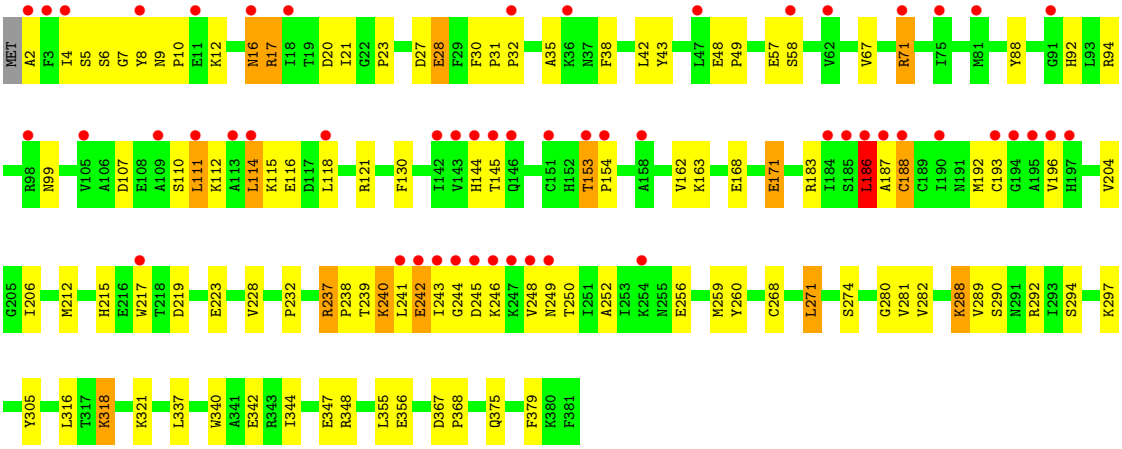
• Molecule 2: SULFITE REDUCTASE, DISSIMILATORY-TYPE SUBUNIT BETA

Chain B:



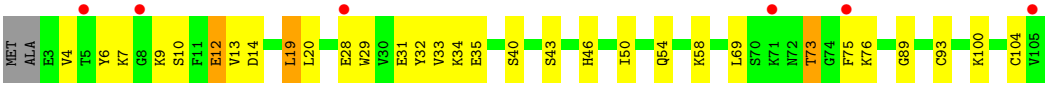
- Molecule 2: SULFITE REDUCTASE, DISSIMILATORY-TYPE SUBUNIT BETA

Chain E:



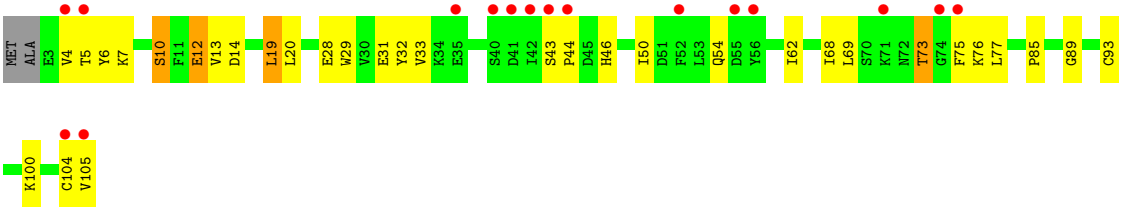
- Molecule 3: SULFITE REDUCTASE, DISSIMILATORY-TYPE SUBUNIT GAMMA

Chain C:



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

Chain F:



4 Data and refinement statistics (i)

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 40.23 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.9 (128.04-2.10) 98.1 (40.23-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 2.10Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, R_{free}	0.190 , 0.219 0.200 , 0.229	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 , 53.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[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: SO3, SH0, SF4, SRM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.34	0/3534	0.56	1/4783 (0.0%)
1	D	0.31	0/3534	0.54	0/4783
2	B	0.36	0/3055	0.58	1/4141 (0.0%)
2	E	0.31	0/3055	0.55	1/4141 (0.0%)
3	C	0.28	0/843	0.46	0/1136
3	F	0.26	0/843	0.45	0/1136
All	All	0.33	0/14864	0.55	3/20120 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	186	LEU	CA-CB-CG	6.39	130.00	115.30
2	E	186	LEU	CA-CB-CG	6.08	129.29	115.30
1	A	178	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

There are no planarity outliers.

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	3443	0	3310	116	0
1	D	3443	0	3310	118	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2975	0	2923	72	0
2	E	2975	0	2923	118	0
3	C	821	0	804	33	0
3	F	821	0	804	35	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	37	0
8	F	27	0	0	3	0
All	All	15816	0	14222	456	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 (456) 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:D:276:ILE:O	8:D:2092:HOH:O	1.60	1.18
1:A:400:VAL:HG13	1:A:402:GLN:HE21	1.04	1.18
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: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
2:E:35:ALA:HB1	8:E:2013:HOH:O	1.53	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:27:ASP:C	8:E:2008:HOH:O	1.92	1.07
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	1.04
1:A:274:PHE:C	8:A:2200:HOH:O	1.97	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
2:E:32:PRO:C	8:E:2010:HOH:O	2.28	0.65
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:5:SER:C	8:E:2003:HOH:O	2.32	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:269:ARG:HG2	1:D:270:ASP:N	2.14	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:ILE:H	1:D:300:ASN:HD21	1.47	0.63
1:D:162:THR:C	8:D:2047:HOH:O	2.29	0.62
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: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
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
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
2:B:256:GLU:CD	2:B:256:GLU:H	2.06	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
2:E:256:GLU:CD	2:E:256:GLU:H	2.05	0.58
1:A:219:ASP:OD1	1:A:226:VAL:HG23	2.03	0.58
2:B:171:GLU:H	2:B:171:GLU:CD	2.06	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
1:D:345:LEU:O	1:D:403:HIS:HE1	1.87	0.57
5:D:503:SH0:H52	5:D:503:SH0: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
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:SH0: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:242:GLU:C	2:B:243:ILE:HG13	2.28	0.53
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
2:E:171:GLU:CD	2:E:171:GLU:H	2.08	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:242:GLU:C	2:E:243:ILE:HG13	2.29	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:427:ASP:OD2	1:D:429:THR:OG1	2.22	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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:6:SER:N	8:E:2003:HOH:O	2.25	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
2:E:297:LYS:NZ	2:E:342:GLU:OE1	2.43	0.47
1:A:251:VAL:O	1:A:255:VAL:HG23	2.13	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
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: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:B:297:LYS:NZ	2:B:342:GLU:OE1	2.43	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:ARG:HD2	1:D:283:ARG:HA	1.83	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
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
1:A:212:TYR:HH	6:B:503:SRM:CED	2.32	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:A:125:ARG:HE	1:A:155:GLU:CD	2.23	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
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
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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:SH0:C11	5:D:503:SH0: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
5:A:503:SH0:C52	5:A:503:SH0:C11	2.99	0.40
1:D:125:ARG:HE	1:D:155:GLU:CD	2.23	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
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
2:B:190:ILE:C	2:B:190:ILE:HD12	2.42	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)

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	434/437 (99%)	422 (97%)	11 (2%)	1 (0%)	47	49
1	D	434/437 (99%)	420 (97%)	13 (3%)	1 (0%)	47	49
2	B	378/381 (99%)	361 (96%)	16 (4%)	1 (0%)	41	41
2	E	378/381 (99%)	362 (96%)	15 (4%)	1 (0%)	41	41
3	C	101/105 (96%)	97 (96%)	4 (4%)	0	100	100
3	F	101/105 (96%)	97 (96%)	4 (4%)	0	100	100
All	All	1826/1846 (99%)	1759 (96%)	63 (4%)	4 (0%)	47	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	387	SER
1	A	387	SER
2	B	153	THR
2	E	153	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	366/367 (100%)	333 (91%)	33 (9%)	9	6
1	D	366/367 (100%)	333 (91%)	33 (9%)	9	6
2	B	322/323 (100%)	291 (90%)	31 (10%)	8	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	E	322/323 (100%)	293 (91%)	29 (9%)	9 6
3	C	90/91 (99%)	82 (91%)	8 (9%)	9 6
3	F	90/91 (99%)	83 (92%)	7 (8%)	12 9
All	All	1556/1562 (100%)	1415 (91%)	141 (9%)	9 6

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	4	HIS
1	A	26	GLN
1	A	38	LEU
1	A	131	ASN
1	A	142	LEU
1	A	146	THR
1	A	149	LEU
1	A	156	LEU
1	A	178	LEU
1	A	184	GLU
1	A	212	TYR
1	A	226	VAL
1	A	241	LYS
1	A	245	LYS
1	A	251	VAL
1	A	262	ASN
1	A	280	VAL
1	A	295	LYS
1	A	315	ARG
1	A	346	VAL
1	A	353	GLU
1	A	400	VAL
1	A	402	GLN
1	A	404	VAL
1	A	416	LYS
1	A	418	GLU
1	A	419	GLU
1	A	426	ARG
1	A	428	ILE
1	A	432	ARG
1	A	434	ARG
1	A	437	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	16	ASN
2	B	17	ARG
2	B	28	GLU
2	B	67	VAL
2	B	71	ARG
2	B	94	ARG
2	B	111	LEU
2	B	114	LEU
2	B	121	ARG
2	B	163	LYS
2	B	171	GLU
2	B	183	ARG
2	B	186	LEU
2	B	188	CYS
2	B	216	GLU
2	B	237	ARG
2	B	239	THR
2	B	240	LYS
2	B	242	GLU
2	B	259	MET
2	B	260	TYR
2	B	271	LEU
2	B	281	VAL
2	B	288	LYS
2	B	289	VAL
2	B	316	LEU
2	B	318	LYS
2	B	347	GLU
2	B	355	LEU
2	B	356	GLU
2	B	375	GLN
3	C	9	LYS
3	C	10	SER
3	C	12	GLU
3	C	19	LEU
3	C	31	GLU
3	C	35	GLU
3	C	73	THR
3	C	76	LYS
1	D	4	HIS
1	D	26	GLN
1	D	38	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	131	ASN
1	D	142	LEU
1	D	146	THR
1	D	149	LEU
1	D	156	LEU
1	D	178	LEU
1	D	184	GLU
1	D	212	TYR
1	D	221	CYS
1	D	226	VAL
1	D	241	LYS
1	D	245	LYS
1	D	251	VAL
1	D	262	ASN
1	D	280	VAL
1	D	295	LYS
1	D	315	ARG
1	D	346	VAL
1	D	353	GLU
1	D	400	VAL
1	D	402	GLN
1	D	404	VAL
1	D	416	LYS
1	D	420	VAL
1	D	426	ARG
1	D	428	ILE
1	D	432	ARG
1	D	433	LYS
1	D	434	ARG
1	D	437	ARG
2	E	16	ASN
2	E	17	ARG
2	E	28	GLU
2	E	71	ARG
2	E	94	ARG
2	E	111	LEU
2	E	114	LEU
2	E	121	ARG
2	E	163	LYS
2	E	171	GLU
2	E	183	ARG
2	E	186	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	188	CYS
2	E	237	ARG
2	E	239	THR
2	E	240	LYS
2	E	242	GLU
2	E	259	MET
2	E	260	TYR
2	E	271	LEU
2	E	281	VAL
2	E	288	LYS
2	E	289	VAL
2	E	316	LEU
2	E	318	LYS
2	E	347	GLU
2	E	355	LEU
2	E	356	GLU
2	E	375	GLN
3	F	4	VAL
3	F	10	SER
3	F	12	GLU
3	F	19	LEU
3	F	31	GLU
3	F	73	THR
3	F	76	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	87	GLN
1	A	98	HIS
1	A	133	HIS
1	A	158	HIS
1	A	191	GLN
1	A	202	GLN
1	A	300	ASN
1	A	308	HIS
1	A	318	HIS
1	A	402	GLN
1	A	403	HIS
2	B	146	GLN
2	B	215	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	220	GLN
2	B	255	ASN
2	B	375	GLN
3	C	46	HIS
1	D	26	GLN
1	D	64	HIS
1	D	87	GLN
1	D	98	HIS
1	D	133	HIS
1	D	158	HIS
1	D	191	GLN
1	D	202	GLN
1	D	300	ASN
1	D	308	HIS
1	D	318	HIS
1	D	402	GLN
1	D	403	HIS
2	E	37	ASN
2	E	99	ASN
2	E	146	GLN
2	E	215	HIS
2	E	255	ASN
2	E	375	GLN
3	F	46	HIS

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)

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	D	502	1	0,12,12	-	-	-		
4	SF4	B	501	2	0,12,12	-	-	-		
4	SF4	A	502	1	0,12,12	-	-	-		
7	SO3	E	504	6	1,3,3	0.12	0	0,3,3	-	-
4	SF4	B	502	2	0,12,12	-	-	-		
6	SRM	B	503	2,3,7	68,70,70	2.36	13 (19%)	81,112,112	1.72	14 (17%)
4	SF4	E	502	2	0,12,12	-	-	-		
4	SF4	E	501	2	0,12,12	-	-	-		
4	SF4	A	501	1	0,12,12	-	-	-		
6	SRM	E	503	2,3,7	68,70,70	2.37	13 (19%)	81,112,112	1.69	14 (17%)
5	SH0	D	503	-	61,66,66	2.58	10 (16%)	60,98,98	2.25	12 (20%)
7	SO3	B	504	6	1,3,3	0.11	0	0,3,3	-	-
5	SH0	A	503	-	61,66,66	2.62	10 (16%)	60,98,98	2.19	11 (18%)
4	SF4	D	501	1	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	D	502	1	-	-	0/6/5/5
4	SF4	B	501	2	-	-	0/6/5/5
4	SF4	A	502	1	-	-	0/6/5/5
4	SF4	B	502	2	-	-	0/6/5/5
6	SRM	B	503	2,3,7	1/1/19/23	15/38/126/126	-
4	SF4	E	502	2	-	-	0/6/5/5
4	SF4	E	501	2	-	-	0/6/5/5
4	SF4	A	501	1	-	-	0/6/5/5
6	SRM	E	503	2,3,7	1/1/19/23	15/38/126/126	-
5	SH0	D	503	-	1/1/24/29	21/52/126/126	0/4/5/5
5	SH0	A	503	-	1/1/24/29	22/52/126/126	0/4/5/5
4	SF4	D	501	1	-	-	0/6/5/5

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	503	SH0	C8-C7	11.55	1.48	1.33
5	A	503	SH0	C8-C7	11.51	1.48	1.33
6	E	503	SRM	C4A-NA	-10.40	1.27	1.35
6	B	503	SRM	C4A-NA	-9.85	1.28	1.35
6	B	503	SRM	CHD-C4C	9.73	1.48	1.35
6	E	503	SRM	CHD-C4C	9.39	1.48	1.35
5	D	503	SH0	C4-N21	-8.40	1.35	1.48
5	A	503	SH0	C4-N21	-8.27	1.36	1.48
5	A	503	SH0	C9-N22	-7.77	1.35	1.47
5	D	503	SH0	C9-N22	-7.60	1.35	1.47
6	E	503	SRM	C3C-C2C	5.71	1.48	1.36
6	B	503	SRM	C3C-C2C	5.62	1.48	1.36
6	B	503	SRM	CHC-C1C	5.40	1.48	1.38
5	A	503	SH0	C13-C14	-5.34	1.50	1.54
6	E	503	SRM	CHC-C1C	5.05	1.48	1.38
5	D	503	SH0	C13-C14	-4.51	1.50	1.54
5	A	503	SH0	C6-N22	4.30	1.35	1.29
5	D	503	SH0	C6-N22	4.13	1.35	1.29
5	D	503	SH0	C10-C6	4.06	1.49	1.40
5	A	503	SH0	C10-C6	4.00	1.49	1.40
6	B	503	SRM	FE-NC	3.98	2.11	1.95
6	E	503	SRM	C3D-C2D	3.94	1.48	1.39
5	D	503	SH0	C20-C1	3.89	1.49	1.40
6	B	503	SRM	C3D-C2D	3.87	1.48	1.39
6	E	503	SRM	FE-NC	3.86	2.10	1.95
5	A	503	SH0	C20-C1	3.77	1.49	1.40
5	A	503	SH0	C16-N24	-3.36	1.33	1.38
5	D	503	SH0	C16-N24	-3.17	1.33	1.38
6	B	503	SRM	C4D-CHA	2.97	1.49	1.41
6	E	503	SRM	C4D-CHA	2.93	1.49	1.41
6	E	503	SRM	C1D-CHD	2.72	1.48	1.41
6	B	503	SRM	C1D-CHD	2.70	1.48	1.41
5	D	503	SH0	C6-C7	2.61	1.49	1.45
6	E	503	SRM	CHB-C4A	2.61	1.46	1.39
6	B	503	SRM	C1C-C2C	2.58	1.49	1.45
5	A	503	SH0	C2-C3	-2.54	1.48	1.54
6	B	503	SRM	CHB-C4A	2.51	1.46	1.39
6	B	503	SRM	C4C-C3C	2.44	1.49	1.45
5	D	503	SH0	C2-C3	-2.38	1.48	1.54
6	E	503	SRM	C1C-C2C	2.37	1.49	1.45
6	E	503	SRM	C1C-NC	-2.36	1.35	1.39
5	A	503	SH0	C6-C7	2.33	1.49	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	503	SRM	C4C-NC	-2.22	1.35	1.39
6	B	503	SRM	C4C-NC	-2.20	1.35	1.39
6	B	503	SRM	C1C-NC	-2.19	1.35	1.39
6	E	503	SRM	C4C-C3C	2.18	1.49	1.45

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	503	SH0	C20-C1-N21	-7.13	112.06	124.73
5	A	503	SH0	C20-C1-N21	-6.29	113.55	124.73
5	D	503	SH0	C31-C3-C2	5.97	126.76	113.73
5	A	503	SH0	C31-C3-C2	5.86	126.52	113.73
5	D	503	SH0	C32-C31-C3	-5.75	107.90	115.72
5	A	503	SH0	C32-C31-C3	-5.70	107.96	115.72
5	A	503	SH0	C19-N24-C16	-5.70	108.55	110.77
6	E	503	SRM	CHC-C1C-NC	-5.64	118.34	124.44
5	D	503	SH0	C10-C6-N22	-5.55	114.69	125.33
5	A	503	SH0	C10-C6-N22	-5.49	114.81	125.33
6	B	503	SRM	CHC-C1C-NC	-5.41	118.59	124.44
5	D	503	SH0	C19-N24-C16	-5.16	108.76	110.77
6	B	503	SRM	C3C-C4C-NC	4.98	115.17	110.32
6	E	503	SRM	C3C-C4C-NC	4.71	114.90	110.32
6	E	503	SRM	C2C-C1C-NC	4.47	114.67	110.32
6	B	503	SRM	C2C-C1C-NC	4.45	114.66	110.32
5	D	503	SH0	C10-C6-C7	-4.06	116.25	124.49
5	A	503	SH0	C10-C6-C7	-3.95	116.46	124.49
6	B	503	SRM	C4C-C3C-C2C	-3.85	102.41	106.86
6	E	503	SRM	C1C-C2C-C3C	-3.79	102.47	106.86
6	E	503	SRM	C4C-C3C-C2C	-3.68	102.61	106.86
6	B	503	SRM	C1C-C2C-C3C	-3.64	102.64	106.86
6	B	503	SRM	C4A-CHB-C1B	-3.59	120.58	125.88
6	E	503	SRM	C4A-CHB-C1B	-3.51	120.70	125.88
6	B	503	SRM	CHD-C4C-NC	-3.23	120.93	124.43
6	E	503	SRM	CDA-C2A-C1A	3.14	116.99	107.12
6	B	503	SRM	CDA-C2A-C1A	3.03	116.64	107.12
6	E	503	SRM	CHD-C4C-NC	-2.91	121.28	124.43
6	E	503	SRM	C1A-NA-C4A	2.89	108.51	105.23
5	A	503	SH0	C42-C41-C8	-2.88	109.35	114.48
5	D	503	SH0	C2-C1-N21	-2.79	108.16	113.17
5	D	503	SH0	C86-C17-C18	2.76	115.79	108.39
5	D	503	SH0	C19-C20-C1	-2.68	123.82	126.44
6	B	503	SRM	C1A-NA-C4A	2.68	108.26	105.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	503	SH0	C2-C1-N21	-2.64	108.43	113.17
5	A	503	SH0	C86-C17-C18	2.62	115.41	108.39
5	D	503	SH0	C42-C41-C8	-2.57	109.90	114.48
6	B	503	SRM	CDD-C3D-C4D	2.52	131.19	127.36
5	A	503	SH0	C61-C18-C17	-2.46	107.36	114.14
6	E	503	SRM	CBD-CAD-C2D	-2.33	108.65	112.62
6	B	503	SRM	O3D-CED-CDD	-2.33	116.40	123.04
5	D	503	SH0	C2-C1-C20	-2.32	117.72	121.92
6	B	503	SRM	C3A-C4A-NA	2.28	115.33	110.85
6	E	503	SRM	CDD-C3D-C4D	2.26	130.80	127.36
5	D	503	SH0	C61-C18-C17	-2.24	107.98	114.14
6	B	503	SRM	CBD-CAD-C2D	-2.23	108.81	112.62
6	B	503	SRM	CMA-C2A-CDA	2.19	114.42	110.80
6	E	503	SRM	O3D-CED-CDD	-2.13	116.97	123.04
6	E	503	SRM	C3A-C4A-NA	2.05	114.87	110.85
6	E	503	SRM	CMA-C2A-CDA	2.04	114.16	110.80
5	A	503	SH0	C12-C11-C10	-2.03	123.43	126.37

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 (73) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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
5	D	503	SH0	C6-C10-C11-N23
5	A	503	SH0	C6-C10-C11-N23
5	D	503	SH0	C4-C5-C9-C8
6	B	503	SRM	C3D-CDD-CED-O3D
6	E	503	SRM	C3D-CDD-CED-O4D
5	A	503	SH0	C2-C3-C31-C32
5	D	503	SH0	C2-C3-C31-C32
5	D	503	SH0	C42-C41-C8-C7
5	A	503	SH0	C17-C86-C87-O1Q
5	A	503	SH0	C17-C86-C87-O2Q
5	D	503	SH0	C17-C86-C87-O1Q
5	D	503	SH0	C17-C86-C87-O2Q
6	E	503	SRM	C3D-CDD-CED-O3D
5	A	503	SH0	C14-C13-C51-C52
5	D	503	SH0	C14-C13-C51-C52
6	B	503	SRM	C3D-CDD-CED-O4D
6	B	503	SRM	CAC-CBC-CCC-O2C
6	E	503	SRM	CAC-CBC-CCC-O2C
5	A	503	SH0	C41-C42-C43-O28
5	D	503	SH0	C61-C62-C63-O2R
6	E	503	SRM	CAC-CBC-CCC-O1C
6	B	503	SRM	C4A-C3A-CAA-CBA
6	E	503	SRM	C4A-C3A-CAA-CBA
5	D	503	SH0	C41-C42-C43-O28
6	E	503	SRM	CAB-CBB-CCB-O1B
6	B	503	SRM	CAC-CBC-CCC-O1C
5	A	503	SH0	C4-C5-C9-C8
5	D	503	SH0	C61-C62-C63-O1R
6	B	503	SRM	CAA-CBA-CCA-O1A
6	E	503	SRM	CAA-CBA-CCA-O1A
5	A	503	SH0	C3-C2-C2A-C2B
6	B	503	SRM	CAA-CBA-CCA-O2A
5	A	503	SH0	C2-C2A-C2B-O12
5	A	503	SH0	C2-C2A-C2B-O22
5	D	503	SH0	C2-C2A-C2B-O22
6	E	503	SRM	CAA-CBA-CCA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	503	SH0	C19-C18-C61-C62
6	B	503	SRM	CAD-CBD-CCD-O2D
5	A	503	SH0	C31-C32-C33-O13
5	A	503	SH0	C61-C62-C63-O2R
5	A	503	SH0	C41-C42-C43-O18
6	B	503	SRM	CAB-CBB-CCB-O1B
6	E	503	SRM	CAB-CBB-CCB-O2B
5	A	503	SH0	C31-C32-C33-O23
6	B	503	SRM	CAB-CBB-CCB-O2B
6	B	503	SRM	CAD-CBD-CCD-O1D
5	D	503	SH0	C2-C2A-C2B-O12
5	A	503	SH0	C61-C62-C63-O1R
5	D	503	SH0	C31-C32-C33-O23
5	D	503	SH0	C41-C42-C43-O18
5	D	503	SH0	C19-C18-C61-C62
5	D	503	SH0	C31-C32-C33-O13
6	E	503	SRM	CAD-CBD-CCD-O2D
6	E	503	SRM	CAD-CBD-CCD-O1D

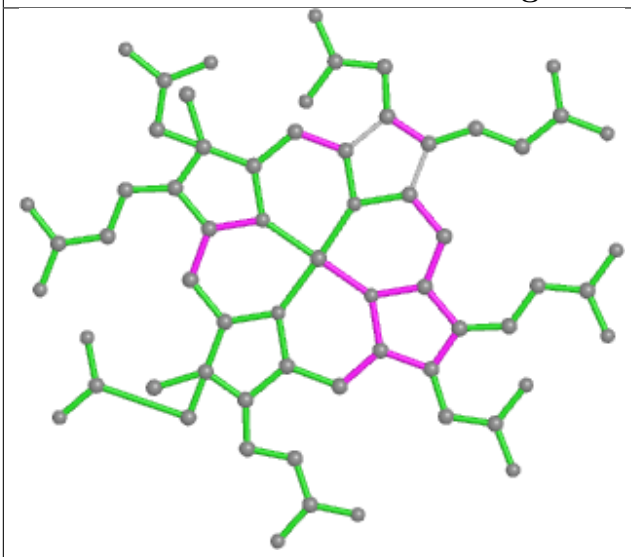
There are no ring outliers.

6 monomers are involved in 28 short contacts:

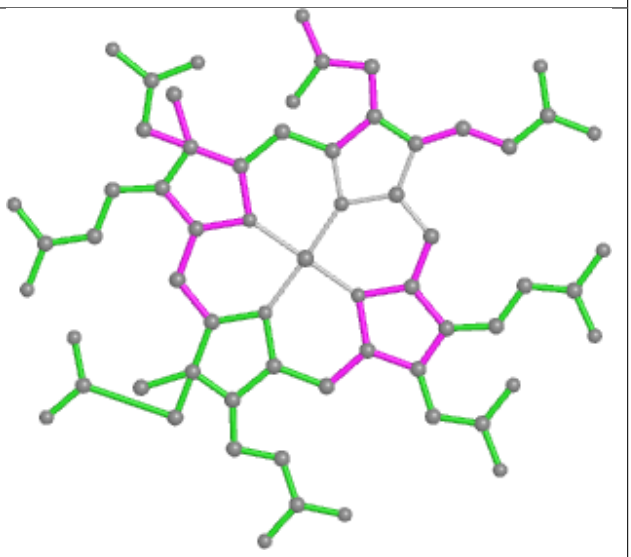
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	503	SRM	8	0
4	A	501	SF4	1	0
6	E	503	SRM	8	0
5	D	503	SH0	6	0
5	A	503	SH0	4	0
4	D	501	SF4	1	0

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

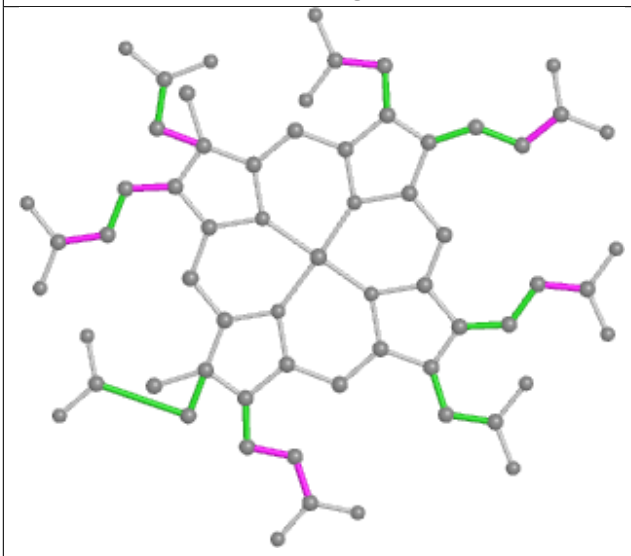
Ligand SRM B 503



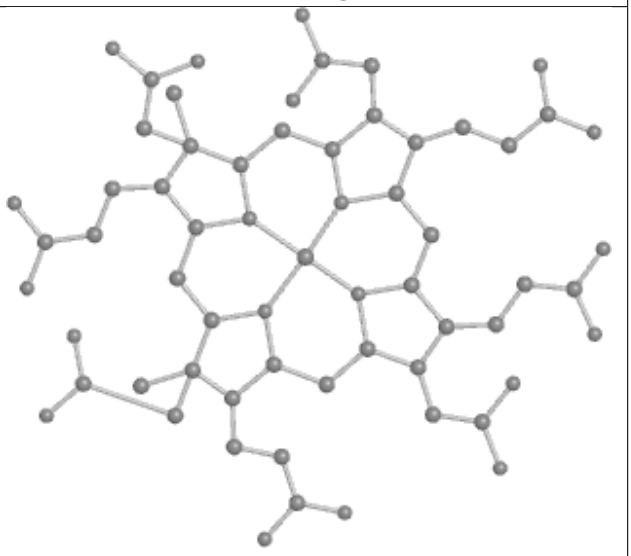
Bond lengths



Bond angles

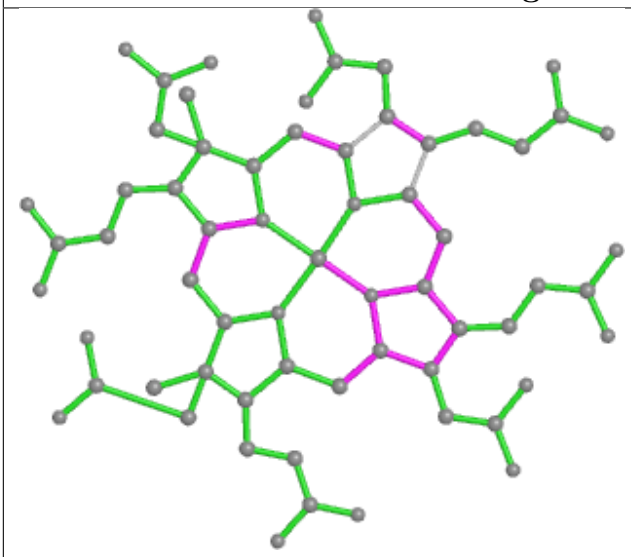


Torsions

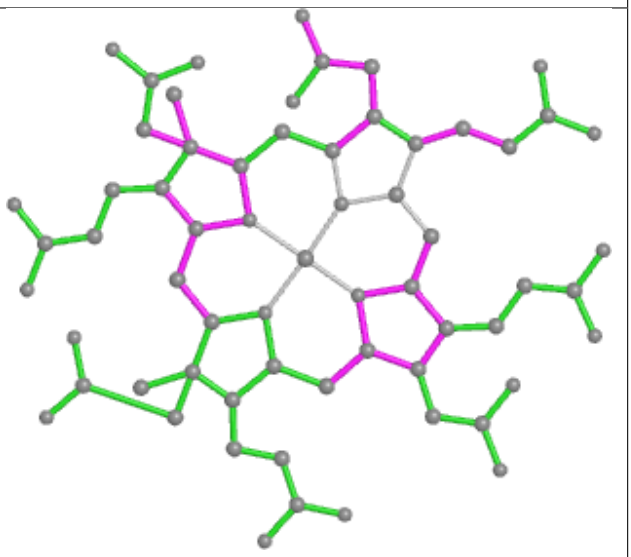


Rings

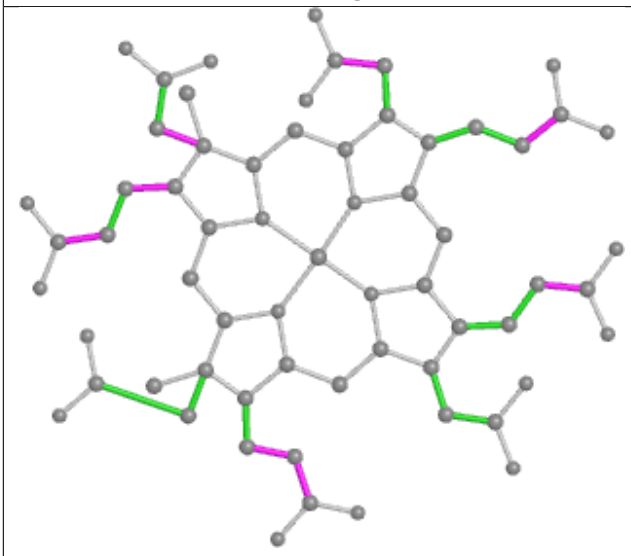
Ligand SRM E 503



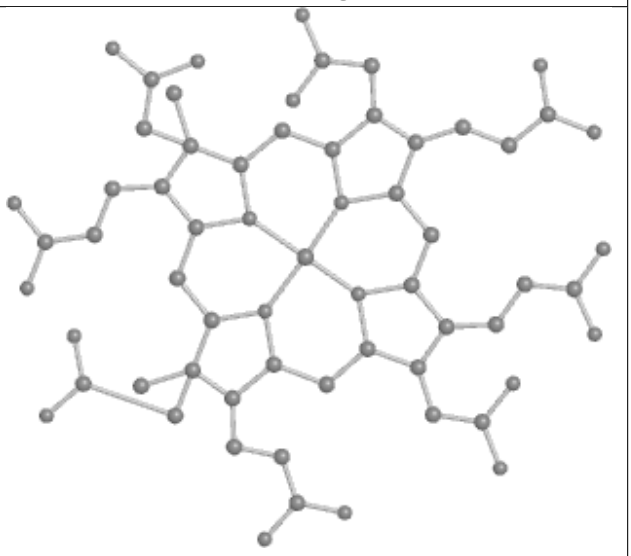
Bond lengths



Bond angles

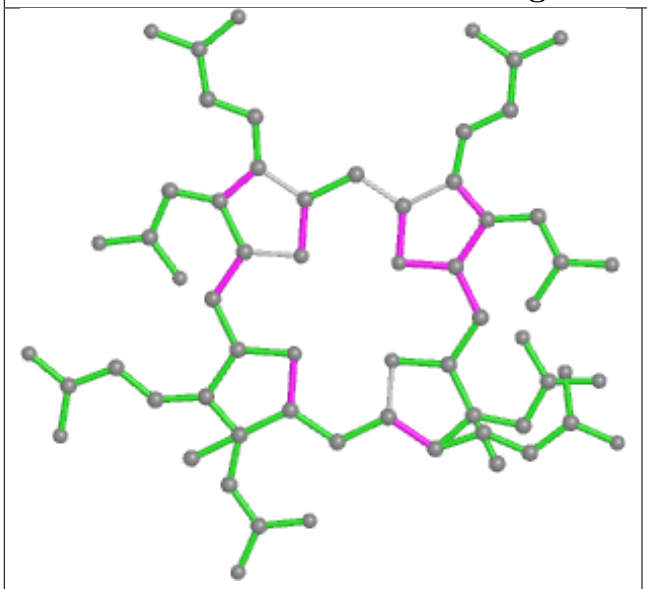


Torsions

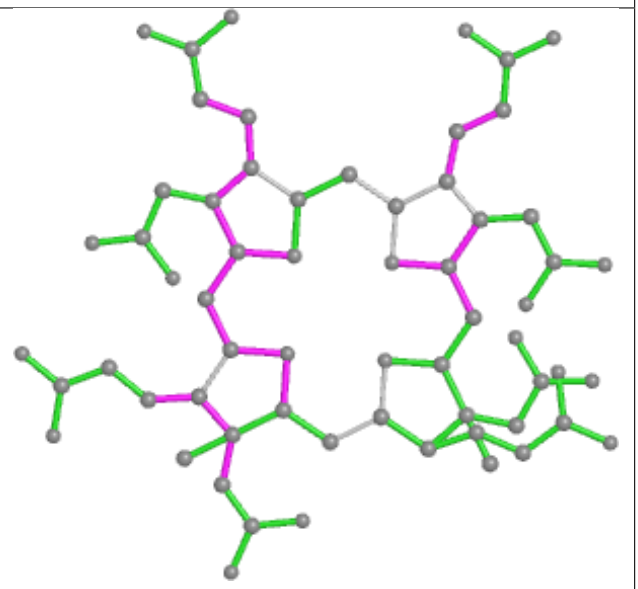


Rings

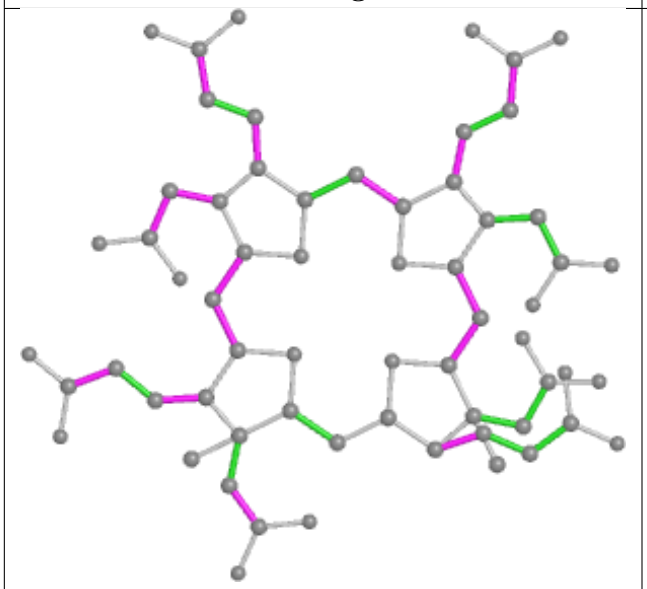
Ligand SH0 D 503



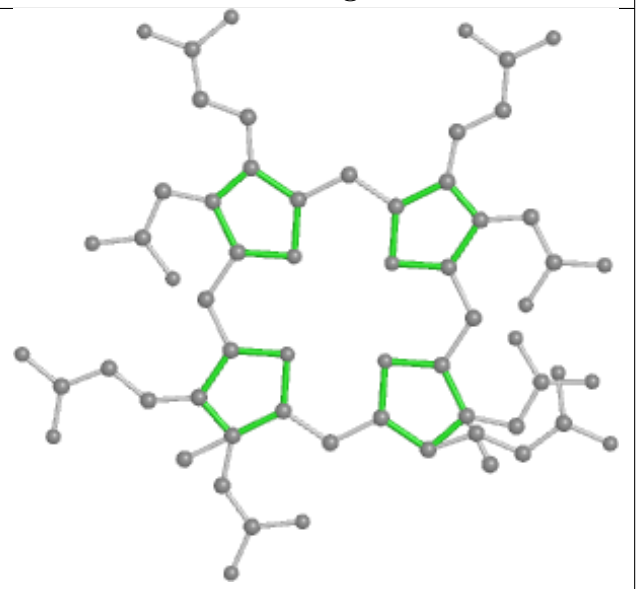
Bond lengths



Bond angles

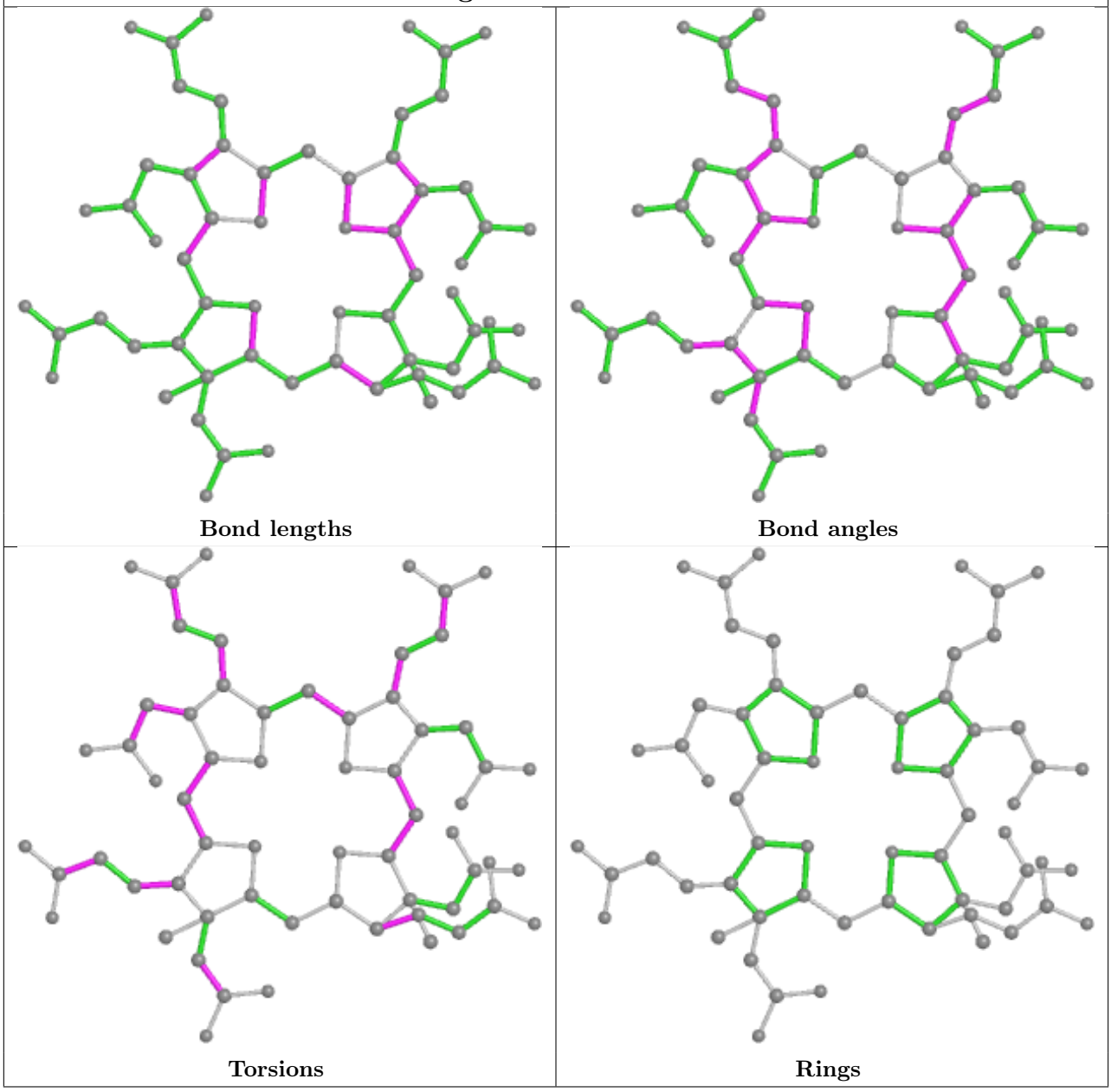


Torsions



Rings

Ligand SH0 A 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 (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	436/437 (99%)	0.12	16 (3%)	41	48	21, 32, 56, 78	0
1	D	436/437 (99%)	0.62	40 (9%)	9	11	26, 50, 67, 79	0
2	B	380/381 (99%)	-0.02	16 (4%)	36	42	21, 31, 53, 88	0
2	E	380/381 (99%)	0.82	54 (14%)	2	3	22, 47, 74, 100	0
3	C	103/105 (98%)	0.24	6 (5%)	23	28	32, 44, 63, 78	0
3	F	103/105 (98%)	0.88	16 (15%)	2	2	45, 59, 76, 82	0
All	All	1838/1846 (99%)	0.40	148 (8%)	12	15	21, 41, 68, 100	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	243	ILE	8.2
2	E	245	ASP	7.0
2	B	245	ASP	6.1
2	E	241	LEU	6.1
2	E	244	GLY	6.0
2	E	248	VAL	5.8
3	C	105	VAL	5.2
2	E	3	PHE	4.5
2	E	105	VAL	4.4
1	D	2	ALA	4.4
1	D	40	TYR	4.4
2	E	246	LYS	4.4
1	D	135	SER	4.4
1	A	2	ALA	4.3
1	D	38	LEU	4.3
2	E	196	VAL	4.2
2	E	186	LEU	4.2
1	D	154	PHE	4.1
2	E	247	LYS	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	142	ILE	4.1
3	F	4	VAL	4.0
2	E	16	ASN	3.9
1	D	35	PRO	3.8
3	C	5	THR	3.7
1	D	140	VAL	3.7
2	E	145	THR	3.7
1	D	124	LEU	3.6
2	E	18	ILE	3.6
2	E	4	ILE	3.5
1	A	226	VAL	3.5
3	F	41	ASP	3.5
1	D	259	PHE	3.5
3	F	104	CYS	3.4
2	E	111	LEU	3.4
2	B	246	LYS	3.4
1	A	227	ALA	3.4
3	F	75	PHE	3.4
3	F	105	VAL	3.3
2	B	244	GLY	3.3
1	D	276	ILE	3.3
1	D	81	ILE	3.2
2	E	98	ARG	3.1
2	E	194	GLY	3.1
1	D	256	ALA	3.0
1	A	225	CYS	3.0
2	E	75	ILE	3.0
1	A	136	THR	3.0
2	B	143	VAL	3.0
2	E	62	VAL	3.0
3	F	44	PRO	3.0
1	A	230	ALA	3.0
2	E	36	LYS	2.9
2	E	242	GLU	2.9
2	E	8	TYR	2.9
1	D	136	THR	2.9
2	E	118	LEU	2.9
1	D	126	GLY	2.9
2	E	197	HIS	2.9
2	E	217	TRP	2.9
1	A	229	ILE	2.9
2	E	32	PRO	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	194	GLY	2.8
1	D	30	TYR	2.8
1	D	231	ARG	2.8
1	D	39	ASP	2.8
2	E	143	VAL	2.8
2	E	195	ALA	2.8
1	D	128	GLY	2.8
3	C	71	LYS	2.8
2	E	71	ARG	2.7
1	D	44	VAL	2.7
2	E	2	ALA	2.7
2	E	187	ALA	2.7
2	E	193	CYS	2.6
1	D	24	ILE	2.6
1	D	227	ALA	2.6
1	D	134	GLY	2.6
1	A	424	TRP	2.6
2	E	185	SER	2.6
3	C	28	GLU	2.6
1	D	260	LYS	2.6
3	F	43	SER	2.6
3	C	75	PHE	2.6
2	B	97	THR	2.5
2	E	184	ILE	2.5
3	F	5	THR	2.5
1	D	91	PHE	2.5
2	B	241	LEU	2.5
2	E	58	SER	2.5
1	D	37	GLY	2.5
2	B	2	ALA	2.5
2	E	188	CYS	2.5
1	D	118	LEU	2.4
1	A	224	GLY	2.4
2	B	193	CYS	2.4
3	F	71	LYS	2.4
3	C	8	GLY	2.4
1	A	221	CYS	2.4
3	F	52	PHE	2.4
2	E	146	GLN	2.4
1	D	230	ALA	2.4
1	D	253	ALA	2.4
1	D	80	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	251	VAL	2.4
1	A	135	SER	2.4
1	D	437	ARG	2.4
1	A	134	GLY	2.4
3	F	55	ASP	2.4
2	E	249	ASN	2.3
2	E	153	THR	2.3
2	E	190	ILE	2.3
1	A	293	GLY	2.3
2	E	91	GLY	2.3
1	D	249	GLU	2.3
1	A	425	ASP	2.3
2	E	254	LYS	2.3
2	E	81	MET	2.3
1	A	137	GLY	2.3
1	D	160	LEU	2.2
1	A	231	ARG	2.2
2	E	144	HIS	2.2
3	F	35	GLU	2.2
2	E	114	LEU	2.2
3	F	56	TYR	2.2
1	D	335	ILE	2.2
2	B	11	GLU	2.2
1	D	139	ILE	2.2
1	D	178	LEU	2.2
1	D	354	PRO	2.2
2	E	151	CYS	2.2
2	B	298	PHE	2.2
3	F	74	GLY	2.2
2	E	47	LEU	2.1
2	B	198	CYS	2.1
2	B	187	ALA	2.1
2	B	243	ILE	2.1
1	D	142	LEU	2.1
2	B	186	LEU	2.1
1	D	217	LYS	2.1
2	E	158	ALA	2.1
2	B	289	VAL	2.1
3	F	42	ILE	2.1
2	E	154	PRO	2.1
2	E	11	GLU	2.1
2	E	113	ALA	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	172	ARG	2.0
3	F	40	SER	2.0
2	E	109	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

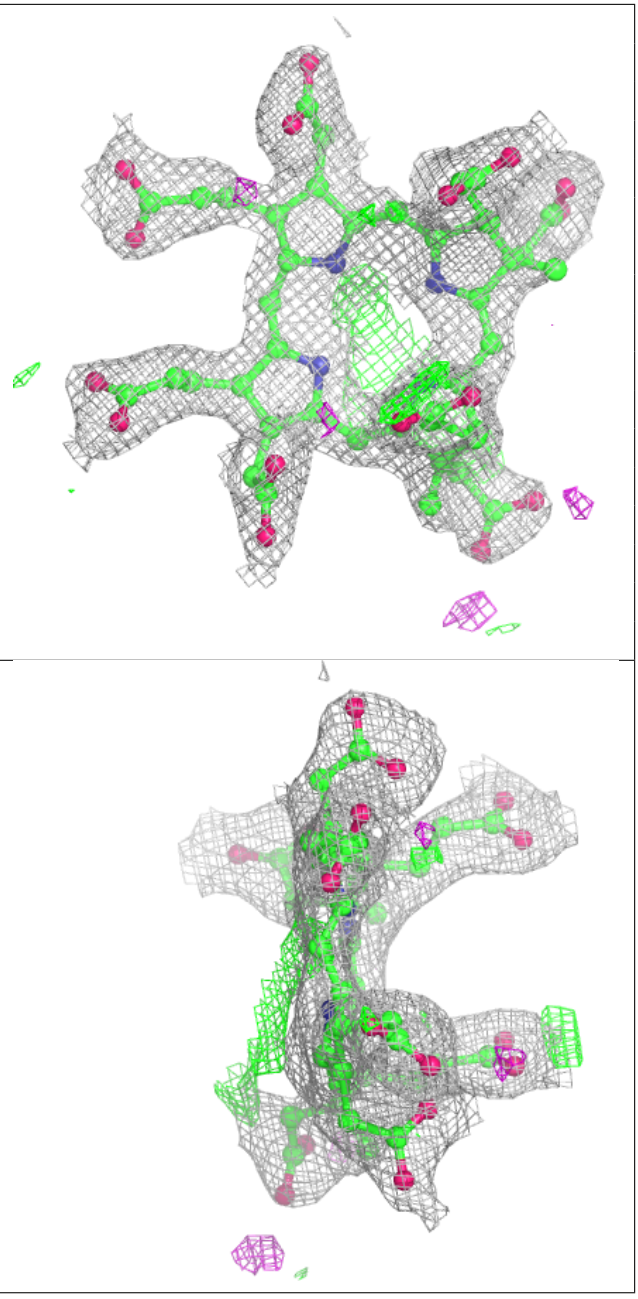
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SH0	D	503	62/62	0.87	0.19	39,47,52,58	0
6	SRM	E	503	63/63	0.94	0.24	35,47,55,60	0
4	SF4	D	501	8/8	0.95	0.10	38,41,44,46	0
5	SH0	A	503	62/62	0.96	0.17	19,24,28,34	0
4	SF4	D	502	8/8	0.96	0.08	38,41,42,46	0
4	SF4	E	501	8/8	0.96	0.08	41,42,45,49	0
6	SRM	B	503	63/63	0.97	0.20	25,29,35,43	0
7	SO3	E	504	4/4	0.97	0.23	76,76,76,77	0
7	SO3	B	504	4/4	0.98	0.13	47,47,47,48	0
4	SF4	E	502	8/8	0.98	0.04	35,37,39,41	0
4	SF4	B	501	8/8	0.99	0.08	28,30,32,37	0
4	SF4	B	502	8/8	0.99	0.08	25,28,29,30	0
4	SF4	A	502	8/8	0.99	0.09	29,30,34,35	0
4	SF4	A	501	8/8	1.00	0.14	23,26,26,27	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.

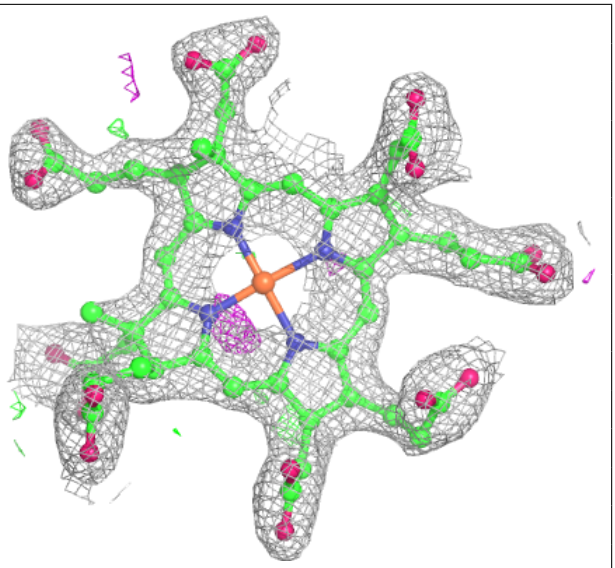
Electron density around SH0 D 503:

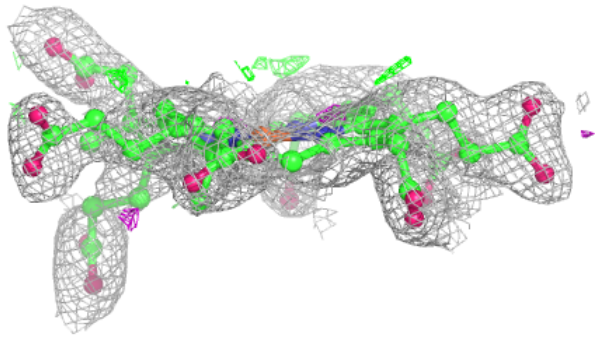
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

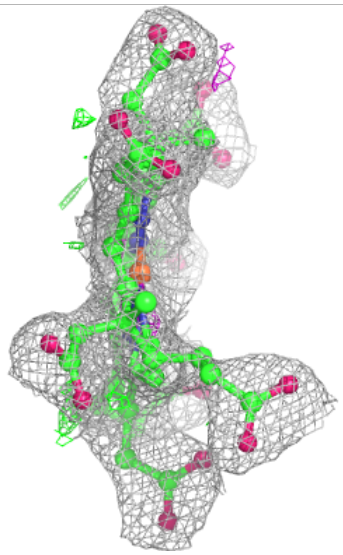


Electron density around SRM E 503:

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

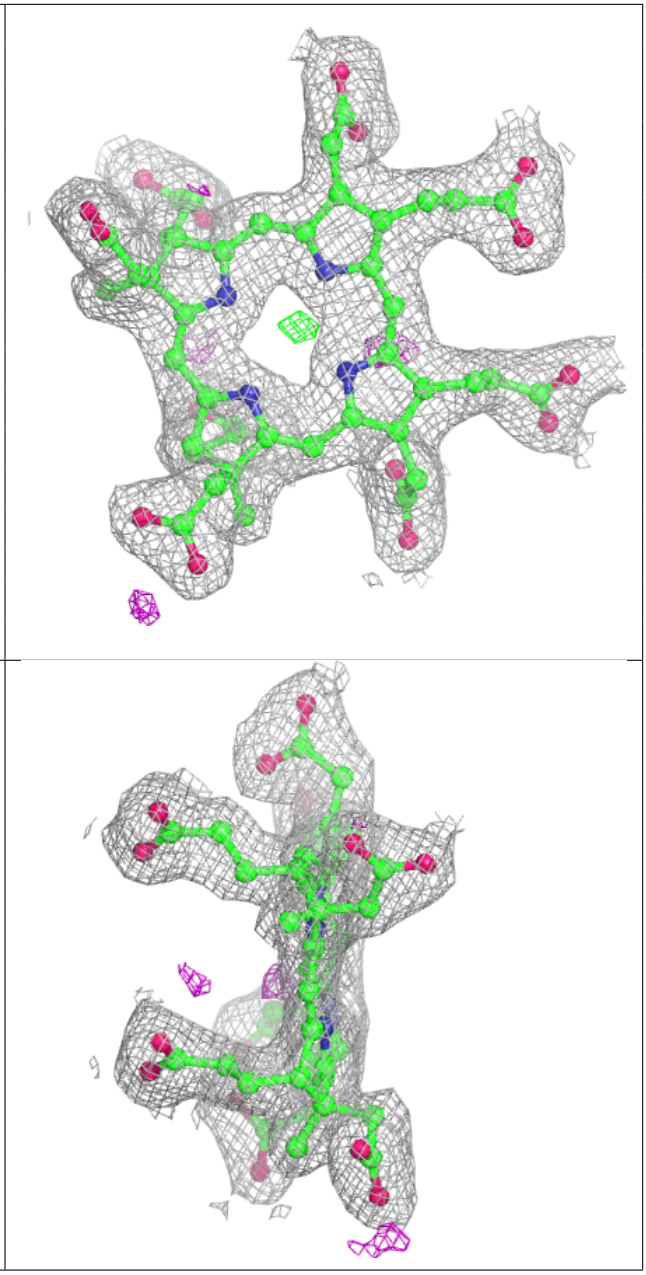






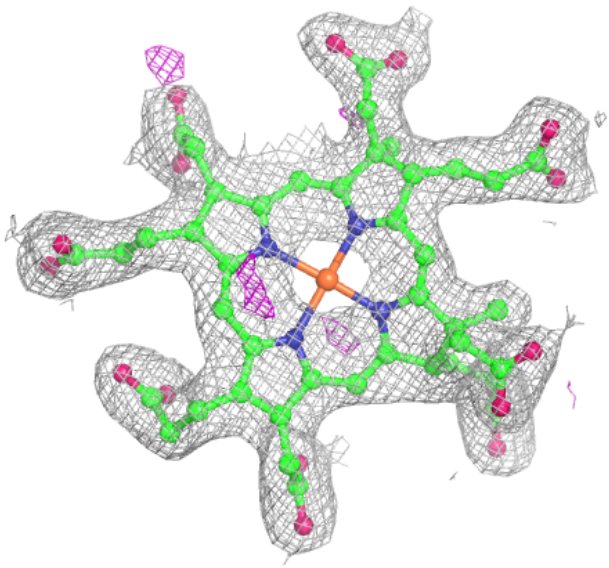
Electron density around SH0 A 503:

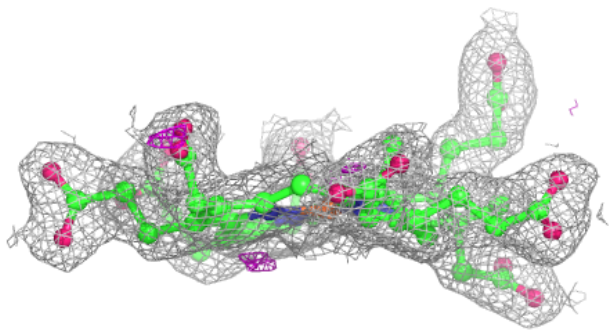
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

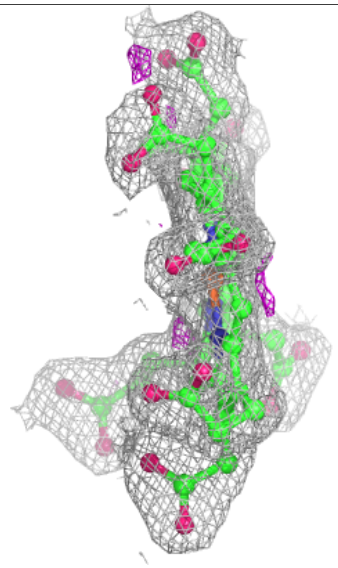


Electron density around SRM B 503:

$2mF_o$-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.