



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2026 – 11:18 AM UTC

PDB ID : 3M32 / pdb_00003m32
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 : 2010-03-08
Resolution : 1.35 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

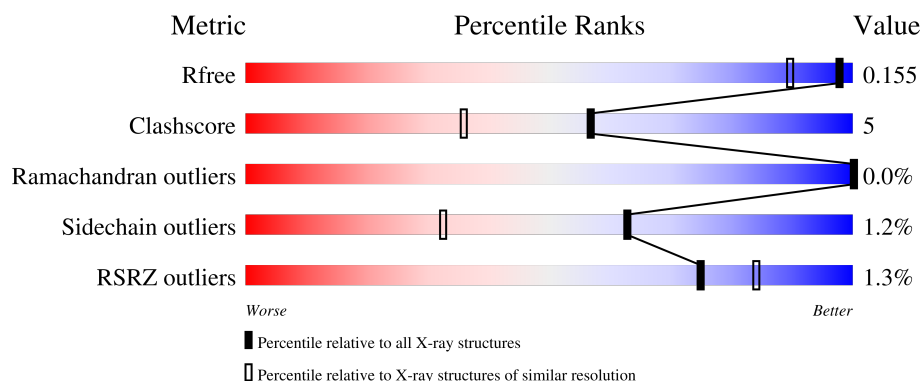
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

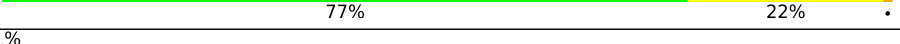
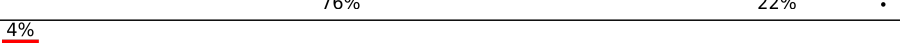
The reported resolution of this entry is 1.35 Å.

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	1216 (1.36-1.36)
Clashscore	190562	1232 (1.36-1.36)
Ramachandran outliers	187476	1220 (1.36-1.36)
Sidechain outliers	187428	1220 (1.36-1.36)
RSRZ outliers	180081	1214 (1.36-1.36)

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	549	
1	D	549	
2	B	442	
2	E	442	
3	C	248	

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Mol	Chain	Length	Quality of chain
3	F	248	3% 61% 36% ..

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 22665 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
1	A	548	Total	C	N	O	S	0	28	0
			4431	2801	735	874	21			
1	D	548	Total	C	N	O	S	0	22	0
			4380	2779	727	853	21			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	442	Total	C	N	O	S	0	24	0
			3462	2211	560	668	23			
2	E	442	Total	C	N	O	S	0	25	0
			3471	2216	564	668	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	247	Total	C	N	O	S	0	10	0
			2056	1276	360	407	13			
3	F	246	Total	C	N	O	S	0	20	0
			2113	1309	372	418	14			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

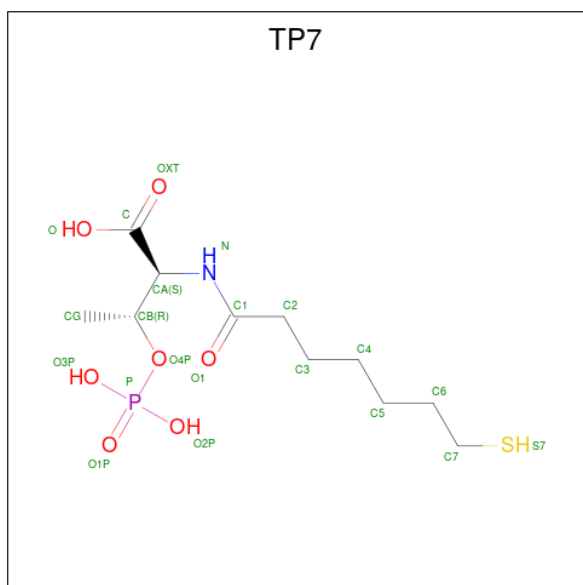
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	2
			2	2		
4	B	2	Total	Mg	0	1
			2	2		
4	C	1	Total	Mg	0	0
			1	1		
4	D	2	Total	Mg	0	0
			2	2		

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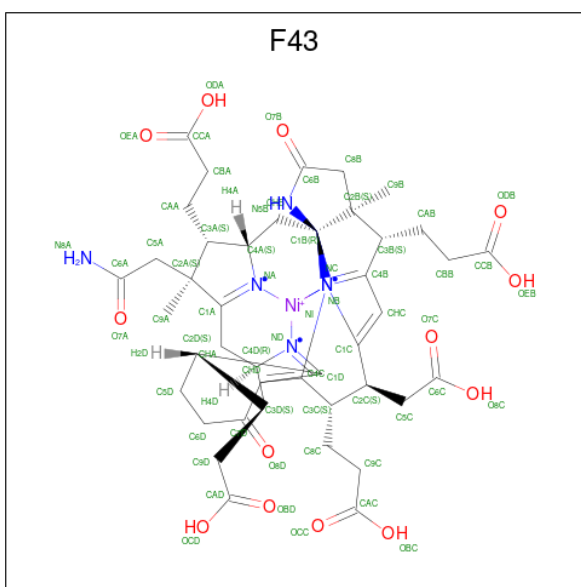
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		

- Molecule 5 is Coenzyme B (CCD ID: TP7) (formula: $C_{11}H_{22}NO_7PS$).



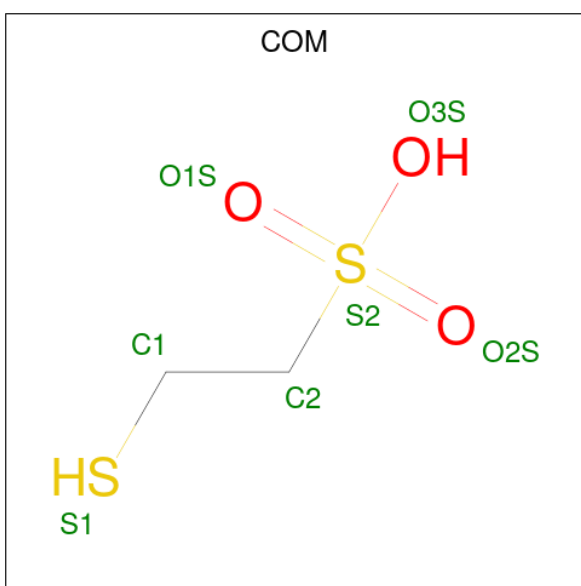
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total 21	C 11	N 1	O 7	P 1	S 1	0	1
5	D	1	Total 21	C 11	N 1	O 7	P 1	S 1	0	1

- Molecule 6 is FACTOR 430 (CCD ID: F43) (formula: $C_{42}H_{51}N_6NiO_{13}$).



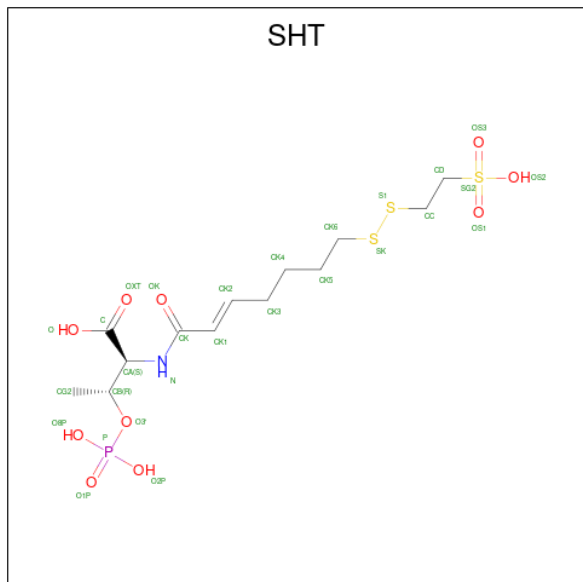
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 62	C 42	N 6	Ni 1	O 13	0	0
6	D	1	Total 62	C 42	N 6	Ni 1	O 13	0	0

- Molecule 7 is 1-THIOETHANESULFONIC ACID (CCD ID: COM) (formula: $\text{C}_2\text{H}_6\text{O}_3\text{S}_2$).



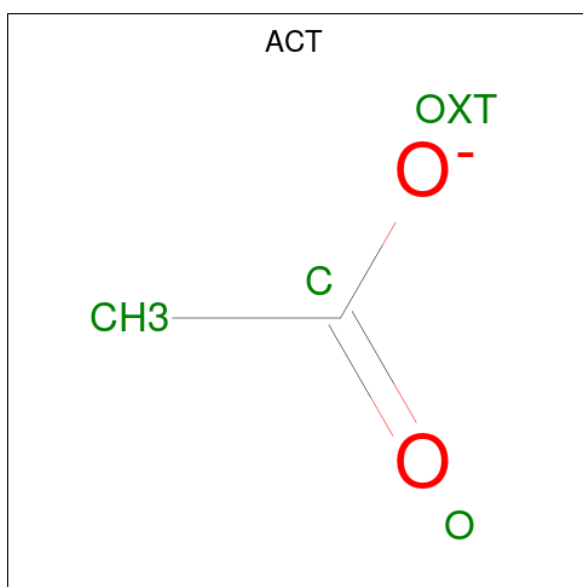
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total 7	C 2	O 3	S 2	0	1
7	D	1	Total 7	C 2	O 3	S 2	0	1

- Molecule 8 is O-PHOSPHONO-N-{(2E)-7-[(2-SULFOETHYL)DITHIO]HEPT-2-ENOYL}-L-THREONINE (CCD ID: SHT) (formula: $C_{13}H_{24}NO_{10}PS_3$).



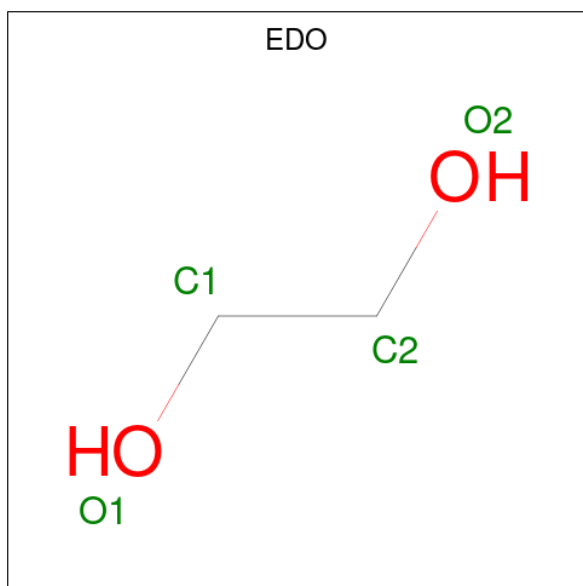
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	A	1	Total 28	C 13	N 1	O 10	P 1	S 3	0	1
8	D	1	Total 28	C 13	N 1	O 10	P 1	S 3	0	1

- Molecule 9 is ACETATE ION (CCD ID: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



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

- Molecule 10 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).

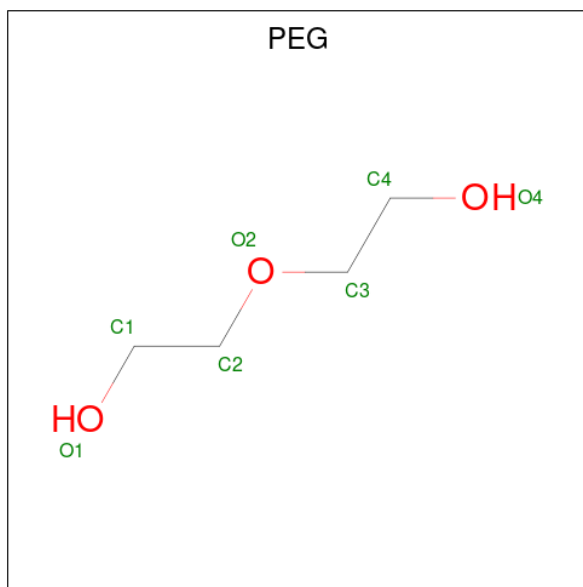


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			4	2	2		
10	B	1	Total	C	O	0	0
			4	2	2		
10	D	1	Total	C	O	0	0
			4	2	2		
10	F	1	Total	C	O	0	0
			4	2	2		
10	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 12 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

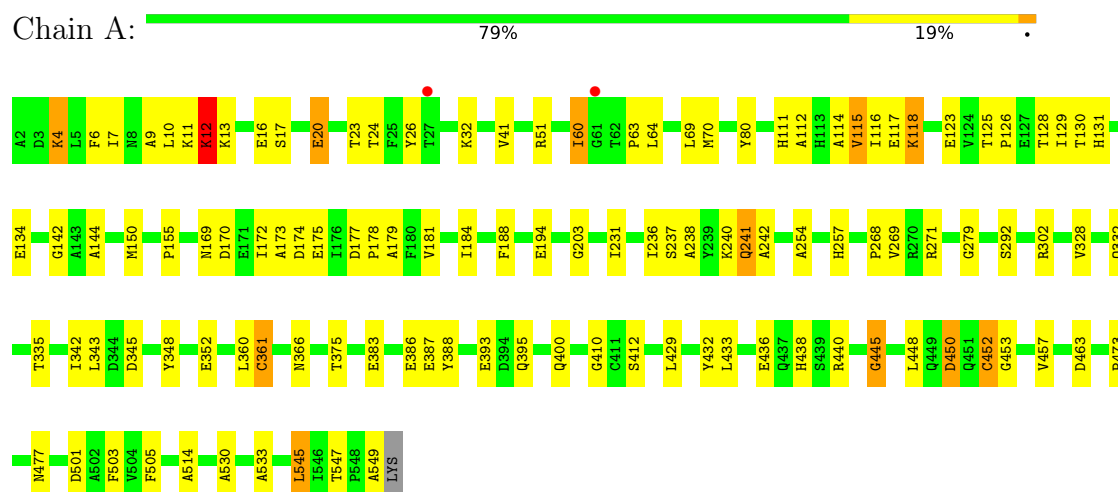
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	507	Total	O	0	28
			522	522		
13	B	462	Total	O	0	24
			477	477		
13	C	254	Total	O	0	12
			262	262		
13	D	529	Total	O	0	20
			539	539		
13	E	414	Total	O	0	16
			421	421		
13	F	250	Total	O	0	8
			254	254		

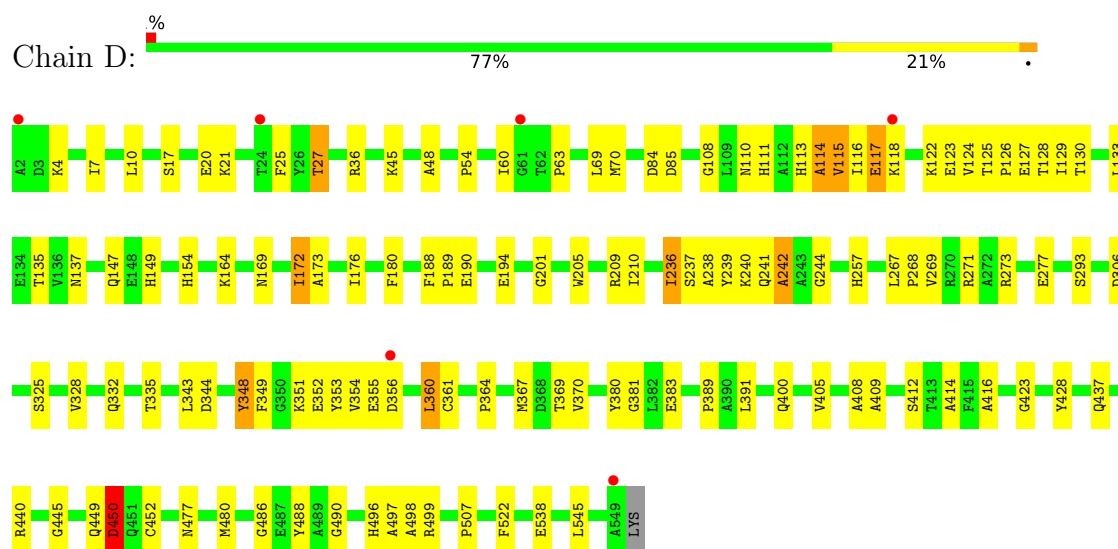
3 Residue-property plots

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

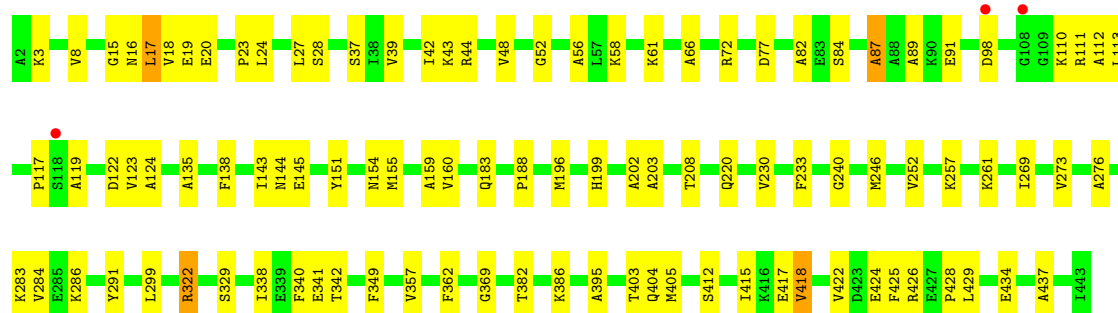


- Molecule 1: Methyl-coenzyme M reductase I subunit alpha



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

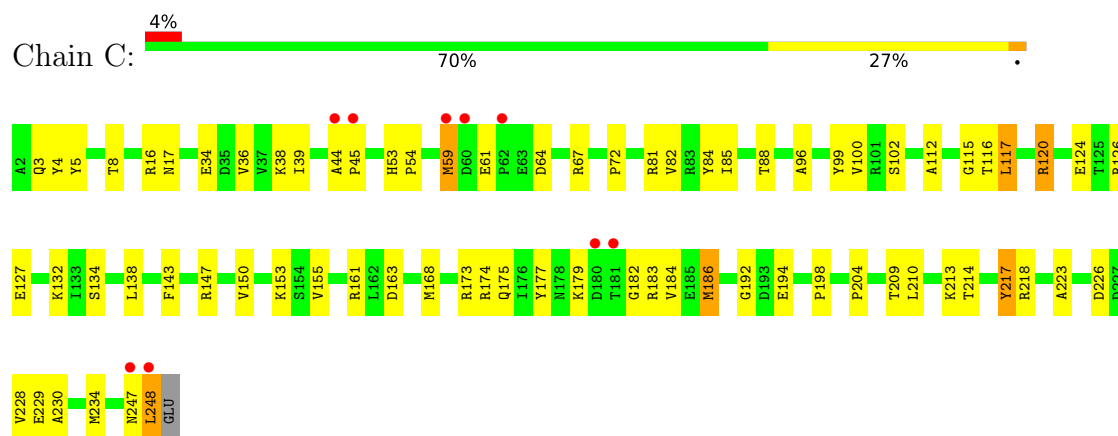




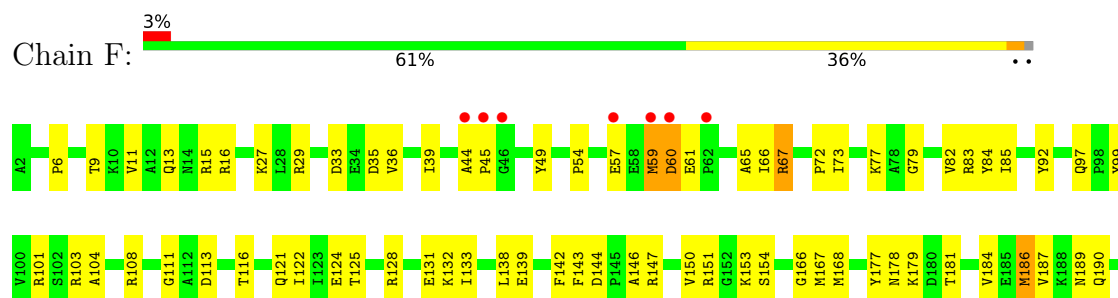
• Molecule 2: Methyl-coenzyme M reductase I subunit beta



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



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



D193		P198		P204		E207		L210		M211		K213		Y217		R218		G221		E222		A223		R225		D226		E229		A230		I233		M234		V239		K247		LEU		GLU
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.02Å 118.26Å 122.39Å 90.00° 91.84° 90.00°	Depositor
Resolution (Å)	20.28 – 1.35 20.28 – 1.35	Depositor EDS
% Data completeness (in resolution range)	92.4 (20.28-1.35) 93.1 (20.28-1.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.55 (at 1.35Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.140 , 0.157 0.139 , 0.155	Depositor DCC
R_{free} test set	23861 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	10.8	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.002 for -h,l,k 0.006 for -h,-l,-k 0.013 for h,-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	22665	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: COM, GL3, F43, ACT, EDO, PEG, MHS, ZN, AGM, MGN, MG, SMC, SHT, TP7

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	1.89	64/4528 (1.4%)	1.60	47/6146 (0.8%)
1	D	1.99	95/4483 (2.1%)	1.64	46/6084 (0.8%)
2	B	1.91	51/3578 (1.4%)	1.58	24/4839 (0.5%)
2	E	2.01	71/3590 (2.0%)	1.58	25/4852 (0.5%)
3	C	2.18	60/2117 (2.8%)	1.69	19/2851 (0.7%)
3	F	2.18	73/2186 (3.3%)	1.76	27/2940 (0.9%)
All	All	2.00	414/20482 (2.0%)	1.63	188/27712 (0.7%)

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	0
1	D	1	0
3	C	0	2
All	All	2	2

All (414) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	85	ILE	N-CA	10.35	1.58	1.46
1	A	269	VAL	CA-CB	9.64	1.66	1.54
3	F	210	LEU	N-CA	9.20	1.57	1.46
1	D	127	GLU	N-CA	-9.19	1.35	1.46
1	A	236	ILE	C-O	9.15	1.34	1.24
2	E	415	ILE	CA-CB	9.03	1.65	1.54
1	D	349	PHE	CA-C	-8.97	1.41	1.52
1	A	450	ASP	CA-CB	-8.97	1.39	1.53
1	D	354	VAL	CA-CB	8.61	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	238	ALA	C-O	8.55	1.35	1.24
2	B	28	SER	CA-C	-8.45	1.44	1.53
1	A	60	ILE	CA-C	8.26	1.63	1.52
1	D	60	ILE	CA-C	8.18	1.62	1.52
1	D	129	ILE	CA-CB	-8.17	1.44	1.54
1	D	240	LYS	CA-C	-8.11	1.42	1.53
3	C	204	PRO	N-CA	8.01	1.56	1.47
3	F	190	GLN	N-CA	8.00	1.56	1.46
2	B	284	VAL	C-O	7.97	1.33	1.24
2	B	286	LYS	N-CA	7.90	1.55	1.45
3	C	247	ASN	CA-C	-7.84	1.43	1.53
1	A	69	LEU	CA-C	-7.83	1.43	1.52
3	F	189	ASN	CA-C	7.79	1.63	1.53
2	B	23	PRO	CA-C	7.78	1.62	1.52
1	D	126	PRO	CA-C	-7.72	1.40	1.52
1	A	60	ILE	CA-CB	7.68	1.64	1.54
1	D	63	PRO	CA-CB	7.64	1.64	1.53
2	E	48	VAL	C-O	7.63	1.32	1.24
3	F	223	ALA	CA-C	-7.45	1.43	1.52
3	C	168	MET	N-CA	7.45	1.55	1.46
3	F	33	ASP	CA-C	-7.42	1.43	1.52
1	D	412	SER	CA-C	-7.41	1.43	1.52
3	C	186	MET	CA-CB	-7.37	1.43	1.53
1	D	4	LYS	N-CA	7.35	1.55	1.46
1	D	496	HIS	C-O	7.33	1.32	1.24
1	D	450	ASP	CA-CB	-7.32	1.41	1.53
2	B	8	VAL	CA-CB	7.23	1.67	1.54
3	C	72	PRO	C-O	7.23	1.32	1.23
1	D	450	ASP	CA-C	-7.23	1.42	1.52
3	C	153	LYS	C-O	7.22	1.32	1.23
3	F	39	ILE	N-CA	7.22	1.55	1.46
1	A	342	ILE	CA-CB	-7.17	1.45	1.54
3	C	184	VAL	N-CA	7.17	1.55	1.46
1	D	149	HIS	CA-C	7.17	1.62	1.53
3	F	72	PRO	C-O	7.16	1.31	1.23
1	D	116	ILE	CA-C	7.14	1.61	1.52
1	A	4[A]	LYS	N-CA	7.07	1.55	1.45
1	A	4[B]	LYS	N-CA	7.07	1.55	1.45
1	D	135	THR	CA-C	7.06	1.61	1.52
1	A	115	VAL	C-O	7.04	1.32	1.24
1	D	111	HIS	CA-C	-7.04	1.43	1.52
2	B	240	GLY	N-CA	7.00	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	143	PHE	C-O	6.96	1.31	1.24
2	B	422	VAL	N-CA	-6.96	1.38	1.46
2	B	87	ALA	CA-CB	6.95	1.64	1.53
3	F	15	ARG	CA-C	-6.94	1.43	1.52
3	F	113	ASP	N-CA	6.93	1.56	1.46
2	B	428	PRO	CA-CB	6.93	1.64	1.53
1	A	131	HIS	CA-C	6.91	1.61	1.52
1	D	54	PRO	CA-C	6.91	1.60	1.52
3	F	204	PRO	C-O	6.90	1.31	1.23
2	E	268	VAL	CA-CB	6.87	1.63	1.54
1	D	117	GLU	N-CA	6.85	1.54	1.46
3	C	209	THR	CA-C	6.82	1.61	1.52
2	E	313	ALA	C-O	-6.80	1.16	1.24
2	E	401	ALA	C-O	6.79	1.33	1.24
3	C	36	VAL	CA-CB	-6.78	1.45	1.54
2	E	341	GLU	C-O	6.77	1.32	1.24
3	F	221	GLY	C-O	6.74	1.33	1.23
2	B	112	ALA	C-O	6.72	1.31	1.23
3	C	175	GLN	C-N	6.72	1.41	1.33
3	C	3	GLN	CA-CB	6.67	1.64	1.53
1	D	351	LYS	CA-C	6.66	1.61	1.52
2	E	306	ALA	CA-C	6.66	1.61	1.52
1	D	205	TRP	N-CA	6.66	1.54	1.46
3	F	233	ILE	CA-C	6.66	1.61	1.52
2	E	240	GLY	N-CA	6.65	1.54	1.45
1	D	383	GLU	CA-C	-6.65	1.43	1.52
2	E	111	ARG	CA-C	-6.62	1.44	1.52
3	F	133	ILE	C-O	6.62	1.32	1.24
1	D	269	VAL	CA-CB	6.62	1.62	1.54
2	B	404	GLN	CA-C	-6.61	1.44	1.52
2	E	352	VAL	C-O	6.58	1.31	1.24
1	A	64	LEU	C-O	6.57	1.31	1.23
1	A	123	GLU	C-O	6.54	1.31	1.23
2	E	103	VAL	C-O	6.52	1.31	1.24
3	F	6	PRO	CA-C	-6.51	1.45	1.52
1	A	112	ALA	N-CA	-6.49	1.38	1.46
1	D	108	GLY	N-CA	6.49	1.53	1.45
2	E	87	ALA	CA-CB	6.47	1.63	1.53
1	D	114	ALA	CA-CB	-6.47	1.43	1.53
1	A	173	ALA	C-O	6.47	1.31	1.24
1	D	176	ILE	CA-CB	6.47	1.62	1.54
3	F	36	VAL	N-CA	6.45	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	356	ASP	CA-CB	-6.43	1.43	1.53
1	A	117	GLU	N-CA	6.40	1.54	1.46
2	B	208	THR	C-O	6.39	1.31	1.24
1	D	110	ASN	CA-CB	-6.39	1.43	1.53
1	D	344	ASP	N-CA	6.38	1.53	1.46
2	B	338	ILE	CA-CB	-6.35	1.45	1.54
1	D	20	GLU	N-CA	6.35	1.53	1.46
2	E	352	VAL	CA-C	-6.35	1.45	1.52
1	A	128	THR	N-CA	6.32	1.54	1.46
1	D	369	THR	CA-C	6.29	1.60	1.52
2	E	274[A]	GLU	C-O	6.28	1.31	1.24
2	E	274[B]	GLU	C-O	6.28	1.31	1.24
1	A	440	ARG	C-O	-6.28	1.17	1.23
1	A	514	ALA	CA-C	-6.26	1.46	1.53
1	D	356	ASP	CA-C	-6.26	1.44	1.52
2	E	409	GLU	C-O	6.25	1.31	1.24
1	D	209	ARG	CA-C	-6.25	1.45	1.52
1	A	388	TYR	C-O	6.25	1.31	1.24
2	E	277	LEU	N-CA	6.25	1.53	1.46
3	C	226	ASP	CA-C	-6.24	1.44	1.52
3	C	223	ALA	N-CA	6.23	1.54	1.46
1	D	352	GLU	C-O	6.23	1.31	1.24
1	A	11	LYS	N-CA	6.21	1.53	1.46
2	B	89	ALA	N-CA	6.20	1.53	1.46
3	C	174	ARG	NE-CZ	6.20	1.39	1.33
2	B	124	ALA	N-CA	6.19	1.53	1.45
1	A	130	THR	N-CA	-6.18	1.38	1.46
2	B	84	SER	CA-C	6.17	1.60	1.52
1	D	173	ALA	N-CA	6.17	1.53	1.46
2	B	426	ARG	CZ-NH2	6.16	1.41	1.33
3	C	213	LYS	CA-C	6.15	1.60	1.52
1	A	203	GLY	CA-C	-6.15	1.46	1.52
1	D	60	ILE	CA-CB	6.14	1.62	1.54
3	C	17	ASN	N-CA	6.14	1.53	1.46
2	E	436	ALA	CA-C	6.12	1.60	1.52
3	F	138	LEU	CA-C	6.12	1.61	1.52
1	D	27	THR	CA-CB	6.11	1.61	1.53
1	D	237	SER	C-O	6.11	1.31	1.24
1	D	244	GLY	C-O	6.11	1.32	1.23
2	E	286	LYS	CA-CB	6.10	1.63	1.53
1	D	367	MET	C-N	6.09	1.42	1.33
1	D	423	GLY	CA-C	6.09	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	114	ALA	N-CA	6.08	1.53	1.46
2	E	277	LEU	C-O	6.07	1.31	1.24
1	D	114	ALA	C-O	6.07	1.31	1.24
3	F	218	ARG	CZ-NH1	6.06	1.41	1.32
3	C	85	ILE	C-O	6.06	1.30	1.24
3	F	85	ILE	CA-C	6.05	1.60	1.52
1	A	111	HIS	CA-C	-6.04	1.45	1.52
3	F	166	GLY	CA-C	6.03	1.59	1.51
1	A	26	TYR	C-N	-6.03	1.25	1.33
3	C	81	ARG	CD-NE	6.01	1.54	1.46
3	F	9	THR	C-N	-6.01	1.26	1.33
1	A	10	LEU	C-O	-5.99	1.17	1.24
2	E	284	VAL	N-CA	-5.99	1.38	1.46
3	F	234	MET	N-CA	5.98	1.53	1.46
2	E	427	GLU	CA-C	-5.97	1.46	1.53
2	E	96	THR	N-CA	5.97	1.53	1.45
2	E	414	LEU	CA-C	-5.97	1.45	1.52
1	A	125	THR	CA-CB	5.96	1.61	1.53
2	E	252	VAL	CA-CB	5.96	1.61	1.54
2	B	39	VAL	CA-C	-5.95	1.45	1.52
3	F	125	THR	CA-C	5.95	1.60	1.52
3	F	101	ARG	NE-CZ	5.94	1.39	1.33
3	F	9	THR	N-CA	-5.94	1.38	1.45
2	E	82	ALA	CA-C	-5.93	1.45	1.52
3	F	214	THR	N-CA	5.93	1.53	1.45
1	D	408	ALA	N-CA	5.91	1.53	1.46
1	A	501	ASP	N-CA	5.91	1.53	1.46
1	D	416	ALA	C-O	5.87	1.30	1.24
2	B	56	ALA	N-CA	5.86	1.53	1.46
3	C	214	THR	N-CA	5.86	1.53	1.45
2	B	16	ASN	N-CA	5.85	1.53	1.46
1	D	164	LYS	CA-C	-5.84	1.45	1.52
3	F	193	ASP	N-CA	5.84	1.53	1.46
1	A	503	PHE	N-CA	5.84	1.53	1.45
1	A	530	ALA	N-CA	5.83	1.53	1.46
3	C	163	ASP	N-CA	5.83	1.53	1.45
2	B	52	GLY	N-CA	5.83	1.53	1.45
1	A	181	VAL	CA-CB	5.82	1.61	1.54
3	F	142	PHE	C-O	5.82	1.31	1.24
3	C	198	PRO	CA-CB	-5.82	1.45	1.53
3	C	214	THR	CA-CB	-5.81	1.43	1.53
2	E	118	SER	CA-CB	5.80	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	226	ASP	N-CA	5.79	1.53	1.46
2	E	10	LEU	C-O	5.79	1.31	1.24
3	C	88	THR	C-O	5.78	1.31	1.24
2	E	58	LYS	CB-CG	-5.76	1.35	1.52
2	E	314	THR	N-CA	5.76	1.53	1.46
3	F	229	GLU	CA-C	5.76	1.60	1.52
1	D	486	GLY	CA-C	5.76	1.59	1.51
3	F	222	GLU	C-O	5.75	1.30	1.24
1	D	349	PHE	C-O	5.75	1.30	1.24
1	D	360	LEU	CA-C	-5.73	1.45	1.52
1	A	60	ILE	C-N	-5.73	1.26	1.33
1	A	231	ILE	N-CA	5.73	1.53	1.46
2	B	82	ALA	CA-CB	-5.73	1.44	1.53
3	F	73	ILE	CA-CB	5.73	1.60	1.54
1	D	48	ALA	N-CA	-5.72	1.39	1.46
2	E	145	GLU	C-O	5.72	1.30	1.24
3	F	217	TYR	C-O	5.72	1.30	1.24
3	F	77	LYS	N-CA	5.71	1.53	1.46
2	B	322	ARG	CZ-NH1	5.71	1.40	1.32
2	E	216	THR	CA-C	-5.71	1.45	1.52
2	B	412	SER	CA-C	5.70	1.60	1.52
1	D	381	GLY	N-CA	5.70	1.52	1.45
1	D	110	ASN	N-CA	5.69	1.53	1.46
2	E	340	PHE	C-O	5.69	1.31	1.24
1	D	348	TYR	N-CA	5.69	1.53	1.46
1	A	240	LYS	N-CA	5.69	1.54	1.46
3	C	204	PRO	C-O	5.69	1.30	1.23
1	D	498	ALA	N-CA	5.68	1.53	1.46
3	F	225	ARG	CZ-NH1	-5.68	1.24	1.32
3	C	173	ARG	N-CA	5.67	1.55	1.46
2	B	291	TYR	N-CA	5.67	1.52	1.46
3	F	186	MET	N-CA	5.67	1.53	1.46
1	D	353	TYR	C-O	5.66	1.30	1.24
1	A	155	PRO	CA-CB	5.66	1.62	1.53
2	E	395	ALA	CA-C	-5.66	1.45	1.52
1	D	498	ALA	C-O	5.65	1.30	1.24
2	E	83	GLU	N-CA	-5.65	1.39	1.46
1	D	352	GLU	N-CA	5.65	1.53	1.46
1	A	436	GLU	C-O	5.64	1.31	1.24
2	B	138	PHE	CA-C	-5.64	1.45	1.52
3	F	144	ASP	CG-OD1	5.64	1.36	1.25
3	F	230	ALA	CA-CB	-5.64	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	293	VAL	CA-C	-5.63	1.45	1.52
1	D	405	VAL	CA-C	-5.63	1.45	1.52
3	F	11	VAL	N-CA	5.62	1.53	1.46
2	E	12	ASP	N-CA	5.62	1.52	1.45
2	E	435	ALA	CA-CB	5.62	1.62	1.53
1	D	128	THR	CA-C	5.61	1.60	1.52
1	D	172	ILE	CA-C	5.61	1.60	1.52
1	A	438	HIS	CE1-NE2	5.61	1.38	1.32
1	A	20	GLU	C-O	5.60	1.30	1.23
2	E	322[A]	ARG	C-N	5.59	1.40	1.33
2	E	322[B]	ARG	C-N	5.59	1.40	1.33
2	E	435	ALA	C-O	-5.59	1.17	1.24
2	E	65	PRO	N-CA	-5.58	1.40	1.47
3	C	124	GLU	CG-CD	5.58	1.66	1.52
1	D	360	LEU	CB-CG	-5.58	1.42	1.53
1	D	389	PRO	C-O	5.58	1.31	1.24
1	D	69	LEU	N-CA	5.57	1.53	1.46
3	F	104	ALA	N-CA	5.57	1.53	1.46
1	A	395	GLN	CA-C	-5.57	1.47	1.53
1	A	63	PRO	C-O	5.56	1.31	1.24
2	E	86	ALA	CA-C	-5.56	1.45	1.52
1	D	440	ARG	N-CA	5.55	1.53	1.46
2	E	213	ALA	CA-CB	5.55	1.61	1.53
2	B	145	GLU	C-O	5.54	1.30	1.24
3	F	125	THR	CA-CB	5.54	1.62	1.53
3	F	116	THR	CA-CB	5.53	1.63	1.53
3	C	228	VAL	CA-CB	5.53	1.62	1.54
3	C	182	GLY	N-CA	5.53	1.53	1.45
1	D	201	GLY	N-CA	5.52	1.54	1.45
3	C	38	LYS	CA-CB	5.51	1.61	1.53
3	C	218	ARG	CZ-NH1	5.51	1.40	1.32
1	D	364	PRO	CA-C	5.51	1.59	1.52
3	C	155	VAL	CA-C	-5.50	1.44	1.52
1	A	142	GLY	N-CA	5.50	1.53	1.45
2	B	220	GLN	C-O	5.50	1.31	1.24
3	C	8	THR	N-CA	5.49	1.52	1.46
3	F	239	VAL	CA-CB	5.49	1.61	1.54
2	B	342	THR	CA-CB	-5.48	1.45	1.54
3	F	226	ASP	CA-C	-5.48	1.45	1.52
2	B	159	ALA	CA-CB	5.47	1.62	1.53
1	D	449	GLN	N-CA	5.47	1.53	1.46
3	C	4	TYR	N-CA	5.45	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	352	GLU	CD-OE2	5.45	1.35	1.25
2	B	382	THR	CA-C	-5.44	1.45	1.52
3	C	183	ARG	CA-C	5.44	1.59	1.52
2	B	19	GLU	CA-C	-5.44	1.46	1.52
1	D	17	SER	CA-C	5.44	1.59	1.53
3	F	104	ALA	CA-CB	-5.44	1.44	1.53
1	D	133	LEU	CA-C	-5.43	1.45	1.52
1	A	386	GLU	N-CA	5.43	1.53	1.46
2	B	143	ILE	C-N	-5.43	1.26	1.34
3	C	155	VAL	CA-CB	5.42	1.61	1.54
1	D	497	ALA	C-N	-5.42	1.26	1.33
3	C	34	GLU	N-CA	-5.42	1.39	1.46
3	C	53	HIS	CA-CB	5.41	1.60	1.53
2	E	289	THR	C-O	5.41	1.30	1.24
2	E	439	ILE	CA-CB	5.41	1.61	1.54
3	C	217	TYR	CA-C	-5.41	1.46	1.52
2	B	151	TYR	C-O	5.40	1.30	1.24
3	C	126	ARG	N-CA	5.40	1.52	1.46
1	A	545	LEU	C-O	5.39	1.30	1.24
3	F	247	ASN	CA-CB	5.39	1.64	1.53
1	A	292	SER	C-O	5.39	1.30	1.24
2	B	117	PRO	C-O	5.39	1.29	1.23
1	D	490	GLY	C-O	5.39	1.30	1.23
3	C	112	ALA	C-O	5.38	1.30	1.24
3	F	154	SER	C-O	5.38	1.31	1.23
3	F	199	VAL	N-CA	-5.38	1.39	1.46
1	D	210	ILE	CA-CB	5.37	1.61	1.54
1	A	393	GLU	C-N	-5.37	1.27	1.33
2	E	353	GLU	N-CA	-5.37	1.39	1.46
1	D	360	LEU	N-CA	5.36	1.52	1.46
2	E	251	LEU	C-O	-5.36	1.18	1.24
1	A	375	THR	N-CA	5.36	1.52	1.46
1	D	369	THR	CB-OG1	5.36	1.52	1.43
1	A	63	PRO	N-CA	-5.36	1.40	1.47
3	F	99	TYR	CA-CB	5.34	1.62	1.53
3	F	92	TYR	N-CA	5.34	1.53	1.46
3	C	183	ARG	CZ-NH1	5.34	1.40	1.32
1	D	110	ASN	C-O	5.34	1.30	1.24
1	A	9	ALA	CA-CB	5.34	1.61	1.53
1	D	488	TYR	C-O	5.34	1.30	1.24
2	E	240	GLY	C-N	-5.33	1.27	1.33
1	D	236	ILE	CA-CB	-5.33	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	239	TYR	C-O	5.33	1.30	1.24
1	D	242	ALA	CA-CB	5.33	1.62	1.53
2	E	278	GLU	N-CA	5.32	1.52	1.46
1	A	348	TYR	CA-C	5.32	1.59	1.52
2	B	43	LYS	CA-C	-5.32	1.45	1.52
1	D	364	PRO	N-CA	-5.31	1.40	1.47
2	B	48	VAL	C-O	5.30	1.29	1.24
3	F	139	GLU	N-CA	5.30	1.53	1.46
3	F	29	ARG	N-CA	-5.30	1.39	1.46
3	F	187	VAL	CA-CB	-5.30	1.48	1.54
2	B	252	VAL	N-CA	5.29	1.52	1.46
1	D	115	VAL	CA-CB	5.29	1.61	1.54
2	E	31	ARG	N-CA	5.29	1.53	1.46
3	F	125	THR	C-O	-5.29	1.18	1.23
2	E	11	TYR	N-CA	5.28	1.52	1.45
2	E	93	ILE	C-N	5.28	1.40	1.33
2	E	269	ILE	CA-C	5.28	1.59	1.52
3	C	247	ASN	CG-ND2	5.27	1.44	1.33
3	C	138	LEU	CA-C	5.27	1.59	1.52
1	D	409	ALA	CA-C	-5.27	1.46	1.52
3	C	120	ARG	CZ-NH1	5.26	1.40	1.32
2	E	250	ASN	CA-CB	5.26	1.61	1.53
1	A	477	ASN	C-O	5.26	1.30	1.24
2	B	77	ASP	CA-CB	5.25	1.59	1.52
1	A	6	PHE	C-O	-5.25	1.17	1.24
2	B	24	LEU	CA-CB	-5.25	1.45	1.53
2	B	17	LEU	C-O	5.25	1.30	1.23
2	B	144	ASN	C-N	-5.25	1.27	1.33
3	F	79	GLY	C-N	5.25	1.40	1.33
3	C	218	ARG	C-N	-5.24	1.27	1.34
3	F	143	PHE	N-CA	-5.23	1.39	1.46
3	C	210	LEU	N-CA	5.22	1.52	1.46
1	A	231	ILE	CA-CB	-5.22	1.48	1.54
1	D	21	LYS	N-CA	-5.22	1.39	1.46
3	C	4	TYR	C-O	5.22	1.30	1.24
1	A	237	SER	C-O	5.21	1.30	1.24
2	E	401	ALA	CA-C	-5.21	1.45	1.52
2	E	437	ALA	N-CA	5.21	1.52	1.46
1	A	150	MET	CA-C	-5.21	1.45	1.52
1	A	10	LEU	CA-C	5.21	1.59	1.52
3	C	3	GLN	CB-CG	-5.20	1.36	1.52
2	E	145	GLU	CA-C	-5.20	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	412	SER	N-CA	5.20	1.52	1.46
3	C	117	LEU	C-O	5.20	1.30	1.23
3	C	155	VAL	C-O	5.19	1.30	1.24
3	C	179	LYS	N-CA	5.19	1.52	1.46
3	F	65	ALA	CA-CB	-5.19	1.45	1.53
2	E	74	LEU	CA-C	-5.19	1.46	1.52
1	D	405	VAL	N-CA	5.18	1.52	1.46
2	E	170	TYR	CA-C	-5.18	1.47	1.53
3	F	226	ASP	N-CA	5.18	1.52	1.46
1	A	23	THR	C-O	-5.18	1.18	1.23
1	A	23	THR	CA-CB	5.17	1.60	1.53
2	E	337	LEU	CA-C	-5.17	1.46	1.52
3	C	230	ALA	CA-CB	-5.17	1.45	1.53
1	D	27	THR	C-N	5.17	1.40	1.33
3	F	146	ALA	CA-C	5.17	1.59	1.52
3	C	5	TYR	C-O	5.17	1.30	1.24
1	D	189	PRO	N-CA	5.17	1.53	1.47
2	E	429	LEU	N-CA	5.16	1.52	1.46
1	D	356	ASP	CG-OD1	5.16	1.35	1.25
1	D	380	TYR	C-N	5.16	1.40	1.33
2	B	135	ALA	CA-CB	5.14	1.61	1.53
1	D	20	GLU	C-O	5.14	1.30	1.23
2	E	430	LYS	N-CA	-5.14	1.40	1.46
1	D	370	VAL	N-CA	5.13	1.52	1.46
2	B	437	ALA	C-O	5.13	1.30	1.24
2	E	409	GLU	N-CA	5.13	1.52	1.46
3	F	49	TYR	N-CA	5.12	1.54	1.46
3	C	102	SER	N-CA	-5.12	1.40	1.46
1	D	111	HIS	C-O	5.12	1.30	1.24
2	B	269	ILE	N-CA	5.11	1.52	1.46
2	E	174	ASN	CA-C	-5.11	1.46	1.53
3	F	16	ARG	CA-C	5.11	1.59	1.52
2	B	202	ALA	C-O	5.11	1.30	1.24
3	F	167	MET	N-CA	5.10	1.52	1.46
1	A	20	GLU	CA-C	-5.10	1.46	1.52
3	F	60	ASP	CA-C	5.10	1.59	1.52
2	E	338	ILE	C-O	5.10	1.30	1.24
3	F	108	ARG	CA-CB	-5.09	1.45	1.53
2	E	250	ASN	C-N	5.09	1.40	1.33
2	B	24	LEU	N-CA	5.09	1.52	1.46
3	C	53	HIS	N-CA	-5.09	1.41	1.46
3	F	124	GLU	C-N	5.08	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	238	ALA	C-O	5.07	1.30	1.24
2	B	403	THR	N-CA	-5.07	1.39	1.46
2	E	31	ARG	NE-CZ	5.07	1.38	1.33
2	E	324	ALA	C-N	-5.07	1.27	1.33
1	A	343	LEU	CA-CB	5.06	1.61	1.53
3	F	11	VAL	CA-C	-5.06	1.46	1.52
3	F	139	GLU	CD-OE2	5.06	1.34	1.25
3	F	193	ASP	CG-OD2	-5.06	1.15	1.25
2	B	111	ARG	CD-NE	5.05	1.53	1.46
3	F	128	ARG	NE-CZ	5.04	1.38	1.33
2	B	154	ASN	N-CA	5.04	1.52	1.46
3	F	198	PRO	C-O	5.04	1.29	1.23
1	A	144	ALA	C-N	-5.03	1.29	1.33
1	A	254	ALA	N-CA	5.03	1.52	1.46
3	F	168	MET	CA-C	-5.03	1.46	1.52
3	C	82	VAL	C-O	5.03	1.29	1.24
3	F	122	ILE	N-CA	5.03	1.51	1.46
3	C	229	GLU	CA-C	5.03	1.59	1.52
3	F	27	LYS	C-O	5.03	1.30	1.24
1	D	124	VAL	N-CA	5.02	1.51	1.46
3	F	122	ILE	CA-C	-5.02	1.46	1.52
2	E	35	ILE	CA-CB	-5.02	1.48	1.54
3	C	100	VAL	N-CA	5.02	1.52	1.46
3	F	213	LYS	N-CA	5.02	1.52	1.46
1	D	306	ASP	C-O	5.01	1.30	1.24
2	B	418	VAL	C-O	5.00	1.29	1.23
1	D	190	GLU	CA-CB	5.00	1.61	1.53

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	ALA	CA-C-O	-8.67	109.56	119.79
1	A	10	LEU	O-C-N	8.65	131.29	122.12
1	A	450	ASP	CB-CA-C	8.19	124.39	110.79
1	D	116	ILE	O-C-N	7.69	129.33	121.87
1	A	128	THR	N-CA-C	-7.59	103.02	111.82
1	D	369	THR	O-C-N	7.44	130.63	122.15
1	D	349	PHE	O-C-N	-7.37	114.48	122.07
1	D	380	TYR	CA-C-O	7.37	128.56	120.82
3	C	177	TYR	CA-C-N	-7.29	113.36	122.84
3	C	177	TYR	C-N-CA	-7.29	113.36	122.84
3	F	177	TYR	O-C-N	-7.29	114.41	123.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	167	MET	O-C-N	7.21	131.52	123.16
2	E	256	VAL	O-C-N	7.18	128.84	121.87
3	C	147	ARG	NE-CZ-NH1	7.14	128.64	121.50
1	A	440	ARG	CA-C-O	7.10	128.88	121.28
1	D	135	THR	O-C-N	7.08	129.74	122.09
3	F	11	VAL	O-C-N	-7.06	114.99	121.91
1	D	351	LYS	O-C-N	7.03	129.31	122.07
2	B	273	VAL	O-C-N	6.99	128.65	121.87
2	E	269	ILE	O-C-N	6.95	128.89	121.94
1	A	450	ASP	N-CA-CB	6.94	120.33	110.12
1	D	111	HIS	O-C-N	-6.91	114.79	122.12
2	B	98	ASP	N-CA-C	6.89	121.27	112.86
2	B	15	GLY	O-C-N	6.87	130.84	122.32
1	A	10	LEU	CA-C-O	-6.74	113.41	120.55
2	B	286	LYS	N-CA-C	-6.71	98.46	108.99
2	B	44	ARG	NE-CZ-NH1	6.61	128.11	121.50
1	D	450	ASP	N-CA-CB	6.54	120.29	110.22
3	C	59	MET	N-CA-C	6.52	121.44	112.90
2	B	341	GLU	CA-C-O	-6.50	113.53	120.42
1	D	70	MET	N-CA-C	6.47	119.69	110.24
1	D	126	PRO	O-C-N	-6.47	114.80	122.24
3	F	184	VAL	O-C-N	6.40	129.71	122.93
2	B	203	ALA	CA-C-O	-6.33	112.68	119.97
1	D	499	ARG	NE-CZ-NH2	-6.32	113.52	119.20
1	D	116	ILE	CA-C-O	-6.31	114.39	120.95
1	D	416	ALA	O-C-N	-6.29	115.30	122.09
1	A	236	ILE	CA-C-O	-6.24	114.56	121.17
3	F	189	ASN	O-C-N	6.23	130.52	122.23
2	B	23	PRO	O-C-N	6.21	130.54	123.03
3	F	39	ILE	CA-C-O	-6.20	114.28	120.85
1	A	16	GLU	N-CA-C	6.19	118.54	110.43
1	D	450	ASP	CB-CA-C	6.14	121.99	110.63
2	E	255	LEU	N-CA-C	6.14	117.97	111.28
3	F	61	GLU	CA-C-N	-6.14	113.95	120.03
3	F	61	GLU	C-N-CA	-6.14	113.95	120.03
1	D	114	ALA	O-C-N	-6.12	115.63	122.12
2	B	341	GLU	N-CA-C	-6.11	104.70	111.36
1	D	477	ASN	CB-CG-ND2	6.07	125.51	116.40
3	F	66	ILE	O-C-N	-6.03	115.63	121.90
1	A	241[A]	GLN	O-C-N	6.02	129.79	122.75
1	A	241[B]	GLN	O-C-N	6.02	129.79	122.75
1	A	345	ASP	CA-CB-CG	-6.02	106.58	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	44	ARG	NE-CZ-NH2	-6.00	113.80	119.20
3	C	16	ARG	O-C-N	6.00	128.47	122.12
2	E	415	ILE	N-CA-C	5.98	116.72	110.62
2	E	212	ALA	O-C-N	-5.95	115.81	122.12
1	D	123	GLU	O-C-N	5.94	129.67	122.96
3	C	174	ARG	O-C-N	5.92	130.26	122.33
1	D	172	ILE	O-C-N	5.92	127.93	121.83
2	E	178	MET	O-C-N	5.92	129.55	122.27
3	F	233	ILE	O-C-N	5.91	127.91	121.83
1	D	10	LEU	O-C-N	5.90	129.53	122.27
1	D	409	ALA	O-C-N	-5.89	115.44	122.15
3	F	35	ASP	CA-C-O	-5.88	112.85	119.79
2	B	18	VAL	N-CA-C	-5.87	106.51	111.56
2	E	273	VAL	O-C-N	5.86	127.56	121.87
1	D	277	GLU	O-C-N	-5.85	116.37	121.35
3	F	147	ARG	NE-CZ-NH1	5.83	127.33	121.50
2	E	437	ALA	N-CA-C	-5.81	105.03	111.36
1	A	547	THR	CA-C-N	-5.80	114.29	120.03
1	A	547	THR	C-N-CA	-5.80	114.29	120.03
1	D	354	VAL	O-C-N	5.80	127.80	121.83
1	D	405	VAL	O-C-N	-5.80	115.86	121.83
3	F	131	GLU	CA-C-O	-5.79	113.56	120.10
1	D	414	ALA	CA-C-O	-5.78	113.32	119.97
2	E	341	GLU	N-CA-C	-5.78	104.94	112.23
1	D	293	SER	CA-C-O	-5.78	114.39	120.63
3	F	13	GLN	CA-C-O	-5.77	114.44	120.55
3	F	226	ASP	O-C-N	-5.76	115.14	122.34
3	C	134	SER	O-C-N	5.75	128.95	122.22
3	C	218	ARG	CA-C-O	-5.75	115.12	121.33
1	D	125	THR	CB-CA-C	-5.75	102.49	110.37
3	C	175	GLN	CA-C-O	5.75	126.45	120.30
1	A	188	PHE	O-C-N	5.74	127.14	121.57
2	B	417	GLU	O-C-N	-5.74	116.03	122.12
3	C	115	GLY	O-C-N	-5.74	118.90	123.49
1	D	7	ILE	N-CA-C	5.72	116.46	110.62
1	A	366	ASN	N-CA-C	5.70	116.61	108.74
3	C	39	ILE	O-C-N	5.68	127.38	121.87
2	B	340	PHE	CA-CB-CG	-5.68	108.12	113.80
1	D	498	ALA	CA-C-O	-5.67	114.41	120.42
1	A	533	ALA	O-C-N	5.66	129.23	122.27
1	A	549	ALA	CA-C-O	-5.66	111.19	120.80
1	D	113	HIS	CA-C-O	-5.65	114.56	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	60	ILE	CB-CA-C	-5.64	103.33	111.34
3	F	233	ILE	CA-C-O	-5.63	114.88	120.85
1	D	538	GLU	CB-CA-C	-5.63	104.59	110.33
2	E	103	VAL	CA-C-O	-5.62	114.59	120.27
3	F	125	THR	O-C-N	5.62	129.01	122.99
2	B	386	LYS	CB-CA-C	5.61	119.79	111.88
2	E	318	GLN	OE1-CD-NE2	5.61	128.21	122.60
3	F	218	ARG	NE-CZ-NH2	5.59	124.23	119.20
2	B	434	GLU	O-C-N	-5.58	116.20	122.12
1	A	412	SER	CA-C-O	-5.56	114.53	120.42
1	A	387	GLU	CB-CG-CD	5.56	122.05	112.60
2	E	178	MET	CA-C-O	-5.56	113.58	119.97
3	F	59	MET	CG-SD-CE	-5.54	88.71	100.90
1	A	41	VAL	O-C-N	5.54	127.34	121.91
2	B	151	TYR	CA-CB-CG	-5.51	103.98	113.90
2	E	84	SER	O-C-N	5.50	127.95	122.12
1	A	231	ILE	N-CA-C	-5.50	105.14	110.42
1	D	135	THR	CA-C-O	-5.50	115.04	120.70
2	E	320	ALA	O-C-N	-5.50	115.89	122.15
1	D	4	LYS	CA-CB-CG	5.49	125.08	114.10
1	D	130	THR	O-C-N	-5.47	115.92	122.15
1	D	180	PHE	O-C-N	-5.46	115.51	122.34
2	E	97	GLU	CA-C-N	-5.45	114.52	122.86
2	E	97	GLU	C-N-CA	-5.45	114.52	122.86
1	A	170	ASP	CA-C-N	-5.45	112.02	120.31
1	A	170	ASP	C-N-CA	-5.45	112.02	120.31
3	C	127	GLU	CA-C-N	-5.45	112.03	120.31
3	C	127	GLU	C-N-CA	-5.45	112.03	120.31
1	D	188	PHE	CA-C-O	-5.44	113.51	120.04
3	F	217	TYR	O-C-N	-5.44	117.02	123.22
1	D	391	LEU	N-CA-C	-5.41	105.47	111.36
3	C	210	LEU	N-CA-C	-5.40	105.39	111.28
1	A	116	ILE	O-C-N	5.40	127.11	121.87
1	A	410	GLY	O-C-N	-5.39	116.97	122.19
1	D	238	ALA	N-CA-C	-5.38	105.45	112.23
2	B	110	LYS	N-CA-C	-5.37	105.47	112.23
2	B	230	VAL	CA-C-O	5.36	126.83	120.72
1	D	147	GLN	N-CA-C	5.36	118.41	110.48
1	A	51	ARG	N-CA-C	5.35	119.97	113.38
3	F	214	THR	CA-C-O	5.35	127.62	121.47
1	A	12[A]	LYS	O-C-N	-5.34	115.70	122.27
1	A	12[B]	LYS	O-C-N	-5.34	115.70	122.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	THR	N-CA-C	-5.33	105.47	111.28
1	A	70	MET	CB-CA-C	-5.32	101.13	109.11
1	A	184	ILE	O-C-N	5.32	127.03	121.87
2	E	188	PRO	O-C-N	-5.30	116.61	123.03
1	A	117	GLU	CB-CG-CD	5.30	121.61	112.60
2	E	248	ALA	CA-C-O	5.30	127.02	121.19
3	C	153	LYS	CG-CD-CE	-5.30	99.12	111.30
1	A	302	ARG	CA-C-O	-5.29	114.94	120.55
1	A	32	LYS	CA-C-O	5.28	125.92	119.05
1	D	490	GLY	CA-C-O	-5.28	115.32	120.75
1	A	128	THR	N-CA-CB	5.23	118.39	110.28
3	C	99	TYR	O-C-N	5.22	128.69	122.27
1	A	70	MET	N-CA-C	5.22	117.86	110.24
2	E	308	ALA	O-C-N	-5.22	116.59	122.12
2	B	426	ARG	N-CA-C	5.21	118.10	111.69
2	B	28	SER	CA-C-O	5.20	125.87	120.25
2	E	317	ASN	OD1-CG-ND2	-5.20	117.40	122.60
1	D	499	ARG	NH1-CZ-NH2	5.19	126.05	119.30
1	A	393	GLU	O-C-N	5.18	129.37	122.43
1	D	343	LEU	O-C-N	5.18	128.28	122.22
3	C	192	GLY	O-C-N	5.18	128.25	122.50
1	D	137	ASN	CB-CG-ND2	5.17	124.16	116.40
3	F	187	VAL	CA-C-O	5.17	124.17	119.20
3	F	103	ARG	O-C-N	5.17	127.40	122.07
1	D	113	HIS	O-C-N	5.17	127.60	122.12
2	E	337	LEU	CA-C-O	-5.16	115.40	120.82
1	D	522	PHE	N-CA-C	5.14	119.17	113.01
1	A	388	TYR	CA-C-N	5.13	124.93	119.28
1	A	388	TYR	C-N-CA	5.13	124.93	119.28
1	A	547	THR	O-C-N	5.13	125.71	121.35
3	F	97	GLN	OE1-CD-NE2	-5.13	117.47	122.60
1	A	32	LYS	O-C-N	-5.13	115.38	122.46
2	B	395	ALA	N-CA-C	-5.13	105.69	111.28
2	B	160	VAL	N-CA-C	5.13	115.79	110.82
2	E	82	ALA	N-CA-C	5.13	116.87	111.28
2	B	329	SER	CA-C-O	-5.12	114.99	120.42
1	A	13	LYS	N-CA-C	5.10	116.92	111.36
1	A	116	ILE	CA-C-O	-5.10	115.64	120.95
1	A	129	ILE	N-CA-C	-5.07	105.76	110.53
3	C	161	ARG	CA-C-O	5.07	126.92	121.55
2	E	106	LEU	O-C-N	-5.07	117.39	123.27
3	C	96	ALA	N-CA-C	-5.06	102.58	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	144	ASP	O-C-N	-5.06	116.89	121.39
1	A	7	ILE	CA-C-O	-5.06	115.69	120.95
3	F	39	ILE	N-CA-C	-5.06	105.61	110.72
2	B	276	ALA	O-C-N	5.06	127.48	122.12
1	A	134	GLU	N-CA-C	-5.05	105.78	111.28
1	D	437	GLN	OE1-CD-NE2	5.03	127.63	122.60
2	E	97	GLU	N-CA-C	5.03	117.50	111.71
3	F	151	ARG	CG-CD-NE	-5.02	100.96	112.00
2	E	397	MET	CA-C-O	-5.01	114.21	119.97

All (2) chirality outliers are listed below:

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

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	120	ARG	Sidechain
3	C	217	TYR	Sidechain

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	4431	0	4224	48	0
1	D	4380	0	4220	29	0
2	B	3462	0	3517	43	0
2	E	3471	0	3532	37	0
3	C	2056	0	2000	25	0
3	F	2113	0	2065	22	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	1	0	0	0	0
5	A	21	0	19	0	0
5	D	21	0	19	0	0
6	A	62	0	43	2	0
6	D	62	0	43	1	0
7	A	7	0	4	0	0
7	D	7	0	5	1	0
8	A	28	0	21	0	0
8	D	28	0	21	1	0
9	A	4	0	3	0	0
10	A	4	0	6	0	0
10	B	4	0	6	0	0
10	D	4	0	6	1	0
10	F	8	0	12	0	0
11	A	1	0	0	0	0
12	C	7	0	10	0	0
13	A	522	0	0	12	0
13	B	477	0	0	15	0
13	C	262	0	0	4	0
13	D	539	0	0	8	0
13	E	421	0	0	10	0
13	F	254	0	0	10	0
All	All	22665	0	19776	184	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 5.

All (184) 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)
3:F:207[B]:GLU:HG3	13:F:3759:HOH:O	1.39	1.23
1:A:429:LEU:HD12	3:C:234[B]:MET:HE1	1.30	1.09
1:A:429:LEU:CD1	3:C:234[B]:MET:HE1	1.85	1.06
1:D:545[A]:LEU:HD12	13:D:2591:HOH:O	1.66	0.93
1:A:433:LEU:HD23	3:C:234[B]:MET:SD	2.08	0.93
2:E:27:LEU:HD22	2:E:246[B]:MET:HE1	1.53	0.91
1:A:432:TYR:HB2	3:C:234[B]:MET:HE3	1.51	0.90
1:A:433:LEU:CD2	3:C:234[B]:MET:SD	2.60	0.88
1:D:36[A]:ARG:HD3	1:D:85:ASP:OD1	1.76	0.86
2:E:27:LEU:CD2	2:E:246[B]:MET:HE1	2.06	0.86
2:E:438[A]:GLU:OE1	2:E:439:ILE:HG23	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196[B]:MET:CE	13:B:3731:HOH:O	2.25	0.83
1:D:545[A]:LEU:CD1	13:D:2591:HOH:O	2.23	0.82
3:C:67[B]:ARG:HG3	3:C:67[B]:ARG:HH11	1.44	0.81
3:C:67[B]:ARG:HH11	3:C:67[B]:ARG:CG	1.95	0.80
3:F:67[A]:ARG:HG2	3:F:67[A]:ARG:HH11	1.48	0.79
13:A:3768:HOH:O	1:D:545[A]:LEU:HD11	1.82	0.79
2:B:196[B]:MET:HE1	13:B:574:HOH:O	1.83	0.77
1:A:24[A]:THR:HG23	13:A:3803:HOH:O	1.84	0.77
2:B:196[B]:MET:CE	13:B:574:HOH:O	2.31	0.77
2:E:27:LEU:HD22	2:E:246[B]:MET:CE	2.16	0.75
1:A:432:TYR:CB	3:C:234[B]:MET:HE3	2.17	0.74
1:A:24[A]:THR:CG2	13:A:3803:HOH:O	2.35	0.73
2:E:261[A]:LYS:HG2	13:F:3664:HOH:O	1.88	0.73
1:A:429:LEU:HD12	3:C:234[B]:MET:CE	2.17	0.70
2:B:27:LEU:HD22	2:B:246[B]:MET:CE	2.21	0.70
1:A:178[A]:PRO:HD3	13:A:1631:HOH:O	1.94	0.67
2:E:17:LEU:HD21	2:E:20[A]:GLU:HG3	1.77	0.67
2:B:299:LEU:HD23	2:B:349[A]:PHE:CE1	2.30	0.65
2:B:196[B]:MET:SD	13:B:3731:HOH:O	2.54	0.64
1:D:194[B]:GLU:HG2	13:D:3701:HOH:O	1.97	0.64
2:E:322[A]:ARG:CZ	3:F:67[A]:ARG:HD2	2.27	0.63
13:B:2205:HOH:O	2:E:188:PRO:HD3	1.98	0.63
1:D:268:PRO:HB3	13:E:1668:HOH:O	1.99	0.62
3:C:67[B]:ARG:NH1	3:C:67[B]:ARG:HB2	2.15	0.61
2:E:322[A]:ARG:NH1	3:F:67[A]:ARG:HD2	2.15	0.61
2:B:27:LEU:HD22	2:B:246[B]:MET:HE1	1.82	0.61
2:E:61[B]:LYS:CE	13:E:2444:HOH:O	2.49	0.61
1:D:169[A]:ASN:CG	1:D:172:ILE:HG12	2.25	0.60
2:E:342:THR:OG1	2:E:344[B]:LEU:HB2	2.02	0.60
2:E:261[B]:LYS:O	2:E:261[B]:LYS:HD2	2.01	0.60
2:E:261[B]:LYS:HG3	2:E:262:GLU:HG3	1.82	0.60
1:A:241[B]:GLN:HA	13:F:4106:HOH:O	2.01	0.59
1:A:241[A]:GLN:HA	13:F:4106:HOH:O	2.02	0.59
2:E:27:LEU:HD22	2:E:246[B]:MET:SD	2.43	0.59
1:A:114:ALA:O	1:A:118:LYS:HD3	2.02	0.59
1:A:60:ILE:HD12	13:D:3878:HOH:O	2.04	0.58
1:A:169[A]:ASN:ND2	1:A:172:ILE:HD12	2.18	0.57
3:C:67[B]:ARG:NH1	3:C:67[B]:ARG:CB	2.68	0.57
3:F:83:ARG:NH2	13:F:4106:HOH:O	2.36	0.57
2:B:261[A]:LYS:HG3	13:B:4130:HOH:O	2.06	0.56
3:C:67[B]:ARG:HH11	3:C:67[B]:ARG:CB	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:ALA:O	1:D:118:LYS:HD3	2.06	0.56
3:F:57:GLU:HG2	13:F:939:HOH:O	2.06	0.56
1:A:241[B]:GLN:HB3	1:A:242:ALA:O	2.06	0.56
3:F:132[A]:LYS:HD2	13:F:1990:HOH:O	2.05	0.56
2:B:37:SER:OG	2:B:424[B]:GLU:OE1	2.21	0.55
2:B:196[B]:MET:HE2	13:B:3731:HOH:O	1.99	0.55
1:D:360:LEU:O	1:D:361[A]:CYS:HB2	2.07	0.55
2:E:299:LEU:HD22	13:E:2973:HOH:O	2.07	0.55
1:A:360:LEU:O	1:A:361[B]:CYS:HB2	2.06	0.54
3:F:44:ALA:HB1	3:F:45:PRO:HD2	1.90	0.54
2:B:257:LYS:NZ	13:B:3430:HOH:O	2.38	0.54
2:B:322:ARG:NH1	3:C:67[A]:ARG:HD3	2.23	0.54
3:C:194[B]:GLU:HG3	13:C:1318:HOH:O	2.08	0.54
2:B:119:ALA:HA	2:B:122[B]:ASP:OD2	2.06	0.53
1:A:17[A]:SER:OG	1:A:20:GLU:HG3	2.09	0.53
1:A:545:LEU:HD11	13:D:1948[B]:HOH:O	2.08	0.53
2:B:27:LEU:CD2	2:B:246[B]:MET:HE1	2.39	0.53
1:D:169[A]:ASN:OD1	1:D:172:ILE:HG12	2.09	0.53
1:A:383[A]:GLU:HG3	13:A:2606:HOH:O	2.09	0.53
2:B:58:LYS:HE2	13:B:3633:HOH:O	2.09	0.52
2:B:299:LEU:HD23	2:B:349[A]:PHE:HE1	1.71	0.52
2:B:233[B]:PHE:CE1	3:C:248:LEU:HG	2.44	0.52
1:D:169[A]:ASN:CG	1:D:172:ILE:CG1	2.83	0.51
1:A:174[A]:ASP:HB2	13:A:1937:HOH:O	2.10	0.51
1:A:194[B]:GLU:HG2	13:A:2095:HOH:O	2.11	0.50
1:A:328:VAL:HB	6:D:552:F43:H9A1	1.92	0.50
1:A:433:LEU:HD21	3:C:234[B]:MET:SD	2.48	0.50
3:F:67[A]:ARG:HH11	3:F:67[A]:ARG:CG	2.20	0.50
1:A:24[B]:THR:HG23	13:A:677:HOH:O	2.11	0.50
2:B:246[A]:MET:HE3	2:B:429:LEU:HD12	1.93	0.50
1:A:268:PRO:HG3	13:A:4030:HOH:O	2.11	0.50
2:E:27:LEU:CD2	2:E:246[B]:MET:CE	2.82	0.49
1:A:242:ALA:HB2	3:F:84:TYR:CE1	2.47	0.49
2:B:199:HIS:CE1	2:B:415[B]:ILE:HD12	2.47	0.49
2:E:344[A]:LEU:HB3	2:E:345:PRO:HD2	1.93	0.49
1:A:177[B]:ASP:C	1:A:179:ALA:N	2.69	0.49
3:F:200[A]:ASP:HB2	13:F:1920:HOH:O	2.11	0.49
3:C:84:TYR:CE1	1:D:242:ALA:HB2	2.47	0.49
1:A:169[A]:ASN:ND2	1:A:172:ILE:CD1	2.76	0.49
2:E:424[B]:GLU:HG3	13:E:3642:HOH:O	2.12	0.49
1:A:126:PRO:HB2	1:A:175[A]:GLU:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:27:LEU:HD21	2:E:246[B]:MET:HE1	1.92	0.48
3:F:178[B]:ASN:HB3	3:F:181[B]:THR:OG1	2.12	0.48
1:D:117:GLU:HB2	1:D:118:LYS:HD2	1.95	0.48
2:B:188:PRO:HD3	13:E:1304:HOH:O	2.12	0.48
2:B:261[A]:LYS:HE3	13:B:4130:HOH:O	2.14	0.48
2:E:113[B]:LEU:C	2:E:113[B]:LEU:HD23	2.39	0.48
2:B:299:LEU:HD23	2:B:349[A]:PHE:CZ	2.48	0.48
1:A:4[A]:LYS:NZ	13:A:2253:HOH:O	2.42	0.47
1:D:236:ILE:HA	1:D:241[A]:GLN:HB2	1.96	0.47
3:F:67[A]:ARG:HG2	3:F:67[A]:ARG:NH1	2.25	0.47
1:D:154:HIS:CE1	1:D:545[A]:LEU:HD21	2.49	0.47
2:B:246[A]:MET:CE	2:B:429:LEU:HD12	2.45	0.47
2:E:299:LEU:CD2	13:E:2973:HOH:O	2.62	0.47
2:B:27:LEU:CD2	2:B:246[B]:MET:CE	2.92	0.47
2:B:113[A]:LEU:HD13	2:B:418:VAL:HG13	1.97	0.46
2:E:61[B]:LYS:HE2	13:E:2444:HOH:O	2.14	0.46
3:F:153[A]:LYS:NZ	13:F:1186:HOH:O	2.27	0.46
1:A:332:GLN:HA	1:A:335:THR:OG1	2.15	0.46
2:E:317:ASN:O	3:F:111:GLY:HA2	2.16	0.46
3:C:67[B]:ARG:HH11	3:C:67[B]:ARG:HB2	1.75	0.46
1:D:332:GLN:HA	1:D:335:THR:OG1	2.16	0.46
1:D:480:MET:O	8:D:555[B]:SHT:HK61	2.16	0.46
3:F:59:MET:O	3:F:60:ASP:C	2.57	0.46
3:F:247:ASN:C	3:F:247:ASN:HD22	2.24	0.45
3:C:64[B]:ASP:HB2	13:C:3620:HOH:O	2.15	0.45
2:E:39:VAL:HG21	2:E:221:THR:HG21	1.98	0.45
3:F:67[A]:ARG:CG	3:F:67[A]:ARG:NH1	2.80	0.45
2:B:196[B]:MET:CE	13:B:1152:HOH:O	2.64	0.45
1:D:36[A]:ARG:HG2	1:D:84:ASP:HB2	1.98	0.45
1:A:115:VAL:HG22	2:E:405[A]:MET:HG3	1.99	0.45
1:A:448:LEU:O	1:A:452:SMC:HCS3	2.17	0.45
1:A:12[A]:LYS:HE2	1:A:80:TYR:CZ	2.52	0.45
3:C:44:ALA:HB1	3:C:45:PRO:HD2	1.98	0.44
1:A:178[A]:PRO:HD2	13:A:1652:HOH:O	2.18	0.44
3:C:132:LYS:HE3	13:C:4098:HOH:O	2.18	0.44
3:F:82:VAL:O	3:F:83:ARG:HD2	2.16	0.44
2:B:87:ALA:O	2:B:91[B]:GLU:HG3	2.17	0.44
1:D:545[A]:LEU:HD11	13:D:2591:HOH:O	2.07	0.44
2:E:374:ILE:C	2:E:374:ILE:HD12	2.43	0.43
1:A:60:ILE:CD1	13:D:3878:HOH:O	2.65	0.43
1:A:169[A]:ASN:HD22	1:A:172:ILE:HD12	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246[B]:MET:HE3	2:B:246[B]:MET:HB3	1.65	0.43
2:B:299:LEU:HD21	13:C:1043:HOH:O	2.17	0.43
6:A:1:F43:H9A1	1:D:328:VAL:HB	2.01	0.43
2:B:42[A]:ILE:HG13	2:B:425:PHE:CE1	2.54	0.43
3:C:67[B]:ARG:CG	3:C:67[B]:ARG:NH1	2.64	0.43
1:D:267:LEU:HD12	1:D:273:ARG:HB2	2.01	0.42
2:E:196[B]:MET:O	2:E:197:VAL:C	2.62	0.42
1:A:12[A]:LYS:HE2	1:A:80:TYR:CE1	2.54	0.42
2:B:17:LEU:HD21	2:B:20[A]:GLU:HG3	2.01	0.42
2:B:424[A]:GLU:HG3	13:B:3930:HOH:O	2.19	0.42
2:E:61[B]:LYS:HE2	2:E:68[B]:LYS:HE3	2.01	0.42
3:F:207[B]:GLU:CG	13:F:3759:HOH:O	2.24	0.42
1:A:505:PHE:CE1	2:E:67:CYS:HB3	2.54	0.42
2:E:20[B]:GLU:HG2	13:E:768:HOH:O	2.19	0.42
2:E:61[B]:LYS:HE3	13:E:2370:HOH:O	2.20	0.42
2:E:261[B]:LYS:HD2	2:E:261[B]:LYS:C	2.43	0.42
1:A:279:GLY:HA2	1:A:473:PRO:HB2	2.01	0.42
2:B:72:ARG:HB3	2:B:155:MET:HE2	2.02	0.42
1:D:241[A]:GLN:HB3	1:D:242:ALA:O	2.20	0.42
2:E:61[A]:LYS:HB3	2:E:61[A]:LYS:HE3	1.95	0.42
2:E:214:LEU:HB2	2:E:428:PRO:HG3	2.02	0.42
3:F:54:PRO:HD2	3:F:59:MET:HE3	2.01	0.42
1:A:12[A]:LYS:HG2	1:A:80:TYR:CD2	2.55	0.42
1:D:45[A]:LYS:HB3	1:D:45[A]:LYS:HE2	1.78	0.42
1:D:348:TYR:CZ	10:D:556:EDO:H11	2.55	0.41
1:A:126:PRO:CB	1:A:175[A]:GLU:HG2	2.51	0.41
1:A:172:ILE:HD12	13:A:3660:HOH:O	2.20	0.41
2:B:61:LYS:NZ	13:B:2541:HOH:O	2.52	0.41
2:B:123[B]:VAL:HG12	2:E:36:LYS:HA	2.01	0.41
1:D:25:PHE:O	1:D:27:THR:HG23	2.21	0.41
2:B:362:PHE:O	2:B:369:GLY:HA3	2.20	0.41
2:B:405[A]:MET:HG3	1:D:115:VAL:HG22	2.02	0.41
3:C:116:THR:C	3:C:117:LEU:HD12	2.45	0.41
1:A:445:GL3:HA2	2:B:357:VAL:HG12	2.02	0.41
2:B:119:ALA:O	2:B:122[B]:ASP:HB2	2.21	0.41
1:A:453:GLY:O	1:A:457:VAL:HG23	2.21	0.41
2:B:122[B]:ASP:HB2	13:B:1261:HOH:O	2.20	0.41
6:A:1:F43:C1C	7:D:554[A]:COM:H12	2.51	0.40
3:C:54:PRO:O	3:C:59:MET:HE3	2.21	0.40
2:E:236[A]:MET:HE2	2:E:236[A]:MET:HB3	1.75	0.40
2:B:183:GLN:HG2	13:E:1668:HOH:O	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:355[B]:GLU:HG2	13:D:1824:HOH:O	2.21	0.40
1:D:428:TYR:HD1	1:D:450:ASP:HB3	1.86	0.40
2:B:66:ALA:O	1:D:507:PRO:HD2	2.22	0.40
2:B:261[A]:LYS:CE	13:B:4130:HOH:O	2.70	0.40
2:E:362:PHE:O	2:E:369:GLY:HA3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	569/549 (104%)	555 (98%)	14 (2%)	0	100	100
1	D	563/549 (103%)	544 (97%)	18 (3%)	1 (0%)	43	19
2	B	465/442 (105%)	457 (98%)	8 (2%)	0	100	100
2	E	466/442 (105%)	457 (98%)	9 (2%)	0	100	100
3	C	255/248 (103%)	247 (97%)	8 (3%)	0	100	100
3	F	264/248 (106%)	258 (98%)	6 (2%)	0	100	100
All	All	2582/2478 (104%)	2518 (98%)	63 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	461/434 (106%)	455 (99%)	6 (1%)	61	30
1	D	455/434 (105%)	453 (100%)	2 (0%)	84	69
2	B	366/341 (107%)	363 (99%)	3 (1%)	73	48
2	E	367/341 (108%)	360 (98%)	7 (2%)	50	17
3	C	225/216 (104%)	221 (98%)	4 (2%)	51	19
3	F	233/216 (108%)	225 (97%)	8 (3%)	32	6
All	All	2107/1982 (106%)	2077 (99%)	30 (1%)	63	28

All (30) 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	118	LYS
1	A	361[A]	CYS
1	A	361[B]	CYS
1	A	450	ASP
2	B	3[A]	LYS
2	B	3[B]	LYS
2	B	283	LYS
3	C	61	GLU
3	C	150	VAL
3	C	186	MET
3	C	248	LEU
1	D	122	LYS
1	D	450	ASP
2	E	58	LYS
2	E	97	GLU
2	E	185	LEU
2	E	283	LYS
2	E	438[A]	GLU
2	E	438[B]	GLU
2	E	440	LYS
3	F	67[A]	ARG
3	F	67[B]	ARG
3	F	121	GLN
3	F	150	VAL
3	F	179[A]	LYS

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Mol	Chain	Res	Type
3	F	179[B]	LYS
3	F	186	MET
3	F	247	ASN

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	42	ASN
1	A	296	ASN
1	A	437	GLN
2	B	102	ASN
2	B	115	GLN
3	C	121	GLN
1	D	296	ASN
1	D	437	GLN
2	E	318	GLN
3	F	121	GLN
3	F	247	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	GL3	A	445	1	2,3,4	2.04	1 (50%)	1,2,4	0.28	0
1	AGM	A	271	1	10,11,12	0.84	0	7,13,15	2.04	2 (28%)
1	MGN	D	400	1	6,9,10	1.84	3 (50%)	7,12,14	1.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	AGM	D	271	1	10,11,12	1.00	0	7,13,15	1.06	1 (14%)
1	MHS	D	257	1	10,11,12	1.50	2 (20%)	5,14,16	9.69	3 (60%)
1	MGN	A	400	1	6,9,10	1.23	1 (16%)	7,12,14	1.00	1 (14%)
1	MHS	A	257	1	10,11,12	1.90	3 (30%)	5,14,16	9.60	3 (60%)
1	SMC	D	452	1	5,6,7	1.20	0	3,6,8	1.58	1 (33%)
1	SMC	A	452	1	5,6,7	1.21	0	3,6,8	1.91	1 (33%)
1	GL3	D	445	1	2,3,4	2.22	1 (50%)	1,2,4	0.31	0

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	GL3	A	445	1	-	1/1/1/2	-
1	AGM	A	271	1	-	2/10/11/13	-
1	MGN	D	400	1	-	0/7/9/12	-
1	AGM	D	271	1	-	1/10/11/13	-
1	MHS	D	257	1	-	0/5/6/8	0/1/1/1
1	MGN	A	400	1	-	0/7/9/12	-
1	MHS	A	257	1	-	0/5/6/8	0/1/1/1
1	SMC	D	452	1	-	1/3/5/7	-
1	SMC	A	452	1	-	1/3/5/7	-
1	GL3	D	445	1	-	1/1/1/2	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	MHS	CE1-NE2	3.77	1.41	1.32
1	D	257	MHS	CE1-NE2	3.41	1.41	1.32
1	D	445	GL3	C-S	-3.14	1.67	1.80
1	D	400	MGN	CB1-CA	-3.09	1.51	1.55
1	A	445	GL3	C-S	-2.88	1.68	1.80
1	A	257	MHS	CG-ND1	-2.85	1.33	1.38
1	A	400	MGN	CB1-CA	2.56	1.57	1.55
1	D	400	MGN	O-C	2.37	1.27	1.20
1	D	257	MHS	CE1-ND1	2.23	1.41	1.35
1	A	257	MHS	O-C	2.22	1.28	1.20
1	D	400	MGN	CB1-CG	2.06	1.57	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	257	MHS	ND1-CE1-NE2	-20.65	100.64	112.94
1	A	257	MHS	ND1-CE1-NE2	-20.64	100.65	112.94
1	D	257	MHS	CD2-NE2-CE1	5.45	112.36	105.24
1	A	257	MHS	CM-ND1-CE1	-4.16	118.51	126.28
1	A	257	MHS	CD2-NE2-CE1	4.05	110.53	105.24
1	D	257	MHS	CM-ND1-CE1	-3.54	119.67	126.28
1	A	271	AGM	NH1-CZ-NE1	3.51	127.31	119.58
1	A	452	SMC	CA-CB-SG	-3.22	108.83	114.04
1	D	452	SMC	CA-CB-SG	-2.47	110.04	114.04
1	A	271	AGM	CD-NE1-CZ	-2.21	119.47	123.59
1	A	400	MGN	CB1-CG-CD	-2.06	108.03	112.13
1	D	271	AGM	CE2-CD-CG	2.04	115.20	111.48

There are no chirality outliers.

All (7) 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	A	445	GL3	S-C-CA-N
1	D	445	GL3	S-C-CA-N
1	A	271	AGM	CE2-CD-NE1-CZ
1	D	271	AGM	CE2-CD-NE1-CZ
1	A	271	AGM	NE1-CD-CG-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	445	GL3	1	0
1	A	452	SMC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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$
10	EDO	A	557	-	3,3,3	0.59	0	2,2,2	0.34	0
10	EDO	F	1	-	3,3,3	0.57	0	2,2,2	0.53	0
7	COM	D	554[A]	6	6,6,6	1.56	1 (16%)	8,8,8	0.85	0
10	EDO	F	251	-	3,3,3	0.65	0	2,2,2	0.44	0
12	PEG	C	1	-	6,6,6	0.56	0	5,5,5	1.14	1 (20%)
8	SHT	A	555[B]	6	26,27,27	2.96	5 (19%)	32,36,36	1.93	7 (21%)
9	ACT	A	556[B]	4	3,3,3	0.94	0	3,3,3	0.40	0
7	COM	A	554[A]	6	6,6,6	1.57	1 (16%)	8,8,8	2.14	2 (25%)
10	EDO	B	445	-	3,3,3	0.73	0	2,2,2	0.24	0
6	F43	D	552	1,7,8	63,71,71	2.75	21 (33%)	73,118,118	2.02	25 (34%)
6	F43	A	1	1,8,7	63,71,71	2.62	16 (25%)	73,118,118	1.70	15 (20%)
8	SHT	D	555[B]	6	26,27,27	2.66	3 (11%)	32,36,36	2.08	7 (21%)
5	TP7	A	553[A]	-	19,20,20	1.04	1 (5%)	24,26,26	1.58	6 (25%)
5	TP7	D	553[A]	-	19,20,20	1.17	1 (5%)	24,26,26	1.26	3 (12%)
10	EDO	D	556	-	3,3,3	0.35	0	2,2,2	0.39	0

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
10	EDO	A	557	-	-	1/1/1/1	-
10	EDO	F	1	-	-	1/1/1/1	-
7	COM	D	554[A]	6	-	0/4/4/4	-
10	EDO	F	251	-	-	1/1/1/1	-
12	PEG	C	1	-	-	0/4/4/4	-
8	SHT	A	555[B]	6	-	5/31/31/31	-
7	COM	A	554[A]	6	-	0/4/4/4	-
10	EDO	B	445	-	-	1/1/1/1	-
6	F43	D	552	1,7,8	-	10/28/185/185	-
6	F43	A	1	1,8,7	-	10/28/185/185	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	SHT	D	555[B]	6	-	3/31/31/31	-
5	TP7	A	553[A]	-	-	2/24/24/24	-
5	TP7	D	553[A]	-	-	1/24/24/24	-
10	EDO	D	556	-	-	1/1/1/1	-

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	555[B]	SHT	CD-SG2	-11.99	1.60	1.77
6	D	552	F43	NI-NB	10.52	2.14	1.89
6	A	1	F43	CHB-C1B	-9.70	1.46	1.53
8	D	555[B]	SHT	CD-SG2	-9.34	1.64	1.77
6	D	552	F43	NI-NA	8.86	2.10	1.89
6	A	1	F43	NI-NB	8.65	2.10	1.89
6	A	1	F43	NI-NA	7.87	2.08	1.89
8	D	555[B]	SHT	CK1-CK2	7.70	1.53	1.32
8	A	555[B]	SHT	CK1-CK2	7.40	1.52	1.32
6	D	552	F43	NI-ND	7.26	2.07	1.89
6	D	552	F43	CHD-C1D	6.32	1.53	1.43
6	A	1	F43	NI-ND	6.08	2.04	1.89
6	A	1	F43	CHA-C4D	4.61	1.57	1.53
6	D	552	F43	C3C-C4C	4.32	1.57	1.50
8	D	555[B]	SHT	OS3-SG2	4.23	1.57	1.45
6	D	552	F43	C6D-C7D	-4.13	1.45	1.50
6	A	1	F43	C3C-C4C	3.56	1.56	1.50
6	D	552	F43	O8D-C7D	3.39	1.30	1.23
6	D	552	F43	OEB-CCB	-3.37	1.19	1.30
6	D	552	F43	CHC-C1C	-3.29	1.29	1.36
7	A	554[A]	COM	C2-S2	-3.13	1.73	1.77
6	A	1	F43	CHB-C4A	3.10	1.56	1.51
6	A	1	F43	OEB-CCB	-3.06	1.20	1.30
6	D	552	F43	C8C-C3C	2.91	1.59	1.54
6	D	552	F43	C1C-NC	2.90	1.44	1.37
6	D	552	F43	C5C-C2C	2.86	1.57	1.53
6	A	1	F43	C5C-C6C	2.82	1.58	1.51
5	D	553[A]	TP7	OXT-C	2.76	1.30	1.22
6	A	1	F43	CHC-C4B	2.73	1.46	1.39
6	D	552	F43	C3C-C2C	-2.68	1.47	1.54
6	A	1	F43	C5D-C2D	2.68	1.58	1.53
6	A	1	F43	O8D-C7D	2.62	1.28	1.23
6	A	1	F43	C4A-NA	2.59	1.53	1.49
6	D	552	F43	CHB-C1B	2.58	1.55	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1	F43	OCC-CAC	2.55	1.30	1.22
6	D	552	F43	CBB-CCB	2.49	1.56	1.50
6	D	552	F43	OBD-CAD	2.38	1.29	1.22
6	D	552	F43	O8C-C6C	-2.26	1.23	1.30
8	A	555[B]	SHT	CG2-CB	2.25	1.57	1.51
6	A	1	F43	OBC-CAC	-2.22	1.23	1.30
7	D	554[A]	COM	C2-S2	-2.19	1.74	1.77
8	A	555[B]	SHT	P-O1P	2.16	1.57	1.50
6	A	1	F43	ODB-CCB	2.13	1.29	1.22
6	D	552	F43	OBC-CAC	-2.10	1.23	1.30
6	D	552	F43	C8C-C9C	2.09	1.59	1.52
5	A	553[A]	TP7	OXT-C	2.08	1.28	1.22
8	A	555[B]	SHT	CC-CD	2.05	1.57	1.51
6	D	552	F43	C4D-ND	-2.04	1.46	1.49
6	D	552	F43	C4A-NA	2.00	1.52	1.49

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	555[B]	SHT	CK3-CK2-CK1	-7.19	110.95	125.92
6	D	552	F43	C5D-C2D-C1D	6.38	118.75	110.43
6	D	552	F43	C2D-C1D-CHD	-5.80	114.66	121.85
8	A	555[B]	SHT	CK3-CK2-CK1	-5.02	115.46	125.92
8	D	555[B]	SHT	CK2-CK1-CK	-4.99	110.26	122.94
7	A	554[A]	COM	C1-C2-S2	4.93	122.79	111.77
6	A	1	F43	CAB-C3B-C2B	-4.37	109.36	119.00
6	D	552	F43	C1D-CHD-C4C	-4.32	113.14	125.28
8	A	555[B]	SHT	CK2-CK1-CK	-4.22	112.21	122.94
6	D	552	F43	C6D-C7D-CHD	4.15	124.60	116.94
6	A	1	F43	OCC-CAC-C9C	-4.14	109.96	123.09
8	A	555[B]	SHT	OS2-SG2-CD	3.96	113.74	106.00
8	A	555[B]	SHT	OS3-SG2-CD	3.95	112.69	106.73
6	A	1	F43	OBC-CAC-C9C	3.78	125.94	114.00
5	A	553[A]	TP7	CB-CA-N	3.76	119.68	111.54
6	D	552	F43	C7D-CHD-C4C	3.71	129.52	121.76
6	A	1	F43	O7C-C6C-C5C	-3.64	111.66	122.84
6	D	552	F43	C2B-C3B-C4B	3.55	105.61	101.64
5	D	553[A]	TP7	CB-CA-N	3.36	118.81	111.54
6	D	552	F43	C4B-CHC-C1C	3.33	131.22	125.84
8	D	555[B]	SHT	OS2-SG2-OS3	3.26	119.56	111.40
8	D	555[B]	SHT	OS2-SG2-CD	3.24	112.34	106.00
8	D	555[B]	SHT	OS1-SG2-OS3	-3.16	103.55	113.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1	F43	C4A-NA-C1A	-3.08	104.89	109.08
6	A	1	F43	C6D-C7D-CHD	2.97	122.43	116.94
6	D	552	F43	O8D-C7D-CHD	-2.87	118.10	122.77
6	D	552	F43	C2B-C1B-NB	2.86	106.10	101.86
7	A	554[A]	COM	O1S-S2-C2	-2.84	102.43	106.73
6	A	1	F43	C3D-C4D-ND	2.83	106.74	102.34
6	D	552	F43	O7C-C6C-C5C	-2.80	114.23	122.84
5	A	553[A]	TP7	C2-C1-N	2.77	120.75	115.86
6	A	1	F43	O8D-C7D-C6D	-2.76	116.34	120.87
6	A	1	F43	C9B-C2B-C3B	2.67	119.70	112.91
6	D	552	F43	C3A-C2A-C1A	2.66	102.64	99.97
6	D	552	F43	CAB-C3B-C2B	-2.63	113.20	119.00
5	A	553[A]	TP7	O4P-P-O1P	-2.61	100.04	109.33
8	A	555[B]	SHT	CK1-CK-N	2.58	119.02	114.61
8	A	555[B]	SHT	OS2-SG2-OS1	-2.55	105.03	111.40
5	A	553[A]	TP7	C-CA-N	-2.52	104.64	110.17
6	D	552	F43	ODB-CCB-CBB	-2.52	115.11	123.09
5	A	553[A]	TP7	CA-N-C1	2.51	126.76	121.80
6	A	1	F43	CHA-C4D-C3D	-2.50	110.84	117.90
6	D	552	F43	OBC-CAC-C9C	2.49	121.87	114.00
6	A	1	F43	C9B-C2B-C8B	-2.48	104.37	110.61
5	D	553[A]	TP7	O4P-P-O1P	-2.46	100.55	109.33
6	D	552	F43	O8C-C6C-C5C	2.39	121.43	114.00
6	A	1	F43	O8C-C6C-C5C	2.38	121.40	114.00
6	A	1	F43	C3B-C4B-CHC	-2.38	118.27	123.33
6	D	552	F43	OEB-CCB-ODB	2.30	129.24	123.33
8	D	555[B]	SHT	CA-N-CK	-2.27	118.51	121.86
6	D	552	F43	C2B-C1B-N5B	-2.27	98.31	105.72
6	D	552	F43	OCD-CAD-OB	-2.23	117.61	123.33
6	D	552	F43	O8D-C7D-C6D	-2.19	117.28	120.87
8	A	555[B]	SHT	P-O3'-CB	-2.18	117.40	123.33
6	D	552	F43	OCC-CAC-C9C	-2.16	116.25	123.09
6	A	1	F43	C2D-C1D-CHD	2.15	124.52	121.85
6	D	552	F43	C2C-C5C-C6C	-2.14	109.95	113.95
12	C	1	PEG	C3-O2-C2	2.13	122.60	113.26
6	D	552	F43	C3D-C2D-C1D	-2.12	98.73	102.47
6	D	552	F43	C6D-C5D-C2D	-2.12	107.21	111.45
8	D	555[B]	SHT	O3'-P-O1P	-2.10	101.86	109.33
6	A	1	F43	C9A-C2A-C3A	2.09	116.00	112.99
5	D	553[A]	TP7	OXT-C-CA	-2.07	114.97	121.86
5	A	553[A]	TP7	O1-C1-N	-2.01	119.55	122.95
6	D	552	F43	C5C-C2C-C3C	-2.01	110.09	115.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	552	F43	OCD-CAD-C9D	2.01	120.23	114.00

There are no chirality outliers.

All (36) torsion outliers are listed below:

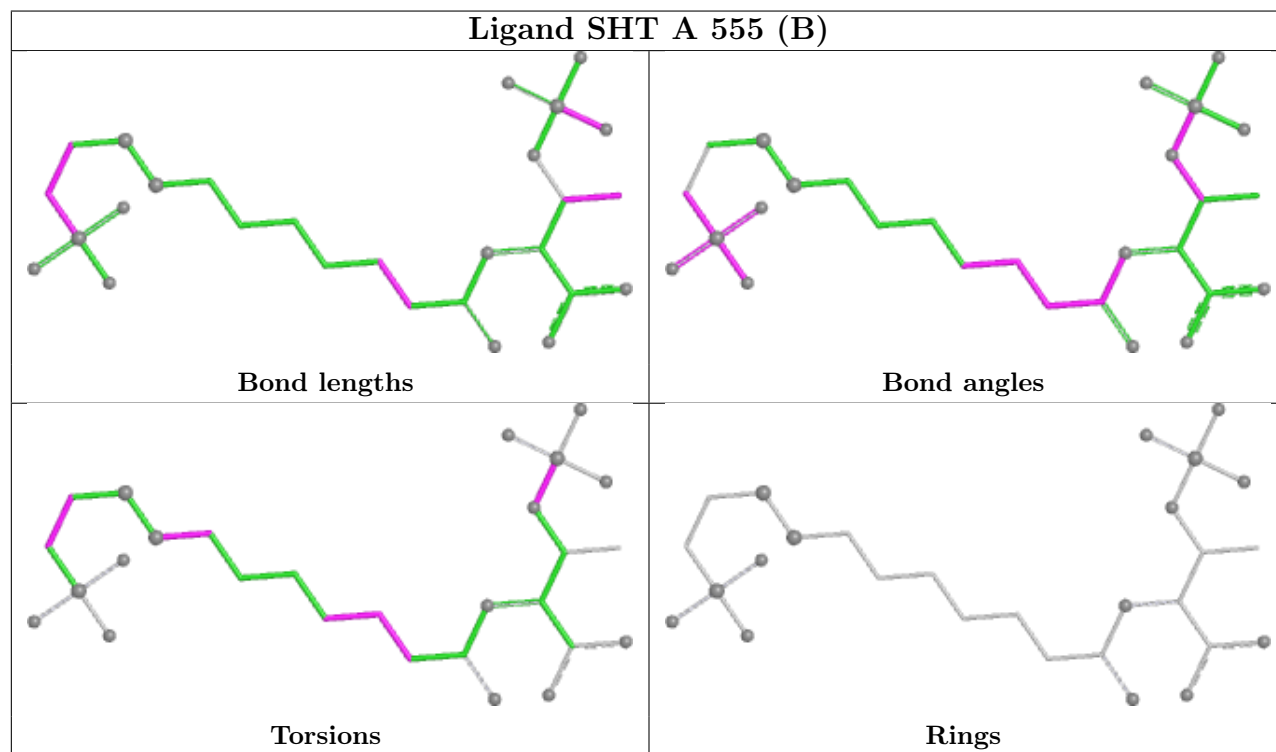
Mol	Chain	Res	Type	Atoms
8	A	555[B]	SHT	S1-CC-CD-SG2
8	A	555[B]	SHT	CK-CK1-CK2-CK3
8	D	555[B]	SHT	CK-CK1-CK2-CK3
6	A	1	F43	C3A-CAA-CBA-CCA
6	D	552	F43	C3A-CAA-CBA-CCA
10	B	445	EDO	O1-C1-C2-O2
10	D	556	EDO	O1-C1-C2-O2
10	F	251	EDO	O1-C1-C2-O2
10	F	1	EDO	O1-C1-C2-O2
8	A	555[B]	SHT	CK1-CK2-CK3-CK4
8	D	555[B]	SHT	CK1-CK2-CK3-CK4
10	A	557	EDO	O1-C1-C2-O2
5	D	553[A]	TP7	C2-C3-C4-C5
8	A	555[B]	SHT	CK5-CK6-SK-S1
8	D	555[B]	SHT	CK5-CK6-SK-S1
6	D	552	F43	C2C-C5C-C6C-O8C
6	D	552	F43	CAA-CBA-CCA-OEA
6	A	1	F43	C2C-C5C-C6C-O8C
6	A	1	F43	CAA-CBA-CCA-OEA
6	A	1	F43	CAB-CBB-CCB-OEB
6	A	1	F43	CAA-CBA-CCA-ODA
6	D	552	F43	CAB-CBB-CCB-OEB
6	D	552	F43	CAA-CBA-CCA-ODA
6	D	552	F43	CAB-CBB-CCB-ODB
5	A	553[A]	TP7	C2-C3-C4-C5
6	D	552	F43	C8C-C9C-CAC-OBC
6	A	1	F43	CAB-CBB-CCB-ODB
6	D	552	F43	C8C-C9C-CAC-OCC
5	A	553[A]	TP7	CB-O4P-P-O3P
8	A	555[B]	SHT	CB-O3'-P-O8P
6	A	1	F43	C2C-C5C-C6C-O7C
6	D	552	F43	C2C-C5C-C6C-O7C
6	D	552	F43	C3D-C9D-CAD-OCD
6	A	1	F43	C3D-C9D-CAD-OB
6	A	1	F43	C3D-C9D-CAD-OCD
6	A	1	F43	C8C-C9C-CAC-OCC

There are no ring outliers.

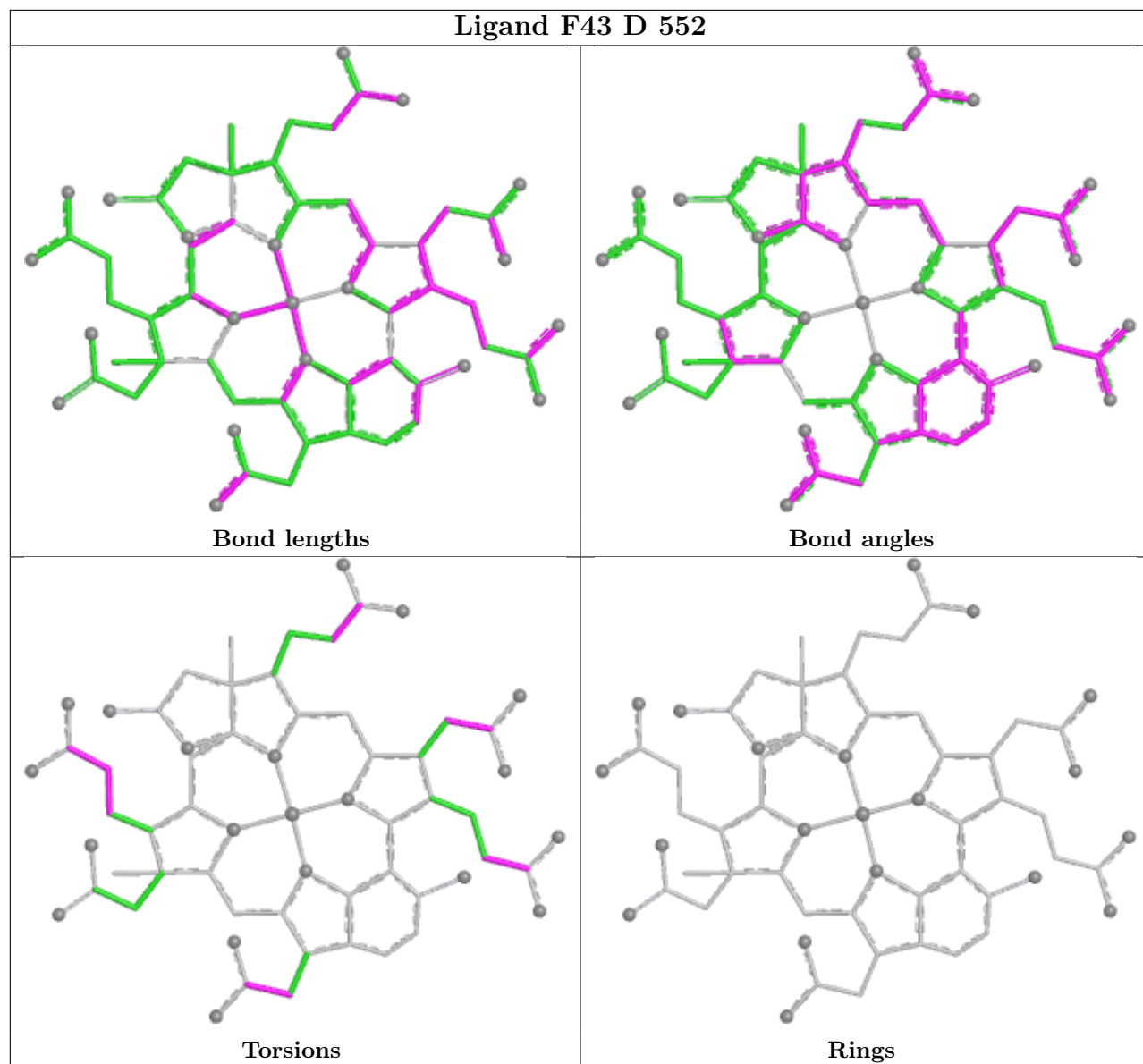
5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	554[A]	COM	1	0
6	D	552	F43	1	0
6	A	1	F43	2	0
8	D	555[B]	SHT	1	0
10	D	556	EDO	1	0

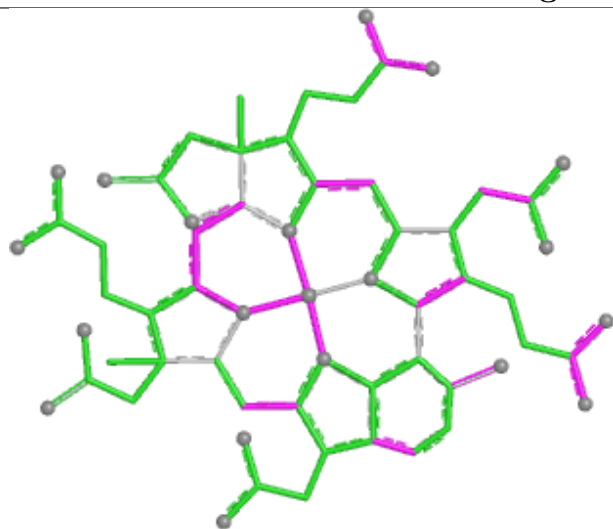
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



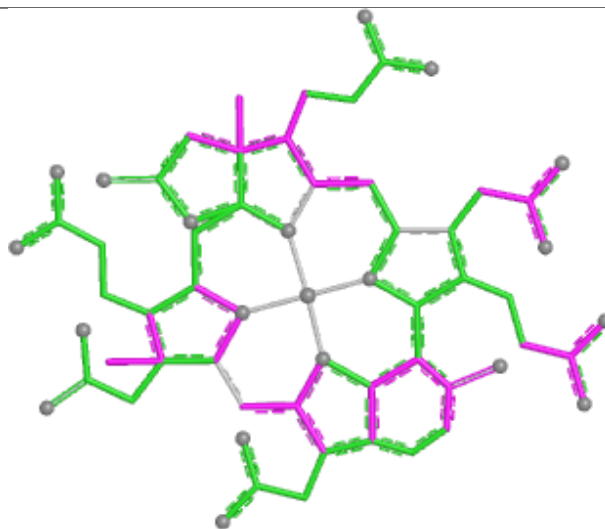
Ligand F43 D 552



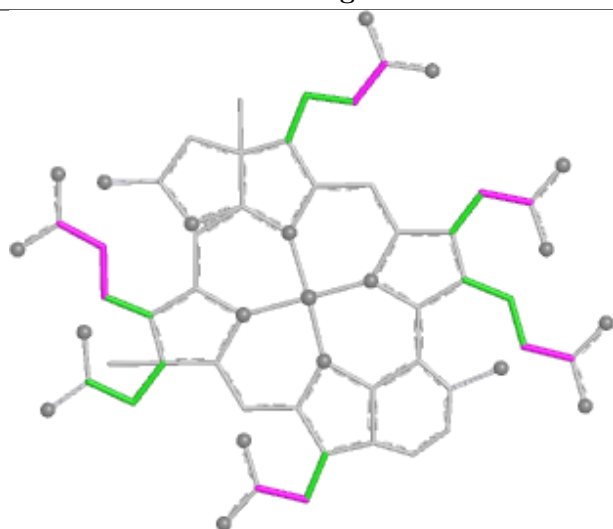
Ligand F43 A 1



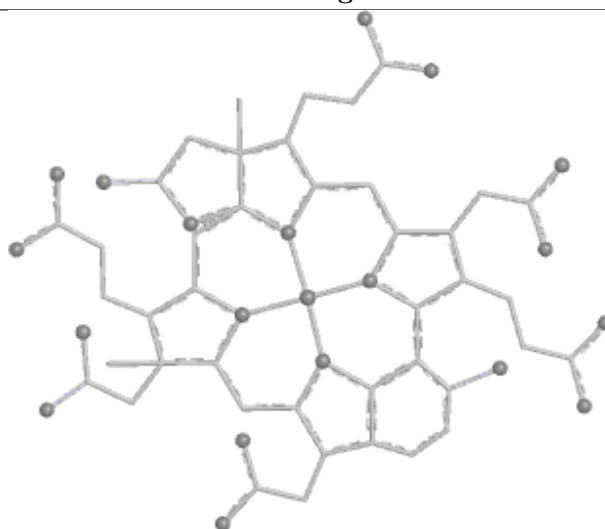
Bond lengths



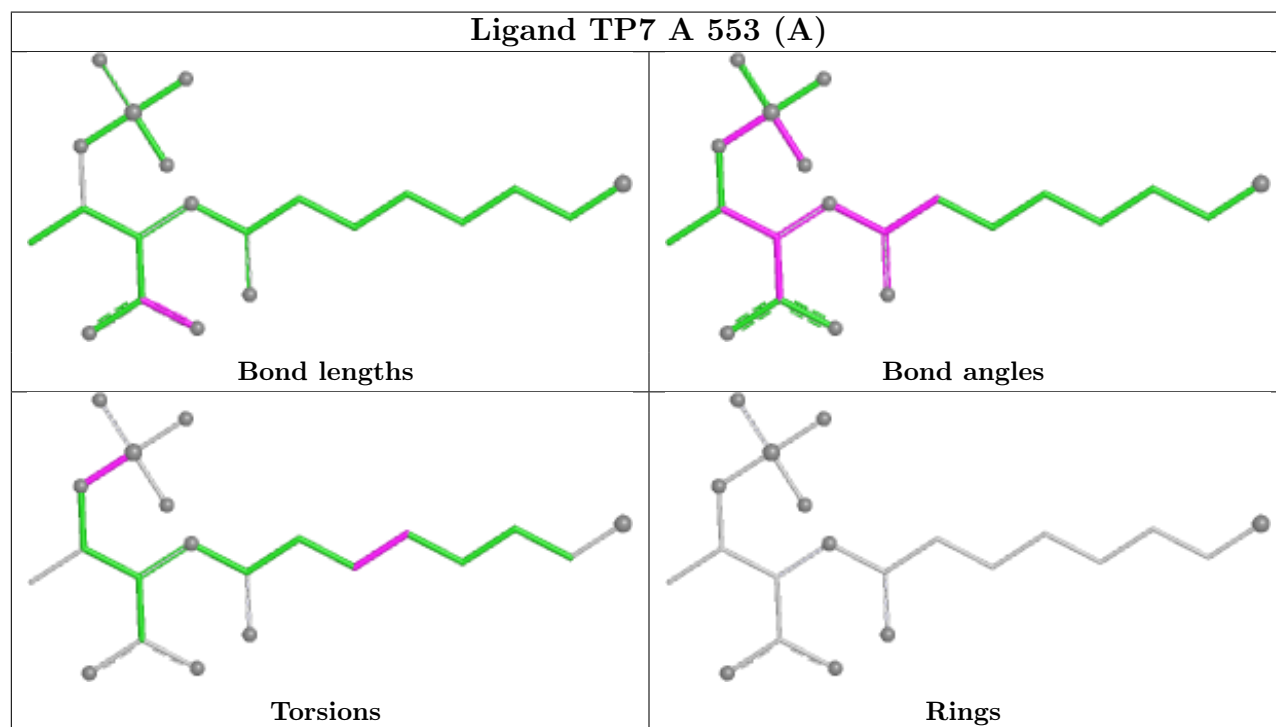
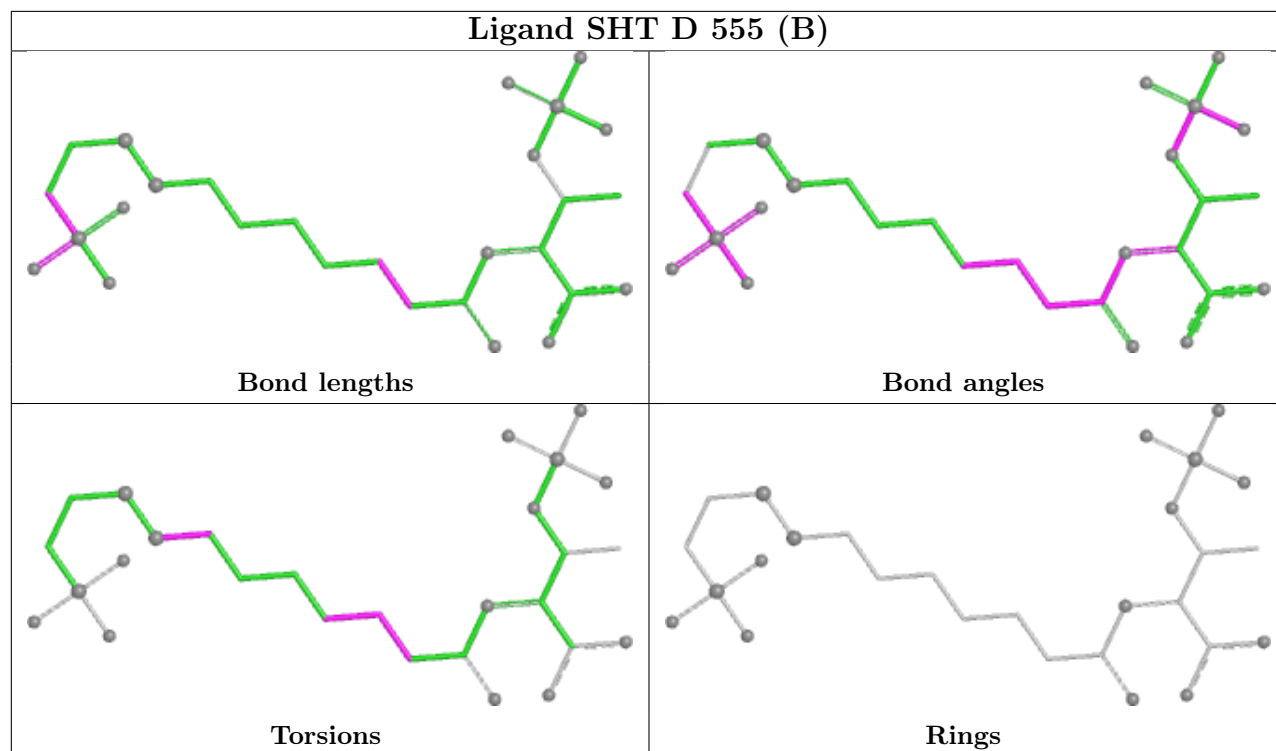
Bond angles

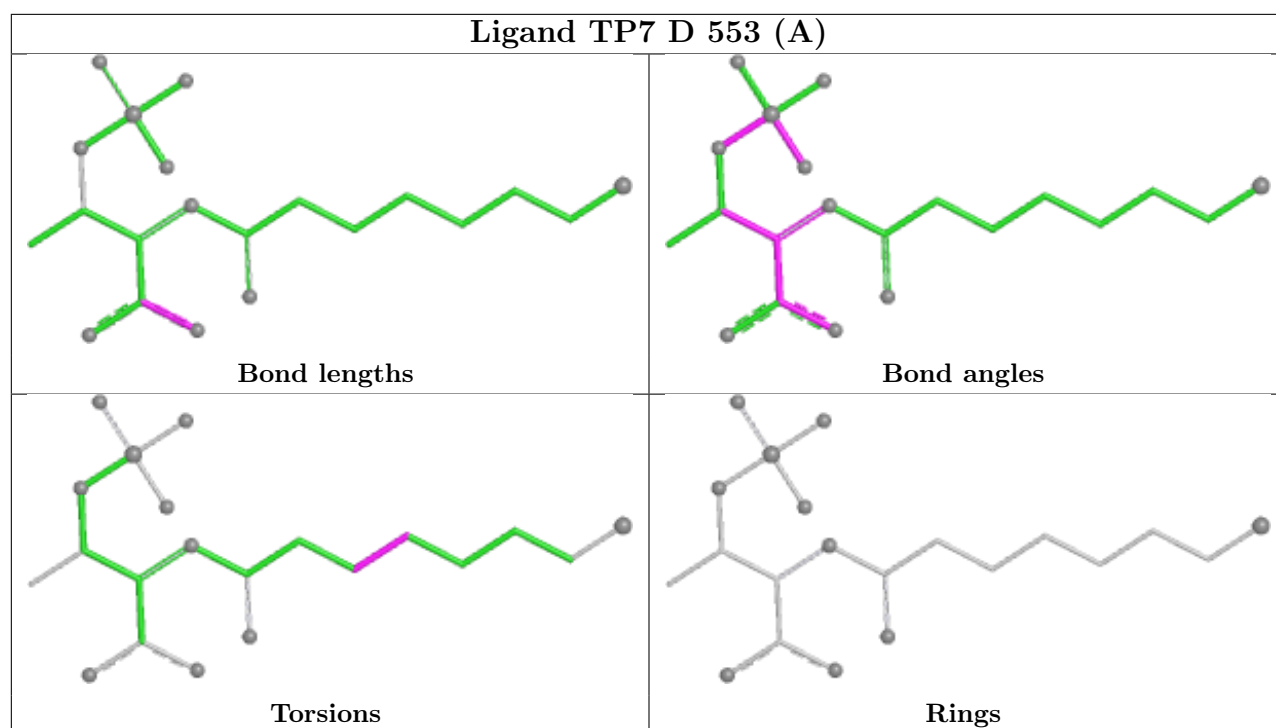


Torsions



Rings





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	543/549 (98%)	-0.44	2 (0%) 88 93	4, 9, 20, 33	27 (4%)
1	D	543/549 (98%)	-0.43	6 (1%) 78 86	4, 10, 20, 37	22 (4%)
2	B	442/442 (100%)	-0.32	3 (0%) 84 90	5, 12, 19, 35	24 (5%)
2	E	442/442 (100%)	-0.24	4 (0%) 81 88	5, 12, 23, 40	25 (5%)
3	C	247/248 (99%)	-0.01	9 (3%) 46 57	6, 14, 32, 47	10 (4%)
3	F	246/248 (99%)	0.03	7 (2%) 55 64	5, 14, 30, 53	20 (8%)
All	All	2463/2478 (99%)	-0.29	31 (1%) 75 84	4, 11, 23, 53	128 (5%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	60	ASP	3.8
1	D	2	ALA	3.7
3	F	45	PRO	3.7
3	C	248	LEU	3.3
3	C	45	PRO	3.2
2	E	97	GLU	3.0
2	B	98	ASP	2.9
1	D	549	ALA	2.8
3	F	62	PRO	2.8
1	D	24	THR	2.6
3	C	181	THR	2.6
3	C	59	MET	2.6
1	D	61	GLY	2.6
3	F	59	MET	2.5
2	E	21	GLN	2.5
3	C	44	ALA	2.5
3	C	180	ASP	2.4
3	C	60	ASP	2.3
3	C	247	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	356	ASP	2.2
1	A	27	THR	2.1
3	F	46	GLY	2.1
3	F	44	ALA	2.1
2	B	118	SER	2.1
2	E	441	ASN	2.1
3	C	62	PRO	2.1
3	F	57	GLU	2.1
1	A	61	GLY	2.1
1	D	118	LYS	2.1
2	E	17	LEU	2.0
2	B	108	GLY	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	MHS	A	257	11/12	0.97	0.06	8,10,14,17	0
1	MHS	D	257	11/12	0.97	0.05	9,10,12,16	0
1	AGM	D	271	12/13	0.97	0.05	6,7,7,8	0
1	MGN	A	400	10/11	0.98	0.04	7,8,9,10	0
1	AGM	A	271	12/13	0.99	0.03	6,6,7,8	0
1	SMC	A	452	7/8	0.99	0.04	7,7,9,10	0
1	MGN	D	400	10/11	0.99	0.04	6,8,8,8	0
1	SMC	D	452	7/8	0.99	0.04	7,8,9,11	0
1	GL3	D	445	4/5	1.00	0.02	6,6,7,7	0
1	GL3	A	445	4/5	1.00	0.04	6,7,7,8	0

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,

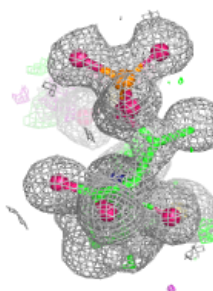
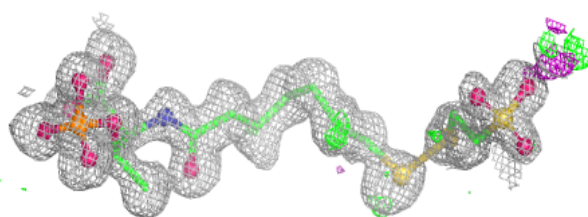
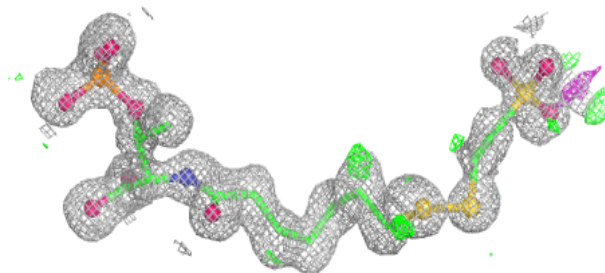
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	EDO	D	556	4/4	0.89	0.10	32,38,40,44	0
12	PEG	C	1	7/7	0.90	0.14	34,38,42,42	0
10	EDO	F	1	4/4	0.91	0.09	38,39,39,39	0
10	EDO	A	557	4/4	0.91	0.11	30,35,39,42	0
10	EDO	B	445	4/4	0.92	0.10	42,42,43,46	0
10	EDO	F	251	4/4	0.92	0.11	39,42,43,48	0
4	MG	B	444	1/1	0.95	0.13	23,23,23,23	0
4	MG	D	1	1/1	0.96	0.14	20,20,20,20	0
9	ACT	A	556[B]	4/4	0.96	0.07	15,16,17,19	4
4	MG	C	250	1/1	0.97	0.09	17,17,17,17	0
4	MG	B	1[B]	1/1	0.98	0.05	21,21,21,21	1
4	MG	A	552[B]	1/1	0.98	0.09	14,14,14,14	1
4	MG	A	551[A]	1/1	0.98	0.10	18,18,18,18	1
4	MG	E	444	1/1	0.98	0.14	22,22,22,22	0
4	MG	F	250	1/1	0.98	0.06	16,16,16,16	0
7	COM	D	554[A]	7/7	0.98	0.05	6,9,10,10	7
8	SHT	A	555[B]	28/28	0.98	0.05	6,7,12,14	28
5	TP7	D	553[A]	21/21	0.99	0.03	4,6,8,8	21
6	F43	A	1	62/62	0.99	0.04	6,8,11,13	0
6	F43	D	552	62/62	0.99	0.03	6,8,11,12	0
7	COM	A	554[A]	7/7	0.99	0.06	8,9,12,12	7
4	MG	D	551	1/1	0.99	0.14	18,18,18,18	0
5	TP7	A	553[A]	21/21	0.99	0.04	5,7,7,8	21
11	ZN	A	558	1/1	0.99	0.04	10,10,10,10	1
8	SHT	D	555[B]	28/28	0.99	0.04	6,7,11,13	28

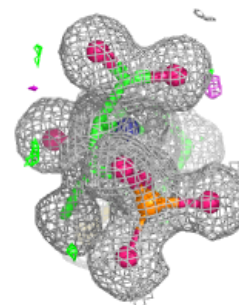
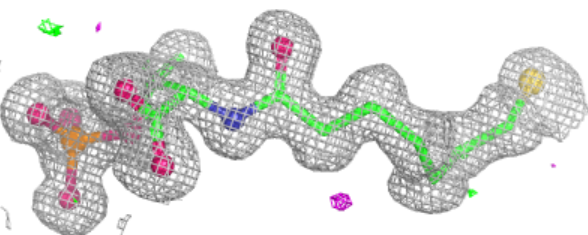
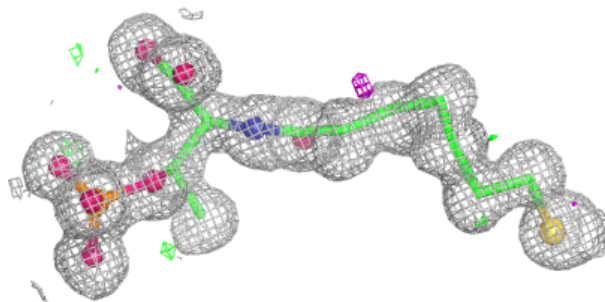
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SHT A 555 (B):

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

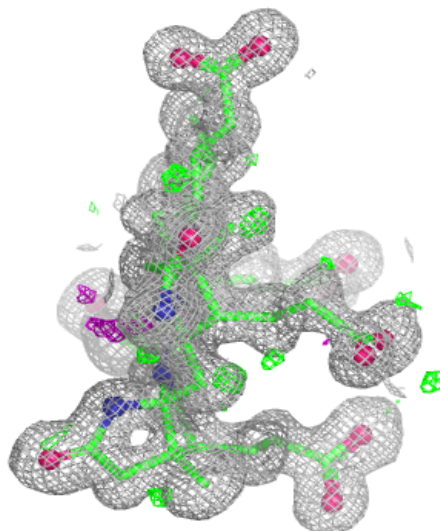
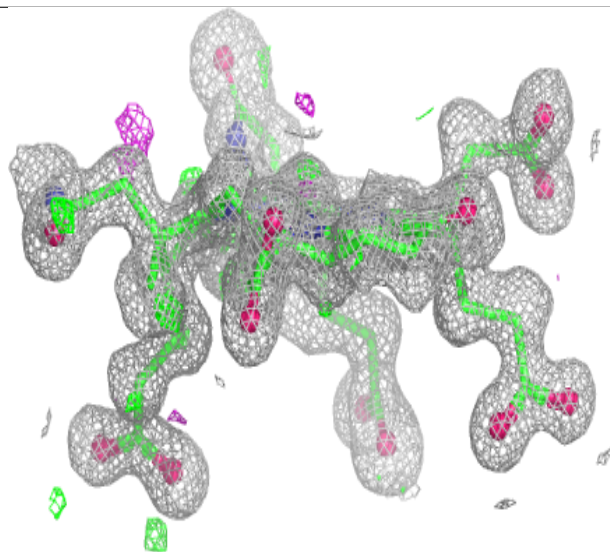
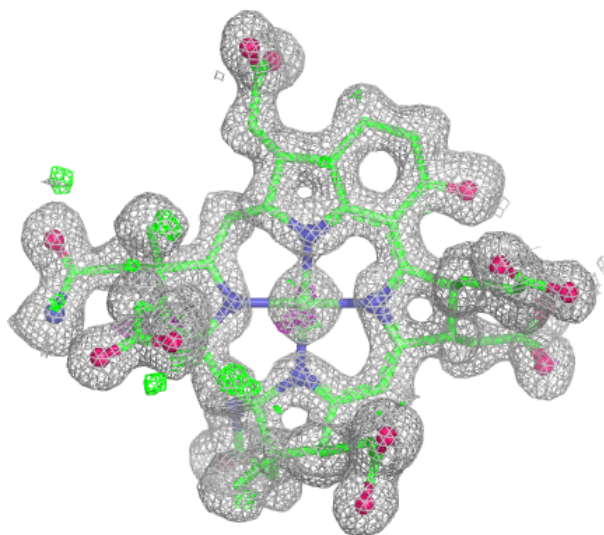
**Electron density around TP7 D 553 (A):**

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



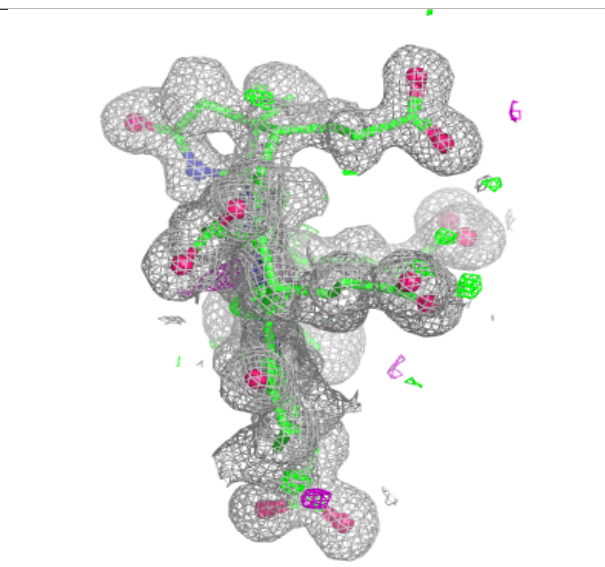
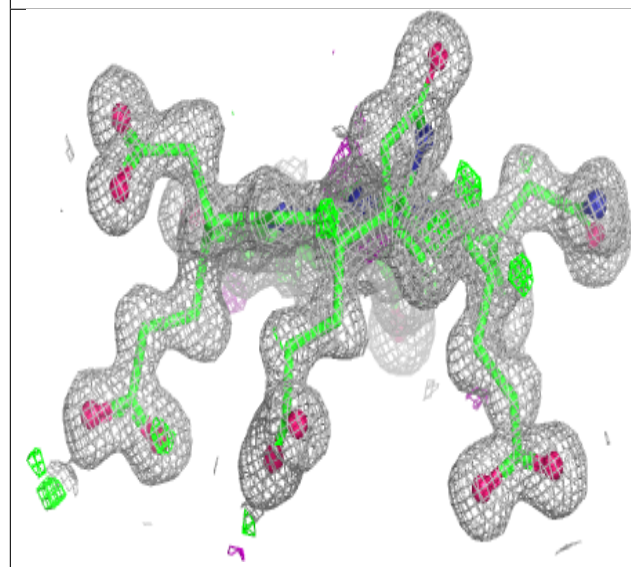
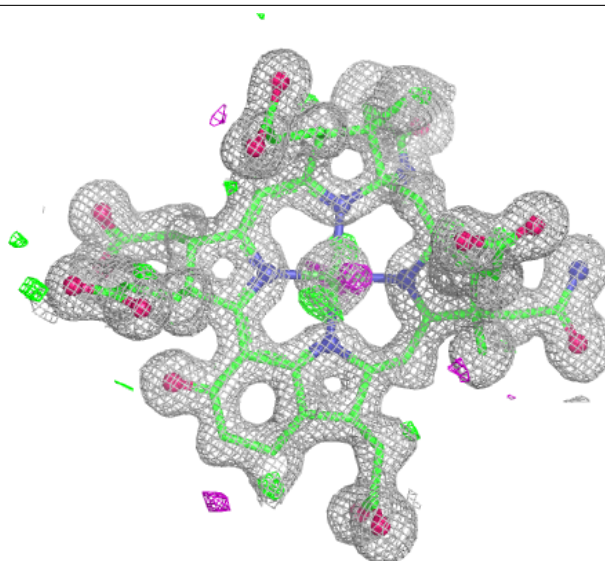
Electron density around F43 A 1:

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



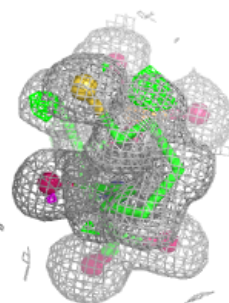
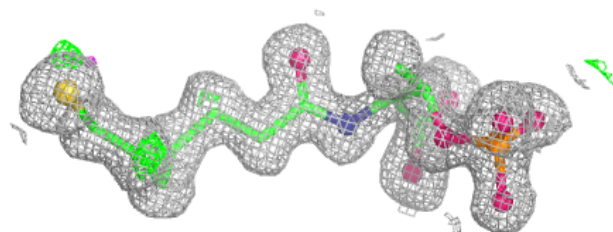
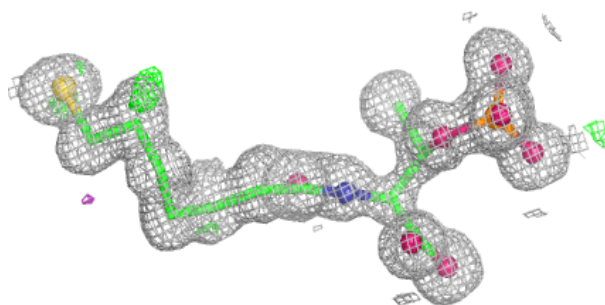
Electron density around F43 D 552:

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

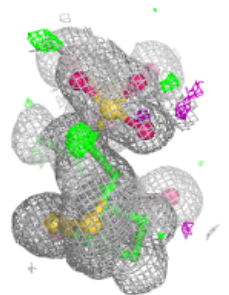
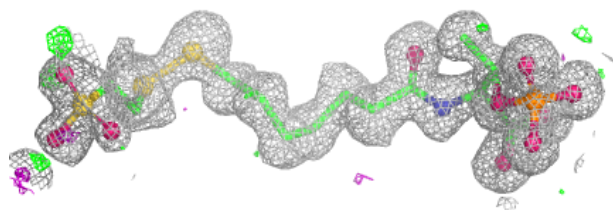
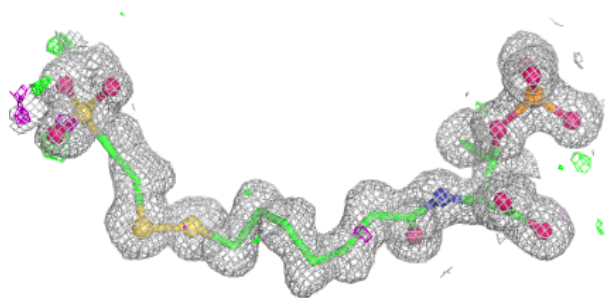


Electron density around TP7 A 553 (A):

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

**Electron density around SHT D 555 (B):**

$2mF_o-DF_c$ (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.