



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 06:20 PM BST

PDB ID : 3M1V  
Title : Structural Insight into Methyl-Coenzyme M Reductase Chemistry using Coenzyme B Analogues  
Authors : Cedervall, P.E.; Dey, M.; Ragsdale, S.W.; Wilmot, C.M.  
Deposited on : 2010-03-05  
Resolution : 1.45 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](mailto: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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13  
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) : 2.13

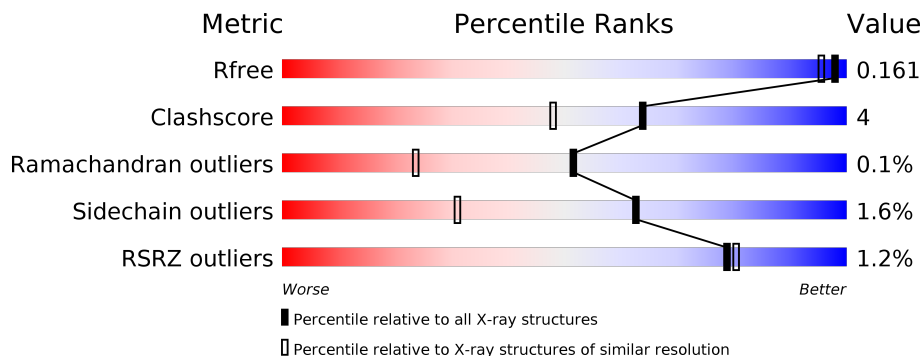
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.45 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	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	549	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 15%, green 84%);"></div> <div style="margin-left: 10px;"> <p>%</p> <p>84% 15% .</p> </div> </div>
1	D	549	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 10%, green 89%);"></div> <div style="margin-left: 10px;"> <p>%</p> <p>89% 10% .</p> </div> </div>
2	B	442	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 89%, yellow 11%);"></div> <div style="margin-left: 10px;"> <p>89% 11%</p> </div> </div>
2	E	442	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 12%, green 88%);"></div> <div style="margin-left: 10px;"> <p>%</p> <p>88% 12%</p> </div> </div>
3	C	248	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 9%, green 89%);"></div> <div style="margin-left: 10px;"> <p>3%</p> <p>89% 9% ..</p> </div> </div>
3	F	248	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 1%, yellow 13%, green 85%);"></div> <div style="margin-left: 10px;"> <p>4%</p> <p>85% 13% ..</p> </div> </div>

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
8	ACT	C	1	-	-	X	-

## 2 Entry composition i

There are 12 unique types of molecules in this entry. The entry contains 23013 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 Methyl-coenzyme M reductase I subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	548	Total	C	N	O	S	0	54	0
			4639	2933	771	914	21			
1	D	548	Total	C	N	O	S	0	30	0
			4423	2816	725	862	20			

- Molecule 2 is a protein called Methyl-coenzyme M reductase I subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	442	Total	C	N	O	S	0	28	0
			3485	2225	566	672	22			
2	E	442	Total	C	N	O	S	0	41	0
			3574	2282	581	689	22			

- Molecule 3 is a protein called Methyl-coenzyme M reductase I subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	246	Total	C	N	O	S	0	12	0
			2063	1279	359	412	13			
3	F	246	Total	C	N	O	S	0	16	0
			2081	1295	362	412	12			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

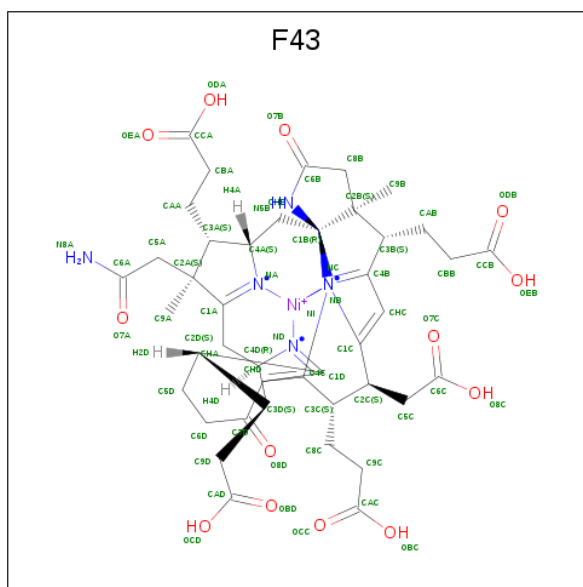
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
4	D	2	Total	Mg	0	0
			2	2		
4	E	1	Total	Mg	0	0
			1	1		
4	B	2	Total	Mg	0	0
			2	2		
4	C	1	Total	Mg	0	0
			1	1		

*Continued on next page...*

Continued from previous page...

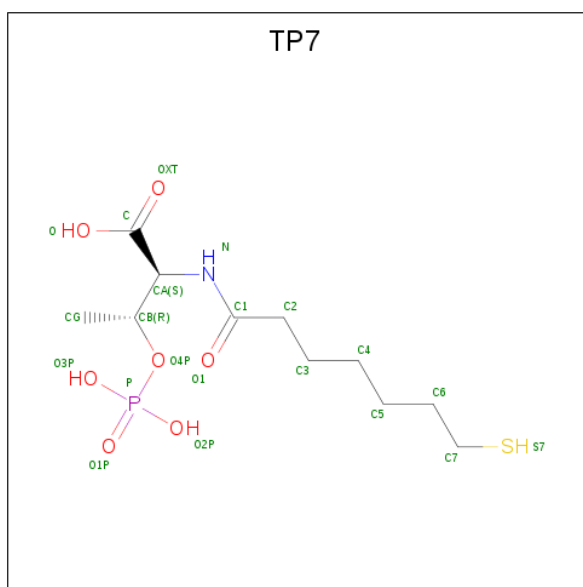
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mg 2 2	0	2
4	F	1	Total Mg 1 1	0	0

- Molecule 5 is FACTOR 430 (three-letter code: F43) (formula:  $C_{42}H_{51}N_6NiO_{13}$ ).



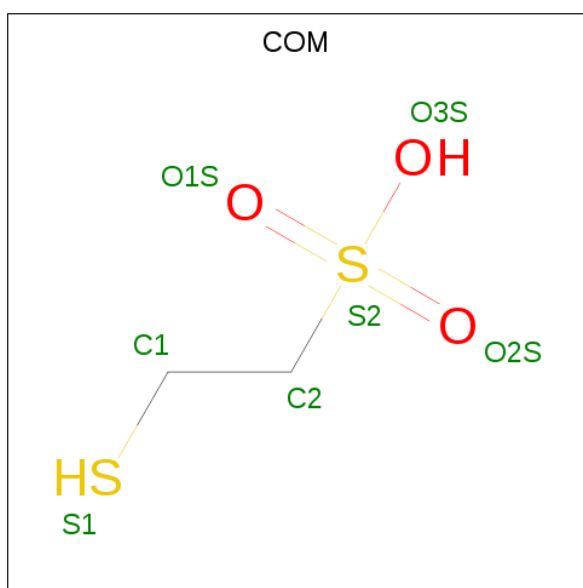
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N Ni O 62 42 6 1 13	0	0
5	D	1	Total C N Ni O 62 42 6 1 13	0	0

- Molecule 6 is Coenzyme B (three-letter code: TP7) (formula:  $C_{11}H_{22}NO_7PS$ ).



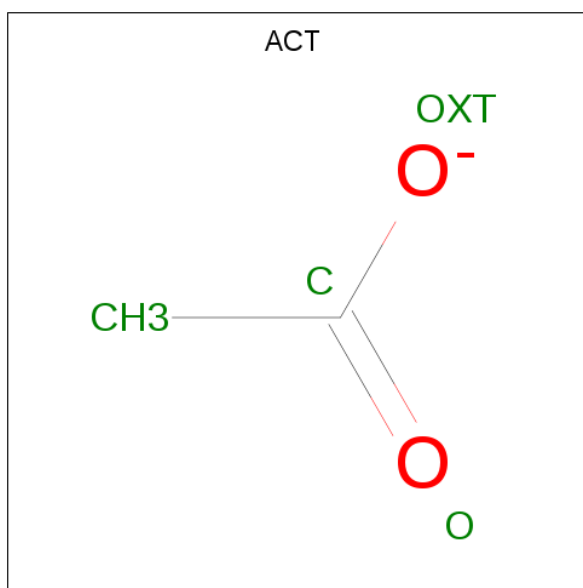
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
6	A	1	21	11	1	7	1	1	0	1
6	D	1	21	11	1	7	1	1	0	1

- Molecule 7 is 1-THIOETHANESULFONIC ACID (three-letter code: COM) (formula:  $C_2H_6O_3S_2$ ).



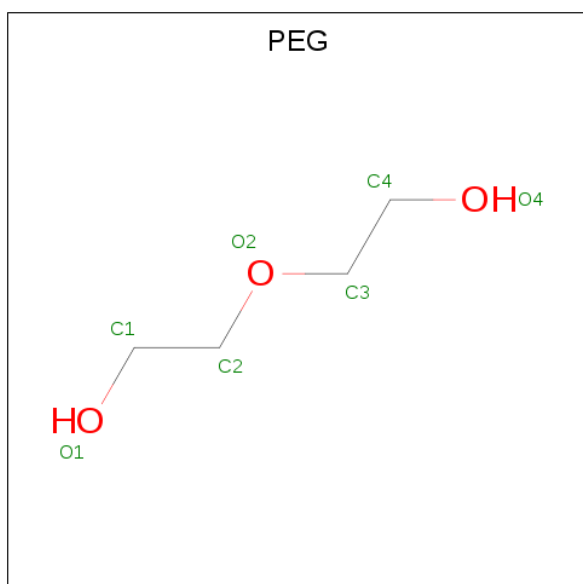
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	O			S
7	A	1	7	2	3	2	0	0
7	D	1	7	2	3	2	0	0

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 4 2 2	0	1
8	A	1	Total C O 4 2 2	0	1
8	B	1	Total C O 4 2 2	0	1
8	C	1	Total C O 4 2 2	0	0

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).

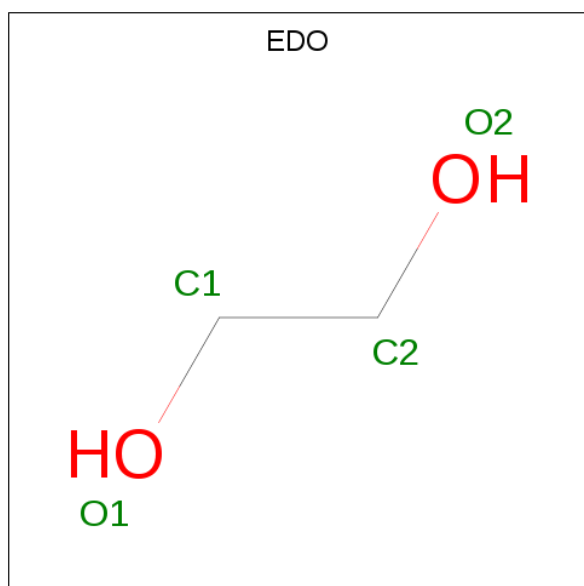


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 7 4 3	0	0
9	C	1	Total C O 7 4 3	0	0

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total Zn 1 1	0	0

- Molecule 11 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	D	1	Total C O 4 2 2	0	0
11	F	1	Total C O 4 2 2	0	0
11	F	1	Total C O 4 2 2	0	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	524	Total O 533 533	0	36

*Continued on next page...*



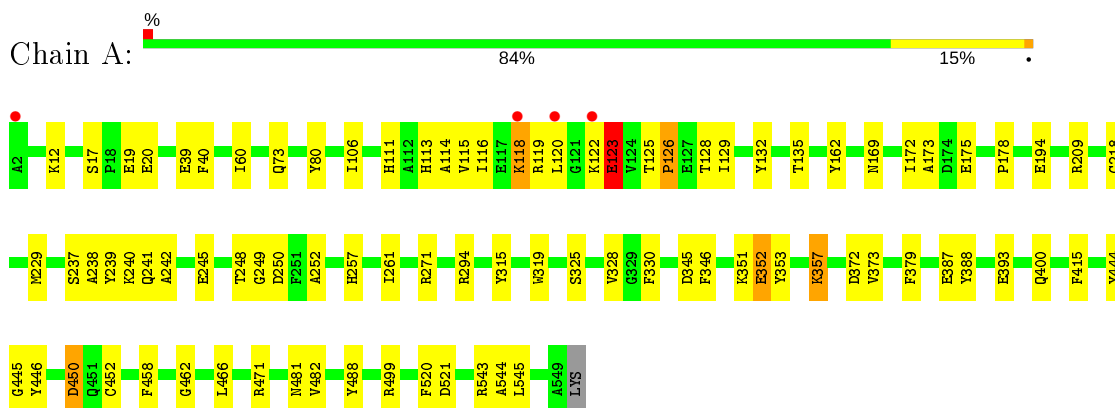
*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
12	B	456	Total 470	O 470	0	27
12	C	262	Total 271	O 271	0	11
12	D	537	Total 547	O 547	0	27
12	E	419	Total 426	O 426	0	16
12	F	264	Total 269	O 269	0	9

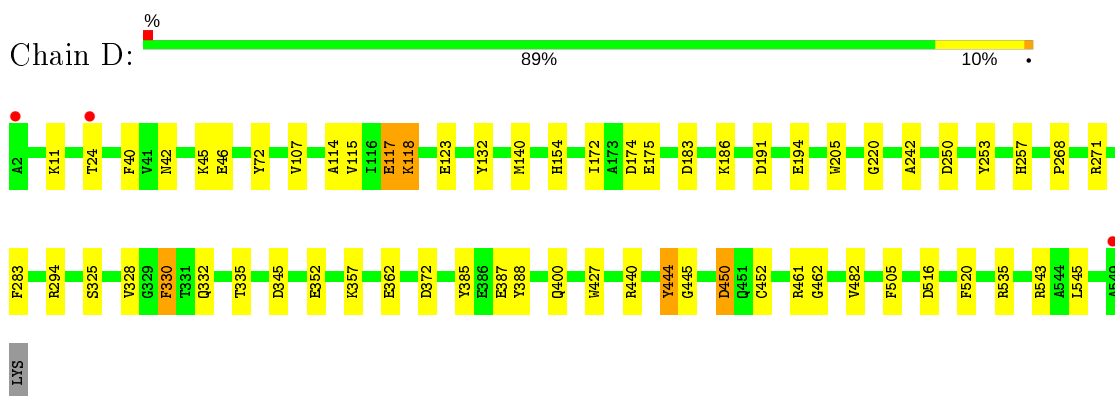
### 3 Residue-property plots

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.

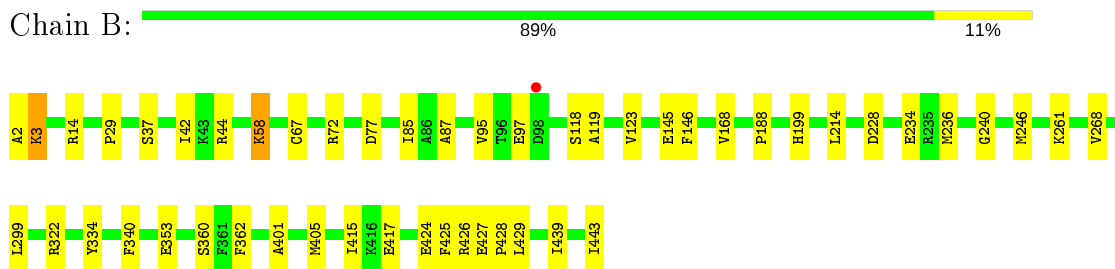
- Molecule 1: Methyl-coenzyme M reductase I subunit alpha



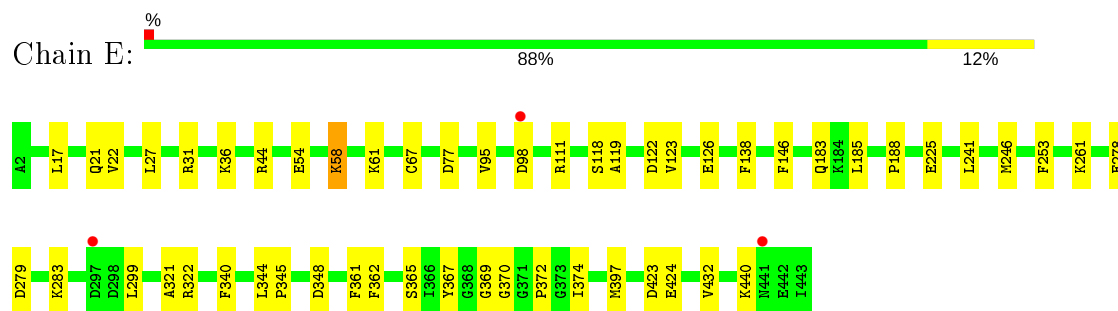
- Molecule 1: Methyl-coenzyme M reductase I subunit alpha



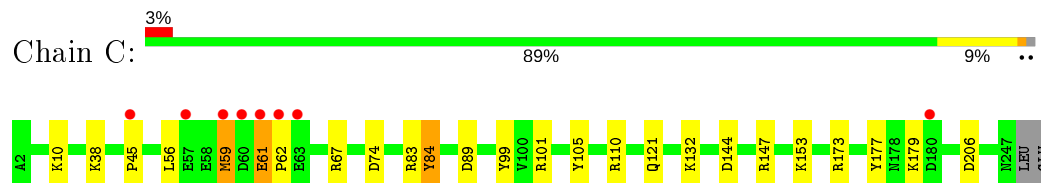
- Molecule 2: Methyl-coenzyme M reductase I subunit beta



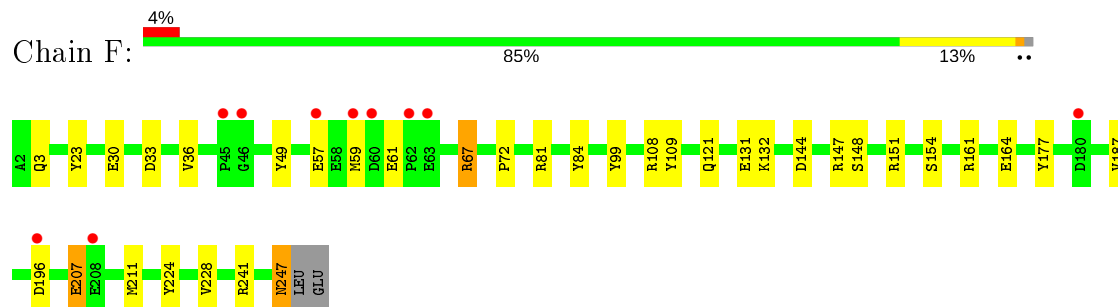
- Molecule 2: Methyl-coenzyme M reductase I subunit beta



- Molecule 3: Methyl-coenzyme M reductase I subunit gamma



- Molecule 3: Methyl-coenzyme M reductase I subunit gamma



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.02Å 118.26Å 122.39Å 90.00° 91.84° 90.00°	Depositor
Resolution (Å)	20.15 – 1.45 20.11 – 1.45	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.15-1.45) 98.8 (20.11-1.45)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.42 (at 1.45Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.135 , 0.162 0.134 , 0.161	Depositor DCC
$R_{free}$ test set	20362 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	10.6	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.009 for -h,-l,-k 0.014 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	23013	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ZN, PEG, SMC, ACT, MG, F43, MGN, TP7, AGM, EDO, GL3, COM, MHS

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	1.56	20/4732 (0.4%)	1.31	22/6422 (0.3%)
1	D	1.53	16/4550 (0.4%)	1.31	17/6173 (0.3%)
2	B	1.50	15/3607 (0.4%)	1.26	9/4877 (0.2%)
2	E	1.55	9/3702 (0.2%)	1.27	11/5003 (0.2%)
3	C	1.52	4/2127 (0.2%)	1.30	11/2864 (0.4%)
3	F	1.56	11/2166 (0.5%)	1.34	15/2914 (0.5%)
All	All	1.54	75/20884 (0.4%)	1.30	85/28253 (0.3%)

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	1	1
1	D	1	0
All	All	2	1

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	340	PHE	CE1-CZ	6.05	1.48	1.37
1	A	319	TRP	CD2-CE2	6.03	1.48	1.41
2	E	54	GLU	CD-OE1	-5.92	1.19	1.25
3	F	30	GLU	CD-OE2	5.91	1.32	1.25
3	F	177	TYR	CD1-CE1	5.90	1.48	1.39
2	E	253	PHE	CD1-CE1	5.85	1.50	1.39
1	A	458	PHE	CE1-CZ	5.84	1.48	1.37
2	E	278	GLU	CG-CD	5.84	1.60	1.51
3	F	161	ARG	CZ-NH1	5.84	1.40	1.33
1	D	117	GLU	CD-OE2	5.75	1.31	1.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	164	GLU	CG-CD	5.75	1.60	1.51
1	D	123	GLU	CG-CD	5.73	1.60	1.51
1	D	362	GLU	CG-CD	-5.71	1.43	1.51
2	E	321	ALA	CA-CB	5.70	1.64	1.52
3	F	3	GLN	CB-CG	-5.68	1.37	1.52
1	A	252	ALA	CA-CB	5.67	1.64	1.52
2	B	2	ALA	N-CA	5.63	1.57	1.46
1	A	123[A]	GLU	CG-CD	5.62	1.60	1.51
1	A	123[B]	GLU	CG-CD	5.62	1.60	1.51
1	D	461	ARG	CZ-NH1	5.61	1.40	1.33
1	A	488	TYR	CD1-CE1	5.60	1.47	1.39
2	B	427	GLU	CG-CD	5.60	1.60	1.51
2	B	362	PHE	CD2-CE2	5.58	1.50	1.39
2	B	240	GLY	N-CA	5.58	1.54	1.46
2	B	87	ALA	CA-CB	5.57	1.64	1.52
1	A	123[A]	GLU	CD-OE2	5.55	1.31	1.25
1	A	123[B]	GLU	CD-OE2	5.55	1.31	1.25
2	B	268	VAL	CB-CG2	5.54	1.64	1.52
1	D	107	VAL	CB-CG1	5.51	1.64	1.52
2	E	67	CYS	CB-SG	5.46	1.91	1.82
1	D	330	PHE	CE2-CZ	5.46	1.47	1.37
1	D	72	TYR	CD1-CE1	5.45	1.47	1.39
3	F	49	TYR	CE2-CZ	5.45	1.45	1.38
2	E	138	PHE	CD2-CE2	5.44	1.50	1.39
2	E	22	VAL	CB-CG2	5.43	1.64	1.52
2	B	168	VAL	CB-CG1	5.43	1.64	1.52
1	D	140	MET	N-CA	5.43	1.57	1.46
1	D	132	TYR	CD1-CE1	5.42	1.47	1.39
1	A	39	GLU	CD-OE2	-5.40	1.19	1.25
2	B	146	PHE	CE1-CZ	5.38	1.47	1.37
1	D	427	TRP	CZ3-CH2	5.37	1.48	1.40
1	A	353	TYR	CE2-CZ	5.35	1.45	1.38
3	C	84	TYR	CD1-CE1	5.35	1.47	1.39
1	A	379	PHE	CE1-CZ	5.33	1.47	1.37
1	D	72	TYR	CG-CD2	5.32	1.46	1.39
1	A	373	VAL	CB-CG2	5.32	1.64	1.52
2	E	146	PHE	CE2-CZ	5.32	1.47	1.37
1	A	123[A]	GLU	C-O	5.27	1.33	1.23
1	A	123[B]	GLU	C-O	5.27	1.33	1.23
1	D	462	GLY	N-CA	5.27	1.53	1.46
1	D	220	GLY	N-CA	5.27	1.53	1.46
1	D	11	LYS	CE-NZ	5.25	1.62	1.49

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	187	VAL	CB-CG1	5.24	1.63	1.52
1	A	20	GLU	CB-CG	5.23	1.62	1.52
3	F	23	TYR	CE1-CZ	5.23	1.45	1.38
1	A	446	TYR	CG-CD2	5.22	1.46	1.39
2	B	353	GLU	CD-OE1	-5.18	1.20	1.25
2	B	145	GLU	CB-CG	5.17	1.61	1.52
1	A	462	GLY	N-CA	5.15	1.53	1.46
3	C	84	TYR	CG-CD2	5.15	1.45	1.39
2	B	360	SER	CB-OG	5.13	1.49	1.42
2	B	85	ILE	CB-CG2	5.13	1.68	1.52
3	F	36	VAL	N-CA	5.12	1.56	1.46
1	A	218	CYS	CB-SG	5.12	1.91	1.82
1	A	19	GLU	CD-OE1	5.11	1.31	1.25
1	D	520	PHE	CE1-CZ	5.09	1.47	1.37
1	D	253	TYR	CD1-CE1	5.07	1.47	1.39
3	F	154	SER	CB-OG	5.06	1.48	1.42
2	B	417	GLU	CD-OE2	5.05	1.31	1.25
3	C	177	TYR	CE2-CZ	-5.05	1.31	1.38
3	C	38	LYS	CE-NZ	5.02	1.61	1.49
3	F	99	TYR	CG-CD1	5.02	1.45	1.39
2	B	340	PHE	CG-CD1	5.01	1.46	1.38
1	A	40	PHE	CE1-CZ	5.01	1.46	1.37
2	B	58	LYS	CB-CG	-5.01	1.39	1.52

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	147	ARG	NE-CZ-NH1	8.59	124.60	120.30
2	B	72	ARG	NE-CZ-NH2	-7.86	116.37	120.30
3	F	131	GLU	OE1-CD-OE2	7.74	132.58	123.30
3	F	147	ARG	NE-CZ-NH1	7.33	123.97	120.30
2	B	44	ARG	NE-CZ-NH1	7.21	123.91	120.30
2	E	279	ASP	CB-CG-OD1	6.47	124.12	118.30
3	C	101	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	D	175	GLU	OE1-CD-OE2	6.24	130.78	123.30
1	A	450	ASP	CB-CA-C	6.09	122.59	110.40
1	D	388	TYR	CD1-CE1-CZ	-6.09	114.32	119.80
3	C	74	ASP	CB-CG-OD1	6.00	123.70	118.30
2	B	77	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	D	345	ASP	CB-CG-OD1	-5.99	112.91	118.30
3	F	144	ASP	CB-CG-OD2	5.92	123.63	118.30
3	F	99	TYR	CG-CD1-CE1	-5.91	116.57	121.30

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	241	ARG	NE-CZ-NH2	5.88	123.24	120.30
2	E	17	LEU	CB-CG-CD2	-5.87	101.03	111.00
1	D	385	TYR	CB-CG-CD2	-5.86	117.49	121.00
2	E	111	ARG	NE-CZ-NH2	5.82	123.21	120.30
1	D	516	ASP	CB-CG-OD1	-5.81	113.07	118.30
1	D	450	ASP	CB-CA-C	5.81	122.02	110.40
2	B	72	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	415	PHE	CB-CG-CD2	-5.79	116.75	120.80
1	D	440	ARG	NE-CZ-NH2	-5.72	117.44	120.30
2	B	14[A]	ARG	NE-CZ-NH2	-5.72	117.44	120.30
2	B	14[B]	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	D	250	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	A	40	PHE	CB-CG-CD2	-5.64	116.85	120.80
1	A	346	PHE	CB-CG-CD2	-5.64	116.85	120.80
3	F	147	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	A	315	TYR	CD1-CE1-CZ	-5.59	114.77	119.80
3	C	173	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	D	385	TYR	CD1-CE1-CZ	-5.58	114.78	119.80
1	A	499	ARG	NE-CZ-NH2	-5.56	117.52	120.30
2	E	361	PHE	CB-CG-CD2	-5.54	116.92	120.80
2	E	225	GLU	OE1-CD-OE2	5.52	129.93	123.30
3	F	81	ARG	NE-CZ-NH1	5.51	123.05	120.30
3	C	206	ASP	CB-CG-OD1	5.49	123.24	118.30
1	D	294	ARG	NE-CZ-NH2	5.47	123.04	120.30
3	C	144	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	162	TYR	CB-CG-CD1	5.45	124.27	121.00
1	A	294	ARG	NE-CZ-NH2	5.44	123.02	120.30
1	A	209	ARG	NE-CZ-NH1	5.43	123.02	120.30
2	E	423	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	A	294	ARG	NE-CZ-NH1	-5.38	117.61	120.30
3	F	144	ASP	CB-CG-OD1	-5.38	113.46	118.30
3	F	196	ASP	CB-CG-OD1	5.37	123.13	118.30
2	B	228	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	A	545[A]	LEU	CB-CG-CD2	-5.34	101.92	111.00
1	A	545[B]	LEU	CB-CG-CD2	-5.34	101.92	111.00
1	A	450	ASP	CB-CG-OD2	5.34	123.10	118.30
1	A	466	LEU	CB-CG-CD2	5.34	120.07	111.00
2	E	241	LEU	CB-CG-CD2	-5.31	101.97	111.00
1	D	444	TYR	CB-CG-CD2	-5.31	117.81	121.00
2	B	426	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	D	283	PHE	CB-CG-CD2	-5.29	117.10	120.80
1	A	471	ARG	NE-CZ-NH1	5.29	122.94	120.30

*Continued on next page...*



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	174	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	388	TYR	CZ-CE2-CD2	-5.28	115.05	119.80
3	F	108	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	162	TYR	CB-CG-CD2	-5.25	117.85	121.00
2	E	77	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	A	357	LYS	CD-CE-NZ	-5.23	99.66	111.70
2	B	334	TYR	CG-CD2-CE2	-5.23	117.12	121.30
1	A	521	ASP	CB-CG-OD2	-5.20	113.62	118.30
3	F	33	ASP	CB-CG-OD1	5.18	122.96	118.30
3	F	151	ARG	CG-CD-NE	-5.17	100.94	111.80
3	C	83	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	A	345	ASP	CB-CG-OD1	-5.14	113.68	118.30
1	D	40	PHE	CB-CG-CD2	-5.12	117.22	120.80
1	D	205	TRP	CD1-CG-CD2	5.12	110.40	106.30
3	C	89	ASP	CB-CG-OD2	5.09	122.88	118.30
2	E	31	ARG	NE-CZ-NH1	5.08	122.84	120.30
3	C	99	TYR	CB-CG-CD1	-5.08	117.95	121.00
3	F	99	TYR	CD1-CG-CD2	5.07	123.48	117.90
1	D	535	ARG	NE-CZ-NH1	-5.07	117.77	120.30
1	A	393	GLU	OE1-CD-OE2	5.06	129.37	123.30
2	E	348	ASP	CB-CG-OD1	5.06	122.85	118.30
1	D	132	TYR	CD1-CE1-CZ	-5.05	115.25	119.80
1	A	520	PHE	CB-CG-CD2	-5.04	117.27	120.80
3	F	109	TYR	CB-CG-CD1	-5.04	117.98	121.00
2	E	44	ARG	NE-CZ-NH1	5.04	122.82	120.30
3	C	105	TYR	CB-CG-CD2	-5.03	117.98	121.00
3	F	224	TYR	CB-CG-CD2	-5.03	117.98	121.00
3	C	110	ARG	NE-CZ-NH1	5.02	122.81	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	450	ASP	CA
1	D	450	ASP	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123[B]	GLU	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4639	0	4437	59	0
1	D	4423	0	4292	30	0
2	B	3485	0	3548	25	0
2	E	3574	0	3636	37	0
3	C	2063	0	1998	20	0
3	F	2081	0	2045	17	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	62	0	43	1	0
5	D	62	0	43	1	0
6	A	21	0	17	3	0
6	D	21	0	17	2	0
7	A	7	0	4	0	0
7	D	7	0	4	0	0
8	A	8	0	5	0	0
8	B	4	0	2	0	0
8	C	4	0	3	2	0
9	A	7	0	10	0	0
9	C	7	0	10	0	0
10	A	1	0	0	0	0
11	D	4	0	6	0	0
11	F	8	0	12	0	0
12	A	533	0	0	7	0
12	B	470	0	0	7	0
12	C	271	0	0	6	0
12	D	547	0	0	13	0
12	E	426	0	0	19	0
12	F	269	0	0	9	0
All	All	23013	0	20132	170	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 4.

All (170) 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)
1:A:169[A]:ASN:ND2	1:A:172:ILE:HD13	1.49	1.27
2:B:322[B]:ARG:NH2	3:C:67[B]:ARG:HG3	1.58	1.19
1:A:126[B]:PRO:CB	1:A:175[B]:GLU:HG2	1.93	0.99
1:A:249:GLY:O	2:E:369[B]:GLY:HA3	1.65	0.95
1:A:169[A]:ASN:ND2	1:A:172:ILE:CD1	2.29	0.94
1:A:122[B]:LYS:HA	12:A:3785:HOH:O	1.68	0.93
1:A:126[B]:PRO:HB2	1:A:175[B]:GLU:HG2	1.50	0.93
12:A:3768:HOH:O	1:D:545[A]:LEU:HD11	1.67	0.92
3:F:67[A]:ARG:HH11	3:F:67[A]:ARG:HG2	1.30	0.92
1:D:545[B]:LEU:CD1	12:D:1687:HOH:O	2.22	0.86
2:B:322[B]:ARG:NH2	3:C:67[B]:ARG:CG	2.39	0.85
2:E:27:LEU:HD22	2:E:246[B]:MET:CE	2.09	0.83
1:A:240[B]:LYS:HE3	12:F:1132:HOH:O	1.78	0.82
1:D:24:THR:HG23	12:F:1497:HOH:O	1.82	0.79
1:A:120[B]:LEU:HD21	1:A:241[B]:GLN:NE2	1.97	0.78
2:B:37[B]:SER:HB3	2:B:424[B]:GLU:OE1	1.84	0.77
3:F:132[A]:LYS:HD2	12:F:1990[A]:HOH:O	1.83	0.76
2:E:27:LEU:HD22	2:E:246[B]:MET:HE1	1.65	0.76
2:E:27:LEU:CD2	2:E:246[B]:MET:HE1	2.16	0.76
1:A:120[B]:LEU:HD11	1:A:241[B]:GLN:OE1	1.89	0.73
1:D:357[A]:LYS:HE2	1:D:372[A]:ASP:OD2	1.89	0.73
1:A:352[A]:GLU:N	1:A:352[A]:GLU:OE1	2.21	0.72
2:E:27:LEU:HD22	2:E:246[B]:MET:SD	2.29	0.72
1:D:42[A]:ASN:ND2	12:D:1802:HOH:O	2.24	0.71
2:B:322[B]:ARG:CZ	3:C:67[B]:ARG:HG3	2.21	0.70
1:A:169[A]:ASN:HD22	1:A:172:ILE:HD13	1.56	0.70
1:A:351:LYS:HD3	1:A:352[A]:GLU:OE1	1.91	0.70
1:A:126[B]:PRO:HB3	1:A:175[B]:GLU:HG2	1.71	0.69
3:F:67[A]:ARG:HH11	3:F:67[A]:ARG:CG	2.03	0.69
2:E:27:LEU:CD2	2:E:246[B]:MET:CE	2.72	0.67
3:C:45:PRO:HB3	12:C:3636:HOH:O	1.94	0.67
1:A:113[B]:HIS:HE1	12:A:731:HOH:O	1.80	0.65
3:F:132[A]:LYS:HE2	12:F:1692:HOH:O	1.96	0.65
2:B:3[A]:LYS:HE2	2:B:234:GLU:OE1	1.96	0.64
1:A:351:LYS:CD	1:A:352[A]:GLU:OE1	2.45	0.64
1:A:60:ILE:HD12	12:D:3878:HOH:O	1.97	0.64
2:B:118[B]:SER:HB3	12:B:1533:HOH:O	1.97	0.64
1:D:330:PHE:CE2	6:D:553[A]:TP7:H71C	2.33	0.64
1:D:268:PRO:HB3	12:E:1668:HOH:O	1.97	0.63
2:E:21:GLN:NE2	12:E:4171:HOH:O	2.32	0.63
1:A:169[A]:ASN:CG	1:A:172:ILE:HD13	2.18	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:545[B]:LEU:HD12	12:D:1687:HOH:O	1.88	0.62
1:D:330:PHE:CD2	1:D:482[A]:VAL:HG11	2.35	0.62
1:A:240[B]:LYS:HA	12:F:1186:HOH:O	1.99	0.61
2:B:188:PRO:HD3	12:E:1304:HOH:O	2.01	0.61
1:D:172[A]:ILE:HD13	12:D:4136:HOH:O	2.00	0.61
1:D:45[B]:LYS:HE3	12:D:1271:HOH:O	2.00	0.60
2:E:61[A]:LYS:HE3	12:E:2470:HOH:O	2.02	0.60
1:A:111[B]:HIS:O	1:A:115[B]:VAL:HG23	2.02	0.60
3:C:45:PRO:HD3	12:C:3778:HOH:O	2.02	0.60
3:C:179:LYS:HG3	12:C:4195:HOH:O	2.01	0.59
2:B:322[B]:ARG:HH21	3:C:67[B]:ARG:HG3	1.64	0.59
2:E:118[B]:SER:HB3	12:E:2658:HOH:O	2.03	0.59
1:D:172[A]:ILE:CD1	12:D:4136:HOH:O	2.51	0.58
2:E:322[A]:ARG:CZ	3:F:67[A]:ARG:HD2	2.33	0.58
2:E:95:VAL:HG21	2:E:119[B]:ALA:HB3	1.85	0.58
1:D:194[B]:GLU:HG2	12:D:3701:HOH:O	2.03	0.58
3:C:10:LYS:HE3	12:C:3969:HOH:O	2.05	0.57
1:A:126[B]:PRO:CB	1:A:175[B]:GLU:CG	2.77	0.57
2:E:261[B]:LYS:HG2	12:F:3664:HOH:O	2.05	0.56
1:A:119[B]:ARG:NH1	1:A:250:ASP:OD2	2.38	0.56
2:B:405[A]:MET:HG3	1:D:115:VAL:HG22	1.88	0.56
1:A:120[B]:LEU:CD2	1:A:241[B]:GLN:NE2	2.67	0.56
1:A:122[B]:LYS:O	1:A:123[B]:GLU:HB2	2.06	0.55
2:E:344[A]:LEU:HB3	2:E:345:PRO:HD2	1.89	0.55
1:A:194[B]:GLU:HG2	12:A:2095:HOH:O	2.07	0.55
1:A:330:PHE:CE2	6:A:553[A]:TP7:H71C	2.43	0.54
1:D:330:PHE:CD2	1:D:482[A]:VAL:CG1	2.91	0.54
1:A:172:ILE:O	1:A:173[A]:ALA:C	2.44	0.54
3:F:67[A]:ARG:NH1	3:F:67[A]:ARG:HG2	2.11	0.54
3:C:61:GLU:HB2	3:C:67[A]:ARG:NH2	2.23	0.54
2:B:424[A]:GLU:HG3	12:B:3930:HOH:O	2.08	0.54
1:A:242[B]:ALA:HB2	3:F:84:TYR:CE1	2.43	0.53
1:A:120[B]:LEU:CD1	1:A:241[B]:GLN:OE1	2.55	0.53
2:E:299:LEU:CD2	12:E:2973:HOH:O	2.57	0.53
1:D:387[A]:GLU:HB2	12:D:3567[A]:HOH:O	2.09	0.53
2:E:61[B]:LYS:CE	12:E:2444:HOH:O	2.57	0.52
2:E:246[B]:MET:HE1	2:E:432:VAL:HG12	1.92	0.51
1:D:172[A]:ILE:HD12	12:D:2242:HOH:O	2.10	0.51
1:A:328:VAL:HB	5:D:552:F43:H9A1	1.91	0.51
1:A:125[B]:THR:HB	1:A:126[B]:PRO:CD	2.41	0.51
2:E:372[B]:PRO:HG2	2:E:397:MET:SD	2.50	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:67[A]:ARG:NH1	3:F:67[A]:ARG:CG	2.67	0.51
1:A:248:THR:HG22	2:E:365[B]:SER:O	2.10	0.51
1:A:352[A]:GLU:OE1	1:A:352[A]:GLU:CA	2.59	0.50
2:B:42[A]:ILE:HG13	2:B:425:PHE:CE1	2.47	0.50
2:B:322[B]:ARG:HH21	3:C:67[B]:ARG:CG	2.18	0.50
1:A:125[B]:THR:HB	1:A:126[B]:PRO:HD2	1.92	0.50
1:A:481:ASN:HA	6:A:553[A]:TP7:S7	2.51	0.50
12:E:3631[A]:HOH:O	3:F:72:PRO:HG3	2.11	0.50
1:A:122[B]:LYS:HE2	1:A:239[B]:TYR:O	2.11	0.50
1:A:178[A]:PRO:HD3	12:A:1631:HOH:O	2.11	0.50
2:B:58:LYS:HE2	12:B:3633:HOH:O	2.11	0.50
3:F:247:ASN:C	3:F:247:ASN:HD22	2.14	0.50
1:A:387[B]:GLU:HG3	12:A:1069:HOH:O	2.11	0.49
1:D:154:HIS:NE2	1:D:545[A]:LEU:HD21	2.28	0.49
2:B:439:ILE:HD12	2:B:443:ILE:HD11	1.94	0.49
3:C:132:LYS:HD2	12:C:4201:HOH:O	2.11	0.49
12:B:3948[A]:HOH:O	3:C:67[A]:ARG:HD3	2.13	0.49
1:A:113[B]:HIS:CE1	12:A:731:HOH:O	2.61	0.49
1:A:330:PHE:CZ	6:A:553[A]:TP7:H71C	2.48	0.49
1:D:154:HIS:CE1	1:D:545[A]:LEU:HD21	2.48	0.48
5:A:1:F43:H9A1	1:D:328:VAL:HB	1.96	0.48
1:A:169[A]:ASN:HD21	1:A:172:ILE:CD1	2.20	0.48
2:E:370[B]:GLY:HA3	2:E:374:ILE:HG12	1.95	0.48
12:E:862:HOH:O	3:F:59:MET:CE	2.61	0.48
3:C:153:LYS:NZ	8:C:1:ACT:H2	2.29	0.47
1:A:242[A]:ALA:HB2	3:F:84:TYR:CE1	2.50	0.47
2:E:424[B]:GLU:HG3	12:E:3642:HOH:O	2.13	0.47
1:D:330:PHE:CE2	1:D:482[A]:VAL:CG1	2.98	0.47
1:A:229:MET:SD	2:E:367[B]:TYR:CE1	3.08	0.46
2:B:95:VAL:HG21	2:B:119[B]:ALA:HB3	1.95	0.46
2:B:401:ALA:O	3:C:59:MET:CE	2.64	0.46
3:C:61:GLU:H	3:C:61:GLU:HG2	1.39	0.46
3:C:84:TYR:CE1	1:D:242:ALA:HB2	2.50	0.46
12:B:2205:HOH:O	2:E:188:PRO:HD3	2.15	0.46
1:D:191:ASP:HB2	12:D:3703:HOH:O	2.14	0.46
1:A:172:ILE:HD12	1:A:172:ILE:N	2.31	0.46
1:A:73:GLN:HB2	1:A:80:TYR:CE2	2.51	0.46
3:C:62:PRO:HD2	12:C:3269:HOH:O	2.15	0.46
2:B:236[C]:MET:HB2	2:B:236[C]:MET:HE2	1.63	0.45
12:E:862:HOH:O	3:F:59:MET:HE2	2.17	0.45
1:A:126[B]:PRO:HB2	1:A:175[B]:GLU:CG	2.35	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120[B]:LEU:CD2	1:A:241[B]:GLN:CD	2.85	0.45
2:B:401:ALA:O	3:C:59:MET:HE1	2.17	0.45
1:A:242[B]:ALA:HB3	1:A:245:GLU:OE2	2.16	0.44
2:E:374:ILE:C	2:E:374:ILE:HD12	2.38	0.44
2:E:58[A]:LYS:HE3	2:E:58[A]:LYS:HB2	1.42	0.44
2:E:283:LYS:HG3	12:E:4160:HOH:O	2.18	0.43
2:B:246[A]:MET:CE	2:B:429:LEU:HD12	2.47	0.43
2:E:299:LEU:HD23	12:E:2973:HOH:O	2.17	0.43
2:E:299:LEU:HD22	12:E:2973:HOH:O	2.18	0.43
1:A:114[A]:ALA:O	1:A:118[A]:LYS:HD3	2.18	0.43
3:C:153:LYS:HZ1	8:C:1:ACT:CH3	2.32	0.43
1:A:135:THR:HG21	1:A:237[B]:SER:OG	2.19	0.43
3:F:228:VAL:HG22	12:F:4180:HOH:O	2.19	0.43
1:A:120[B]:LEU:HD21	1:A:241[B]:GLN:CD	2.39	0.43
3:F:132[A]:LYS:CE	12:F:1692:HOH:O	2.63	0.43
3:F:207[A]:GLU:HG3	12:F:3759[A]:HOH:O	2.18	0.43
1:A:357:LYS:NZ	1:A:372[B]:ASP:OD1	2.46	0.43
2:B:29:PRO:O	2:E:123[B]:VAL:HG11	2.18	0.42
1:A:351:LYS:HD2	1:A:352[A]:GLU:OE1	2.17	0.42
2:B:214:LEU:HB2	2:B:428:PRO:HG3	2.01	0.42
1:A:126[B]:PRO:HG2	1:A:175[B]:GLU:CD	2.39	0.42
2:E:283:LYS:HG2	12:E:4240:HOH:O	2.19	0.42
2:E:122[B]:ASP:HB2	12:E:1158:HOH:O	2.19	0.42
12:B:769:HOH:O	2:E:183:GLN:HG2	2.20	0.42
1:A:330:PHE:CD2	1:A:482[A]:VAL:HG11	2.55	0.42
2:E:61[B]:LYS:HE2	12:E:2444:HOH:O	2.19	0.42
2:E:362:PHE:O	2:E:369[A]:GLY:HA3	2.19	0.42
2:E:61[A]:LYS:CE	12:E:2470:HOH:O	2.65	0.42
3:C:56:LEU:O	3:C:59:MET:HB2	2.19	0.41
2:E:362:PHE:CE1	2:E:367[B]:TYR:HB3	2.55	0.41
1:D:114:ALA:HA	1:D:118[A]:LYS:HE3	2.03	0.41
1:D:183:ASP:OD2	1:D:186[B]:LYS:HG3	2.20	0.41
2:E:61[B]:LYS:HE3	12:E:2370:HOH:O	2.21	0.41
1:A:128[B]:THR:O	1:A:129[B]:ILE:C	2.57	0.41
2:B:199:HIS:CE1	2:B:415[B]:ILE:HD12	2.56	0.41
1:D:330:PHE:HE2	6:D:553[A]:TP7:H71C	1.84	0.41
1:A:132:TYR:HA	1:A:238[B]:ALA:CB	2.51	0.41
2:B:299:LEU:HD22	12:B:2183:HOH:O	2.19	0.41
1:A:544:ALA:HB2	12:D:3604[A]:HOH:O	2.21	0.41
1:D:332:GLN:HA	1:D:335:THR:OG1	2.21	0.41
1:D:46[B]:GLU:HG3	12:D:696:HOH:O	2.20	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ILE:HB	1:A:261:ILE:HB	2.03	0.40
1:D:117:GLU:HB2	1:D:118[A]:LYS:HE3	2.02	0.40
1:A:116[B]:ILE:HG23	1:A:122[B]:LYS:HB2	2.03	0.40
2:B:123[B]:VAL:HG12	2:E:36[B]:LYS:HA	2.02	0.40
2:B:67:CYS:HB3	1:D:505:PHE:CE1	2.56	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	595/549 (108%)	570 (96%)	24 (4%)	1 (0%)	47	22
1	D	571/549 (104%)	548 (96%)	22 (4%)	1 (0%)	47	22
2	B	469/442 (106%)	462 (98%)	7 (2%)	0	100	100
2	E	482/442 (109%)	473 (98%)	9 (2%)	0	100	100
3	C	256/248 (103%)	249 (97%)	7 (3%)	0	100	100
3	F	260/248 (105%)	255 (98%)	5 (2%)	0	100	100
All	All	2633/2478 (106%)	2557 (97%)	74 (3%)	2 (0%)	51	24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	325	SER
1	D	325	SER

### 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	481/434 (111%)	468 (97%)	13 (3%)	44	12
1	D	463/434 (107%)	456 (98%)	7 (2%)	65	35
2	B	369/341 (108%)	364 (99%)	5 (1%)	67	37
2	E	378/341 (111%)	372 (98%)	6 (2%)	62	31
3	C	226/216 (105%)	223 (99%)	3 (1%)	69	40
3	F	230/216 (106%)	219 (95%)	11 (5%)	25	2
All	All	2147/1982 (108%)	2102 (98%)	45 (2%)	62	19

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12[A]	LYS
1	A	12[B]	LYS
1	A	17[A]	SER
1	A	17[B]	SER
1	A	118[A]	LYS
1	A	118[B]	LYS
1	A	126[A]	PRO
1	A	126[B]	PRO
1	A	352[A]	GLU
1	A	352[B]	GLU
1	A	444	TYR
1	A	450	ASP
1	A	543	ARG
2	B	3[A]	LYS
2	B	3[B]	LYS
2	B	97	GLU
2	B	261[A]	LYS
2	B	261[B]	LYS
3	C	59	MET
3	C	61	GLU
3	C	121	GLN
1	D	118[A]	LYS
1	D	118[B]	LYS
1	D	352[A]	GLU
1	D	352[B]	GLU
1	D	444	TYR

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	D	450	ASP
1	D	543	ARG
2	E	58[A]	LYS
2	E	58[B]	LYS
2	E	98	ASP
2	E	126	GLU
2	E	185	LEU
2	E	440	LYS
3	F	57[A]	GLU
3	F	57[B]	GLU
3	F	61	GLU
3	F	67[A]	ARG
3	F	67[B]	ARG
3	F	121	GLN
3	F	148[A]	SER
3	F	148[B]	SER
3	F	207[A]	GLU
3	F	207[B]	GLU
3	F	247	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
3	C	121	GLN
1	D	241	GLN
3	F	121	GLN
3	F	247	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues 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
1	MHS	A	257	1	7,11,12	1.81	3 (42%)	6,14,16	4.07	3 (50%)
1	SMC	A	452	1	5,6,7	1.32	0	2,6,8	2.08	1 (50%)
1	GL3	A	445	1	2,3,4	2.54	1 (50%)	1,2,4	0.26	0
1	GL3	D	445	1	2,3,4	2.66	1 (50%)	1,2,4	0.09	0
1	AGM	D	271	1	10,11,12	1.66	2 (20%)	6,13,15	1.51	1 (16%)
1	MHS	D	257	1	7,11,12	1.82	2 (28%)	6,14,16	2.77	2 (33%)
1	MGN	A	400	1	6,9,10	1.74	3 (50%)	5,12,14	1.12	0
1	AGM	A	271	1	10,11,12	1.37	1 (10%)	6,13,15	1.43	1 (16%)
1	MGN	D	400	1	6,9,10	1.73	1 (16%)	5,12,14	0.66	0
1	SMC	D	452	1	5,6,7	1.51	1 (20%)	2,6,8	2.64	1 (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
1	MHS	A	257	1	-	0/5/6/8	0/1/1/1
1	SMC	A	452	1	-	1/3/5/7	-
1	GL3	A	445	1	-	0/1/1/2	-
1	GL3	D	445	1	-	0/1/1/2	-
1	AGM	D	271	1	-	2/10/11/13	-
1	MHS	D	257	1	-	0/5/6/8	0/1/1/1
1	MGN	A	400	1	-	0/7/9/12	-
1	AGM	A	271	1	-	2/10/11/13	-
1	MGN	D	400	1	-	0/7/9/12	-
1	SMC	D	452	1	-	1/3/5/7	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	445	GL3	C-S	-3.73	1.67	1.80
1	D	271	AGM	CB-CA	3.67	1.58	1.53
1	A	445	GL3	C-S	-3.59	1.68	1.80
1	D	400	MGN	O-C	3.45	1.31	1.19
1	D	257	MHS	CD2-NE2	3.18	1.45	1.35

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	MHS	CE1-NE2	3.05	1.41	1.34
1	D	452	SMC	CB-SG	2.89	1.84	1.80
1	D	257	MHS	CE1-NE2	2.71	1.40	1.34
1	A	400	MGN	CB1-CA	2.68	1.58	1.55
1	D	271	AGM	CG-CB	2.48	1.60	1.53
1	A	257	MHS	CM-ND1	2.46	1.53	1.47
1	A	271	AGM	CB-CA	2.39	1.56	1.53
1	A	257	MHS	O-C	2.28	1.29	1.19
1	A	400	MGN	CB1-CG	2.25	1.58	1.53
1	A	400	MGN	O-C	2.24	1.27	1.19

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	MHS	NE2-CE1-ND1	-8.46	99.69	112.26
1	D	257	MHS	NE2-CE1-ND1	-5.56	104.00	112.26
1	A	257	MHS	CD2-NE2-CE1	3.96	111.96	105.78
1	D	452	SMC	CA-CB-SG	-3.72	108.03	114.04
1	A	452	SMC	CA-CB-SG	-2.91	109.34	114.04
1	D	257	MHS	CM-ND1-CG	2.76	128.11	124.44
1	A	257	MHS	CM-ND1-CG	2.58	127.87	124.44
1	A	271	AGM	NE1-CZ-NH2	-2.52	116.19	120.59
1	D	271	AGM	CG-CD-NE1	-2.36	106.33	110.49

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	452	SMC	CA-CB-SG-CS
1	D	452	SMC	CA-CB-SG-CS
1	D	271	AGM	CE2-CD-NE1-CZ
1	A	271	AGM	CE2-CD-NE1-CZ
1	D	271	AGM	NE1-CD-CG-CB
1	A	271	AGM	NE1-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 10 are monoatomic - leaving 15 for Mogul analysis.

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
5	F43	A	1	1,7	46,71,71	3.04	11 (23%)	48,118,118	1.63	10 (20%)
11	EDO	F	252	-	3,3,3	0.59	0	2,2,2	0.61	0
9	PEG	A	557	-	6,6,6	0.44	0	5,5,5	0.71	0
7	COM	D	554	5	6,6,6	0.67	0	7,8,8	0.64	0
7	COM	A	554	5	6,6,6	1.62	2 (33%)	7,8,8	0.82	0
8	ACT	B	446[B]	-	1,3,3	0.02	0	0,3,3	0.00	-
6	TP7	A	553[A]	-	16,20,20	0.89	1 (6%)	18,26,26	1.15	1 (5%)
11	EDO	F	251	-	3,3,3	0.59	0	2,2,2	0.70	0
6	TP7	D	553[A]	-	16,20,20	0.88	1 (6%)	18,26,26	1.40	3 (16%)
8	ACT	C	1	-	1,3,3	1.22	0	0,3,3	0.00	-
8	ACT	A	555[B]	-	1,3,3	1.24	0	0,3,3	0.00	-
11	EDO	D	555	-	3,3,3	0.44	0	2,2,2	0.34	0
9	PEG	C	251	-	6,6,6	0.47	0	5,5,5	0.68	0
8	ACT	A	556[B]	-	1,3,3	0.32	0	0,3,3	0.00	-
5	F43	D	552	1,7	46,71,71	2.87	16 (34%)	48,118,118	1.68	15 (31%)

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
5	F43	A	1	1,7	-	1/18/185/185	-
11	EDO	F	252	-	-	1/1/1/1	-
9	PEG	A	557	-	-	3/4/4/4	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	COM	D	554	5	-	0/4/4/4	-
6	TP7	A	553[A]	-	-	0/20/24/24	-
7	COM	A	554	5	-	0/4/4/4	-
11	EDO	F	251	-	-	1/1/1/1	-
6	TP7	D	553[A]	-	-	1/20/24/24	-
11	EDO	D	555	-	-	1/1/1/1	-
9	PEG	C	251	-	-	2/4/4/4	-
5	F43	D	552	1,7	-	1/18/185/185	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1	F43	NI-NA	10.40	2.11	1.89
5	A	1	F43	NI-NB	10.39	2.11	1.89
5	D	552	F43	NI-NB	9.71	2.10	1.89
5	D	552	F43	NI-NA	8.73	2.08	1.89
5	A	1	F43	NI-ND	8.04	2.06	1.89
5	D	552	F43	NI-ND	7.20	2.05	1.89
5	A	1	F43	CHB-C1B	6.40	1.57	1.53
5	D	552	F43	CHB-C1B	5.44	1.57	1.53
5	A	1	F43	CHA-C4D	5.07	1.58	1.53
5	D	552	F43	C3C-C4C	4.31	1.57	1.50
5	D	552	F43	C4A-NA	3.49	1.54	1.49
5	A	1	F43	CHC-C4B	3.42	1.48	1.39
5	A	1	F43	C3C-C4C	3.26	1.55	1.50
5	A	1	F43	C6B-N5B	3.11	1.39	1.34
6	D	553[A]	TP7	P-O4P	2.92	1.64	1.59
5	D	552	F43	CAA-C3A	2.88	1.58	1.53
7	A	554	COM	C2-S2	-2.85	1.73	1.77
5	D	552	F43	CHC-C4B	2.79	1.47	1.39
5	D	552	F43	CHA-C4D	2.76	1.55	1.53
5	A	1	F43	C4C-NC	2.69	1.39	1.35
5	D	552	F43	C5C-C2C	2.62	1.58	1.54
5	D	552	F43	CHD-C1D	2.56	1.47	1.43
5	D	552	F43	C1C-NC	2.40	1.42	1.37
5	D	552	F43	C3A-C4A	2.37	1.57	1.53
6	A	553[A]	TP7	P-O3P	-2.32	1.45	1.54
5	D	552	F43	C8C-C3C	2.31	1.58	1.54
5	A	1	F43	C4A-NA	2.15	1.52	1.49
5	D	552	F43	C9B-C2B	2.14	1.58	1.54
5	D	552	F43	CAB-C3B	2.07	1.59	1.54
5	A	1	F43	C8B-C6B	2.05	1.54	1.50

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	554	COM	C1-S1	2.01	1.87	1.80

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1	F43	O8D-C7D-C6D	-3.58	114.99	120.86
5	D	552	F43	O8D-C7D-C6D	-3.53	115.07	120.86
5	A	1	F43	C5D-C2D-C1D	3.31	114.91	110.45
5	D	552	F43	C2B-C1B-NB	3.27	106.73	101.84
5	D	552	F43	C6D-C7D-CHD	3.21	122.98	116.95
5	D	552	F43	C1D-CHD-C4C	-3.07	116.60	125.31
6	A	553[A]	TP7	CB-CA-N	2.96	117.99	111.38
5	A	1	F43	C3D-C4D-ND	2.95	106.93	102.34
5	A	1	F43	CAB-C3B-C2B	-2.89	112.97	119.09
5	D	552	F43	CAB-C3B-C2B	-2.76	113.25	119.09
5	D	552	F43	C5D-C2D-C1D	2.67	114.04	110.45
6	D	553[A]	TP7	O1-C1-N	2.64	127.41	122.95
5	D	552	F43	C9A-C2A-C3A	2.62	116.86	112.98
6	D	553[A]	TP7	C5-C6-C7	2.60	117.71	113.09
5	D	552	F43	CAB-CBB-CCB	-2.56	108.08	113.59
5	A	1	F43	C2B-C3B-C4B	-2.49	98.81	101.63
5	D	552	F43	C4B-CHC-C1C	2.48	129.90	125.84
5	A	1	F43	C1B-C2B-C3B	2.34	104.97	101.51
5	D	552	F43	C3C-C4C-NC	2.32	113.64	110.05
5	D	552	F43	C4A-NA-C1A	-2.32	106.16	108.97
5	A	1	F43	C9A-C2A-C1A	2.28	113.49	107.65
5	D	552	F43	C2D-C1D-CHD	-2.22	119.00	121.85
5	A	1	F43	C4B-CHC-C1C	2.21	129.45	125.84
5	A	1	F43	C3B-C4B-CHC	-2.17	118.64	123.32
5	D	552	F43	C3D-C4D-ND	2.17	105.71	102.34
6	D	553[A]	TP7	O4P-P-O1P	-2.09	101.34	109.39
5	D	552	F43	C5C-C2C-C3C	-2.08	109.61	114.94
5	D	552	F43	C3D-C2D-C1D	-2.05	99.22	102.69
5	A	1	F43	CAD-C9D-C3D	-2.04	111.74	115.91

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1	F43	C3A-CAA-CBA-CCA
5	D	552	F43	C3A-CAA-CBA-CCA
9	A	557	PEG	O1-C1-C2-O2

Continued on next page...

*Continued from previous page...*

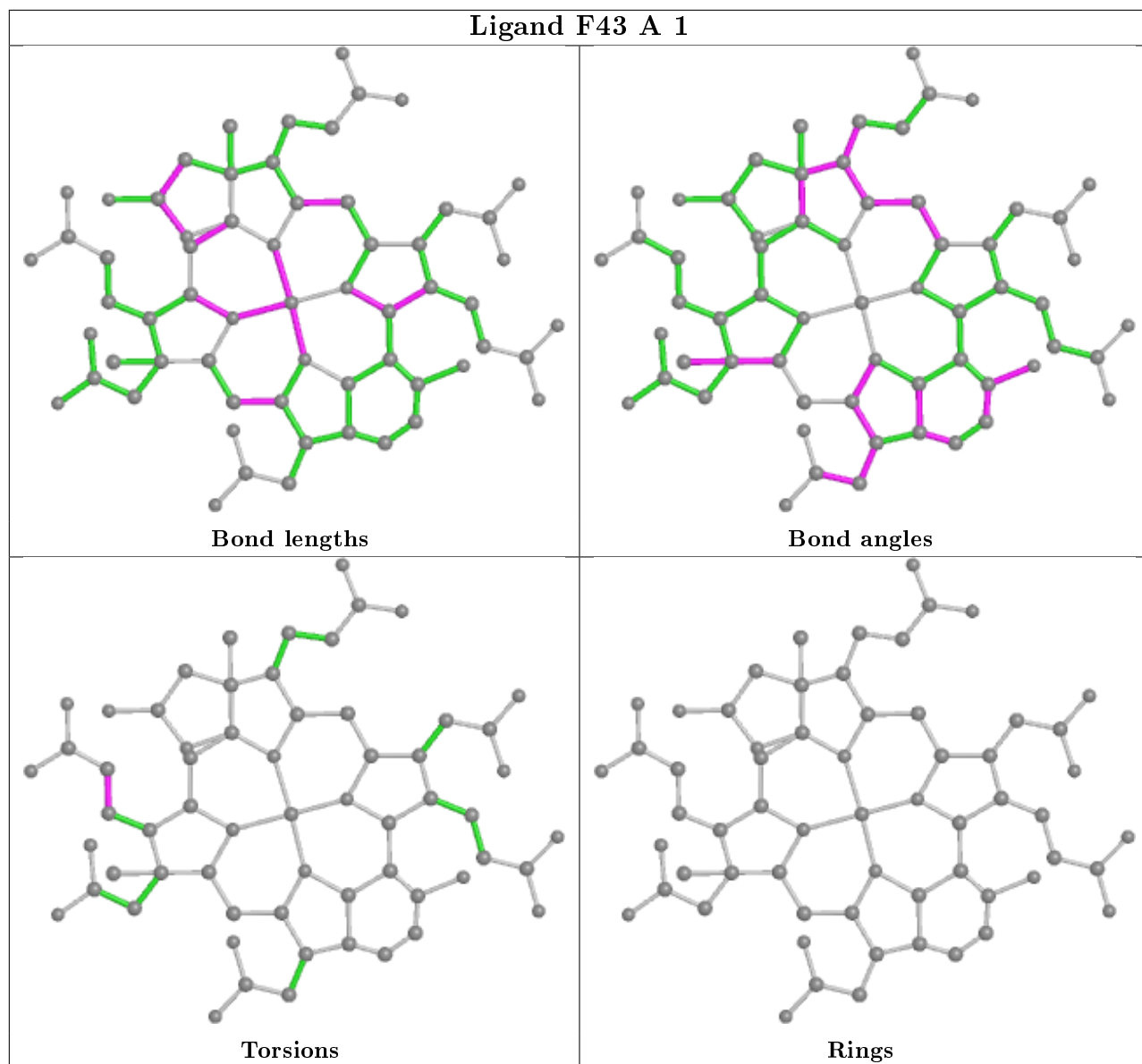
Mol	Chain	Res	Type	Atoms
9	C	251	PEG	O2-C3-C4-O4
9	A	557	PEG	O2-C3-C4-O4
9	C	251	PEG	O1-C1-C2-O2
11	F	252	EDO	O1-C1-C2-O2
11	F	251	EDO	O1-C1-C2-O2
6	D	553[A]	TP7	C1-C2-C3-C4
9	A	557	PEG	C1-C2-O2-C3
11	D	555	EDO	O1-C1-C2-O2

There are no ring outliers.

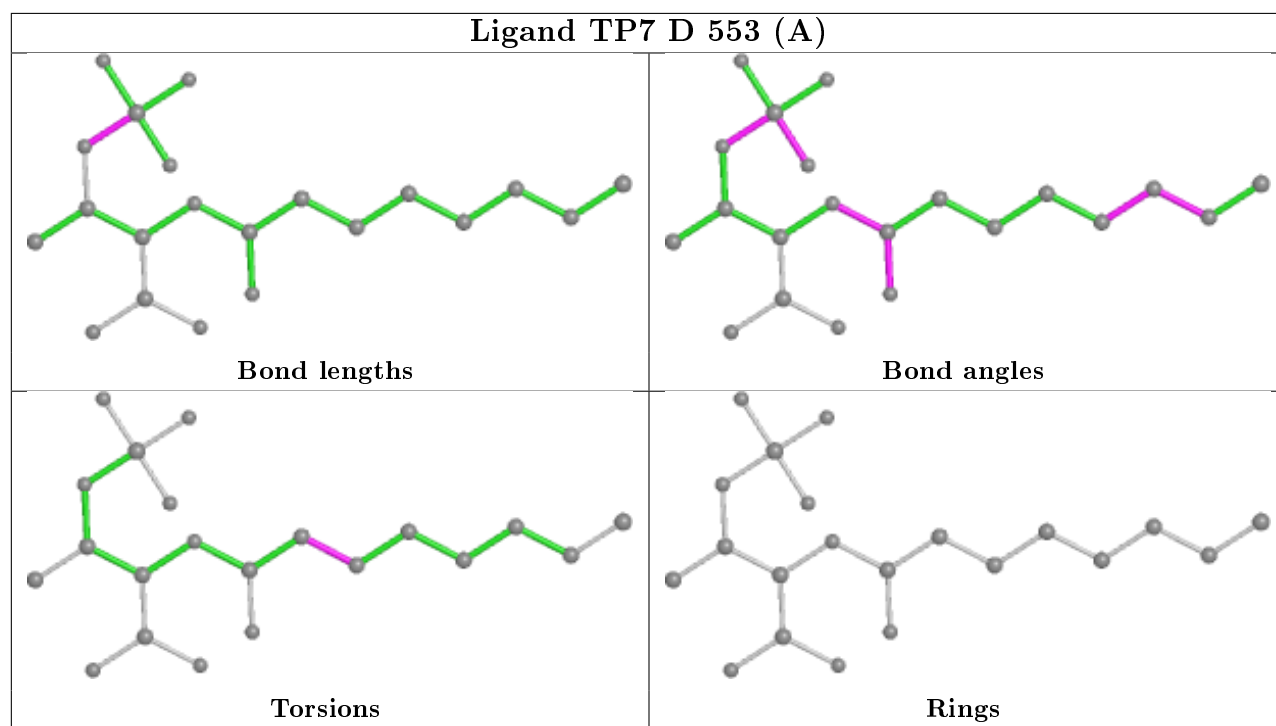
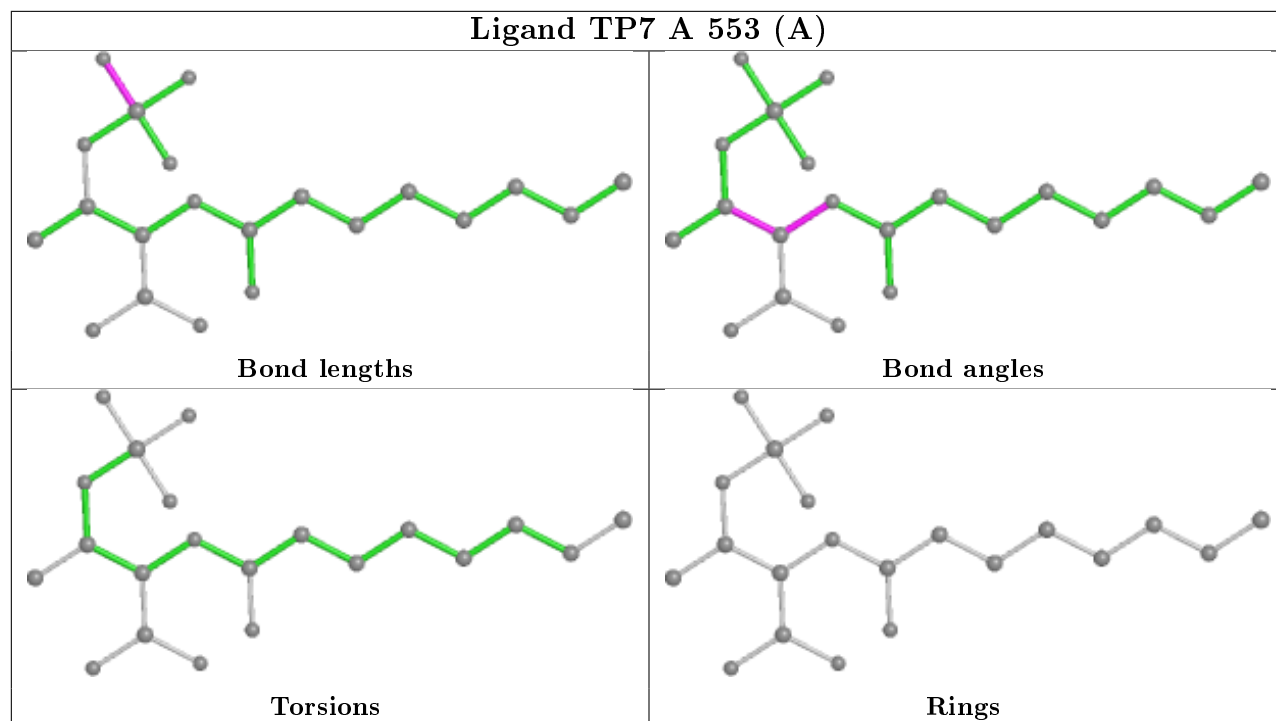
5 monomers are involved in 9 short contacts:

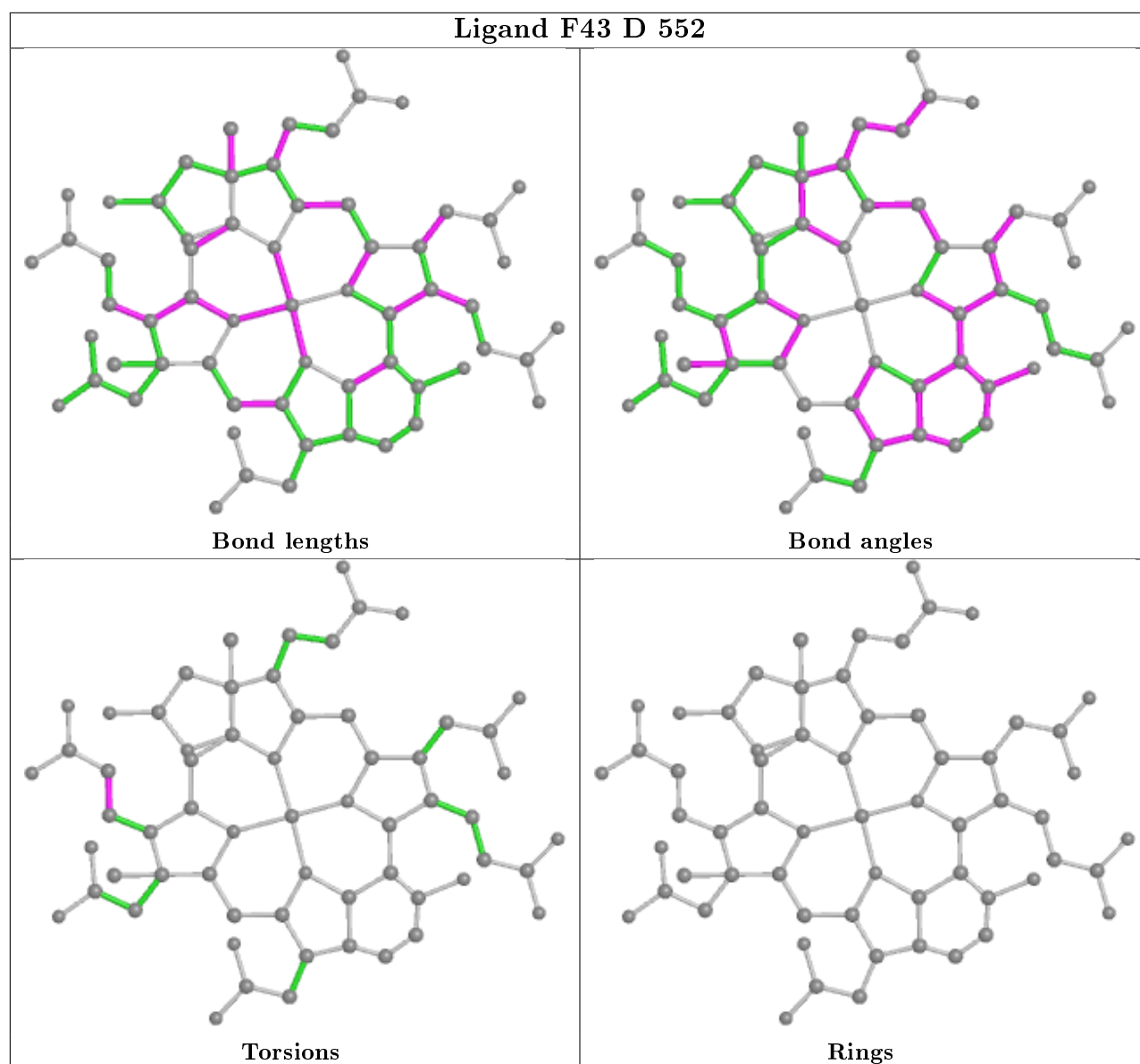
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1	F43	1	0
6	A	553[A]	TP7	3	0
6	D	553[A]	TP7	2	0
8	C	1	ACT	2	0
5	D	552	F43	1	0

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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	543/549 (98%)	-0.66	4 (0%) 87 89	5, 9, 19, 35	0
1	D	543/549 (98%)	-0.71	3 (0%) 89 91	6, 9, 19, 39	0
2	B	442/442 (100%)	-0.69	1 (0%) 95 95	6, 11, 20, 39	0
2	E	442/442 (100%)	-0.57	3 (0%) 87 89	7, 12, 23, 41	0
3	C	246/248 (99%)	-0.48	8 (3%) 46 48	7, 12, 28, 53	0
3	F	246/248 (99%)	-0.42	10 (4%) 37 40	7, 13, 32, 56	0
All	All	2462/2478 (99%)	-0.62	29 (1%) 79 80	5, 10, 21, 56	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	60	ASP	6.4
3	C	60	ASP	5.7
3	C	45	PRO	4.8
1	D	549	ALA	4.5
3	F	45	PRO	4.4
3	C	59	MET	3.9
3	F	62	PRO	3.7
3	F	57[A]	GLU	3.4
1	A	120[A]	LEU	3.3
2	E	98	ASP	3.3
3	C	62	PRO	3.3
3	F	46	GLY	3.1
2	B	98	ASP	3.0
1	D	2	ALA	2.9
3	C	57	GLU	2.8
2	E	441	ASN	2.7
3	C	180	ASP	2.6
2	E	297[A]	ASP	2.5
3	F	196	ASP	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	F	59	MET	2.4
3	F	180	ASP	2.4
3	C	61	GLU	2.3
1	A	122[A]	LYS	2.3
3	F	63	GLU	2.2
3	F	208	GLU	2.2
3	C	63	GLU	2.1
1	A	118[A]	LYS	2.1
1	D	24	THR	2.1
1	A	2	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	MHS	A	257	11/12	0.96	0.06	14,16,21,24	0
1	MHS	D	257	11/12	0.97	0.07	10,13,19,21	0
1	AGM	D	271	12/13	0.98	0.06	5,6,7,7	0
1	MGN	A	400	10/11	0.98	0.04	5,7,8,8	0
1	AGM	A	271	12/13	0.98	0.06	5,6,7,7	0
1	SMC	A	452	7/8	0.99	0.05	6,7,9,10	0
1	SMC	D	452	7/8	0.99	0.06	6,7,8,10	0
1	MGN	D	400	10/11	0.99	0.05	5,6,7,8	0
1	GL3	A	445	4/5	0.99	0.06	6,6,6,7	0
1	GL3	D	445	4/5	1.00	0.04	5,6,6,6	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

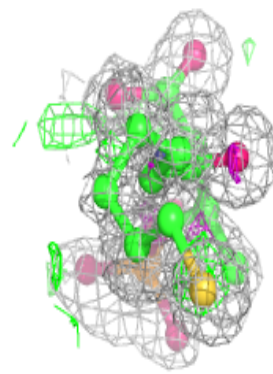
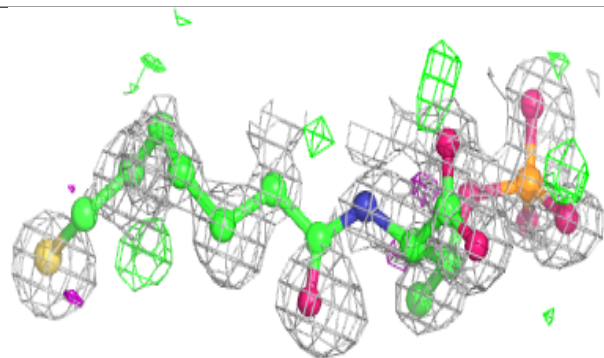
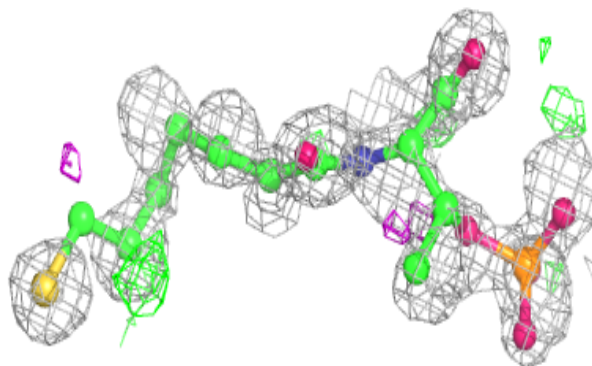
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
11	EDO	F	251	4/4	0.84	0.17	31,32,33,37	0
9	PEG	C	251	7/7	0.86	0.13	36,38,44,45	0
11	EDO	D	555	4/4	0.87	0.08	40,43,43,45	0
9	PEG	A	557	7/7	0.90	0.20	28,31,35,37	0
11	EDO	F	252	4/4	0.91	0.15	30,30,36,39	0
8	ACT	C	1	4/4	0.93	0.14	26,28,31,34	0
4	MG	B	444	1/1	0.95	0.16	26,26,26,26	0
8	ACT	A	556[B]	4/4	0.95	0.12	15,15,17,17	4
8	ACT	B	446[B]	4/4	0.95	0.09	13,14,14,16	4
4	MG	A	552[A]	1/1	0.96	0.15	13,13,13,13	1
8	ACT	A	555[B]	4/4	0.96	0.09	14,15,17,18	4
6	TP7	D	553[A]	21/21	0.97	0.09	4,6,8,18	21
4	MG	B	445	1/1	0.97	0.29	25,25,25,25	1
4	MG	F	250	1/1	0.98	0.09	14,14,14,14	0
6	TP7	A	553[A]	21/21	0.98	0.09	4,7,9,12	21
4	MG	C	250	1/1	0.98	0.08	16,16,16,16	0
4	MG	D	551	1/1	0.99	0.28	29,29,29,29	0
7	COM	A	554	7/7	0.99	0.04	6,7,8,9	0
4	MG	E	444	1/1	0.99	0.17	17,17,17,17	0
5	F43	A	1	62/62	0.99	0.05	4,6,8,12	0
4	MG	D	1	1/1	0.99	0.17	23,23,23,23	0
4	MG	A	551[B]	1/1	0.99	0.19	18,18,18,18	1
5	F43	D	552	62/62	0.99	0.05	4,6,8,12	0
7	COM	D	554	7/7	1.00	0.04	7,7,8,9	0
10	ZN	A	558	1/1	1.00	0.03	11,11,11,11	1

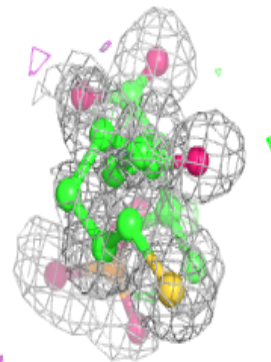
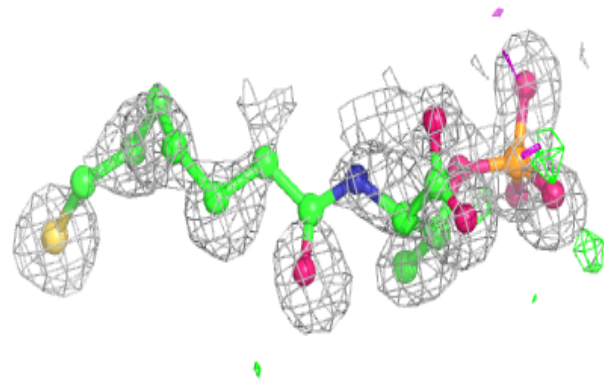
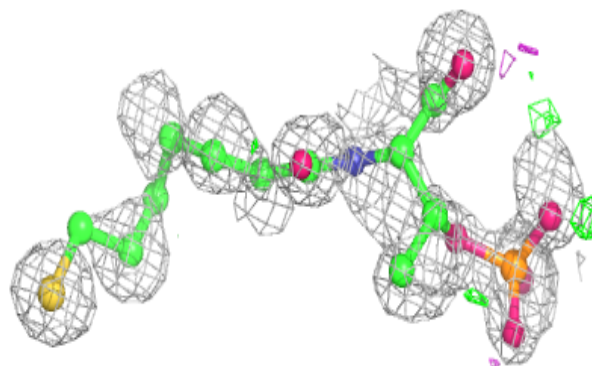
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around TP7 D 553 (A):**

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

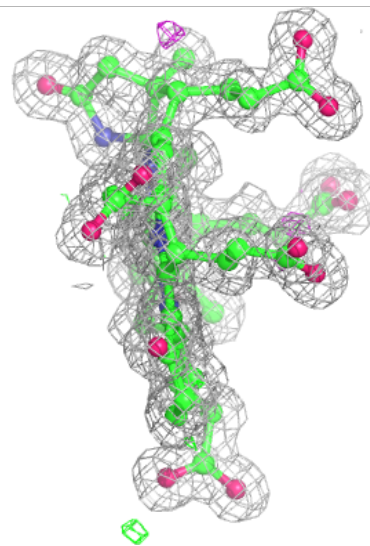
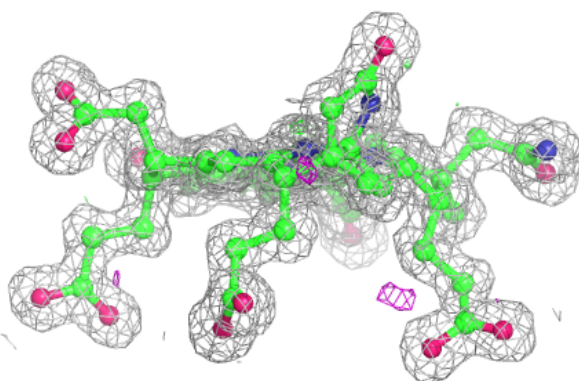
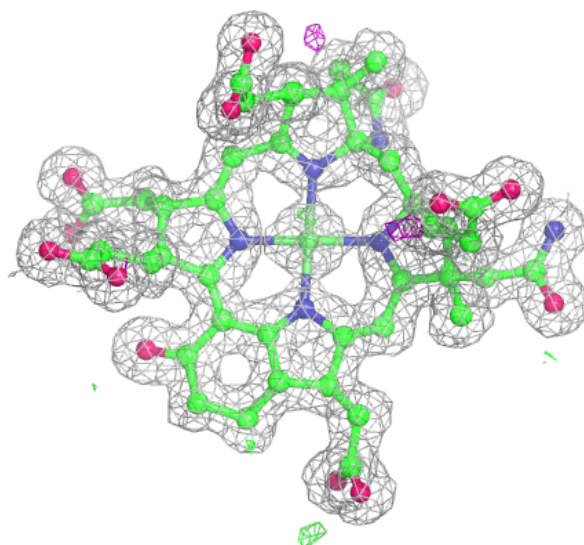
**Electron density around TP7 A 553 (A):**

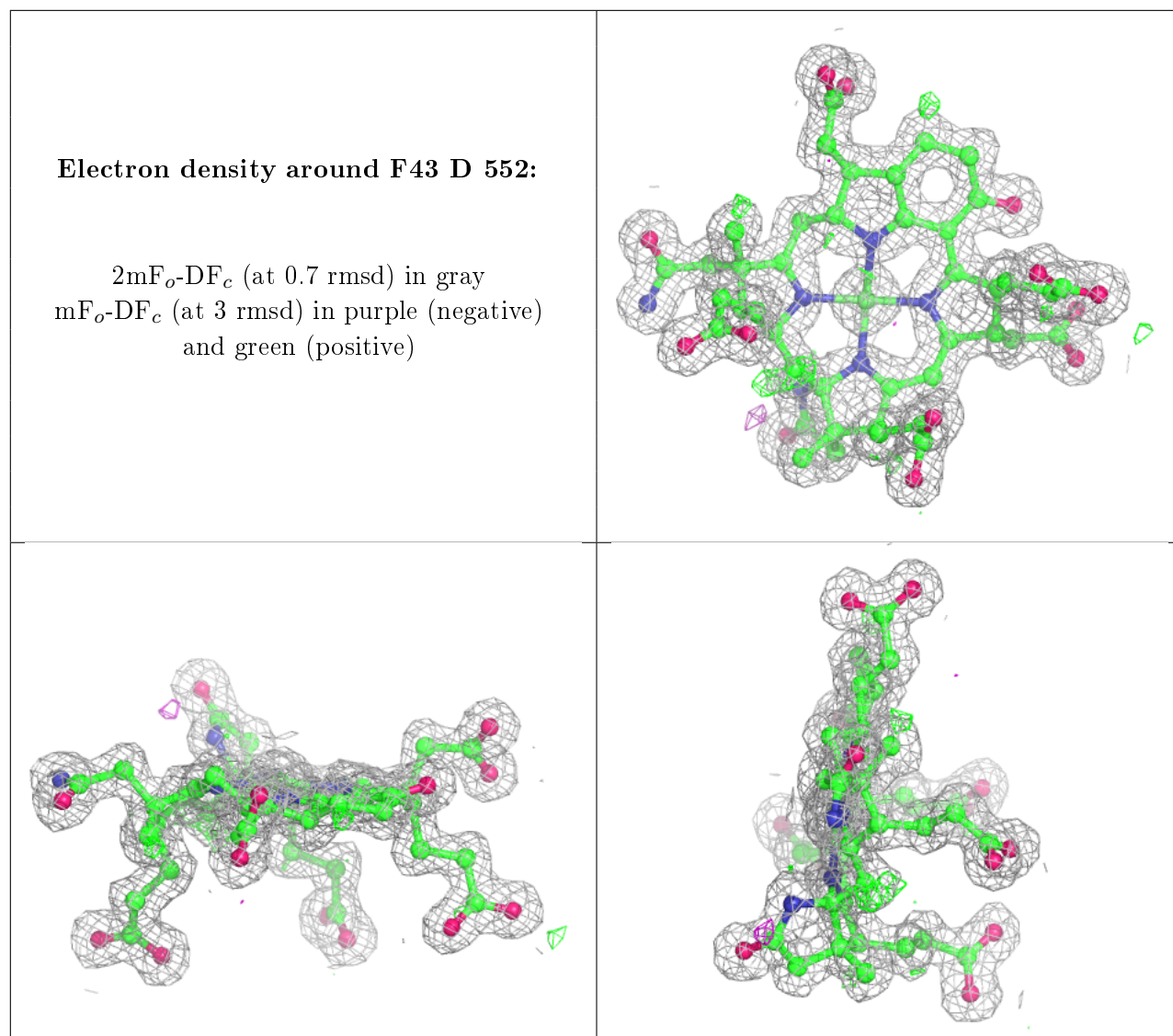
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around F43 A 1:**

$2mF_o-DF_c$  (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.