



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 08:21 PM EDT

PDB ID : 3MM7 / pdb_00003mm7
Title : Dissimilatory sulfite reductase carbon monoxide complex
Authors : Parey, K.; Warkentin, E.; Kroneck, P.M.H.; Ermler, U.
Deposited on : 2010-04-19
Resolution : 1.90 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

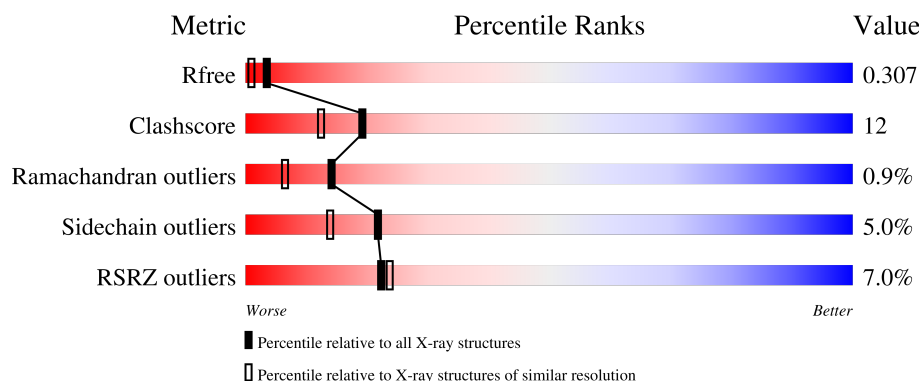
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	418	16% 74% 21% 5%
1	D	418	16% 83% 16%
2	B	366	76% 21%
2	E	366	10% 57% 31% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SRM	A	580	X	-	-	-
3	SRM	B	570	X	-	-	-
3	SRM	D	580	X	-	-	-
3	SRM	E	570	X	-	-	-
4	SF4	B	585	-	-	X	-
4	SF4	E	585	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13292 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

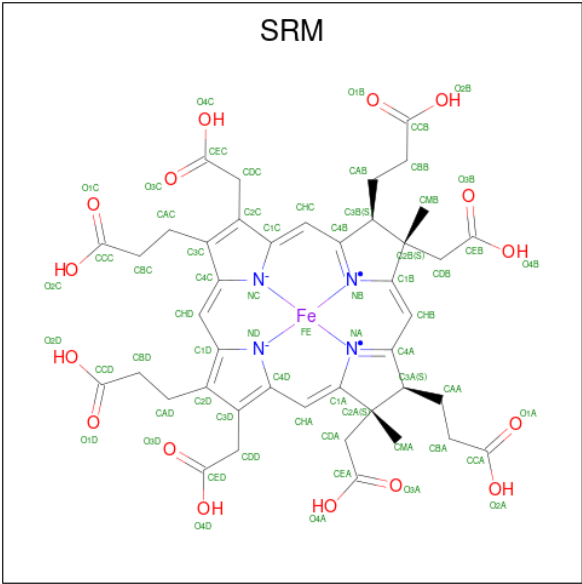
- Molecule 1 is a protein called Sulfite reductase, dissimilatory-type subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3330	2134	557	613	26			
1	D	417	Total	C	N	O	S	0	0	0
			3330	2134	557	613	26			

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

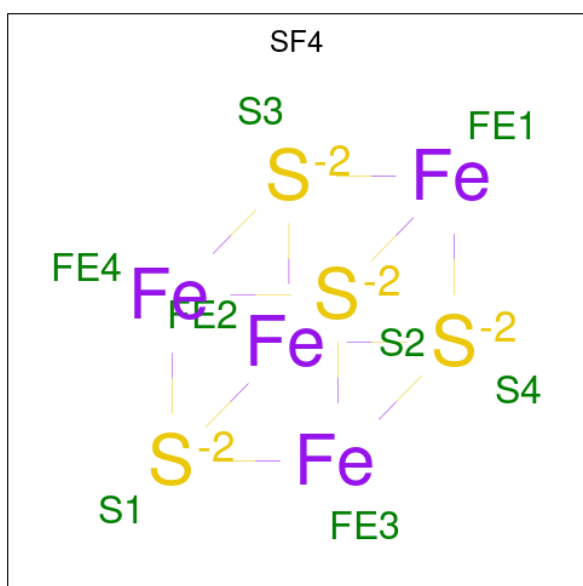
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	363	Total	C	N	O	S	0	0	0
			2901	1862	491	526	22			
2	E	363	Total	C	N	O	S	0	0	0
			2901	1862	491	526	22			

- Molecule 3 is SIROHEME (CCD ID: SRM) (formula: C₄₂H₄₄FeN₄O₁₆).



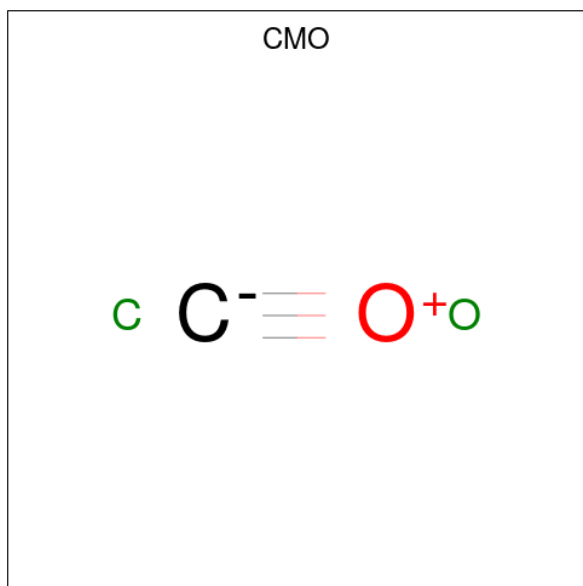
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	
			63	42	1	4	16	
3	B	1	Total	C	Fe	N	O	
			63	42	1	4	16	
3	D	1	Total	C	Fe	N	O	
			63	42	1	4	16	
3	E	1	Total	C	Fe	N	O	
			63	42	1	4	16	

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 5 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			2	1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	226	Total	O	0	0
			226	226		
6	B	209	Total	O	0	0
			209	209		
6	D	56	Total	O	0	0
			56	56		
6	E	21	Total	O	0	0
			21	21		

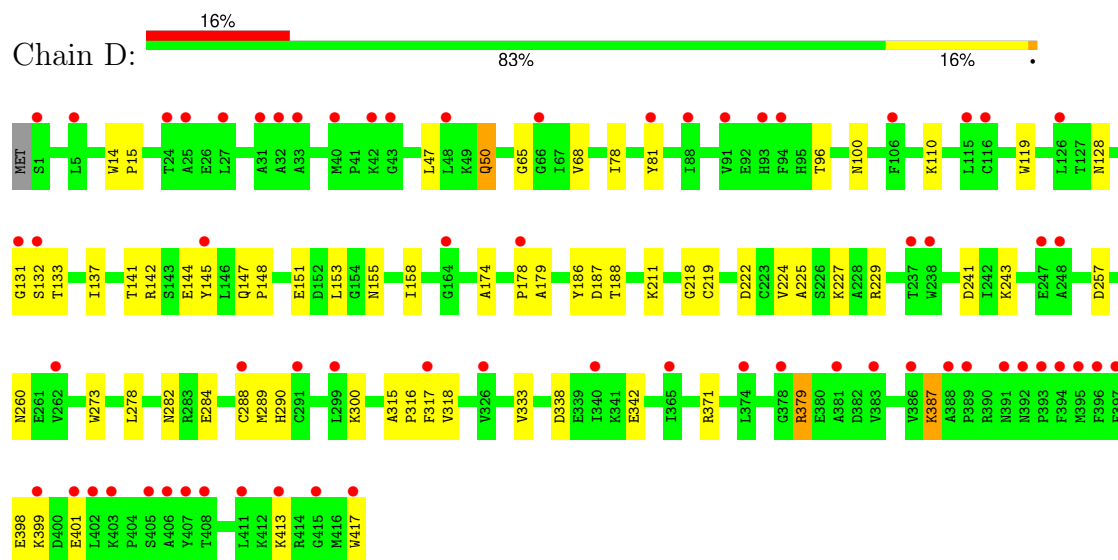
3 Residue-property plots

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.

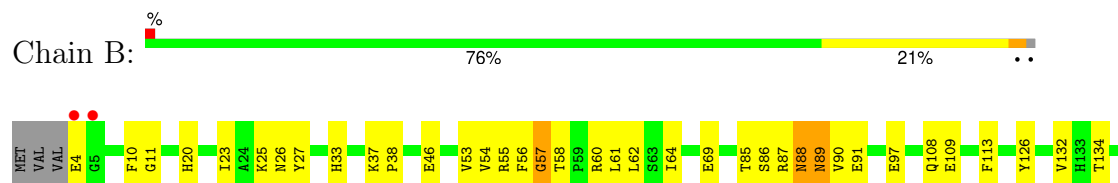
- Molecule 1: Sulfite reductase, dissimilatory-type subunit alpha

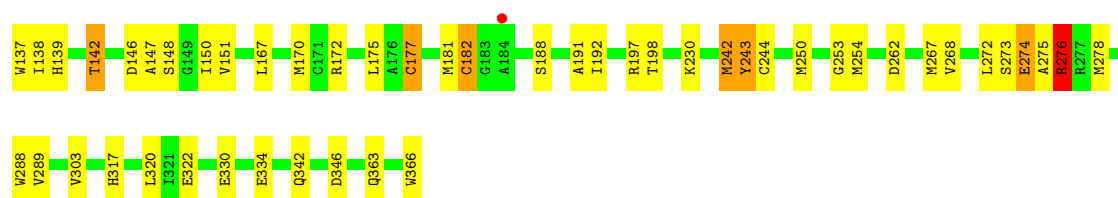


- Molecule 1: Sulfite reductase, dissimilatory-type subunit alpha

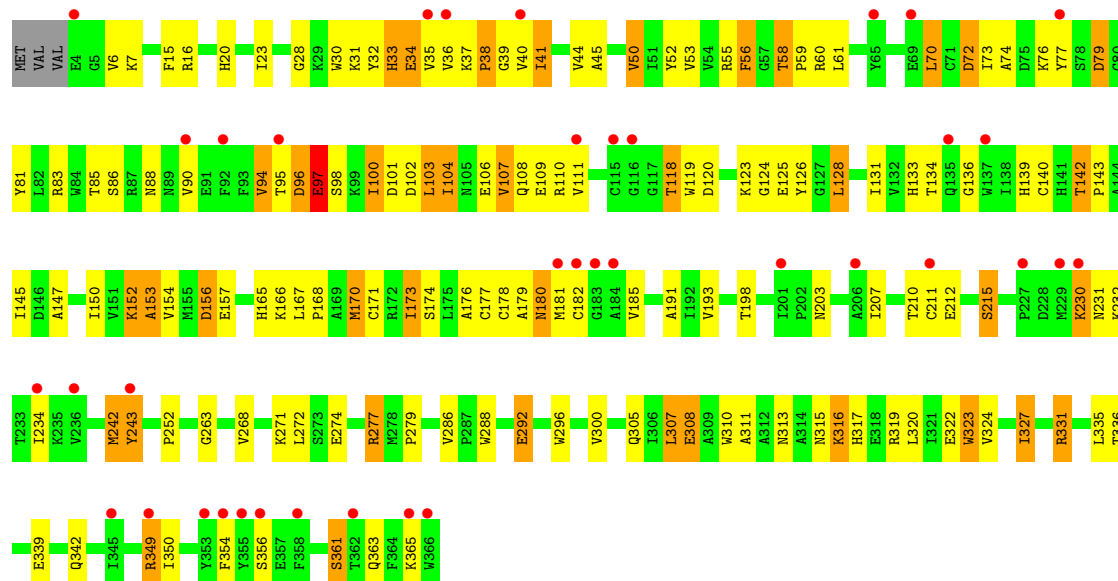


- Molecule 2: Sulfite reductase, dissimilatory-type subunit beta





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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.84Å 69.28Å 146.33Å 90.00° 107.68° 90.00°	Depositor
Resolution (Å)	49.14 – 1.90 49.14 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.14-1.90) 98.6 (49.14-1.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.6.0046	Depositor
R, R_{free}	0.215 , 0.261 0.268 , 0.307	Depositor DCC
R_{free} test set	7021 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13292	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.57	42/3417 (1.2%)	1.41	33/4610 (0.7%)
1	D	0.79	0/3417	1.01	4/4610 (0.1%)
2	B	1.56	30/2984 (1.0%)	1.40	24/4058 (0.6%)
2	E	1.10	14/2984 (0.5%)	1.26	25/4058 (0.6%)
All	All	1.29	86/12802 (0.7%)	1.28	86/17336 (0.5%)

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

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

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	72	ASP	CB-CG	12.86	1.84	1.52
2	B	85	THR	N-CA	12.75	1.61	1.45
2	E	79	ASP	C-N	12.42	1.49	1.33
1	A	270	ALA	CA-CB	11.62	1.73	1.53
1	A	113	ARG	C-O	11.38	1.38	1.24
2	B	274	GLU	C-O	11.36	1.39	1.24
1	A	326	VAL	CA-CB	10.24	1.66	1.53
1	A	285	CYS	N-CA	8.97	1.57	1.45
2	E	98	SER	C-O	-8.80	1.12	1.24
1	A	263	VAL	N-CA	-8.74	1.36	1.46
2	B	58	THR	CA-CB	8.64	1.64	1.53
1	A	287	ARG	CA-C	-8.54	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	225	ALA	CA-CB	8.42	1.65	1.53
1	A	111	ALA	CA-CB	8.29	1.66	1.53
2	E	331	ARG	N-CA	7.83	1.56	1.46
2	E	70	LEU	C-N	7.81	1.43	1.33
1	A	223	CYS	C-O	7.69	1.35	1.24
1	A	103	SER	C-O	7.69	1.32	1.23
2	B	53	VAL	N-CA	7.67	1.55	1.46
1	A	224	VAL	N-CA	7.48	1.54	1.46
2	B	303	VAL	CA-CB	7.41	1.63	1.54
2	E	79	ASP	CG-OD2	7.29	1.39	1.25
1	A	285	CYS	C-N	6.94	1.43	1.33
1	A	219	CYS	N-CA	6.90	1.52	1.46
2	E	97	GLU	C-N	6.81	1.43	1.33
2	E	72	ASP	CG-OD1	-6.69	1.12	1.25
2	B	55	ARG	CG-CD	6.66	1.72	1.52
1	A	219	CYS	CA-CB	6.64	1.63	1.54
2	B	132	VAL	C-O	-6.57	1.17	1.24
1	A	115	LEU	C-O	6.41	1.31	1.24
2	B	142	THR	CA-CB	6.33	1.63	1.53
2	B	56	PHE	CA-C	6.27	1.60	1.52
1	A	266	CYS	CA-CB	6.23	1.63	1.53
1	A	287	ARG	CZ-NH1	6.22	1.41	1.32
2	E	98	SER	CA-CB	6.16	1.63	1.53
1	A	189	LEU	C-O	6.13	1.31	1.24
2	B	55	ARG	CB-CG	6.10	1.70	1.52
1	A	235	ILE	CA-CB	6.04	1.62	1.54
2	B	62	LEU	CA-C	-5.99	1.45	1.52
2	B	268	VAL	CA-CB	5.92	1.64	1.55
2	B	87	ARG	CB-CG	5.85	1.70	1.52
2	B	88	ASN	N-CA	5.83	1.54	1.46
1	A	177	GLY	N-CA	-5.81	1.36	1.44
2	E	38	PRO	CA-CB	5.80	1.61	1.53
2	B	192	ILE	CA-CB	5.71	1.61	1.54
1	A	385	MET	C-O	-5.70	1.16	1.24
1	A	214	ILE	CA-CB	5.70	1.61	1.54
1	A	222	ASP	N-CA	5.69	1.54	1.46
1	A	222	ASP	C-O	5.66	1.30	1.23
2	B	262	ASP	CA-C	5.63	1.60	1.52
2	B	253	GLY	C-O	-5.63	1.17	1.23
2	B	181	MET	C-O	5.62	1.31	1.24
2	B	87	ARG	CA-CB	-5.60	1.44	1.53
2	B	198	THR	CA-C	5.57	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	96	ASP	CA-C	5.55	1.59	1.52
2	E	98	SER	C-N	-5.52	1.24	1.33
1	A	225	ALA	C-O	5.44	1.30	1.23
2	B	148	SER	C-O	-5.42	1.17	1.24
1	A	219	CYS	CB-SG	-5.42	1.63	1.81
2	B	167	LEU	C-O	-5.38	1.17	1.23
1	A	289	MET	CB-CG	5.38	1.68	1.52
1	A	185	CYS	C-O	-5.37	1.16	1.24
1	A	25	ALA	N-CA	5.36	1.52	1.46
2	B	54	VAL	CA-C	5.33	1.59	1.52
1	A	126	LEU	CA-C	-5.28	1.46	1.52
2	B	151	VAL	CA-CB	5.27	1.60	1.54
1	A	79	GLY	N-CA	5.26	1.52	1.45
1	A	117	ASP	N-CA	5.25	1.52	1.46
2	B	181	MET	N-CA	5.25	1.52	1.46
2	E	79	ASP	C-O	5.22	1.30	1.24
2	B	289	VAL	CA-CB	5.20	1.63	1.54
1	A	271	ILE	CA-CB	5.17	1.61	1.54
2	B	113	PHE	CA-C	-5.17	1.45	1.52
1	A	126	LEU	C-N	5.13	1.39	1.33
2	B	273	SER	N-CA	-5.13	1.39	1.45
2	B	274	GLU	N-CA	5.10	1.52	1.46
2	B	276	ARG	NE-CZ	-5.06	1.27	1.33
1	A	33	ALA	C-O	5.05	1.30	1.24
1	A	8	GLU	C-O	5.05	1.30	1.24
1	A	136	ILE	CA-C	5.04	1.58	1.52
1	A	111	ALA	C-O	-5.03	1.18	1.24
1	A	158	ILE	CA-C	5.03	1.58	1.52
1	A	328	VAL	C-O	-5.02	1.18	1.24
2	E	327	ILE	CA-CB	-5.02	1.47	1.54
1	A	270	ALA	N-CA	5.02	1.52	1.46
1	A	269	GLY	C-O	-5.01	1.18	1.24

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	167	LEU	CA-C-N	14.98	134.77	119.64
2	E	167	LEU	C-N-CA	14.98	134.77	119.64
1	A	219	CYS	CA-C-N	-13.51	105.13	120.12
1	A	219	CYS	C-N-CA	-13.51	105.13	120.12
2	E	292	GLU	CA-C-N	-8.51	113.44	119.66
2	E	292	GLU	C-N-CA	-8.51	113.44	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	295	MET	CA-C-N	8.38	128.11	119.56
1	A	295	MET	C-N-CA	8.38	128.11	119.56
2	B	58	THR	CA-C-N	8.37	129.37	120.83
2	B	58	THR	C-N-CA	8.37	129.37	120.83
1	A	222	ASP	N-CA-C	8.14	122.65	111.17
2	B	273	SER	N-CA-C	-7.86	100.15	110.53
2	E	154	VAL	N-CA-C	7.84	118.60	110.36
2	B	55	ARG	CG-CD-NE	-7.77	94.91	112.00
2	E	350	ILE	N-CA-C	7.48	118.27	110.72
1	A	289	MET	N-CA-C	7.47	126.71	110.80
1	A	220	PRO	N-CA-C	7.38	123.05	114.20
2	B	57	GLY	N-CA-C	-7.25	99.57	112.54
1	A	269	GLY	CA-C-N	-7.25	107.45	121.58
1	A	269	GLY	C-N-CA	-7.25	107.45	121.58
2	B	89	ASN	N-CA-C	7.19	119.85	110.43
1	A	131	GLY	N-CA-C	-7.13	103.41	112.54
2	B	254	MET	CA-C-N	-7.09	112.69	119.85
2	B	254	MET	C-N-CA	-7.09	112.69	119.85
2	E	211	CYS	N-CA-C	7.07	119.42	110.24
2	B	33	HIS	N-CA-C	-7.00	98.67	109.52
2	B	69	GLU	N-CA-C	-6.95	103.47	112.23
2	E	74	ALA	N-CA-C	6.85	119.59	111.71
2	E	327	ILE	N-CA-C	6.79	119.57	111.09
2	E	323	TRP	N-CA-C	-6.76	103.15	111.40
1	A	241	ASP	N-CA-C	6.74	119.79	110.35
2	B	109	GLU	N-CA-C	6.48	118.42	111.36
2	E	349	ARG	N-CA-C	6.46	118.32	111.28
2	B	278	MET	CA-C-N	6.45	126.82	119.92
2	B	278	MET	C-N-CA	6.45	126.82	119.92
2	E	126	TYR	N-CA-C	6.30	119.78	109.06
1	A	233	ALA	CA-C-N	-6.30	114.84	122.90
1	A	233	ALA	C-N-CA	-6.30	114.84	122.90
2	E	286	VAL	CA-C-N	-6.09	112.23	119.84
2	E	286	VAL	C-N-CA	-6.09	112.23	119.84
1	A	270	ALA	N-CA-C	6.08	120.53	113.18
1	D	387	LYS	N-CA-C	-6.08	105.69	113.23
1	A	136	ILE	CB-CA-C	-6.05	102.74	111.34
1	A	234	ILE	CA-C-N	-5.99	114.47	122.98
1	A	234	ILE	C-N-CA	-5.99	114.47	122.98
1	D	219	CYS	CA-C-N	-5.95	114.76	120.83
1	D	219	CYS	C-N-CA	-5.95	114.76	120.83
2	E	168	PRO	CB-CA-C	-5.85	101.89	111.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	VAL	CA-C-N	-5.85	113.11	120.77
1	A	262	VAL	C-N-CA	-5.85	113.11	120.77
1	A	40	MET	CA-C-N	5.78	125.40	119.56
1	A	40	MET	C-N-CA	5.78	125.40	119.56
2	B	89	ASN	CA-C-N	-5.75	113.01	122.67
2	B	89	ASN	C-N-CA	-5.75	113.01	122.67
2	B	148	SER	CA-C-N	5.66	126.38	119.99
2	B	148	SER	C-N-CA	5.66	126.38	119.99
2	B	272	LEU	N-CA-C	5.64	120.29	112.45
2	E	95	THR	N-CA-C	-5.51	105.34	113.61
2	B	25	LYS	N-CA-C	5.47	117.68	111.11
1	A	226	SER	N-CA-C	5.46	117.31	111.36
2	E	230	LYS	CA-C-N	5.46	131.52	121.70
2	E	230	LYS	C-N-CA	5.46	131.52	121.70
1	A	348	TRP	N-CA-C	5.42	117.61	111.11
2	E	98	SER	CA-CB-OG	-5.41	100.29	111.10
2	E	308	GLU	O-C-N	5.39	129.91	122.46
1	A	323	ILE	N-CA-C	-5.39	100.65	108.36
2	B	86	SER	CA-CB-OG	-5.38	100.35	111.10
2	B	85	THR	N-CA-C	-5.30	102.17	110.17
1	A	327	ALA	N-CA-C	-5.23	105.97	112.93
1	A	126	LEU	CA-C-O	-5.19	115.15	121.28
1	A	114	GLY	N-CA-C	-5.19	106.22	112.49
1	A	229	ARG	N-CA-C	5.17	118.70	111.56
2	B	172	ARG	NE-CZ-NH2	-5.17	114.55	119.20
2	E	111	VAL	N-CA-C	-5.17	107.79	112.96
2	B	276	ARG	NE-CZ-NH1	-5.15	116.35	121.50
1	A	290	HIS	N-CA-C	5.14	121.75	110.80
2	E	56	PHE	N-CA-C	5.14	117.62	109.50
2	E	32	TYR	N-CA-C	5.08	116.97	108.99
1	A	164	GLY	N-CA-C	5.08	119.48	112.37
2	E	98	SER	CB-CA-C	5.08	118.13	109.24
1	A	218	GLY	N-CA-C	-5.07	108.03	114.16
1	A	22	LYS	N-CA-C	5.03	116.76	111.28
2	E	154	VAL	CB-CA-C	-5.02	105.45	111.88
1	A	222	ASP	CB-CA-C	-5.01	104.20	112.06
2	B	61	LEU	CD1-CG-CD2	-5.01	99.78	110.80
1	D	155	ASN	CB-CG-ND2	5.00	123.91	116.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	280	ILE	Peptide
1	A	288	CYS	Mainchain
2	B	88	ASN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3330	0	3276	72	0
1	D	3330	0	3277	53	0
2	B	2901	0	2838	53	0
2	E	2901	0	2840	122	0
3	A	63	0	34	11	0
3	B	63	0	34	9	0
3	D	63	0	34	11	0
3	E	63	0	34	10	0
4	A	16	0	0	2	0
4	B	16	0	0	2	0
4	D	16	0	0	1	0
4	E	16	0	0	7	0
5	A	2	0	0	1	0
6	A	226	0	0	14	0
6	B	209	0	0	11	0
6	D	56	0	0	1	0
6	E	21	0	0	8	0
All	All	13292	0	12367	292	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 12.

All (292) 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:72:ASP:CG	2:E:72:ASP:CB	1.84	1.49
2:E:134:THR:HG21	2:E:182:CYS:HB2	1.15	1.12
3:E:570:SRM:HBD2	3:E:570:SRM:HDD2	1.37	1.04
2:E:230:LYS:CB	2:E:231:ASN:HB2	1.89	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:CYS:SG	6:A:522:HOH:O	2.17	1.02
3:A:580:SRM:O1A	2:B:139:HIS:HD2	1.41	1.01
2:E:230:LYS:HB2	2:E:231:ASN:HB2	1.41	1.00
3:D:580:SRM:HMB2	3:D:580:SRM:HBB2	1.46	0.97
1:A:197:MET:SD	6:B:567:HOH:O	2.23	0.97
2:B:11:GLY:HA3	6:B:567:HOH:O	1.67	0.95
2:E:134:THR:HG21	2:E:182:CYS:CB	2.00	0.92
2:E:134:THR:CG2	2:E:182:CYS:HB2	1.99	0.92
1:A:289:MET:SD	6:A:522:HOH:O	2.28	0.91
1:A:266:CYS:SG	1:A:270:ALA:N	2.44	0.91
1:A:290:HIS:HB2	2:B:275:ALA:HB1	1.53	0.90
1:A:288:CYS:O	1:A:288:CYS:SG	2.27	0.90
1:A:379:ARG:HG3	1:A:379:ARG:HH11	1.35	0.89
3:D:580:SRM:HBB2	3:D:580:SRM:CMB	2.03	0.88
2:B:275:ALA:O	2:B:276:ARG:HB2	1.71	0.86
2:E:123:LYS:O	2:E:123:LYS:HG3	1.73	0.86
2:E:177:CYS:HB2	4:E:585:SF4:S3	2.17	0.85
1:A:289:MET:HE2	6:A:522:HOH:O	1.76	0.84
2:E:124:GLY:HA3	2:E:316:LYS:HD2	1.61	0.82
1:D:379:ARG:HH11	1:D:379:ARG:HG3	1.46	0.80
3:A:580:SRM:O1A	2:B:139:HIS:CD2	2.32	0.80
1:D:128:ASN:HB2	1:D:137:ILE:HB	1.64	0.79
1:A:289:MET:CE	6:A:522:HOH:O	2.30	0.78
1:D:211:LYS:NZ	3:D:580:SRM:HDD2	1.98	0.78
2:E:131:ILE:HG12	2:E:173:ILE:HB	1.66	0.77
2:E:55:ARG:HH22	3:E:570:SRM:HBA2	1.49	0.77
2:E:140:CYS:SG	4:E:585:SF4:FE2	1.75	0.76
2:E:60:ARG:HD3	2:E:133:HIS:CE1	2.21	0.76
1:A:262:VAL:O	1:A:263:VAL:C	2.26	0.76
2:E:140:CYS:SG	4:E:585:SF4:S3	2.83	0.74
3:A:580:SRM:CBB	3:A:580:SRM:HMB1	2.20	0.71
1:D:398:GLU:HB2	1:D:401:GLU:HG3	1.73	0.70
2:E:94:VAL:HG12	2:E:96:ASP:H	1.55	0.70
2:E:263:GLY:HA3	2:E:288:TRP:NE1	2.07	0.70
1:A:94:PHE:O	2:B:139:HIS:HE1	1.74	0.70
1:A:229:ARG:NH1	6:A:594:HOH:O	1.92	0.70
2:E:41:ILE:HG13	2:E:53:VAL:O	1.91	0.70
1:A:5:LEU:HD11	1:A:56:LYS:HE2	1.74	0.69
2:E:313:ASN:HB3	6:E:378:HOH:O	1.92	0.69
1:A:80:ARG:NH2	3:A:580:SRM:O2A	2.21	0.69
1:A:120:GLU:HB2	2:B:64:ILE:CD1	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:HIS:HB3	2:B:23:ILE:HD12	1.76	0.67
1:A:225:ALA:O	1:A:229:ARG:HG2	1.94	0.67
1:A:379:ARG:HH11	1:A:379:ARG:CG	2.08	0.67
2:E:134:THR:HB	4:E:585:SF4:S4	2.35	0.66
2:E:323:TRP:CE2	2:E:327:ILE:HD13	2.31	0.66
2:E:107:VAL:C	6:E:498:HOH:O	2.38	0.66
1:D:379:ARG:HH11	1:D:379:ARG:CG	2.09	0.66
1:A:220:PRO:HD3	1:A:236:GLY:O	1.97	0.65
3:B:570:SRM:HMA3	3:B:570:SRM:CBA	2.14	0.65
1:D:211:LYS:HZ1	3:D:580:SRM:HDD2	1.60	0.65
1:A:371:ARG:HD3	6:E:372:HOH:O	1.96	0.64
2:E:109:GLU:N	6:E:498:HOH:O	2.30	0.64
2:E:142:THR:N	2:E:143:PRO:CD	2.61	0.64
3:D:580:SRM:HMB2	3:D:580:SRM:CBB	2.20	0.64
3:E:570:SRM:HDD2	3:E:570:SRM:CBD	2.22	0.63
1:A:284:GLU:HG3	6:A:629:HOH:O	1.99	0.63
1:A:417:TRP:CD1	1:A:417:TRP:C	2.76	0.63
1:D:78:ILE:HG21	3:D:580:SRM:HBA1	1.81	0.62
2:E:274:GLU:HB3	2:E:363:GLN:HE21	1.64	0.62
3:A:580:SRM:C4C	2:B:182:CYS:HA	2.28	0.62
1:D:14:TRP:CD2	1:D:15:PRO:HD2	2.34	0.62
3:A:580:SRM:HMB1	3:A:580:SRM:HBB1	1.81	0.62
2:E:182:CYS:HG	4:E:585:SF4:FE3	1.15	0.62
1:D:243:LYS:HE3	1:D:300:LYS:HE3	1.81	0.61
2:E:37:LYS:HB2	2:E:38:PRO:HD2	1.82	0.61
2:B:170:MET:SD	3:B:570:SRM:HBD1	2.41	0.61
2:E:52:TYR:CE1	2:E:97:GLU:HB3	2.35	0.61
2:E:263:GLY:HA3	2:E:288:TRP:CD1	2.36	0.61
1:A:270:ALA:HB3	4:A:576:SF4:S3	2.40	0.60
2:B:274:GLU:OE1	2:B:363:GLN:HG3	2.02	0.60
1:D:15:PRO:HB2	2:E:59:PRO:HG3	1.82	0.60
2:B:242:MET:SD	2:B:244:CYS:HB3	2.42	0.60
1:A:288:CYS:O	2:B:275:ALA:HA	2.02	0.59
2:E:56:PHE:CE2	2:E:107:VAL:HG11	2.37	0.59
2:E:44:VAL:HG22	2:E:50:VAL:HG22	1.85	0.59
2:E:52:TYR:HE1	2:E:97:GLU:HB3	1.66	0.59
2:B:134:THR:OG1	2:B:177:CYS:SG	2.34	0.59
2:E:176:ALA:HB2	2:E:185:VAL:HG21	1.85	0.59
2:E:123:LYS:O	2:E:123:LYS:CG	2.47	0.59
2:E:58:THR:HG22	2:E:90:VAL:HG12	1.85	0.59
1:D:315:ALA:HB1	1:D:316:PRO:CD	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:182:CYS:SG	4:E:585:SF4:S2	2.97	0.58
2:B:330:GLU:O	2:B:334:GLU:HG3	2.02	0.58
2:E:305:GLN:NE2	2:E:336:THR:O	2.34	0.58
1:A:94:PHE:O	2:B:139:HIS:CE1	2.56	0.58
2:B:276:ARG:NH1	2:B:276:ARG:HG3	2.18	0.57
2:E:272:LEU:HB2	3:E:570:SRM:CCC	2.34	0.57
1:A:56:LYS:NZ	6:A:546:HOH:O	2.23	0.57
1:A:98:ARG:C	1:A:99:ILE:HD13	2.28	0.57
1:D:128:ASN:ND2	2:E:61:LEU:HD12	2.19	0.57
2:E:33:HIS:CD2	2:E:34:GLU:N	2.72	0.57
2:B:170:MET:CE	3:B:570:SRM:HBD1	2.34	0.57
2:E:86:SER:OG	3:E:570:SRM:HAB1	2.04	0.57
3:B:570:SRM:C1A	3:B:570:SRM:HBA1	2.35	0.57
1:A:14:TRP:CD2	1:A:15:PRO:HD2	2.41	0.56
2:E:76:LYS:HD3	2:E:77:TYR:CE1	2.40	0.56
2:E:185:VAL:HG11	2:E:193:VAL:HG22	1.87	0.56
1:A:186:TYR:OH	1:A:216:CYS:HB3	2.05	0.56
1:D:151:GLU:HG2	2:E:6:VAL:HG22	1.87	0.56
2:E:323:TRP:NE1	2:E:327:ILE:HD13	2.21	0.56
2:E:97:GLU:O	2:E:100:ILE:HD11	2.06	0.56
2:E:145:ILE:HB	2:E:150:ILE:HD11	1.87	0.56
1:D:96:THR:HG23	2:E:139:HIS:CE1	2.41	0.55
2:B:366:TRP:HA	2:B:366:TRP:CE3	2.40	0.55
2:B:320:LEU:N	6:B:489:HOH:O	2.32	0.55
2:E:106:GLU:C	6:E:498:HOH:O	2.48	0.55
1:A:223:CYS:HB3	3:B:570:SRM:C4B	2.37	0.55
2:B:134:THR:HB	4:B:585:SF4:S4	2.46	0.55
2:E:108:GLN:N	6:E:498:HOH:O	2.39	0.55
1:D:128:ASN:HD22	2:E:61:LEU:HA	1.72	0.55
2:E:157:GLU:HG3	2:E:300:VAL:HG11	1.87	0.55
1:D:147:GLN:HB3	1:D:148:PRO:HD3	1.89	0.55
1:D:178:PRO:HG3	1:D:187:ASP:HA	1.89	0.54
1:A:170:ARG:HH12	5:A:590:CMO:C	2.20	0.54
2:E:279:PRO:HD2	2:E:361:SER:HB2	1.88	0.54
2:B:11:GLY:CA	6:B:567:HOH:O	2.38	0.54
1:A:99:ILE:HD13	1:A:99:ILE:N	2.22	0.54
1:A:69:SER:HB2	6:A:544:HOH:O	2.08	0.54
2:E:153:ALA:O	2:E:156:ASP:HB2	2.07	0.53
3:A:580:SRM:CBB	3:A:580:SRM:CMB	2.87	0.53
2:B:11:GLY:N	6:B:567:HOH:O	2.40	0.53
1:D:211:LYS:HZ2	3:D:580:SRM:HDD2	1.70	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:ALA:HB2	2:B:177:CYS:SG	2.49	0.53
2:E:56:PHE:CD2	2:E:107:VAL:HG11	2.44	0.53
1:A:374:LEU:HD21	1:A:385:MET:HE1	1.91	0.53
3:A:580:SRM:HBA1	3:A:580:SRM:HHB	1.90	0.52
1:D:399:LYS:HD3	1:D:417:TRP:O	2.10	0.52
1:A:223:CYS:HB3	3:B:570:SRM:CHC	2.39	0.52
1:A:379:ARG:HG3	1:A:379:ARG:NH1	2.15	0.52
2:B:275:ALA:O	2:B:276:ARG:CB	2.44	0.52
1:A:289:MET:HG3	6:A:522:HOH:O	2.10	0.51
2:E:6:VAL:HG12	2:E:7:LYS:O	2.11	0.51
1:D:151:GLU:HG2	2:E:6:VAL:CG2	2.40	0.51
1:D:288:CYS:O	1:D:289:MET:HB2	2.11	0.51
2:E:210:THR:HG21	2:E:252:PRO:HG3	1.93	0.51
2:E:39:GLY:N	2:E:118:THR:OG1	2.37	0.51
1:A:96:THR:HG23	2:B:139:HIS:NE2	2.25	0.51
1:D:186:TYR:CD1	1:D:333:VAL:HG11	2.46	0.51
2:E:320:LEU:O	2:E:324:VAL:HG23	2.10	0.51
1:A:289:MET:CG	6:A:522:HOH:O	2.57	0.50
2:E:170:MET:O	2:E:319:ARG:HG2	2.11	0.50
2:B:177:CYS:HB2	4:B:585:SF4:S3	2.51	0.50
3:D:580:SRM:CMB	3:D:580:SRM:CBB	2.78	0.50
1:A:56:LYS:CE	6:A:546:HOH:O	2.57	0.50
1:A:300:LYS:HD3	6:B:571:HOH:O	2.10	0.50
2:E:110:ARG:N	6:E:498:HOH:O	2.28	0.50
1:D:338:ASP:O	1:D:342:GLU:HB2	2.12	0.50
1:A:257:ASP:O	1:A:261:GLU:HB2	2.12	0.49
2:E:263:GLY:HA3	2:E:288:TRP:HE1	1.74	0.49
1:D:387:LYS:HE3	2:E:356:SER:O	2.12	0.49
3:A:580:SRM:C1C	2:B:182:CYS:HA	2.42	0.49
1:D:179:ALA:O	2:E:30:TRP:HZ2	1.96	0.49
2:E:103:LEU:O	2:E:106:GLU:N	2.45	0.49
2:E:230:LYS:CA	2:E:231:ASN:HB2	2.42	0.49
1:D:128:ASN:HD21	2:E:61:LEU:HD12	1.78	0.49
2:E:310:TRP:O	2:E:311:ALA:C	2.55	0.49
3:D:580:SRM:HBD1	3:D:580:SRM:HHD	1.94	0.49
2:B:134:THR:HG21	2:B:182:CYS:HB2	1.95	0.49
2:E:103:LEU:O	2:E:104:ILE:C	2.56	0.48
2:B:276:ARG:HG3	2:B:276:ARG:HH11	1.78	0.48
1:A:223:CYS:HA	3:B:570:SRM:C1C	2.44	0.48
2:E:72:ASP:CG	2:E:72:ASP:CA	2.76	0.48
1:A:382:ASP:O	1:A:385:MET:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:315:ASN:O	2:E:316:LYS:C	2.56	0.48
3:A:580:SRM:NC	2:B:182:CYS:HA	2.28	0.48
2:E:125:GLU:HB3	2:E:165:HIS:HB3	1.96	0.48
1:A:147:GLN:HB3	1:A:148:PRO:HD3	1.95	0.48
2:B:342:GLN:HG2	1:D:371:ARG:HG3	1.96	0.48
2:E:58:THR:C	2:E:60:ARG:H	2.22	0.48
2:E:30:TRP:HA	2:E:45:ALA:HA	1.95	0.48
2:E:44:VAL:HG22	2:E:50:VAL:CG2	2.44	0.47
2:B:175:LEU:HD23	2:B:175:LEU:C	2.39	0.47
1:D:273:TRP:HB2	1:D:278:LEU:HD12	1.97	0.47
1:A:219:CYS:HB2	6:A:522:HOH:O	2.12	0.47
1:A:132:SER:O	1:A:229:ARG:NH2	2.48	0.47
2:E:20:HIS:HA	2:E:81:TYR:CD1	2.49	0.47
1:D:119:TRP:CH2	1:D:141:THR:HB	2.50	0.47
2:E:85:THR:HB	3:E:570:SRM:HAB2	1.98	0.46
2:E:131:ILE:HG23	2:E:174:SER:HA	1.97	0.46
3:B:570:SRM:HMB2	3:B:570:SRM:HHB	1.50	0.46
2:B:134:THR:CG2	2:B:182:CYS:HB2	2.45	0.46
2:E:97:GLU:O	2:E:100:ILE:CD1	2.63	0.46
2:E:185:VAL:HG13	2:E:191:ALA:HB1	1.96	0.46
1:A:417:TRP:C	1:A:417:TRP:HD1	2.22	0.46
2:E:136:GLY:N	2:E:177:CYS:SG	2.89	0.46
1:A:120:GLU:HB2	2:B:64:ILE:HD11	1.97	0.46
1:A:197:MET:CE	6:B:567:HOH:O	2.57	0.46
2:E:307:LEU:HD23	2:E:308:GLU:N	2.31	0.46
2:B:64:ILE:HD13	2:B:64:ILE:HG21	1.70	0.45
2:E:271:LYS:NZ	2:E:277:ARG:O	2.46	0.45
2:E:320:LEU:C	2:E:320:LEU:HD23	2.41	0.45
2:B:138:ILE:HG13	6:B:379:HOH:O	2.15	0.45
2:E:15:PHE:CG	2:E:16:ARG:N	2.84	0.45
1:A:81:TYR:HE2	1:A:93:HIS:CE1	2.34	0.45
3:E:570:SRM:HMA2	3:E:570:SRM:HHA	1.72	0.45
1:A:241:ASP:OD1	1:A:241:ASP:N	2.47	0.45
1:D:50:GLN:HE21	1:D:50:GLN:HB2	1.60	0.45
1:D:225:ALA:HB3	1:D:229:ARG:HD3	1.97	0.45
2:E:55:ARG:NH2	3:E:570:SRM:HBA2	2.25	0.45
1:A:326:VAL:HB	1:A:385:MET:HA	1.98	0.45
2:E:134:THR:CG2	2:E:182:CYS:CB	2.77	0.45
2:E:277:ARG:HG2	2:E:322:GLU:HG2	1.99	0.45
1:D:131:GLY:HA3	3:D:580:SRM:HBB1	1.99	0.45
2:E:342:GLN:C	2:E:342:GLN:OE1	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ARG:C	1:A:289:MET:H	2.24	0.45
2:B:250:MET:HB3	2:B:250:MET:HE3	1.67	0.44
1:A:169:LEU:O	1:A:203:LEU:HA	2.17	0.44
2:E:292:GLU:HB2	2:E:296:TRP:HA	1.99	0.44
1:A:379:ARG:CG	1:A:379:ARG:NH1	2.72	0.44
2:E:142:THR:N	2:E:143:PRO:HD3	2.33	0.44
1:A:25:ALA:O	1:A:29:GLU:HB2	2.17	0.44
2:E:33:HIS:CD2	2:E:33:HIS:C	2.95	0.44
1:A:40:MET:HE3	1:A:40:MET:HB3	1.79	0.44
1:D:379:ARG:CG	1:D:379:ARG:NH1	2.73	0.44
2:B:346:ASP:HB3	2:E:354:PHE:HB2	1.99	0.44
1:D:65:GLY:HA2	1:D:81:TYR:CD1	2.53	0.44
1:D:218:GLY:HA3	4:D:575:SF4:S2	2.58	0.44
1:D:222:ASP:OD1	1:D:227:LYS:HG2	2.18	0.44
1:A:39:LYS:HG2	1:A:121:LYS:O	2.18	0.44
2:B:322:GLU:OE1	6:B:420:HOH:O	2.21	0.43
2:E:73:ILE:HD11	2:E:110:ARG:HD3	2.00	0.43
2:E:33:HIS:HD2	2:E:34:GLU:N	2.16	0.43
1:A:220:PRO:HG2	1:A:287:ARG:O	2.18	0.43
1:D:142:ARG:HB2	1:D:145:TYR:CD2	2.54	0.43
1:D:153:LEU:HD23	1:D:153:LEU:HA	1.88	0.43
1:D:387:LYS:HE2	1:D:387:LYS:HB2	1.79	0.43
2:E:230:LYS:HE3	2:E:231:ASN:OD1	2.19	0.43
1:D:317:PHE:HA	1:D:318:VAL:HA	1.73	0.43
1:A:197:MET:HE1	6:B:567:HOH:O	2.17	0.43
1:D:110:LYS:HD2	1:D:158:ILE:HD12	2.00	0.43
1:D:178:PRO:O	2:E:28:GLY:N	2.48	0.43
1:D:257:ASP:OD2	1:D:260:ASN:HB2	2.18	0.43
2:E:86:SER:H	3:E:570:SRM:HAB1	1.84	0.43
1:A:315:ALA:HB1	1:A:316:PRO:HD2	2.01	0.43
1:A:81:TYR:CE2	1:A:93:HIS:ND1	2.87	0.43
2:E:339:GLU:HG2	6:E:381:HOH:O	2.18	0.43
2:E:37:LYS:HB2	2:E:38:PRO:CD	2.49	0.42
2:E:212:GLU:HB3	2:E:215:SER:OG	2.19	0.42
1:A:221:ASN:HA	6:A:511:HOH:O	2.19	0.42
2:B:242:MET:C	2:B:243:TYR:CG	2.97	0.42
2:B:126:TYR:OH	2:B:317:HIS:ND1	2.50	0.42
2:B:197:ARG:HD3	2:B:288:TRP:CD1	2.54	0.42
3:A:580:SRM:C3C	2:B:182:CYS:HA	2.50	0.42
1:D:174:ALA:HB1	1:D:188:THR:HB	2.02	0.42
2:B:10:PHE:C	6:B:567:HOH:O	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:ASP:O	2:B:150:ILE:HD12	2.19	0.42
2:B:366:TRP:O	2:E:331:ARG:NH2	2.53	0.42
3:B:570:SRM:HMA3	3:B:570:SRM:HBA1	2.00	0.42
1:A:37:ASP:OD2	1:A:121:LYS:HE3	2.19	0.42
1:A:176:MET:HG2	4:A:575:SF4:S1	2.60	0.42
1:D:316:PRO:HG2	2:E:181:MET:HE3	2.01	0.42
2:E:133:HIS:HB2	2:E:147:ALA:HB1	2.00	0.42
1:A:83:ASP:C	1:A:83:ASP:OD1	2.63	0.41
2:B:137:TRP:CE3	2:B:146:ASP:HB2	2.55	0.41
1:D:241:ASP:CG	1:D:282:ASN:ND2	2.78	0.41
2:B:90:VAL:HG22	2:B:91:GLU:N	2.35	0.41
1:D:290:HIS:N	6:D:540:HOH:O	2.36	0.41
2:E:58:THR:HG23	2:E:88:ASN:O	2.20	0.41
2:E:128:LEU:HD12	2:E:171:CYS:O	2.19	0.41
1:D:187:ASP:OD1	1:D:187:ASP:C	2.62	0.41
2:E:203:ASN:O	2:E:207:ILE:HG13	2.19	0.41
2:E:307:LEU:HD23	2:E:308:GLU:HG3	2.02	0.41
3:E:570:SRM:HMA3	3:E:570:SRM:HAA2	1.56	0.41
1:A:319:GLU:OE1	2:E:349:ARG:NH1	2.53	0.41
2:B:26:ASN:O	2:B:27:TYR:C	2.62	0.41
1:D:399:LYS:HE3	1:D:399:LYS:HB2	1.77	0.41
2:E:178:CYS:SG	2:E:180:ASN:HB2	2.61	0.41
1:A:219:CYS:CB	6:A:522:HOH:O	2.52	0.41
1:D:128:ASN:HD21	2:E:61:LEU:CD1	2.33	0.41
2:E:242:MET:C	2:E:243:TYR:CG	2.98	0.41
1:A:394:PHE:CE2	2:E:179:ALA:HB1	2.56	0.41
1:D:284:GLU:HA	2:E:365:LYS:HE2	2.03	0.41
1:D:110:LYS:HD2	1:D:158:ILE:CD1	2.50	0.41
1:A:222:ASP:OD2	1:A:227:LYS:NZ	2.54	0.41
2:B:37:LYS:O	2:B:38:PRO:C	2.62	0.41
2:E:35:VAL:HB	2:E:120:ASP:OD1	2.20	0.41
2:E:70:LEU:HD23	2:E:70:LEU:HA	1.83	0.41
2:E:152:LYS:O	2:E:153:ALA:C	2.64	0.41
2:E:323:TRP:CE2	2:E:327:ILE:CD1	3.02	0.41
1:D:78:ILE:HG21	3:D:580:SRM:CBA	2.50	0.41
1:A:271:ILE:HA	1:A:279:THR:O	2.21	0.40
2:B:57:GLY:HA2	2:B:89:ASN:OD1	2.21	0.40
1:A:186:TYR:CD1	1:A:333:VAL:HG11	2.56	0.40
2:E:177:CYS:CB	4:E:585:SF4:S3	2.99	0.40
2:E:316:LYS:HG3	2:E:317:HIS:CD2	2.56	0.40
2:B:191:ALA:HB3	2:B:267:MET:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:35:VAL:HG21	2:E:119:TRP:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	415/418 (99%)	394 (95%)	19 (5%)	2 (0%)	24	16
1	D	415/418 (99%)	391 (94%)	24 (6%)	0	100	100
2	B	361/366 (99%)	339 (94%)	18 (5%)	4 (1%)	11	4
2	E	361/366 (99%)	309 (86%)	44 (12%)	8 (2%)	5	1
All	All	1552/1568 (99%)	1433 (92%)	105 (7%)	14 (1%)	14	6

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	103	LEU
2	E	104	ILE
1	A	289	MET
2	E	34	GLU
2	E	79	ASP
2	E	153	ALA
2	E	232	LYS
2	B	182	CYS
1	A	290	HIS
2	B	60	ARG
2	E	156	ASP
2	B	276	ARG
2	B	142	THR
2	E	142	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	353/354 (100%)	338 (96%)	15 (4%)	26	19
1	D	353/354 (100%)	343 (97%)	10 (3%)	38	32
2	B	314/317 (99%)	305 (97%)	9 (3%)	37	31
2	E	314/317 (99%)	281 (90%)	33 (10%)	6	2
All	All	1334/1342 (99%)	1267 (95%)	67 (5%)	22	14

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LYS
1	A	38	VAL
1	A	40	MET
1	A	50	GLN
1	A	68	VAL
1	A	144	GLU
1	A	216	CYS
1	A	243	LYS
1	A	271	ILE
1	A	278	LEU
1	A	279	THR
1	A	286	VAL
1	A	383	VAL
1	A	409	GLU
1	A	417	TRP
2	B	4	GLU
2	B	46	GLU
2	B	97	GLU
2	B	108	GLN
2	B	177	CYS
2	B	188	SER
2	B	230	LYS
2	B	242	MET
2	B	243	TYR

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Mol	Chain	Res	Type
1	D	47	LEU
1	D	50	GLN
1	D	68	VAL
1	D	100	ASN
1	D	132	SER
1	D	133	THR
1	D	144	GLU
1	D	224	VAL
1	D	379	ARG
1	D	413	LYS
2	E	23	ILE
2	E	31	LYS
2	E	33	HIS
2	E	36	VAL
2	E	40	VAL
2	E	41	ILE
2	E	50	VAL
2	E	58	THR
2	E	83	ARG
2	E	94	VAL
2	E	97	GLU
2	E	100	ILE
2	E	101	ASP
2	E	102	ASP
2	E	107	VAL
2	E	118	THR
2	E	128	LEU
2	E	152	LYS
2	E	166	LYS
2	E	170	MET
2	E	173	ILE
2	E	180	ASN
2	E	198	THR
2	E	215	SER
2	E	234	ILE
2	E	242	MET
2	E	243	TYR
2	E	268	VAL
2	E	277	ARG
2	E	307	LEU
2	E	316	LYS
2	E	335	LEU

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Mol	Chain	Res	Type
2	E	361	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	221	ASN
1	A	293	ASN
2	B	139	HIS
1	D	50	GLN
1	D	93	HIS
1	D	100	ASN
1	D	128	ASN
2	E	33	HIS
2	E	180	ASN
2	E	363	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SF4	D	575	1	0,12,12	-	-	-		
3	SRM	E	570	1	68,70,70	2.16	15 (22%)	86,112,112	2.92	31 (36%)
4	SF4	A	576	1	0,12,12	-	-	-		
4	SF4	E	585	2	0,12,12	-	-	-		
4	SF4	E	586	2	0,12,12	-	-	-		
4	SF4	A	575	1	0,12,12	-	-	-		
4	SF4	B	585	2	0,12,12	-	-	-		
5	CMO	A	590	-	0,1,1	-	-	-		
4	SF4	B	586	2	0,12,12	-	-	-		
3	SRM	A	580	2	68,70,70	2.32	17 (25%)	86,112,112	2.78	34 (39%)
3	SRM	D	580	-	68,70,70	2.18	18 (26%)	86,112,112	2.63	26 (30%)
4	SF4	D	576	6,1	0,12,12	-	-	-		
3	SRM	B	570	1	68,70,70	3.23	25 (36%)	86,112,112	4.54	43 (50%)

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	575	1	-	-	0/6/5/5
3	SRM	E	570	1	1/1/19/23	22/38/126/126	-
4	SF4	A	576	1	-	-	0/6/5/5
4	SF4	E	585	2	-	-	0/6/5/5
4	SF4	E	586	2	-	-	0/6/5/5
4	SF4	A	575	1	-	-	0/6/5/5
4	SF4	B	585	2	-	-	0/6/5/5
4	SF4	B	586	2	-	-	0/6/5/5
3	SRM	A	580	2	2/2/19/23	13/38/126/126	-
3	SRM	D	580	-	2/2/19/23	19/38/126/126	-
4	SF4	D	576	6,1	-	-	0/6/5/5
3	SRM	B	570	1	1/1/19/23	21/38/126/126	-

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	570	SRM	C4B-NB	-14.07	1.25	1.35
3	E	570	SRM	C3C-C2C	7.59	1.52	1.36
3	B	570	SRM	C1D-C2D	7.15	1.58	1.44
3	A	580	SRM	C3C-C2C	6.94	1.51	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	570	SRM	CHC-C1C	-6.65	1.25	1.38
3	B	570	SRM	C1D-ND	-6.54	1.27	1.39
3	D	580	SRM	C3C-C2C	6.38	1.50	1.36
3	B	570	SRM	C4C-NC	-6.25	1.27	1.39
3	E	570	SRM	C4A-NA	-6.21	1.30	1.35
3	A	580	SRM	FE-NA	6.09	2.13	1.94
3	D	580	SRM	C3A-C4A	-5.72	1.39	1.51
3	A	580	SRM	FE-NB	5.69	2.12	1.94
3	B	570	SRM	C2B-C3B	-5.57	1.40	1.55
3	A	580	SRM	C3A-C4A	-5.34	1.39	1.51
3	D	580	SRM	C3B-C4B	-5.32	1.39	1.51
3	D	580	SRM	FE-NB	5.13	2.10	1.94
3	A	580	SRM	C4D-C3D	5.05	1.54	1.44
3	E	570	SRM	C1C-NC	-4.99	1.30	1.39
3	B	570	SRM	C3C-C2C	4.87	1.46	1.36
3	D	580	SRM	FE-NA	4.84	2.09	1.94
3	E	570	SRM	C4C-NC	-4.82	1.30	1.39
3	A	580	SRM	C3B-C4B	-4.77	1.41	1.51
3	A	580	SRM	C1D-C2D	4.66	1.53	1.44
3	B	570	SRM	C4A-NA	-4.64	1.31	1.35
3	B	570	SRM	CDC-CEC	4.47	1.58	1.51
3	B	570	SRM	C4D-ND	-4.37	1.31	1.39
3	E	570	SRM	C4D-C3D	4.36	1.53	1.44
3	B	570	SRM	C4D-C3D	4.31	1.53	1.44
3	D	580	SRM	FE-NC	4.30	2.09	1.95
3	B	570	SRM	CDD-C3D	4.25	1.57	1.51
3	A	580	SRM	C4C-C3C	4.09	1.52	1.45
3	E	570	SRM	C1D-C2D	4.09	1.52	1.44
3	B	570	SRM	C2B-C1B	4.05	1.63	1.54
3	E	570	SRM	C1C-C2C	4.03	1.52	1.45
3	D	580	SRM	C1D-C2D	4.01	1.52	1.44
3	B	570	SRM	C3B-C4B	3.93	1.59	1.51
3	B	570	SRM	C4C-C3C	3.90	1.52	1.45
3	A	580	SRM	C1C-C2C	3.79	1.51	1.45
3	B	570	SRM	CHB-C4A	3.72	1.49	1.39
3	B	570	SRM	CDB-CEB	3.65	1.61	1.50
3	E	570	SRM	CDD-C3D	3.54	1.56	1.51
3	E	570	SRM	C3D-C2D	3.39	1.55	1.40
3	D	580	SRM	C1C-C2C	3.35	1.51	1.45
3	D	580	SRM	C3D-C2D	3.20	1.54	1.40
3	A	580	SRM	C3D-C2D	3.12	1.54	1.40
3	D	580	SRM	C4D-C3D	3.08	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	570	SRM	O1B-CCB	3.08	1.32	1.22
3	B	570	SRM	CHD-C1D	-3.08	1.32	1.39
3	E	570	SRM	C4C-C3C	2.99	1.50	1.45
3	B	570	SRM	O4B-CEB	-2.99	1.20	1.30
3	E	570	SRM	CDC-C2C	2.97	1.55	1.51
3	A	580	SRM	FE-NC	2.95	2.04	1.95
3	D	580	SRM	C4C-NC	-2.81	1.34	1.39
3	D	580	SRM	C4C-C3C	2.81	1.50	1.45
3	A	580	SRM	O2C-CCC	-2.81	1.21	1.30
3	A	580	SRM	CDD-C3D	2.79	1.55	1.51
3	A	580	SRM	C4D-ND	-2.78	1.34	1.39
3	B	570	SRM	CBD-CCD	2.78	1.57	1.50
3	B	570	SRM	C1C-C2C	2.75	1.50	1.45
3	D	580	SRM	C4A-NA	-2.67	1.33	1.35
3	B	570	SRM	O2C-CCC	-2.52	1.22	1.30
3	D	580	SRM	C4D-ND	-2.46	1.35	1.39
3	D	580	SRM	C1C-NC	-2.45	1.35	1.39
3	D	580	SRM	C1D-ND	-2.40	1.35	1.39
3	B	570	SRM	CBC-CAC	2.38	1.60	1.51
3	E	570	SRM	CAD-C2D	2.36	1.57	1.51
3	D	580	SRM	FE-ND	-2.22	1.87	1.95
3	E	570	SRM	C2B-C3B	-2.20	1.49	1.55
3	D	580	SRM	CAA-C3A	-2.20	1.49	1.54
3	A	580	SRM	O3A-CEA	2.15	1.29	1.22
3	E	570	SRM	C2A-C1A	-2.11	1.49	1.54
3	A	580	SRM	C4B-NB	2.09	1.36	1.35
3	B	570	SRM	O3D-CED	2.04	1.28	1.22
3	E	570	SRM	O3A-CEA	2.02	1.28	1.22
3	A	580	SRM	CBD-CCD	2.02	1.55	1.50

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	570	SRM	CMB-C2B-C3B	13.86	137.63	112.05
3	B	570	SRM	C3C-C4C-NC	11.81	121.72	110.32
3	B	570	SRM	C2B-C3B-C4B	11.60	115.58	100.89
3	B	570	SRM	C2C-C1C-NC	11.43	121.35	110.32
3	B	570	SRM	CHC-C1C-NC	-10.86	112.63	124.45
3	B	570	SRM	C2B-C1B-CHB	-10.66	113.96	123.54
3	B	570	SRM	C4B-NB-C1B	10.39	118.17	105.34
3	D	580	SRM	C2A-C3A-C4A	10.37	114.03	100.89
3	A	580	SRM	CAA-C3A-C4A	9.78	128.25	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	570	SRM	CAB-C3B-C4B	9.72	128.15	111.19
3	A	580	SRM	C2A-C3A-C4A	9.47	112.89	100.89
3	D	580	SRM	CAA-C3A-C4A	9.36	127.52	111.19
3	E	570	SRM	C2B-C1B-CHB	-9.30	115.19	123.54
3	B	570	SRM	C4A-CHB-C1B	-8.17	113.82	125.84
3	B	570	SRM	C1C-C2C-C3C	-7.80	98.12	106.84
3	B	570	SRM	C1A-NA-C4A	-7.68	95.85	105.34
3	E	570	SRM	C2A-C1A-CHA	-7.42	116.88	123.54
3	A	580	SRM	CMB-C2B-C3B	7.37	125.66	112.05
3	E	570	SRM	C4C-C3C-C2C	-6.83	99.20	106.84
3	B	570	SRM	CHD-C4C-NC	-6.52	117.36	124.45
3	D	580	SRM	C2B-C3B-C4B	6.51	109.14	100.89
3	E	570	SRM	C1D-C2D-C3D	-6.46	100.03	106.81
3	B	570	SRM	C3B-C2B-C1B	-6.46	89.96	100.92
3	B	570	SRM	CBD-CAD-C2D	6.33	130.05	112.53
3	E	570	SRM	C2B-C3B-C4B	6.24	108.79	100.89
3	B	570	SRM	C3B-C4B-NB	-6.17	98.78	110.83
3	E	570	SRM	C2D-C1D-ND	6.07	116.89	110.15
3	B	570	SRM	CHD-C1D-ND	5.99	134.72	123.86
3	B	570	SRM	C3A-C4A-NA	5.74	122.03	110.83
3	B	570	SRM	C4C-NC-C1C	-5.65	96.61	105.82
3	A	580	SRM	C2B-C1B-CHB	-5.65	118.47	123.54
3	A	580	SRM	C2B-C3B-C4B	5.59	107.97	100.89
3	A	580	SRM	C4C-C3C-C2C	-5.27	100.95	106.84
3	A	580	SRM	C3C-C4C-NC	5.15	115.29	110.32
3	D	580	SRM	C4D-ND-C1D	5.07	114.08	105.82
3	D	580	SRM	C3C-C4C-NC	4.93	115.08	110.32
3	B	570	SRM	C1C-CHC-C4B	4.91	138.47	126.62
3	B	570	SRM	C1D-C2D-C3D	-4.87	101.71	106.81
3	B	570	SRM	CHD-C1D-C2D	-4.86	114.65	125.30
3	B	570	SRM	C4C-C3C-C2C	-4.81	101.46	106.84
3	A	580	SRM	CBA-CAA-C3A	4.80	128.25	114.65
3	E	570	SRM	C3C-C4C-NC	4.80	114.95	110.32
3	B	570	SRM	CAA-C3A-C2A	-4.77	101.06	114.19
3	D	580	SRM	C1A-NA-C4A	4.71	111.16	105.34
3	D	580	SRM	CMA-C2A-CDA	4.70	118.72	110.74
3	E	570	SRM	CDA-C2A-C1A	4.64	121.48	107.11
3	B	570	SRM	C4D-CHA-C1A	4.58	134.31	125.87
3	B	570	SRM	CMA-C2A-CDA	4.50	118.38	110.74
3	D	580	SRM	CBB-CAB-C3B	4.48	127.35	114.65
3	D	580	SRM	C2C-C1C-NC	4.43	114.60	110.32
3	E	570	SRM	CAD-C2D-C1D	-4.42	116.30	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	580	SRM	CBD-CAD-C2D	4.36	124.60	112.53
3	A	580	SRM	CBB-CAB-C3B	4.20	126.54	114.65
3	E	570	SRM	CBD-CAD-C2D	4.19	124.12	112.53
3	D	580	SRM	C1C-C2C-C3C	-4.17	102.18	106.84
3	B	570	SRM	C4D-ND-C1D	4.15	112.59	105.82
3	A	580	SRM	C1D-C2D-C3D	-4.14	102.47	106.81
3	A	580	SRM	C4D-ND-C1D	4.07	112.45	105.82
3	D	580	SRM	C4D-C3D-C2D	-3.96	102.66	106.81
3	A	580	SRM	CAC-C3C-C4C	3.94	132.87	124.85
3	B	570	SRM	C4D-C3D-C2D	-3.91	102.71	106.81
3	E	570	SRM	CAC-C3C-C2C	-3.89	120.11	129.24
3	D	580	SRM	C4C-C3C-C2C	-3.87	102.51	106.84
3	B	570	SRM	CEC-CDC-C2C	-3.79	104.24	113.76
3	D	580	SRM	C2D-C1D-ND	-3.74	106.00	110.15
3	E	570	SRM	C3B-C2B-C1B	-3.74	94.58	100.92
3	E	570	SRM	C3A-C4A-NA	3.71	118.08	110.83
3	B	570	SRM	CAB-C3B-C2B	-3.66	104.10	114.19
3	E	570	SRM	C3D-C4D-ND	3.65	114.20	110.15
3	A	580	SRM	CMA-C2A-C3A	-3.63	105.34	112.05
3	A	580	SRM	C3A-C2A-C1A	-3.63	94.75	100.92
3	E	570	SRM	C1C-C2C-C3C	-3.57	102.85	106.84
3	E	570	SRM	CED-CDD-C3D	3.56	122.71	113.76
3	D	580	SRM	C3A-C2A-C1A	-3.54	94.90	100.92
3	E	570	SRM	C4D-C3D-C2D	-3.50	103.14	106.81
3	D	580	SRM	C1D-C2D-C3D	-3.45	103.19	106.81
3	E	570	SRM	CMB-C2B-C3B	3.35	118.23	112.05
3	A	580	SRM	C1A-NA-C4A	3.26	109.37	105.34
3	B	570	SRM	CAC-CBC-CCC	-3.24	105.07	113.67
3	D	580	SRM	CMB-C2B-C3B	3.22	118.00	112.05
3	B	570	SRM	C3A-C2A-C1A	-3.19	95.50	100.92
3	D	580	SRM	CHD-C4C-NC	-3.18	120.99	124.45
3	A	580	SRM	O2B-CCB-CBB	3.13	123.90	114.00
3	B	570	SRM	O2D-CCD-CBD	3.12	123.84	114.00
3	A	580	SRM	CAB-C3B-C4B	-3.11	105.76	111.19
3	D	580	SRM	CAD-C2D-C3D	-3.09	115.71	125.30
3	B	570	SRM	CDA-C2A-C3A	-3.06	100.28	108.37
3	B	570	SRM	CMA-C2A-C3A	-2.95	106.60	112.05
3	E	570	SRM	O4B-CEB-CDB	2.92	123.60	114.35
3	D	580	SRM	CHC-C1C-NC	-2.91	121.29	124.45
3	E	570	SRM	C4A-CHB-C1B	-2.90	121.57	125.84
3	E	570	SRM	C3A-C4A-CHB	-2.87	117.21	123.33
3	E	570	SRM	CBC-CAC-C3C	-2.85	104.66	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	580	SRM	CBD-CAD-C2D	2.84	120.39	112.53
3	D	580	SRM	C2A-C1A-CHA	2.83	126.08	123.54
3	E	570	SRM	CAC-C3C-C4C	-2.82	119.13	124.85
3	B	570	SRM	C3A-C4A-CHB	-2.81	117.35	123.33
3	B	570	SRM	CHD-C4C-C3C	-2.80	120.44	124.86
3	A	580	SRM	CAB-C3B-C2B	-2.78	106.55	114.19
3	A	580	SRM	C4D-CHA-C1A	2.77	130.98	125.87
3	B	570	SRM	CDA-C2A-C1A	2.73	115.58	107.11
3	B	570	SRM	O3A-CEA-CDA	-2.73	115.21	122.95
3	B	570	SRM	CBC-CAC-C3C	-2.72	105.02	112.53
3	B	570	SRM	CAC-C3C-C4C	2.69	130.33	124.85
3	D	580	SRM	C3A-C4A-CHB	2.59	128.85	123.33
3	D	580	SRM	C3B-C2B-C1B	-2.58	96.54	100.92
3	B	570	SRM	O1D-CCD-CBD	-2.58	114.91	123.09
3	A	580	SRM	CMA-C2A-CDA	2.55	115.07	110.74
3	E	570	SRM	CHD-C4C-C3C	-2.50	120.92	124.86
3	A	580	SRM	O4B-CEB-CDB	2.49	122.25	114.35
3	E	570	SRM	C4D-CHA-C1A	-2.39	121.47	125.87
3	E	570	SRM	CEC-CDC-C2C	-2.34	107.88	113.76
3	E	570	SRM	C1A-NA-C4A	-2.33	102.45	105.34
3	E	570	SRM	O3B-CEB-CDB	-2.33	116.36	122.95
3	A	580	SRM	CMB-C2B-CDB	-2.31	106.80	110.74
3	B	570	SRM	CHA-C4D-C3D	-2.31	120.24	125.30
3	E	570	SRM	O2A-CCA-CBA	2.30	121.25	114.00
3	A	580	SRM	C3A-C4A-CHB	2.24	128.10	123.33
3	A	580	SRM	O2C-CCC-O1C	-2.24	117.57	123.33
3	B	570	SRM	O4A-CEA-O3A	2.24	129.09	123.33
3	A	580	SRM	O2D-CCD-CBD	2.23	121.03	114.00
3	D	580	SRM	CAD-C2D-C1D	-2.18	120.68	124.94
3	A	580	SRM	C3B-C2B-C1B	-2.18	97.22	100.92
3	B	570	SRM	CMB-C2B-C1B	-2.17	98.81	109.59
3	A	580	SRM	CED-CDD-C3D	2.17	119.22	113.76
3	A	580	SRM	O2C-CCC-CBC	2.17	120.85	114.00
3	E	570	SRM	CAB-C3B-C2B	2.17	120.15	114.19
3	A	580	SRM	CDA-C2A-C1A	2.15	113.78	107.11
3	D	580	SRM	C3A-C4A-NA	-2.15	106.63	110.83
3	A	580	SRM	C2C-C1C-NC	2.13	112.38	110.32
3	A	580	SRM	O3B-CEB-CDB	-2.11	116.97	122.95
3	D	580	SRM	CBA-CAA-C3A	2.10	120.59	114.65
3	A	580	SRM	CHD-C4C-C3C	-2.09	121.56	124.86
3	A	580	SRM	CAC-CBC-CCC	-2.09	108.13	113.67

All (6) chirality outliers are listed below:

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

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	580	SRM	C4A-C3A-CAA-CBA
3	B	570	SRM	CMA-C2A-CDA-CEA
3	B	570	SRM	C4A-C3A-CAA-CBA
3	D	580	SRM	C1A-C2A-CDA-CEA
3	D	580	SRM	CMA-C2A-CDA-CEA
3	D	580	SRM	C3A-C2A-CDA-CEA
3	D	580	SRM	C1B-C2B-CDB-CEB
3	D	580	SRM	C2B-C3B-CAB-CBB
3	D	580	SRM	C2D-C3D-CDD-CED
3	E	570	SRM	C4A-C3A-CAA-CBA
3	E	570	SRM	C2B-C3B-CAB-CBB
3	E	570	SRM	C4C-C3C-CAC-CBC
3	E	570	SRM	C2D-C3D-CDD-CED
3	E	570	SRM	C4D-C3D-CDD-CED
3	E	570	SRM	C3D-C2D-CAD-CBD
3	D	580	SRM	C2A-C3A-CAA-CBA
3	E	570	SRM	C4B-C3B-CAB-CBB
3	D	580	SRM	C1D-C2D-CAD-CBD
3	E	570	SRM	C3A-CAA-CBA-CCA
3	E	570	SRM	C3B-CAB-CBB-CCB
3	D	580	SRM	C3C-CAC-CBC-CCC
3	A	580	SRM	C4D-C3D-CDD-CED
3	B	570	SRM	C4D-C3D-CDD-CED
3	A	580	SRM	C2B-CDB-CEB-O3B
3	A	580	SRM	C3B-CAB-CBB-CCB
3	A	580	SRM	C2B-C3B-CAB-CBB
3	D	580	SRM	C3A-CAA-CBA-CCA
3	B	570	SRM	C3B-C2B-CDB-CEB
3	B	570	SRM	C2B-CDB-CEB-O3B
3	E	570	SRM	C1B-C2B-CDB-CEB
3	A	580	SRM	C1D-C2D-CAD-CBD
3	A	580	SRM	C3D-CDD-CED-O3D
3	B	570	SRM	C3D-CDD-CED-O3D

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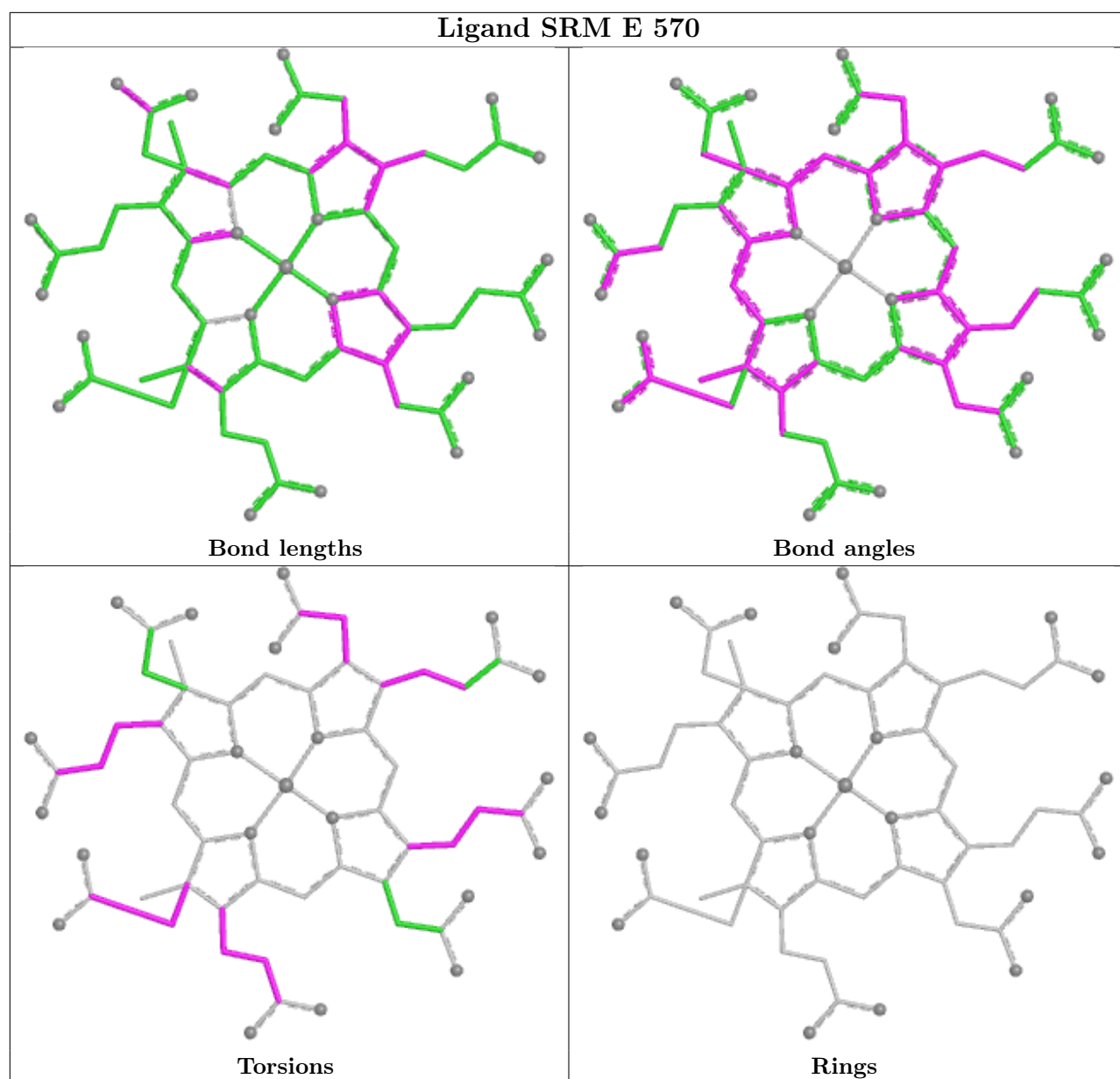
Mol	Chain	Res	Type	Atoms
3	A	580	SRM	C2B-CDB-CEB-O4B
3	E	570	SRM	C2B-CDB-CEB-O3B
3	E	570	SRM	C2B-CDB-CEB-O4B
3	B	570	SRM	C3D-C2D-CAD-CBD
3	E	570	SRM	C2D-CAD-CBD-CCD
3	A	580	SRM	C3D-CDD-CED-O4D
3	B	570	SRM	C3D-CDD-CED-O4D
3	E	570	SRM	C3D-CDD-CED-O4D
3	E	570	SRM	C1D-C2D-CAD-CBD
3	A	580	SRM	CAB-CBB-CCB-O1B
3	B	570	SRM	C3C-CAC-CBC-CCC
3	E	570	SRM	C3C-CAC-CBC-CCC
3	B	570	SRM	CAA-CBA-CCA-O1A
3	B	570	SRM	CAA-CBA-CCA-O2A
3	D	580	SRM	C3B-C2B-CDB-CEB
3	A	580	SRM	CAB-CBB-CCB-O2B
3	B	570	SRM	CAB-CBB-CCB-O1B
3	D	580	SRM	CAA-CBA-CCA-O2A
3	D	580	SRM	CAA-CBA-CCA-O1A
3	B	570	SRM	CAB-CBB-CCB-O2B
3	A	580	SRM	CAC-CBC-CCC-O2C
3	B	570	SRM	C2B-CDB-CEB-O4B
3	A	580	SRM	CAC-CBC-CCC-O1C
3	B	570	SRM	CAD-CBD-CCD-O2D
3	D	580	SRM	C2C-C3C-CAC-CBC
3	D	580	SRM	C4C-C3C-CAC-CBC
3	D	580	SRM	CAB-CBB-CCB-O1B
3	D	580	SRM	CAB-CBB-CCB-O2B
3	D	580	SRM	CAD-CBD-CCD-O2D
3	B	570	SRM	CAC-CBC-CCC-O1C
3	D	580	SRM	CAD-CBD-CCD-O1D
3	E	570	SRM	CAB-CBB-CCB-O2B
3	E	570	SRM	CAB-CBB-CCB-O1B
3	B	570	SRM	CAD-CBD-CCD-O1D
3	E	570	SRM	CAC-CBC-CCC-O1C
3	E	570	SRM	CAC-CBC-CCC-O2C
3	E	570	SRM	C3D-CDD-CED-O3D
3	B	570	SRM	C3A-C2A-CDA-CEA
3	B	570	SRM	CAC-CBC-CCC-O2C
3	B	570	SRM	C2D-C3D-CDD-CED
3	B	570	SRM	C2D-CAD-CBD-CCD
3	E	570	SRM	CAA-CBA-CCA-O2A

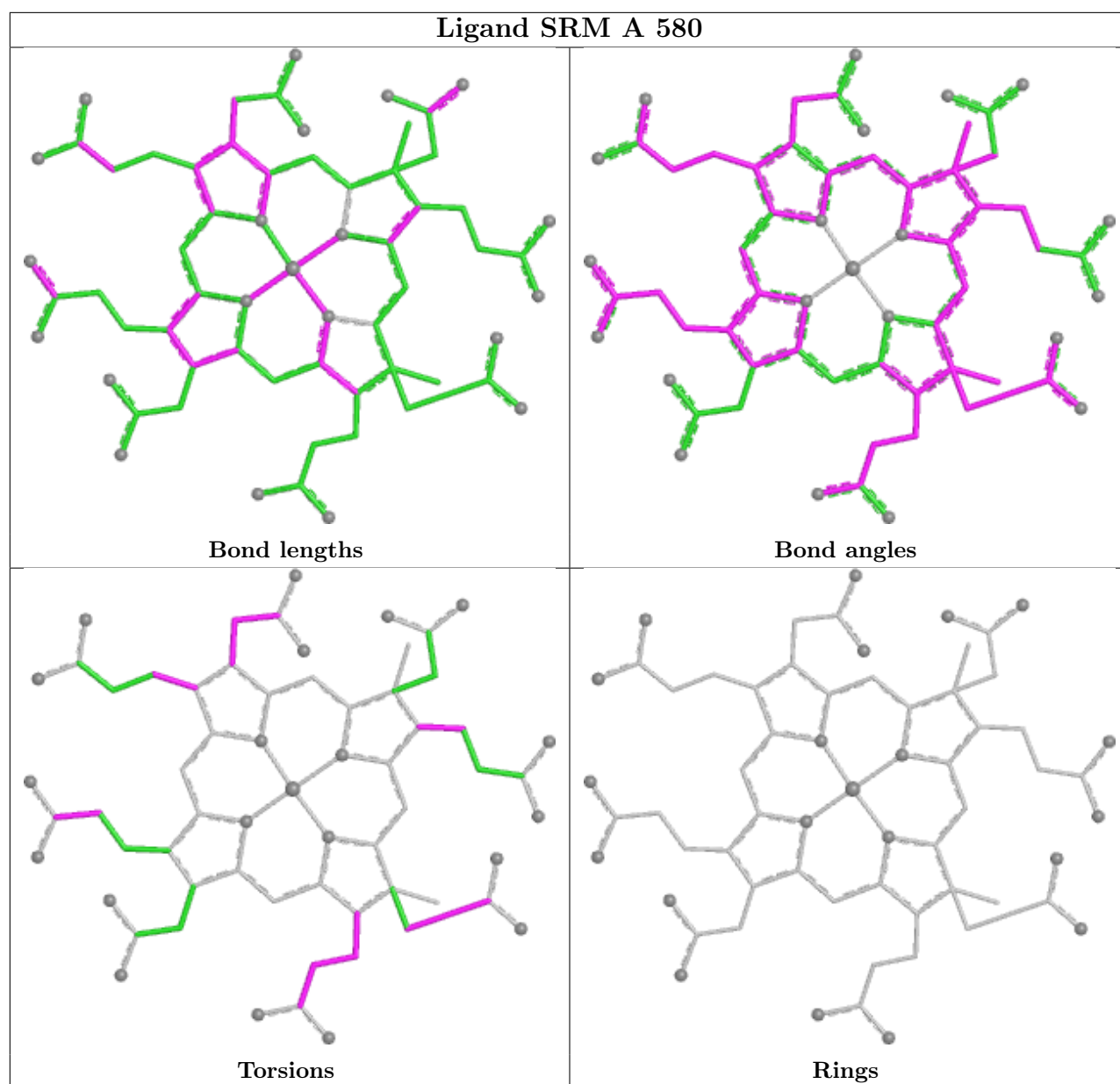
There are no ring outliers.

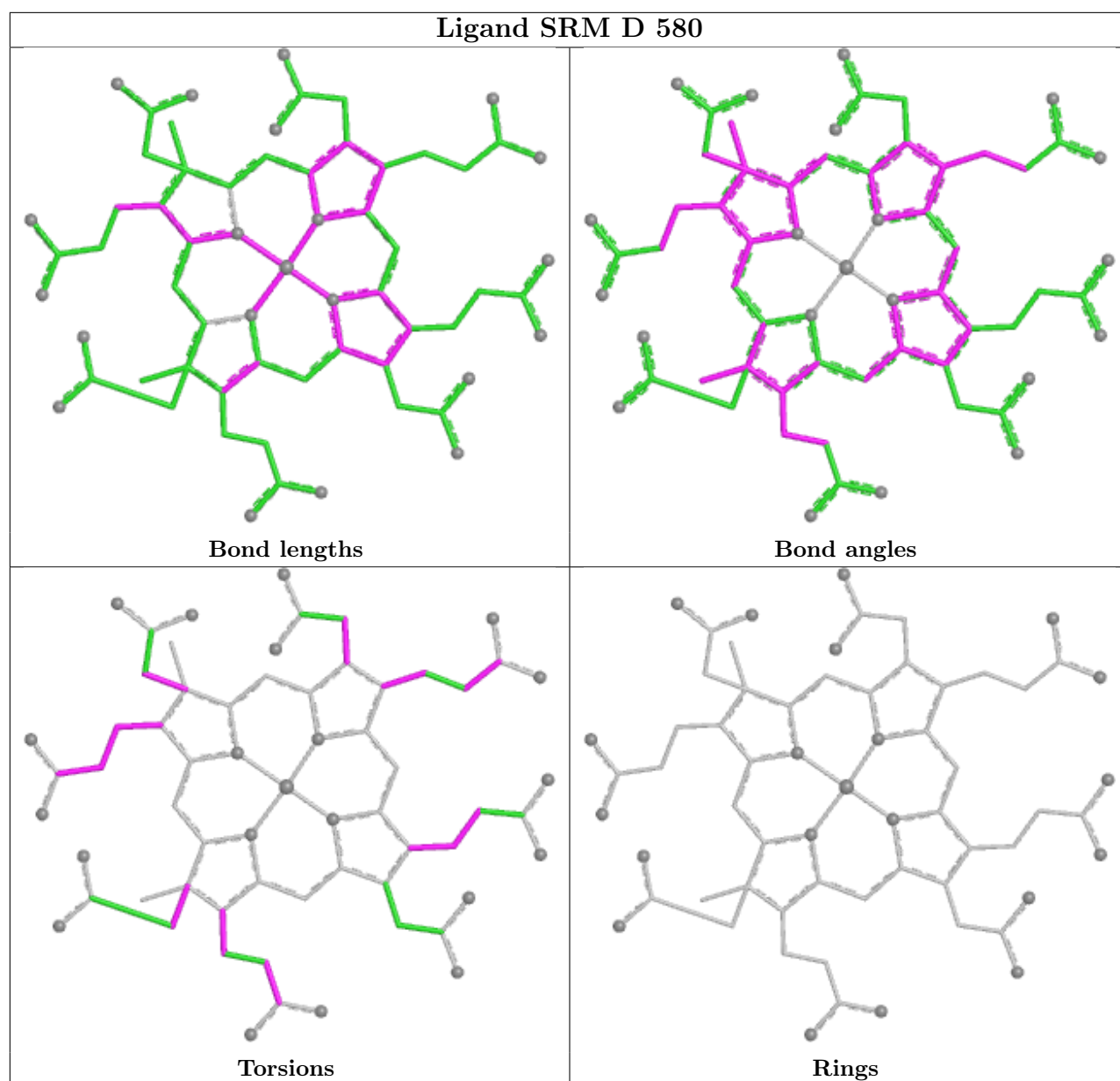
10 monomers are involved in 54 short contacts:

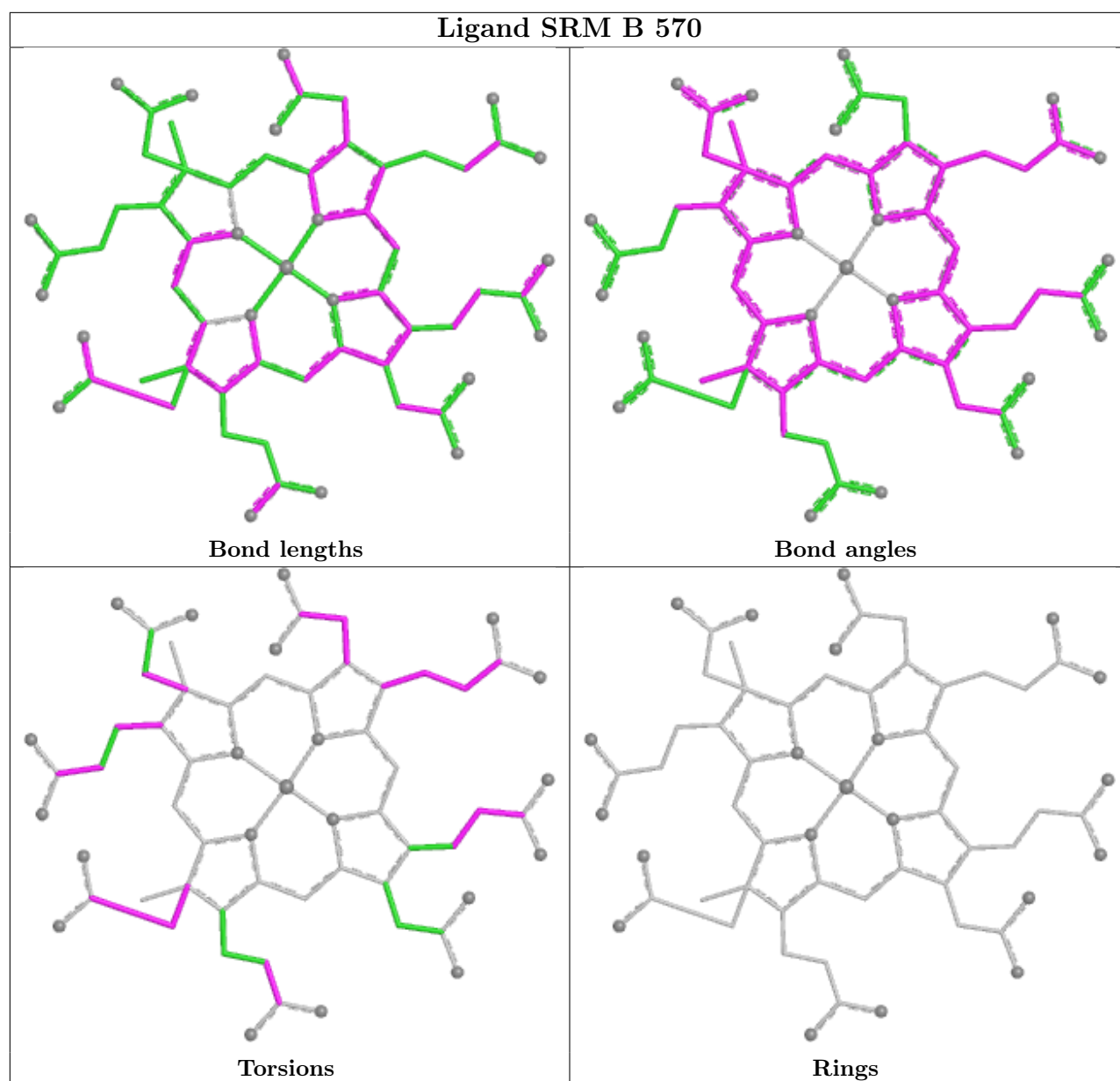
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	575	SF4	1	0
3	E	570	SRM	10	0
4	A	576	SF4	1	0
4	E	585	SF4	7	0
4	A	575	SF4	1	0
4	B	585	SF4	2	0
5	A	590	CMO	1	0
3	A	580	SRM	11	0
3	D	580	SRM	11	0
3	B	570	SRM	9	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	417/418 (99%)	0.17	3 (0%) 84 86	4, 17, 30, 66	0
1	D	417/418 (99%)	1.18	65 (15%) 5 5	7, 15, 28, 38	0
2	B	363/366 (99%)	0.10	3 (0%) 82 85	8, 17, 26, 51	0
2	E	363/366 (99%)	0.83	38 (10%) 11 12	2, 12, 36, 55	0
All	All	1560/1568 (99%)	0.58	109 (6%) 22 24	2, 16, 30, 66	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	406	ALA	5.2
2	B	184	ALA	5.0
1	A	417	TRP	4.8
1	D	25	ALA	4.7
1	D	383	VAL	4.7
1	D	407	TYR	4.7
1	D	402	LEU	4.7
1	D	131	GLY	4.6
1	D	408	THR	4.6
1	D	43	GLY	4.4
1	D	94	PHE	4.4
1	D	415	GLY	4.4
1	D	91	VAL	4.1
1	D	88	ILE	4.0
1	D	386	VAL	3.8
1	D	405	SER	3.8
1	D	393	PRO	3.7
1	D	31	ALA	3.6
1	D	389	PRO	3.5
1	D	411	LEU	3.5
2	E	206	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	392	ASN	3.4
1	D	115	LEU	3.4
2	E	111	VAL	3.4
1	D	388	ALA	3.4
1	D	33	ALA	3.3
2	E	35	VAL	3.3
2	E	354	PHE	3.3
1	D	403	LYS	3.2
2	E	95	THR	3.2
2	E	4	GLU	3.2
1	D	299	LEU	3.2
2	E	358	PHE	3.2
1	D	391	ASN	3.1
1	D	417	TRP	3.1
1	D	395	MET	3.0
1	D	378	GLY	3.0
1	D	381	ALA	3.0
1	D	81	TYR	3.0
2	B	5	GLY	3.0
2	E	115	CYS	3.0
1	D	413	LYS	2.9
2	E	182	CYS	2.9
1	A	406	ALA	2.9
2	E	366	TRP	2.9
1	D	1	SER	2.9
1	D	394	PHE	2.9
1	D	27	LEU	2.8
2	E	69	GLU	2.8
2	B	4	GLU	2.8
1	D	317	PHE	2.7
1	A	66	GLY	2.7
1	D	24	THR	2.7
2	E	229	MET	2.7
1	D	32	ALA	2.7
2	E	184	ALA	2.7
2	E	201	ILE	2.7
1	D	248	ALA	2.6
2	E	92	PHE	2.6
1	D	42	LYS	2.6
2	E	353	TYR	2.6
2	E	365	LYS	2.6
2	E	181	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	116	CYS	2.5
1	D	340	ILE	2.5
1	D	326	VAL	2.5
2	E	356	SER	2.5
1	D	401	GLU	2.5
2	E	135	GLN	2.5
1	D	396	PHE	2.4
1	D	238	TRP	2.4
2	E	137	TRP	2.4
1	D	399	LYS	2.4
2	E	236	VAL	2.4
1	D	106	PHE	2.4
2	E	234	ILE	2.4
1	D	5	LEU	2.3
1	D	145	TYR	2.3
2	E	227	PRO	2.3
2	E	230	LYS	2.3
1	D	48	LEU	2.3
1	D	374	LEU	2.3
2	E	349	ARG	2.3
1	D	164	GLY	2.2
1	D	247	GLU	2.2
1	D	365	ILE	2.2
1	D	40	MET	2.2
2	E	362	THR	2.2
1	D	132	SER	2.2
1	D	291	CYS	2.2
2	E	211	CYS	2.2
1	D	66	GLY	2.2
2	E	183	GLY	2.2
2	E	77	TYR	2.1
2	E	40	VAL	2.1
2	E	116	GLY	2.1
1	D	93	HIS	2.1
2	E	65	TYR	2.1
2	E	345	ILE	2.1
2	E	355	TYR	2.1
1	D	237	THR	2.1
1	D	178	PRO	2.1
1	D	262	VAL	2.0
2	E	36	VAL	2.0
2	E	90	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	126	LEU	2.0
1	D	288	CYS	2.0
1	D	397	PHE	2.0
2	E	243	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](#)

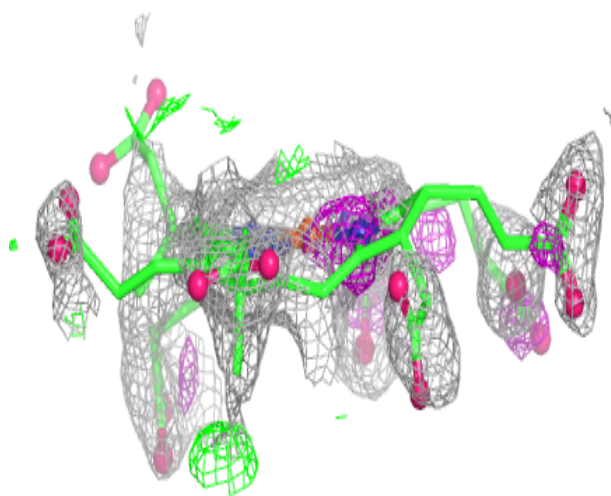
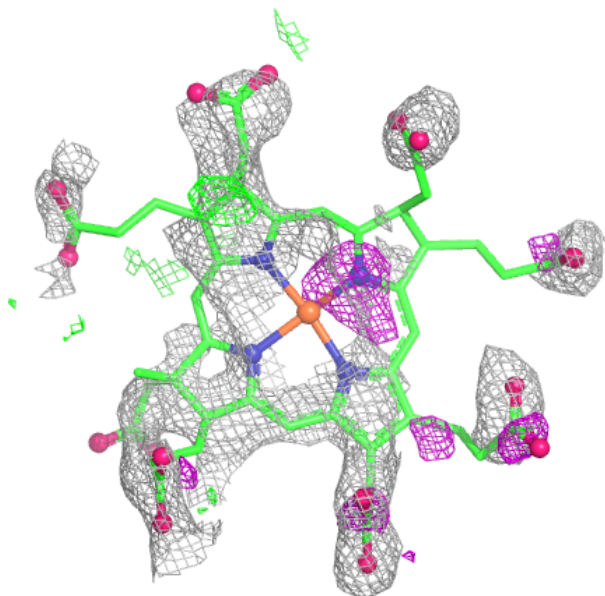
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	SRM	D	580	63/63	0.66	0.18	37,81,97,102	0
5	CMO	A	590	2/2	0.71	0.29	29,29,29,42	0
4	SF4	E	585	8/8	0.79	0.15	3,3,3,4	8
3	SRM	E	570	63/63	0.87	0.11	8,12,19,21	0
4	SF4	A	576	8/8	0.89	0.12	2,4,9,9	0
4	SF4	D	576	8/8	0.91	0.14	11,12,14,15	0
4	SF4	D	575	8/8	0.92	0.17	12,14,15,16	0
3	SRM	A	580	63/63	0.93	0.09	17,28,42,48	0
3	SRM	B	570	63/63	0.95	0.07	4,10,20,32	0
4	SF4	A	575	8/8	0.96	0.06	9,16,18,18	0
4	SF4	E	586	8/8	0.96	0.15	21,26,28,29	0
4	SF4	B	585	8/8	0.96	0.05	16,20,22,26	8
4	SF4	B	586	8/8	0.97	0.04	15,18,21,22	0

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

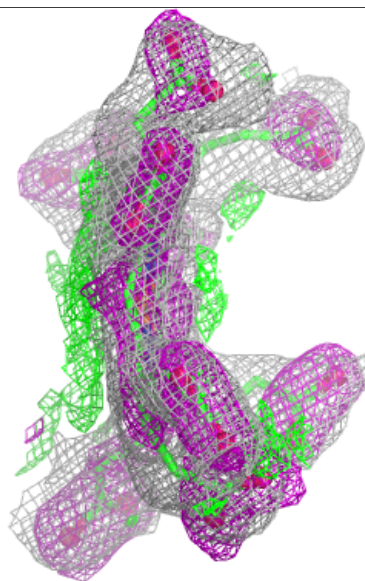
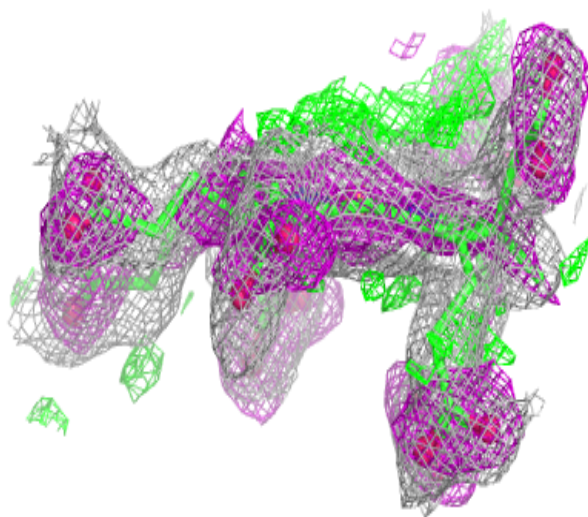
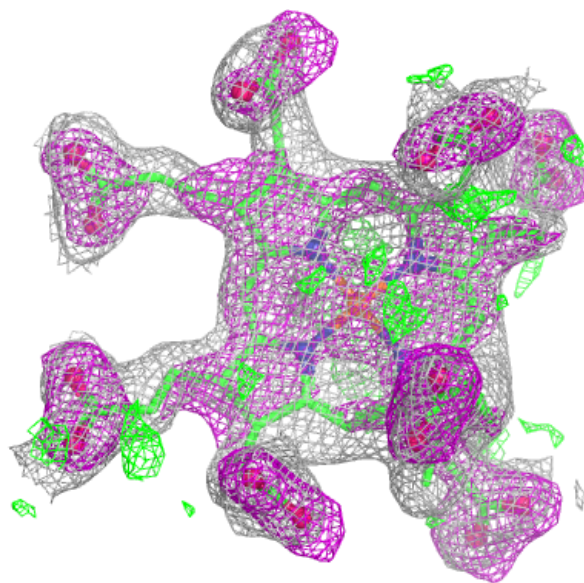
Electron density around SRM D 580:

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



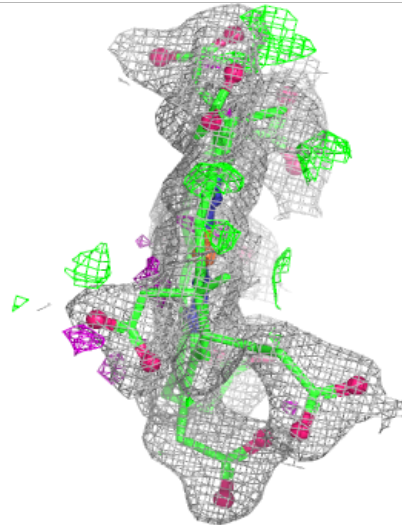
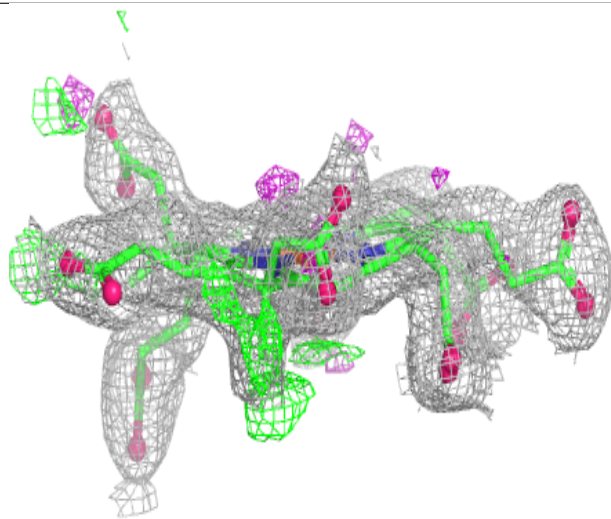
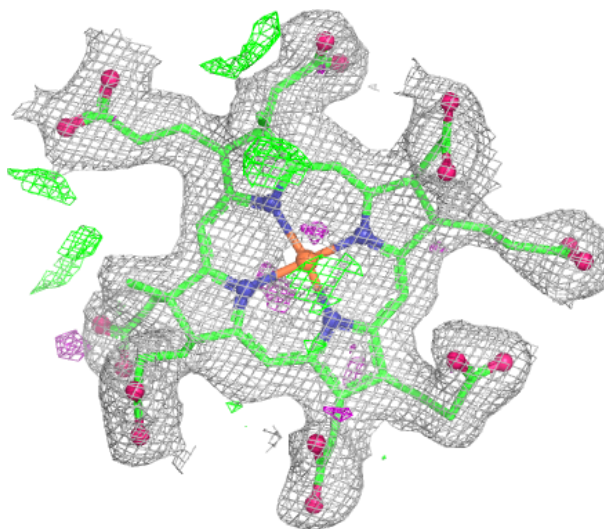
Electron density around SRM E 570:

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



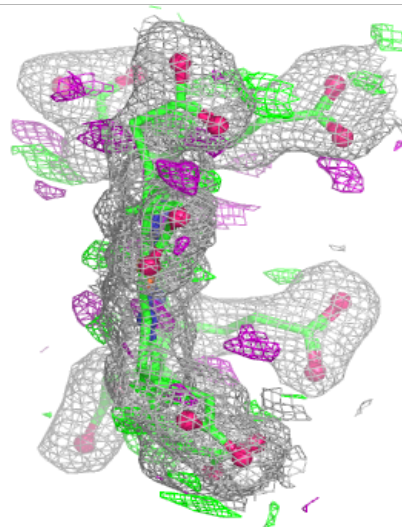
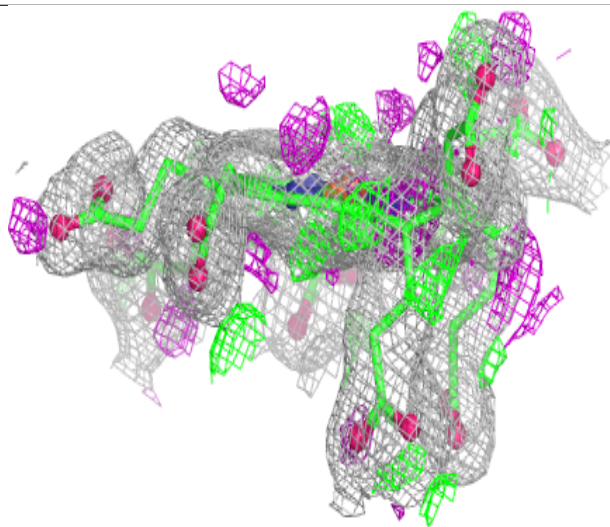
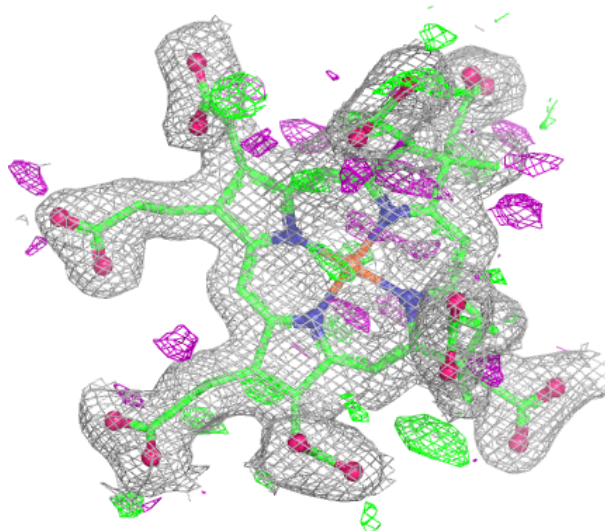
Electron density around SRM A 580:

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



Electron density around SRM B 570:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.