



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:08 PM UTC

PDB ID : 3M2U / pdb_00003m2u
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 : 1.40 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

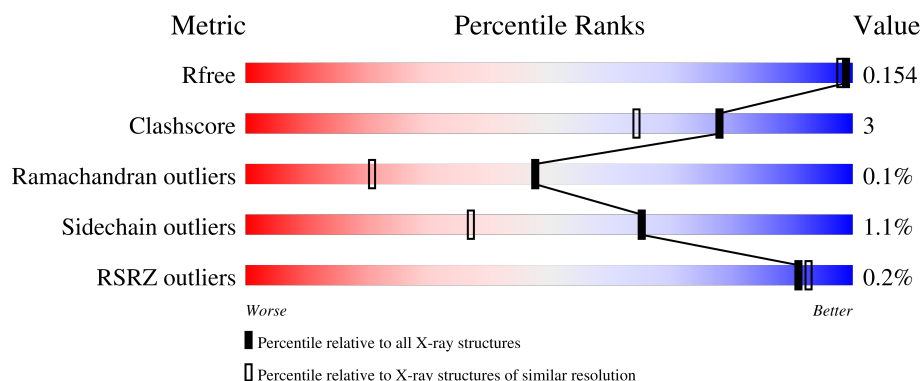
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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	 83% 15% .
1	D	549	 82% 17% .
2	B	442	 85% 14% .
2	E	442	 79% 20% .
3	C	248	 79% 19% ..

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Mol	Chain	Length	Quality of chain
3	F	248	% 81% 15% ..

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 22594 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	31	0
			4446	2817	734	874	21			
1	D	548	Total	C	N	O	S	0	28	0
			4410	2799	724	867	20			

- 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
			3464	2212	563	666	23			
2	E	442	Total	C	N	O	S	0	34	0
			3527	2250	571	683	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	246	Total	C	N	O	S	0	14	0
			2072	1287	359	412	14			
3	F	246	Total	C	N	O	S	0	10	0
			2041	1268	356	404	13			

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

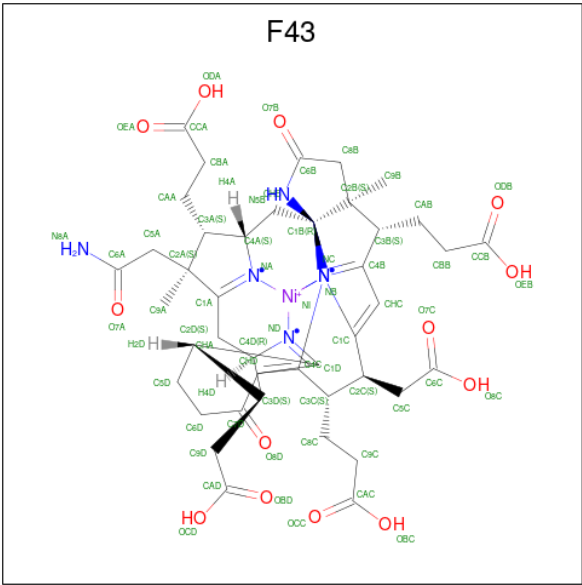
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	2
			2	2		
4	B	2	Total	Mg	0	1
			2	2		
4	C	1	Total	Mg	0	0
			1	1		
4	D	3	Total	Mg	0	0
			3	3		

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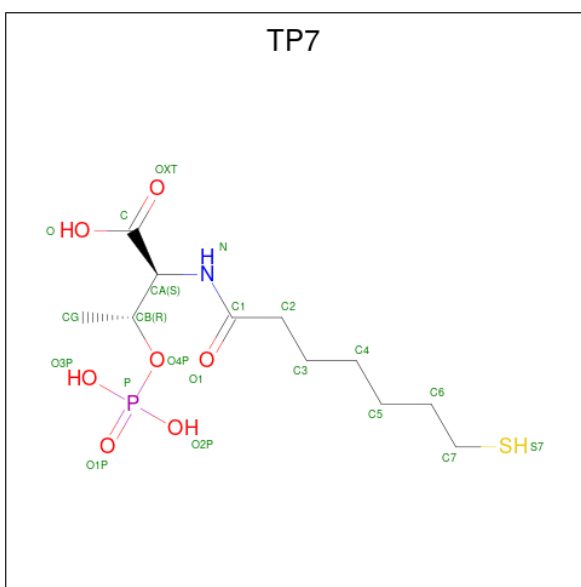
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	2	Total	Mg	0	1
			2	2		
4	F	1	Total	Mg	0	0
			1	1		

- Molecule 5 is FACTOR 430 (CCD ID: F43) (formula: C₄₂H₅₁N₆NiO₁₃).



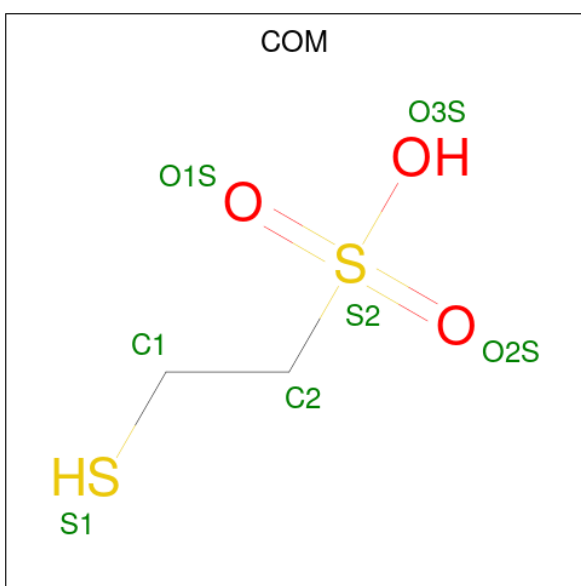
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		
5	D	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		

- Molecule 6 is Coenzyme B (CCD ID: TP7) (formula: C₁₁H₂₂NO₇PS).



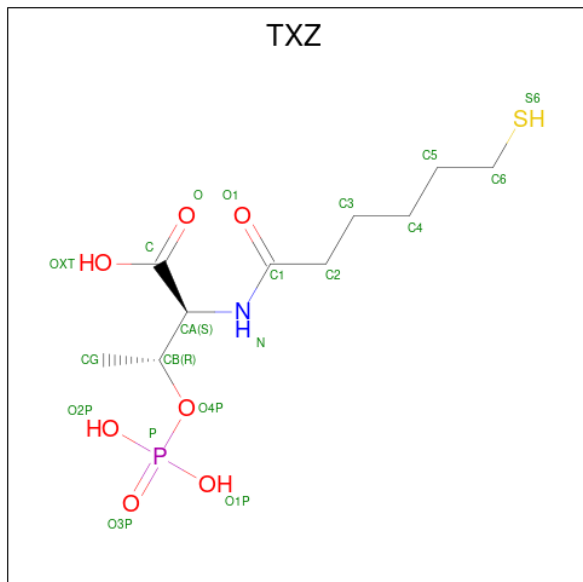
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	S	0	1
			21	11	1	7	1	1		
6	D	1	Total	C	N	O	P	S	0	1
			21	11	1	7	1	1		

- Molecule 7 is 1-THIOETHANESULFONIC ACID (CCD ID: COM) (formula: $C_2H_6O_3S_2$).



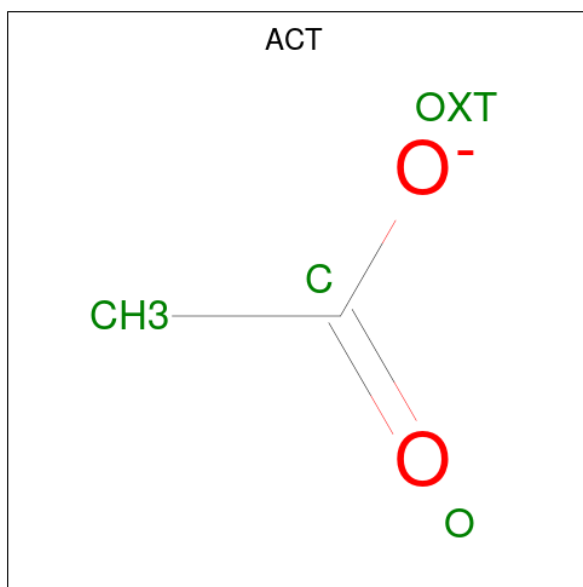
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	S	0	1
			7	2	3	2		
7	D	1	Total	C	O	S	0	1
			7	2	3	2		

- Molecule 8 is O-phosphono-N-(6-sulfanylhexanoyl)-L-threonine (CCD ID: TXZ) (formula: $C_{10}H_{20}NO_7PS$).



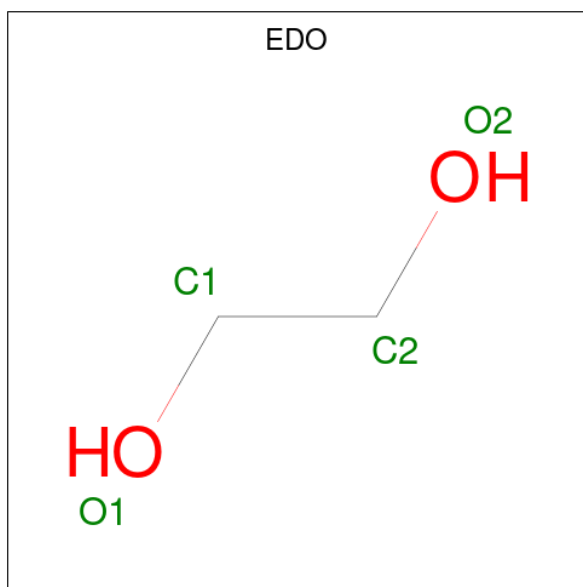
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	S	0	1
			20	10	1	7	1	1		
8	D	1	Total	C	N	O	P	S	0	1
			20	10	1	7	1	1		

- Molecule 9 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



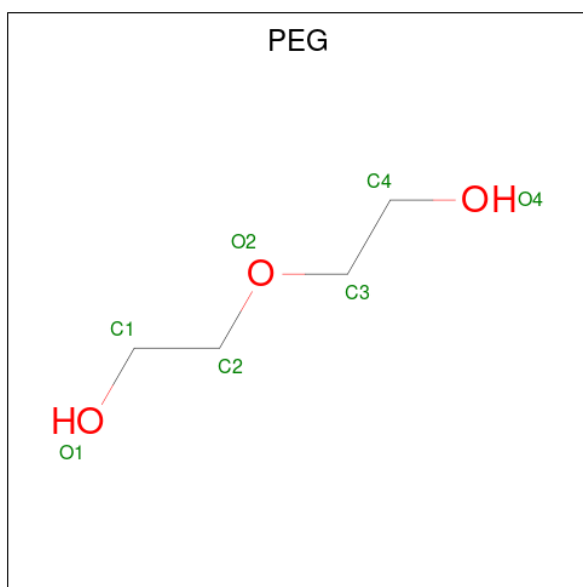
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	1
			4	2	2		
9	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			4	2	2		
10	A	1	Total	C	O	0	0
			4	2	2		
10	C	1	Total	C	O	0	0
			4	2	2		
10	D	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 DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

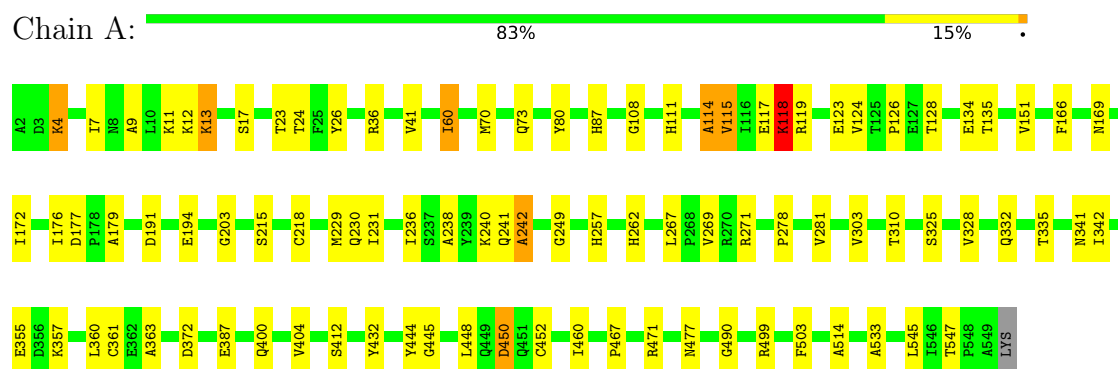
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	482	Total	O	0	24
			491	491		
13	B	436	Total	O	0	26
			454	454		
13	C	245	Total	O	0	15
			255	255		
13	D	488	Total	O	0	23
			502	502		
13	E	393	Total	O	0	11
			400	400		
13	F	246	Total	O	0	10
			250	250		

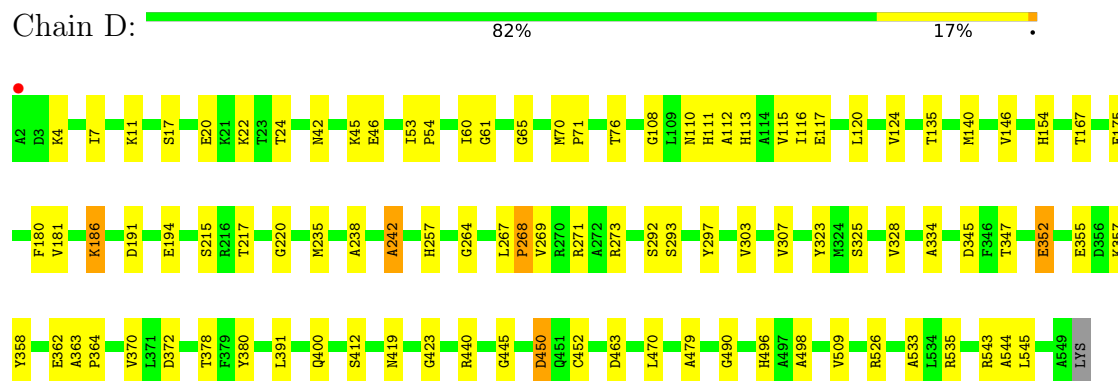
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

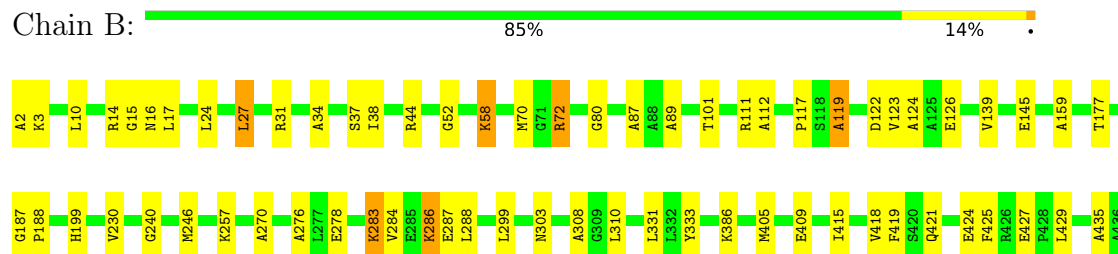
- Molecule 1: Methyl-coenzyme M reductase I subunit alpha



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



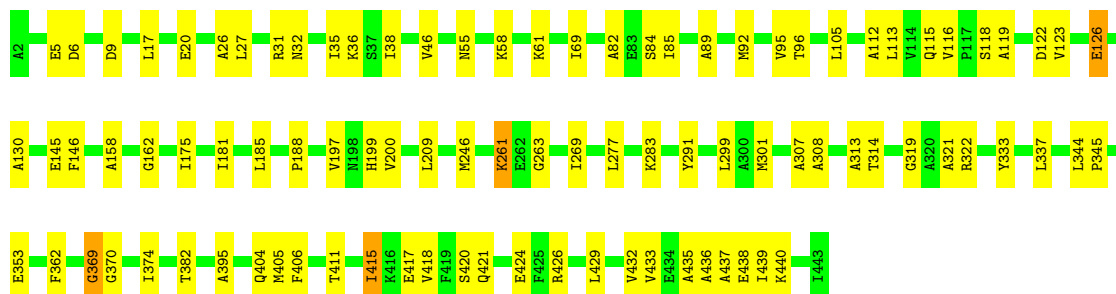
- Molecule 2: Methyl-coenzyme M reductase I subunit beta





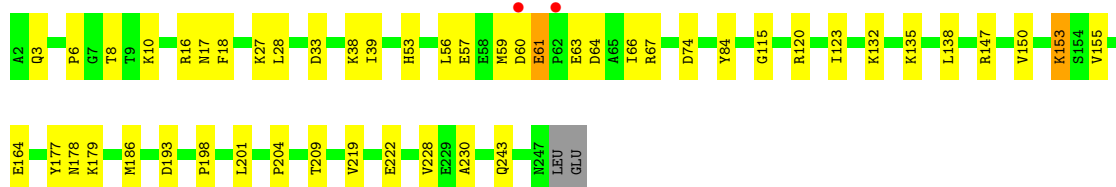
- Molecule 2: Methyl-coenzyme M reductase I subunit beta

Chain E: 79% 20%



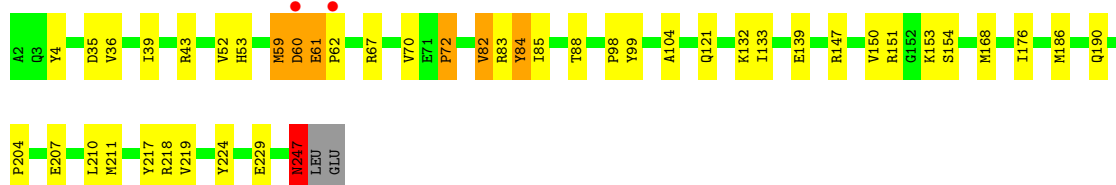
- Molecule 3: Methyl-coenzyme M reductase I subunit gamma

Chain C: 79% 19%



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

Chain F: 81% 15%



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)	19.89 – 1.40 19.89 – 1.40	Depositor EDS
% Data completeness (in resolution range)	98.5 (19.89-1.40) 98.5 (19.89-1.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.77 (at 1.40Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.130 , 0.155 0.129 , 0.154	Depositor DCC
R_{free} test set	22348 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	11.7	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.007 for -h,-l,-k 0.013 for h,-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	22594	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 3.36% 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, MG, PEG, ZN, SMC, MHS, TXZ, MGN, EDO, ACT, TP7, AGM, GL3, F43

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	1.84	56/4555 (1.2%)	1.47	21/6181 (0.3%)
1	D	1.87	62/4531 (1.4%)	1.51	19/6148 (0.3%)
2	B	1.86	45/3580 (1.3%)	1.47	11/4841 (0.2%)
2	E	1.88	61/3656 (1.7%)	1.51	16/4943 (0.3%)
3	C	1.92	34/2143 (1.6%)	1.50	8/2885 (0.3%)
3	F	1.95	28/2105 (1.3%)	1.55	8/2833 (0.3%)
All	All	1.88	286/20570 (1.4%)	1.50	83/27831 (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
2	B	0	2
2	E	0	1
All	All	2	4

All (286) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	269	VAL	CA-CB	10.35	1.67	1.54
1	D	269	VAL	CA-CB	9.23	1.68	1.54
2	B	286	LYS	N-CA	8.94	1.56	1.46
1	D	111	HIS	CA-C	-8.78	1.41	1.52
2	B	117	PRO	C-O	8.71	1.33	1.23
1	D	117	GLU	N-CA	8.27	1.56	1.46
2	B	284	VAL	C-O	8.16	1.32	1.24
2	B	3	LYS	CD-CE	-8.06	1.28	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	72	PRO	C-O	8.06	1.32	1.23
3	C	6	PRO	N-CA	7.86	1.54	1.46
2	B	58	LYS	CB-CG	-7.84	1.28	1.52
1	D	264	GLY	N-CA	7.73	1.53	1.45
2	B	87	ALA	CA-CB	7.56	1.65	1.53
2	E	321	ALA	CA-CB	7.51	1.66	1.53
1	A	117	GLU	N-CA	7.49	1.55	1.46
3	C	198	PRO	C-O	7.41	1.32	1.23
1	A	450	ASP	CA-C	-7.38	1.43	1.52
3	C	153	LYS	CE-NZ	7.31	1.71	1.49
2	E	175	ILE	C-O	7.28	1.31	1.23
2	E	437	ALA	N-CA	7.27	1.55	1.46
3	F	70	VAL	CA-CB	7.26	1.62	1.53
2	E	145	GLU	C-O	7.22	1.32	1.24
2	B	145	GLU	C-O	7.21	1.32	1.24
1	D	11	LYS	CA-C	-7.19	1.43	1.52
2	B	38	ILE	C-O	7.17	1.32	1.24
2	E	435	ALA	CA-CB	7.16	1.64	1.53
2	B	435	ALA	CA-CB	7.13	1.64	1.53
3	C	8	THR	N-CA	7.05	1.54	1.46
1	A	310	THR	N-CA	7.04	1.54	1.46
2	B	278	GLU	C-O	7.03	1.32	1.24
3	C	243	GLN	CA-C	-6.98	1.43	1.52
1	A	60	ILE	CA-C	6.98	1.61	1.52
3	C	10	LYS	CA-C	6.93	1.61	1.52
2	B	159	ALA	CA-CB	6.89	1.64	1.53
1	A	342	ILE	CA-CB	-6.87	1.45	1.54
3	F	39	ILE	N-CA	6.86	1.54	1.46
1	D	242	ALA	C-O	6.82	1.32	1.23
1	A	13[A]	LYS	CA-C	-6.81	1.43	1.52
1	A	13[B]	LYS	CA-C	-6.81	1.43	1.52
1	D	4	LYS	CG-CD	-6.75	1.32	1.52
1	D	544	ALA	CA-CB	6.75	1.63	1.53
1	A	124	VAL	C-O	6.71	1.31	1.24
3	C	209	THR	CA-C	6.65	1.61	1.52
2	E	263	GLY	N-CA	6.65	1.53	1.45
2	E	69	ILE	CA-C	6.62	1.60	1.52
2	B	409	GLU	C-O	6.57	1.31	1.24
1	D	450	ASP	CA-CB	-6.53	1.43	1.53
1	D	533	ALA	N-CA	6.51	1.54	1.46
2	E	291	TYR	N-CA	6.48	1.53	1.46
3	F	82	VAL	N-CA	6.48	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	112	ALA	C-O	6.48	1.31	1.24
2	E	130	ALA	C-O	6.41	1.30	1.24
1	A	60	ILE	CA-CB	6.40	1.62	1.54
3	C	138	LEU	CA-C	6.40	1.61	1.52
3	F	36	VAL	N-CA	6.40	1.54	1.46
2	E	308	ALA	CA-CB	6.36	1.63	1.53
3	F	247	ASN	CA-CB	6.36	1.66	1.53
3	F	52	VAL	CA-CB	6.35	1.62	1.54
1	D	146	VAL	N-CA	6.35	1.51	1.46
2	B	418	VAL	C-O	6.29	1.30	1.23
3	F	218	ARG	CZ-NH1	6.25	1.41	1.32
1	D	76	THR	N-CA	6.24	1.54	1.46
2	B	119	ALA	CA-CB	-6.22	1.43	1.53
2	B	437	ALA	C-O	6.21	1.31	1.24
2	E	85	ILE	N-CA	6.19	1.53	1.46
2	E	415[A]	ILE	CA-CB	6.19	1.62	1.54
2	E	415[B]	ILE	CA-CB	6.19	1.62	1.54
1	A	514	ALA	CA-CB	6.16	1.60	1.52
1	A	60	ILE	C-N	-6.13	1.22	1.33
3	F	224	TYR	CA-CB	6.13	1.62	1.53
2	E	32	ASN	C-O	6.12	1.31	1.24
1	D	215	SER	C-O	6.11	1.31	1.24
2	B	72	ARG	CA-CB	6.10	1.63	1.53
1	D	297	TYR	C-O	6.07	1.31	1.24
2	E	269	ILE	CA-C	6.07	1.60	1.52
2	B	89	ALA	C-N	6.05	1.41	1.33
2	E	322[A]	ARG	C-N	6.05	1.41	1.33
2	E	322[B]	ARG	C-N	6.05	1.41	1.33
2	B	101	THR	C-O	6.03	1.31	1.23
1	D	112	ALA	CA-C	6.02	1.60	1.52
2	E	26	ALA	CA-CB	6.02	1.63	1.53
1	D	378	THR	N-CA	6.02	1.53	1.46
1	D	60	ILE	CA-C	6.01	1.59	1.52
1	A	460	ILE	CA-CB	6.01	1.61	1.54
2	E	96	THR	N-CA	6.00	1.53	1.46
1	A	114	ALA	C-O	6.00	1.31	1.24
3	C	204	PRO	N-CA	5.99	1.54	1.47
1	D	60	ILE	CA-CB	5.96	1.61	1.54
3	C	153	LYS	C-O	5.95	1.30	1.23
1	A	134	GLU	CD-OE1	5.93	1.36	1.25
2	E	404	GLN	C-O	5.93	1.30	1.23
2	B	2	ALA	N-CA	5.92	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	110	ASN	N-CA	5.91	1.53	1.46
1	D	146	VAL	CA-C	-5.90	1.46	1.52
2	B	240	GLY	N-CA	5.90	1.53	1.45
1	A	203	GLY	N-CA	5.88	1.52	1.45
1	D	391	LEU	C-O	5.87	1.31	1.24
1	D	54	PRO	CA-C	5.86	1.59	1.52
1	A	11	LYS	N-CA	5.85	1.53	1.46
3	F	133	ILE	C-O	5.85	1.31	1.24
3	F	190	GLN	N-CA	5.84	1.53	1.46
3	F	210	LEU	N-CA	5.84	1.53	1.46
1	A	262	HIS	C-O	5.84	1.31	1.23
2	E	130	ALA	N-CA	5.83	1.51	1.46
3	F	84	TYR	N-CA	5.83	1.53	1.45
1	D	11	LYS	N-CA	5.83	1.53	1.46
3	F	99	TYR	CA-CB	5.82	1.62	1.53
2	E	411	THR	CA-CB	5.82	1.62	1.53
3	C	53	HIS	CA-CB	5.82	1.61	1.53
2	E	84	SER	CA-C	5.82	1.60	1.52
3	F	204	PRO	C-O	5.82	1.30	1.23
1	A	166	PHE	N-CA	5.80	1.53	1.45
1	D	53	ILE	CA-CB	5.80	1.61	1.54
2	E	200	VAL	C-O	5.79	1.31	1.24
1	D	235	MET	C-O	5.78	1.30	1.24
3	C	193	ASP	N-CA	5.77	1.53	1.46
1	A	404	VAL	N-CA	5.77	1.53	1.46
2	E	307	ALA	C-N	5.77	1.41	1.33
2	E	82	ALA	CA-C	-5.76	1.45	1.52
1	A	238	ALA	C-O	5.76	1.31	1.24
2	E	35	ILE	N-CA	5.76	1.53	1.46
1	D	440	ARG	N-CA	5.75	1.53	1.46
2	E	116	VAL	N-CA	-5.75	1.41	1.47
2	B	283	LYS	N-CA	5.73	1.53	1.45
3	C	60	ASP	CA-C	5.73	1.60	1.52
2	B	286	LYS	CA-CB	5.72	1.63	1.53
2	B	80	GLY	N-CA	5.72	1.53	1.45
1	D	362	GLU	N-CA	5.71	1.53	1.46
2	E	209	LEU	CA-CB	5.71	1.62	1.53
3	F	67	ARG	CZ-NH2	5.71	1.40	1.33
1	A	503	PHE	N-CA	5.70	1.53	1.45
1	A	151	VAL	C-O	5.68	1.30	1.24
1	A	115	VAL	C-O	5.68	1.30	1.24
2	E	436	ALA	C-O	-5.68	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	355	GLU	C-O	5.67	1.30	1.24
2	B	177	THR	N-CA	5.66	1.53	1.45
1	D	370	VAL	N-CA	5.63	1.53	1.46
2	E	126	GLU	C-O	5.63	1.31	1.24
1	A	203	GLY	CA-C	-5.62	1.47	1.52
3	C	123	ILE	C-O	5.62	1.29	1.24
3	F	60	ASP	CA-C	5.62	1.60	1.52
1	D	509	VAL	N-CA	5.62	1.53	1.46
2	B	10	LEU	CA-C	-5.61	1.46	1.52
2	E	418	VAL	CA-CB	5.61	1.62	1.54
2	E	9	ASP	C-O	5.61	1.30	1.23
2	B	27	LEU	N-CA	5.60	1.53	1.46
1	D	543	ARG	CB-CG	5.60	1.69	1.52
1	D	303	VAL	C-O	5.59	1.30	1.24
1	D	496	HIS	C-O	5.58	1.30	1.24
3	C	204	PRO	C-O	5.57	1.30	1.23
2	E	313	ALA	CA-CB	5.57	1.61	1.53
1	D	180	PHE	C-O	5.56	1.31	1.23
2	B	425	PHE	N-CA	5.53	1.53	1.46
1	D	479	ALA	N-CA	5.52	1.53	1.46
2	E	92	MET	C-O	5.52	1.30	1.24
1	D	71	PRO	C-O	5.51	1.30	1.23
2	B	16	ASN	N-CA	5.50	1.52	1.46
1	A	87	HIS	N-CA	5.50	1.52	1.46
1	A	123	GLU	C-O	5.48	1.30	1.23
1	D	419	ASN	CA-C	5.48	1.59	1.52
3	C	115	GLY	N-CA	5.47	1.51	1.45
1	A	36	ARG	CZ-NH1	5.47	1.40	1.32
1	A	444	TYR	CZ-OH	5.46	1.49	1.38
1	D	470	LEU	N-CA	5.46	1.53	1.46
1	A	4[A]	LYS	N-CA	5.46	1.53	1.45
1	A	4[B]	LYS	N-CA	5.46	1.53	1.45
1	A	412	SER	C-O	5.46	1.30	1.24
2	B	112	ALA	C-O	5.46	1.30	1.23
3	F	104	ALA	N-CA	5.45	1.52	1.46
1	A	387	GLU	CA-C	-5.44	1.45	1.52
3	C	3	GLN	CG-CD	5.44	1.65	1.52
2	E	420	SER	N-CA	5.44	1.53	1.46
1	A	471	ARG	CZ-NH2	5.43	1.40	1.33
3	C	155	VAL	C-O	5.43	1.31	1.24
3	C	222	GLU	C-O	5.42	1.30	1.24
1	A	281	VAL	N-CA	5.42	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	303	ASN	N-CA	5.42	1.52	1.46
2	E	319	GLY	N-CA	5.42	1.52	1.45
3	F	219	VAL	C-O	5.41	1.30	1.24
1	A	278	PRO	C-O	5.40	1.30	1.24
2	B	270	ALA	N-CA	5.38	1.52	1.46
1	A	236	ILE	C-O	5.37	1.30	1.24
2	E	38	ILE	N-CA	5.37	1.52	1.46
1	D	135	THR	CA-C	5.35	1.59	1.52
1	A	23	THR	C-O	-5.35	1.18	1.23
2	B	257	LYS	N-CA	5.35	1.52	1.46
3	F	154	SER	C-O	5.34	1.31	1.23
3	F	168	MET	N-CA	5.34	1.52	1.45
2	B	230	VAL	C-O	5.33	1.29	1.24
1	A	363	ALA	C-O	5.33	1.30	1.23
1	D	61	GLY	N-CA	5.33	1.54	1.45
2	B	111	ARG	C-O	5.33	1.30	1.23
2	E	417	GLU	CA-C	-5.33	1.45	1.52
2	B	31	ARG	N-CA	5.33	1.53	1.46
2	B	270	ALA	C-O	5.32	1.30	1.24
3	C	18	PHE	CA-CB	5.32	1.61	1.53
2	E	31	ARG	N-CA	5.32	1.53	1.46
2	E	301	MET	CA-CB	5.32	1.61	1.53
2	E	369	GLY	C-O	5.31	1.30	1.24
3	F	139	GLU	N-CA	5.31	1.53	1.46
1	D	364	PRO	CA-C	5.30	1.59	1.52
2	E	432	VAL	C-O	-5.30	1.17	1.24
3	C	228	VAL	CA-CB	5.30	1.62	1.54
1	D	268	PRO	CA-CB	-5.30	1.46	1.53
1	D	380	TYR	N-CA	-5.30	1.40	1.46
2	E	382	THR	C-O	5.29	1.31	1.23
2	E	277	LEU	C-O	5.29	1.30	1.24
1	D	108	GLY	N-CA	5.29	1.51	1.45
2	E	337	LEU	C-O	5.28	1.30	1.24
1	A	7	ILE	N-CA	5.28	1.52	1.46
1	A	240	LYS	CA-CB	5.27	1.61	1.53
2	B	421	GLN	CA-C	-5.27	1.45	1.52
1	A	108	GLY	N-CA	5.26	1.51	1.45
2	B	419	PHE	CA-CB	5.26	1.61	1.53
2	E	321	ALA	CA-C	5.25	1.59	1.52
2	E	158	ALA	N-CA	5.25	1.52	1.46
2	B	308	ALA	CA-CB	5.25	1.61	1.53
2	B	52	GLY	N-CA	5.24	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	5	GLU	N-CA	5.23	1.52	1.46
1	D	292	SER	C-O	5.23	1.30	1.24
3	F	176	ILE	CA-CB	5.23	1.60	1.54
3	C	74	ASP	C-N	5.22	1.40	1.33
1	D	490	GLY	C-O	5.22	1.30	1.23
1	D	167	THR	N-CA	5.21	1.52	1.45
3	C	38	LYS	CE-NZ	5.21	1.65	1.49
1	D	423	GLY	CA-C	5.21	1.57	1.51
1	A	467	PRO	N-CA	5.20	1.53	1.47
2	B	70	MET	N-CA	5.20	1.52	1.46
1	A	545	LEU	C-O	5.20	1.30	1.24
1	D	113	HIS	N-CA	5.19	1.52	1.46
2	E	395	ALA	C-O	5.18	1.30	1.24
3	C	66	ILE	C-O	5.18	1.29	1.24
1	A	41	VAL	N-CA	5.18	1.52	1.46
3	C	57	GLU	N-CA	5.17	1.52	1.46
1	D	120	LEU	CA-C	5.17	1.59	1.52
1	A	490	GLY	N-CA	5.17	1.52	1.45
2	E	181	ILE	N-CA	5.16	1.52	1.46
1	D	412	SER	C-O	5.16	1.30	1.24
2	E	421	GLN	C-O	5.16	1.30	1.24
3	C	230	ALA	N-CA	5.16	1.52	1.46
1	D	135	THR	C-O	5.16	1.30	1.24
1	D	220	GLY	N-CA	5.15	1.52	1.45
3	C	16	ARG	N-CA	5.15	1.52	1.46
2	E	115	GLN	C-O	5.15	1.29	1.24
3	C	27	LYS	CA-C	-5.15	1.46	1.52
3	C	17	ASN	C-O	-5.14	1.18	1.24
3	F	229	GLU	CA-C	5.14	1.59	1.52
1	D	181	VAL	CA-CB	5.14	1.60	1.54
3	C	219	VAL	N-CA	5.13	1.52	1.46
1	D	124	VAL	N-CA	5.13	1.52	1.46
2	B	17	LEU	C-O	5.12	1.29	1.23
2	E	433	VAL	N-CA	5.12	1.52	1.46
1	A	128	THR	C-O	5.12	1.30	1.24
1	D	140	MET	N-CA	5.11	1.51	1.46
2	E	89	ALA	N-CA	5.11	1.52	1.46
1	D	334	ALA	N-CA	5.10	1.52	1.46
1	D	217	THR	C-N	5.10	1.37	1.32
1	D	363	ALA	CA-CB	5.10	1.60	1.53
2	E	46	VAL	C-O	5.09	1.29	1.24
3	F	4	TYR	N-CA	5.08	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	498	ALA	N-CA	5.08	1.52	1.46
1	A	387	GLU	N-CA	5.08	1.52	1.46
1	A	70	MET	C-O	5.07	1.30	1.23
1	A	341	ASN	CA-CB	5.07	1.61	1.53
1	D	347	THR	CA-C	5.07	1.59	1.52
3	C	28	LEU	CA-CB	5.07	1.61	1.54
3	C	178	ASN	N-CA	5.07	1.52	1.46
3	F	139	GLU	CA-C	-5.06	1.45	1.52
1	A	230	GLN	C-O	5.06	1.30	1.24
2	B	124	ALA	N-CA	5.06	1.51	1.45
1	D	535	ARG	CA-C	5.05	1.59	1.53
2	B	24	LEU	C-O	5.05	1.30	1.24
2	B	139	VAL	CA-CB	5.05	1.60	1.54
2	E	105	LEU	C-O	5.04	1.30	1.23
2	E	277	LEU	N-CA	5.04	1.52	1.46
1	D	526	ARG	N-CA	5.03	1.52	1.46
1	A	119	ARG	CB-CG	-5.03	1.37	1.52
3	F	85	ILE	CA-CB	5.03	1.62	1.54
2	E	162	GLY	N-CA	5.03	1.52	1.45
1	A	242	ALA	C-O	5.02	1.30	1.23
1	A	547	THR	CA-C	5.02	1.57	1.52
2	E	146	PHE	N-CA	5.02	1.52	1.46
1	A	432	TYR	C-O	5.02	1.30	1.24
3	F	43	ARG	N-CA	5.01	1.52	1.45
3	C	135	LYS	C-O	5.01	1.29	1.24
3	C	120	ARG	CZ-NH1	5.01	1.39	1.32

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	147	ARG	NE-CZ-NH1	8.25	129.75	121.50
3	F	59	MET	CG-SD-CE	-7.53	84.33	100.90
1	A	26	TYR	O-C-N	7.01	129.38	121.88
1	D	450	ASP	N-CA-CB	7.01	120.43	110.12
1	A	450	ASP	N-CA-C	6.98	118.89	111.28
2	E	353	GLU	OE1-CD-OE2	6.97	139.64	122.90
2	E	32	ASN	O-C-N	-6.95	115.40	121.31
3	F	35	ASP	CA-C-O	-6.88	113.13	120.42
1	A	450	ASP	CB-CA-C	6.83	122.12	110.79
3	F	151	ARG	CG-CD-NE	-6.56	97.56	112.00
2	E	435	ALA	N-CA-C	6.47	118.33	111.28
3	F	217	TYR	O-C-N	-6.27	116.07	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	391	LEU	N-CA-C	-6.27	104.53	111.36
1	D	293	SER	CA-C-O	-6.23	113.23	120.20
1	D	307	VAL	N-CA-C	-6.22	104.69	110.53
1	A	303	VAL	N-CA-C	-6.20	104.70	110.53
2	B	44	ARG	NE-CZ-NH1	6.14	127.64	121.50
1	A	547	THR	O-C-N	6.09	126.30	121.55
2	E	261	LYS	N-CA-C	6.06	117.96	111.36
2	E	32	ASN	CA-C-O	6.05	124.12	119.46
2	E	314	THR	O-C-N	6.01	128.26	122.07
1	D	238	ALA	CA-C-O	-5.90	112.83	119.79
2	B	38	ILE	CA-C-O	-5.89	114.60	120.85
3	C	38	LYS	CG-CD-CE	5.85	124.76	111.30
1	A	448	LEU	N-CA-C	-5.82	104.63	110.97
1	D	7	ILE	N-CA-C	5.82	116.55	110.62
1	D	450	ASP	CB-CA-C	5.81	120.44	110.79
2	B	230	VAL	CA-C-O	5.81	127.47	120.67
1	A	242	ALA	N-CA-C	-5.80	102.47	110.35
2	B	15	GLY	O-C-N	5.79	129.50	122.32
3	F	147	ARG	NE-CZ-NH1	5.76	127.26	121.50
1	D	450	ASP	N-CA-C	5.75	117.55	111.28
1	A	547	THR	CA-C-N	-5.63	113.90	119.92
1	A	547	THR	C-N-CA	-5.63	113.90	119.92
3	F	53	HIS	CA-C-N	-5.57	114.64	120.38
3	F	53	HIS	C-N-CA	-5.57	114.64	120.38
1	A	229	MET	N-CA-C	-5.57	105.29	111.36
1	D	146	VAL	O-C-N	-5.56	117.70	121.98
2	B	230	VAL	O-C-N	-5.56	117.18	123.18
2	B	427	GLU	O-C-N	-5.51	116.05	121.17
2	E	197	VAL	CA-C-O	-5.47	115.26	120.95
2	E	269	ILE	O-C-N	5.45	127.16	121.87
1	D	412	SER	O-C-N	-5.44	115.95	122.15
2	B	276	ALA	CA-C-O	-5.42	114.80	120.55
1	D	345	ASP	CA-C-O	5.42	126.51	120.82
2	E	439	ILE	N-CA-C	5.40	117.37	112.29
3	C	147	ARG	NE-CZ-NH2	-5.40	114.34	119.20
1	A	231	ILE	N-CA-C	-5.39	105.24	110.42
2	B	187	GLY	N-CA-C	-5.39	101.35	112.34
3	C	3	GLN	N-CA-C	5.38	120.12	113.50
1	D	533	ALA	O-C-N	5.36	127.80	122.12
1	A	267	LEU	CA-C-N	5.35	125.33	120.03
1	A	267	LEU	C-N-CA	5.35	125.33	120.03
1	A	450	ASP	N-CA-CB	5.30	117.92	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	135	THR	O-C-N	5.28	127.80	122.09
1	A	477	ASN	CB-CG-ND2	5.28	124.32	116.40
1	A	118	LYS	CB-CG-CD	5.28	123.43	111.30
3	F	88	THR	CA-C-O	-5.26	115.13	120.71
3	C	177	TYR	CA-C-N	-5.24	116.03	122.84
3	C	177	TYR	C-N-CA	-5.24	116.03	122.84
1	A	215	SER	CA-C-O	5.23	126.09	120.55
2	E	439	ILE	CB-CA-C	-5.22	104.73	111.88
1	A	135	THR	CA-C-O	-5.21	115.35	120.82
2	E	426	ARG	O-C-N	5.20	129.30	122.33
1	D	543	ARG	CA-CB-CG	5.18	124.46	114.10
3	C	222	GLU	CA-C-O	-5.16	114.81	120.43
2	B	34	ALA	CA-C-O	-5.16	114.95	120.42
1	D	112	ALA	O-C-N	5.15	127.37	122.07
1	D	70	MET	CB-CA-C	-5.12	101.49	108.86
2	E	353	GLU	CG-CD-OE2	-5.11	106.65	118.40
1	A	36	ARG	NE-CZ-NH2	5.10	123.79	119.20
2	E	6	ASP	CB-CA-C	-5.09	100.94	109.65
1	A	450	ASP	CA-CB-CG	5.08	117.68	112.60
1	D	65	GLY	CA-C-O	-5.08	113.47	119.46
2	B	270	ALA	CA-C-O	-5.06	115.19	120.55
1	D	116	ILE	O-C-N	5.04	126.85	121.91
2	E	35	ILE	N-CA-C	-5.04	105.58	110.42
2	E	370	GLY	N-CA-C	-5.04	103.93	110.38
3	C	33	ASP	O-C-N	-5.03	116.78	122.12
1	D	175	GLU	N-CA-C	5.03	119.47	113.23
2	B	386	LYS	CB-CA-C	5.02	118.96	111.88
1	A	533	ALA	O-C-N	5.01	127.43	122.12
2	E	406	PHE	CA-CB-CG	-5.00	108.80	113.80

All (2) chirality outliers are listed below:

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

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	499	ARG	Sidechain
2	B	333	TYR	Sidechain
2	B	72	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	E	333	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	4446	0	4260	24	0
1	D	4410	0	4245	24	0
2	B	3464	0	3524	18	0
2	E	3527	0	3584	27	0
3	C	2072	0	2014	13	0
3	F	2041	0	1991	14	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	3	0	0	0	0
4	E	2	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	19	0	0
6	D	21	0	19	0	0
7	A	7	0	5	0	0
7	D	7	0	5	0	0
8	A	20	0	17	0	0
8	D	20	0	17	0	0
9	A	4	0	3	0	0
9	C	4	0	3	0	0
10	A	8	0	12	1	0
10	C	4	0	6	0	0
10	D	8	0	12	2	0
10	F	8	0	12	0	0
11	A	7	0	10	0	0
11	C	7	0	10	0	0
12	A	1	0	0	0	0
13	A	491	0	0	5	0
13	B	454	0	0	4	0
13	C	255	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	D	502	0	0	7	0
13	E	400	0	0	10	0
13	F	250	0	0	5	0
All	All	22594	0	19854	112	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 3.

All (112) 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:C:153:LYS:CE	3:C:153:LYS:NZ	1.71	1.54
3:C:186[B]:MET:HE2	3:C:201:LEU:HD11	1.15	1.13
2:E:27:LEU:HD22	2:E:246[B]:MET:HE1	1.47	0.93
2:E:27:LEU:CD2	2:E:246[B]:MET:HE1	2.02	0.89
3:C:186[B]:MET:CE	3:C:201:LEU:HD11	2.02	0.87
1:A:24:THR:HG23	13:C:3803:HOH:O	1.73	0.87
2:E:27:LEU:HD22	2:E:246[B]:MET:CE	2.10	0.81
3:F:132[A]:LYS:HE2	13:F:1692:HOH:O	1.86	0.75
3:C:153:LYS:NZ	3:C:153:LYS:CD	2.50	0.73
2:B:188:PRO:HD3	13:E:1304:HOH:O	1.89	0.72
1:D:22:LYS:NZ	10:D:558:EDO:H12	2.03	0.72
3:F:153[A]:LYS:NZ	13:F:1186:HOH:O	2.22	0.71
3:F:61:GLU:HB2	3:F:62:PRO:CD	2.20	0.71
13:A:3768:HOH:O	1:D:545[A]:LEU:HD11	1.89	0.71
1:A:194[B]:GLU:HG2	13:A:2095:HOH:O	1.92	0.68
2:E:27:LEU:HD22	2:E:246[B]:MET:SD	2.34	0.68
2:B:246[A]:MET:HE3	2:B:429:LEU:HD12	1.77	0.67
1:D:24[A]:THR:HG23	13:F:1497:HOH:O	1.97	0.65
1:D:194[B]:GLU:HG2	13:D:3701:HOH:O	1.99	0.63
3:C:179:LYS:HG3	13:C:4173:HOH:O	1.99	0.62
1:D:22:LYS:HZ1	10:D:558:EDO:H12	1.64	0.62
2:E:17:LEU:HD21	2:E:20[A]:GLU:HG3	1.82	0.61
1:D:357[A]:LYS:HE2	1:D:372[A]:ASP:OD2	2.01	0.61
1:D:268:PRO:HB3	13:E:1668:HOH:O	2.00	0.60
13:E:3631[A]:HOH:O	3:F:72:PRO:HG3	2.02	0.60
1:A:357:LYS:NZ	1:A:372[B]:ASP:OD1	2.34	0.60
3:C:132:LYS:HD2	13:C:4122[B]:HOH:O	2.02	0.58
3:F:59:MET:O	3:F:60:ASP:C	2.46	0.58
1:A:191:ASP:HB2	13:A:4177:HOH:O	2.03	0.57
2:B:286:LYS:HE2	2:B:288:LEU:HD21	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:207:GLU:O	3:F:211[A]:MET:HG2	2.04	0.57
1:A:60:ILE:HD12	13:D:3878:HOH:O	2.04	0.56
3:C:64[A]:ASP:HB3	3:C:67[A]:ARG:HB2	1.87	0.56
1:D:42[A]:ASN:ND2	13:D:1802:HOH:O	2.39	0.55
2:E:118[B]:SER:HB3	13:E:2658:HOH:O	2.07	0.55
2:B:246[A]:MET:CE	2:B:429:LEU:HD12	2.36	0.54
1:D:46[B]:GLU:HG3	13:D:700:HOH:O	2.08	0.54
2:E:95:VAL:HG21	2:E:119[B]:ALA:HB3	1.91	0.53
1:D:352[A]:GLU:OE2	1:D:355[A]:GLU:OE1	2.27	0.52
1:D:24[A]:THR:CG2	13:F:1497:HOH:O	2.58	0.51
1:A:114:ALA:O	1:A:118:LYS:HD3	2.11	0.50
2:E:58[B]:LYS:HE3	13:E:1433:HOH:O	2.10	0.50
1:A:177[B]:ASP:C	1:A:179:ALA:N	2.69	0.50
2:B:405[A]:MET:HG3	1:D:115:VAL:HG22	1.94	0.50
2:E:344[A]:LEU:HB3	2:E:345:PRO:HD2	1.94	0.50
1:D:191:ASP:HB2	13:D:3703:HOH:O	2.11	0.49
1:A:328:VAL:HB	5:D:553:F43:H9A1	1.94	0.49
1:D:45:LYS:NZ	13:D:2225:HOH:O	2.46	0.49
1:A:360:LEU:O	1:A:361[A]:CYS:HB2	2.13	0.49
2:B:123[B]:VAL:HG12	2:E:36:LYS:HA	1.94	0.49
3:F:61:GLU:HB2	3:F:62:PRO:HD2	1.95	0.48
1:A:9:ALA:O	1:A:13[B]:LYS:HG3	2.14	0.48
2:E:55:ASN:HA	2:E:58[A]:LYS:HG2	1.97	0.47
2:E:119[B]:ALA:O	2:E:123[B]:VAL:HG22	2.13	0.47
1:A:242:ALA:HB2	3:F:84:TYR:CE1	2.50	0.47
1:A:249:GLY:HA3	13:A:3685:HOH:O	2.14	0.47
2:B:119:ALA:HA	2:B:122[B]:ASP:OD2	2.14	0.47
2:B:299:LEU:HD22	13:B:2183:HOH:O	2.13	0.47
1:D:154:HIS:CE1	1:D:545[A]:LEU:HD21	2.50	0.47
1:D:17:SER:OG	1:D:20[B]:GLU:HG3	2.14	0.47
5:A:1:F43:H9A1	1:D:328:VAL:HB	1.97	0.47
3:C:61:GLU:OE1	13:C:4106[B]:HOH:O	2.21	0.46
2:E:299:LEU:HD22	13:E:4196:HOH:O	2.14	0.46
1:A:241[A]:GLN:HB3	1:A:242:ALA:O	2.15	0.46
2:B:199:HIS:CE1	2:B:415[B]:ILE:HD12	2.51	0.46
3:F:247:ASN:C	3:F:247:ASN:HD22	2.22	0.46
2:E:374:ILE:C	2:E:374:ILE:HD12	2.41	0.45
3:F:61:GLU:H	3:F:61:GLU:HG2	1.57	0.45
2:B:310:LEU:HD11	2:B:331:LEU:HD23	1.98	0.45
3:C:56:LEU:O	3:C:59[A]:MET:HB2	2.16	0.45
1:A:169:ASN:OD1	1:A:172[B]:ILE:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172[A]:ILE:HG22	1:A:176[A]:ILE:HD12	1.98	0.45
2:B:119:ALA:O	2:B:122[B]:ASP:HB2	2.17	0.45
1:A:115:VAL:HG22	2:E:405[A]:MET:HG3	1.98	0.44
2:B:58:LYS:HE2	13:B:3633:HOH:O	2.15	0.44
3:C:39:ILE:HG12	3:C:186[B]:MET:HG2	1.99	0.44
3:F:61:GLU:HB2	3:F:62:PRO:HD3	1.98	0.44
1:A:172[A]:ILE:HG22	1:A:176[A]:ILE:CD1	2.48	0.44
2:B:424[A]:GLU:HG3	13:B:3930:HOH:O	2.16	0.44
13:B:2205:HOH:O	2:E:188:PRO:HD3	2.17	0.44
3:C:164[A]:GLU:HG2	13:C:1182:HOH:O	2.18	0.44
2:E:113[B]:LEU:C	2:E:113[B]:LEU:HD23	2.43	0.43
1:A:241[B]:GLN:H	1:A:241[B]:GLN:HG3	1.46	0.43
2:B:27:LEU:HD22	2:B:246[B]:MET:SD	2.59	0.43
3:F:61:GLU:CB	3:F:62:PRO:CD	2.90	0.43
2:E:27:LEU:CD2	2:E:246[B]:MET:CE	2.80	0.43
2:E:61[B]:LYS:CE	13:E:2444:HOH:O	2.67	0.43
3:F:82:VAL:O	3:F:83:ARG:HD2	2.18	0.43
2:B:37:SER:OG	2:B:424[B]:GLU:OE1	2.25	0.43
2:E:424[B]:GLU:HG3	13:E:3642:HOH:O	2.19	0.43
1:A:73:GLN:HB2	1:A:80:TYR:CE2	2.54	0.42
3:C:84:TYR:CE1	1:D:242:ALA:HB2	2.54	0.42
1:A:4[A]:LYS:NZ	13:A:2253:HOH:O	2.43	0.42
1:A:332:GLN:HA	1:A:335:THR:OG1	2.18	0.42
1:D:352[B]:GLU:OE1	13:D:831:HOH:O	2.22	0.42
1:D:358:TYR:OH	1:D:372[A]:ASP:OD2	2.34	0.42
2:E:199:HIS:CE1	2:E:415[B]:ILE:HD12	2.55	0.42
2:B:14[A]:ARG:NH1	3:C:63:GLU:HG2	2.35	0.42
2:E:246[A]:MET:CE	2:E:429:LEU:HD12	2.50	0.42
1:D:267:LEU:HD12	1:D:273:ARG:HB2	2.02	0.41
1:D:186[A]:LYS:HB2	1:D:186[A]:LYS:NZ	2.35	0.41
1:A:111:HIS:CE1	10:A:558:EDO:H12	2.55	0.41
2:B:246[B]:MET:HE2	2:B:246[B]:MET:HB3	1.61	0.41
2:E:122[B]:ASP:HB2	13:E:1158:HOH:O	2.21	0.41
2:E:362:PHE:O	2:E:369:GLY:HA3	2.21	0.41
3:F:61:GLU:CB	3:F:62:PRO:HD3	2.50	0.41
2:E:261:LYS:HG2	13:F:3664:HOH:O	2.20	0.41
1:A:218:CYS:HA	1:D:323:TYR:CZ	2.57	0.40
2:B:126:GLU:HB3	2:E:126:GLU:HB3	2.03	0.40
2:E:20[B]:GLU:HG2	13:E:768:HOH:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	572/549 (104%)	553 (97%)	18 (3%)	1 (0%)	43	19
1	D	569/549 (104%)	555 (98%)	13 (2%)	1 (0%)	43	19
2	B	465/442 (105%)	454 (98%)	11 (2%)	0	100	100
2	E	475/442 (108%)	463 (98%)	12 (2%)	0	100	100
3	C	258/248 (104%)	251 (97%)	7 (3%)	0	100	100
3	F	254/248 (102%)	247 (97%)	7 (3%)	0	100	100
All	All	2593/2478 (105%)	2523 (97%)	68 (3%)	2 (0%)	48	21

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	463/434 (107%)	457 (99%)	6 (1%)	61	30
1	D	460/434 (106%)	455 (99%)	5 (1%)	65	37
2	B	366/341 (107%)	364 (100%)	2 (0%)	81	61
2	E	375/341 (110%)	370 (99%)	5 (1%)	61	30
3	C	228/216 (106%)	226 (99%)	2 (1%)	70	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	224/216 (104%)	218 (97%)	6 (3%)	39	10
All	All	2116/1982 (107%)	2090 (99%)	26 (1%)	65	34

All (26) 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	SER
1	A	118	LYS
1	A	126	PRO
1	A	450	ASP
2	B	283	LYS
2	B	287	GLU
3	C	61	GLU
3	C	150	VAL
1	D	186[A]	LYS
1	D	186[B]	LYS
1	D	352[A]	GLU
1	D	352[B]	GLU
1	D	450	ASP
2	E	185	LEU
2	E	283	LYS
2	E	438[A]	GLU
2	E	438[B]	GLU
2	E	440	LYS
3	F	61	GLU
3	F	98	PRO
3	F	121	GLN
3	F	150	VAL
3	F	186	MET
3	F	247	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
2	B	21	GLN
2	B	102	ASN
2	B	115	GLN
2	B	404	GLN

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Mol	Chain	Res	Type
3	C	121	GLN
1	D	73	GLN
1	D	296	ASN
1	D	384	GLN
2	E	115	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	AGM	D	271	1	10,11,12	1.57	2 (20%)	7,13,15	0.49	0
1	MGN	A	400	1	6,9,10	1.12	1 (16%)	7,12,14	1.34	1 (14%)
1	MHS	D	257	1	10,11,12	1.80	3 (30%)	5,14,16	8.34	5 (100%)
1	GL3	A	445	1	2,3,4	2.12	1 (50%)	1,2,4	0.37	0
1	MGN	D	400	1	6,9,10	1.91	2 (33%)	7,12,14	0.93	0
1	AGM	A	271	1	10,11,12	1.40	2 (20%)	7,13,15	1.85	3 (42%)
1	SMC	A	452	1	5,6,7	1.07	0	3,6,8	1.63	1 (33%)
1	SMC	D	452	1	5,6,7	0.56	0	3,6,8	1.92	1 (33%)
1	MHS	A	257	1	10,11,12	1.62	2 (20%)	5,14,16	8.32	4 (80%)
1	GL3	D	445	1	2,3,4	1.89	1 (50%)	1,2,4	0.36	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	AGM	D	271	1	-	1/10/11/13	-
1	MGN	A	400	1	-	0/7/9/12	-
1	MHS	D	257	1	-	0/5/6/8	0/1/1/1
1	GL3	A	445	1	-	1/1/1/2	-
1	MGN	D	400	1	-	0/7/9/12	-
1	AGM	A	271	1	-	1/10/11/13	-
1	SMC	A	452	1	-	1/3/5/7	-
1	SMC	D	452	1	-	1/3/5/7	-
1	MHS	A	257	1	-	0/5/6/8	0/1/1/1
1	GL3	D	445	1	-	1/1/1/2	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	400	MGN	O-C	3.21	1.30	1.20
1	D	271	AGM	CG-CD	3.20	1.58	1.53
1	A	445	GL3	C-S	-2.99	1.68	1.80
1	D	400	MGN	CB1-CG	2.88	1.59	1.53
1	D	445	GL3	C-S	-2.66	1.69	1.80
1	A	257	MHS	CE1-NE2	2.65	1.39	1.32
1	D	257	MHS	CD2-CG	2.58	1.40	1.36
1	A	257	MHS	CE1-ND1	2.57	1.42	1.35
1	D	257	MHS	CG-ND1	-2.30	1.34	1.38
1	A	400	MGN	O-C	2.26	1.27	1.20
1	D	257	MHS	O-C	2.21	1.28	1.20
1	A	271	AGM	CZ-NE1	2.08	1.36	1.33
1	D	271	AGM	CB-CA	2.03	1.56	1.53
1	A	271	AGM	O-C	2.02	1.27	1.20

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	MHS	ND1-CE1-NE2	-17.36	102.61	112.94
1	D	257	MHS	ND1-CE1-NE2	-17.00	102.82	112.94
1	D	257	MHS	CD2-NE2-CE1	5.50	112.44	105.24
1	A	257	MHS	CM-ND1-CE1	-4.85	117.21	126.28
1	D	257	MHS	CM-ND1-CE1	-4.18	118.45	126.28
1	A	257	MHS	CD2-NE2-CE1	3.68	110.06	105.24
1	A	257	MHS	CM-ND1-CG	2.77	129.64	126.69
1	D	452	SMC	CA-CB-SG	-2.73	109.63	114.04
1	A	452	SMC	CA-CB-SG	-2.65	109.76	114.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	400	MGN	CB1-CG-CD	-2.64	106.86	112.13
1	A	271	AGM	NH1-CZ-NE1	2.51	125.11	119.58
1	D	257	MHS	CM-ND1-CG	2.35	129.19	126.69
1	D	257	MHS	CG-CD2-NE2	-2.33	104.86	109.79
1	A	271	AGM	CD-NE1-CZ	-2.30	119.30	123.59
1	A	271	AGM	CE2-CD-NE1	-2.13	104.92	110.31

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	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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 12 are monoatomic - leaving 19 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$
6	TP7	A	553[A]	-	19,20,20	1.29	1 (5%)	24,26,26	1.28	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	EDO	D	557	-	3,3,3	0.59	0	2,2,2	0.10	0
10	EDO	A	557	-	3,3,3	0.35	0	2,2,2	0.14	0
5	F43	D	553	13,7,1	63,71,71	2.46	14 (22%)	73,118,118	1.75	18 (24%)
9	ACT	C	1	-	3,3,3	1.22	0	3,3,3	1.62	1 (33%)
5	F43	A	1	1,7,13	63,71,71	2.60	18 (28%)	73,118,118	1.70	14 (19%)
6	TP7	D	554[A]	-	19,20,20	1.07	0	24,26,26	1.58	4 (16%)
9	ACT	A	556[A]	4	3,3,3	0.88	0	3,3,3	1.55	1 (33%)
11	PEG	A	559	-	6,6,6	0.95	0	5,5,5	2.09	2 (40%)
8	TXZ	A	555[B]	-	18,19,19	1.31	3 (16%)	23,25,25	1.15	1 (4%)
8	TXZ	D	556[B]	-	18,19,19	1.21	1 (5%)	23,25,25	1.15	1 (4%)
10	EDO	C	251	-	3,3,3	0.34	0	2,2,2	0.72	0
10	EDO	D	558	-	3,3,3	0.64	0	2,2,2	0.67	0
10	EDO	F	251	-	3,3,3	0.54	0	2,2,2	0.46	0
7	COM	D	555[A]	5	6,6,6	2.63	3 (50%)	8,8,8	1.32	1 (12%)
10	EDO	F	252	-	3,3,3	0.53	0	2,2,2	0.42	0
10	EDO	A	558	-	3,3,3	0.48	0	2,2,2	0.80	0
7	COM	A	554[A]	5	6,6,6	2.00	2 (33%)	8,8,8	1.76	2 (25%)
11	PEG	C	252	-	6,6,6	0.60	0	5,5,5	0.79	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
5	F43	D	553	13,7,1	-	10/28/185/185	-
8	TXZ	A	555[B]	-	-	2/23/23/23	-
11	PEG	C	252	-	-	0/4/4/4	-
6	TP7	A	553[A]	-	-	3/24/24/24	-
10	EDO	D	557	-	-	1/1/1/1	-
10	EDO	D	558	-	-	1/1/1/1	-
10	EDO	F	251	-	-	1/1/1/1	-
7	COM	D	555[A]	5	-	1/4/4/4	-
5	F43	A	1	1,7,13	-	9/28/185/185	-
6	TP7	D	554[A]	-	-	0/24/24/24	-
10	EDO	A	557	-	-	1/1/1/1	-
10	EDO	F	252	-	-	1/1/1/1	-
10	EDO	A	558	-	-	1/1/1/1	-
8	TXZ	D	556[B]	-	-	2/23/23/23	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	COM	A	554[A]	5	-	0/4/4/4	-
10	EDO	C	251	-	-	1/1/1/1	-
11	PEG	A	559	-	-	2/4/4/4	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	553	F43	NI-NB	10.17	2.13	1.89
5	D	553	F43	NI-NA	9.62	2.12	1.89
5	A	1	F43	NI-NA	9.20	2.11	1.89
5	A	1	F43	NI-NB	8.41	2.09	1.89
5	D	553	F43	NI-ND	7.21	2.06	1.89
5	A	1	F43	NI-ND	7.03	2.06	1.89
5	A	1	F43	CHA-C4D	5.69	1.58	1.53
5	A	1	F43	CHB-C1B	5.19	1.56	1.53
5	A	1	F43	CHB-C4A	4.74	1.58	1.51
7	D	555[A]	COM	O1S-S2	-4.48	1.32	1.45
5	A	1	F43	C3C-C4C	3.77	1.56	1.50
5	A	1	F43	C4C-NC	3.61	1.41	1.35
5	D	553	F43	C3C-C4C	3.57	1.56	1.50
5	A	1	F43	C4A-NA	3.20	1.54	1.49
7	A	554[A]	COM	C2-S2	-3.19	1.73	1.77
7	D	555[A]	COM	O3S-S2	3.17	1.59	1.47
5	A	1	F43	CHC-C4B	3.12	1.48	1.39
5	A	1	F43	OEB-CCB	-3.04	1.20	1.30
5	A	1	F43	O8D-C7D	2.98	1.29	1.23
5	D	553	F43	CHD-C1D	2.95	1.48	1.43
5	A	1	F43	OCC-CAC	2.80	1.31	1.22
5	A	1	F43	C1C-NC	2.79	1.43	1.37
7	A	554[A]	COM	C1-C2	-2.70	1.44	1.51
5	D	553	F43	O8D-C7D	2.68	1.28	1.23
6	A	553[A]	TP7	OXT-C	2.63	1.29	1.22
5	A	1	F43	CAA-CBA	2.63	1.60	1.52
8	A	555[B]	TXZ	O-C	2.62	1.29	1.22
5	D	553	F43	OBD-CAD	2.54	1.30	1.22
5	D	553	F43	C5C-C2C	2.38	1.57	1.53
5	D	553	F43	C4A-NA	2.36	1.52	1.49
5	D	553	F43	CAA-C3A	2.34	1.57	1.53
5	A	1	F43	O8C-C6C	-2.30	1.23	1.30
5	D	553	F43	CAA-CBA	2.28	1.59	1.52
5	D	553	F43	C3A-C4A	2.25	1.57	1.53
8	A	555[B]	TXZ	CA-N	2.24	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	553	F43	CHC-C4B	2.23	1.45	1.39
5	A	1	F43	OBD-CAD	2.23	1.29	1.22
7	D	555[A]	COM	C1-C2	-2.16	1.46	1.51
5	A	1	F43	OCD-CAD	-2.14	1.23	1.30
8	D	556[B]	TXZ	C3-C2	2.08	1.59	1.52
5	D	553	F43	OCC-CAC	2.03	1.28	1.22
8	A	555[B]	TXZ	CG-CB	2.02	1.56	1.51

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	553	F43	O8D-C7D-C6D	-6.00	111.03	120.87
6	D	554[A]	TP7	C5-C6-C7	-4.89	104.38	113.09
5	A	1	F43	O8D-C7D-C6D	-4.89	112.86	120.87
5	A	1	F43	C4A-NA-C1A	-4.15	103.44	109.08
5	D	553	F43	C6D-C7D-CHD	4.04	124.39	116.94
5	A	1	F43	C2B-C1B-NB	3.76	107.45	101.86
5	A	1	F43	OBC-CAC-C9C	3.74	125.83	114.00
11	A	559	PEG	O4-C4-C3	3.59	132.97	111.82
7	D	555[A]	COM	C1-C2-S2	3.57	119.75	111.77
5	A	1	F43	C6D-C7D-CHD	3.53	123.46	116.94
5	A	1	F43	C3D-C4D-ND	3.44	107.68	102.34
5	A	1	F43	O7C-C6C-C5C	-3.36	112.53	122.84
5	D	553	F43	OBC-CAC-C9C	3.24	124.23	114.00
7	A	554[A]	COM	O2S-S2-C2	3.04	111.32	106.73
5	D	553	F43	CAB-C3B-C2B	-3.04	112.29	119.00
5	D	553	F43	C2D-C1D-CHD	-3.01	118.12	121.85
5	A	1	F43	C5D-C2D-C1D	2.98	114.31	110.43
5	A	1	F43	OBD-CAD-C9D	-2.92	113.87	122.84
5	D	553	F43	C1D-CHD-C4C	-2.86	117.24	125.28
5	D	553	F43	C9A-C2A-C3A	2.84	117.07	112.99
5	A	1	F43	OCC-CAC-C9C	-2.73	114.43	123.09
6	A	553[A]	TP7	O1-C1-C2	-2.72	117.09	122.02
8	A	555[B]	TXZ	C4-C5-C6	-2.67	108.33	113.09
7	A	554[A]	COM	O3S-S2-O2S	-2.63	104.81	111.40
5	D	553	F43	C2C-C5C-C6C	-2.61	109.06	113.95
5	D	553	F43	C3D-C4D-ND	2.56	106.32	102.34
5	D	553	F43	OCD-CAD-C9D	2.50	121.78	114.00
5	A	1	F43	C3B-C4B-CHC	-2.49	118.03	123.33
5	D	553	F43	C3A-C2A-C1A	2.48	102.46	99.97
6	D	554[A]	TP7	CB-CA-N	2.46	116.86	111.54
5	A	1	F43	C9B-C2B-C8B	-2.44	104.47	110.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	553	F43	OCC-CAC-C9C	-2.43	115.37	123.09
5	D	553	F43	C1B-C2B-C3B	2.39	104.99	101.51
6	D	554[A]	TP7	O4P-P-O1P	-2.38	100.84	109.33
11	A	559	PEG	C3-O2-C2	2.37	123.65	113.26
5	D	553	F43	C3D-C2D-C1D	-2.35	98.32	102.47
5	D	553	F43	C4B-CHC-C1C	2.34	129.63	125.84
6	D	554[A]	TP7	O1-C1-N	2.32	126.89	122.95
5	D	553	F43	C5D-C2D-C1D	2.23	113.34	110.43
5	A	1	F43	OCD-CAD-C9D	2.20	120.83	114.00
5	D	553	F43	C5C-C2C-C3C	-2.19	109.64	115.05
9	A	556[A]	ACT	OXT-C-CH3	2.17	124.13	115.05
9	C	1	ACT	OXT-C-O	-2.15	114.07	122.03
5	A	1	F43	CAB-C3B-C2B	-2.11	114.34	119.00
5	D	553	F43	O8C-C6C-C5C	2.02	120.28	114.00
8	D	556[B]	TXZ	CB-CA-C	-2.01	106.41	110.80

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	553	F43	C3A-CAA-CBA-CCA
5	A	1	F43	C3A-CAA-CBA-CCA
10	D	557	EDO	O1-C1-C2-O2
8	A	555[B]	TXZ	C3-C4-C5-C6
10	A	557	EDO	O1-C1-C2-O2
10	A	558	EDO	O1-C1-C2-O2
10	D	558	EDO	O1-C1-C2-O2
10	F	252	EDO	O1-C1-C2-O2
7	D	555[A]	COM	C1-C2-S2-O2S
8	A	555[B]	TXZ	C2-C3-C4-C5
11	A	559	PEG	O1-C1-C2-O2
8	D	556[B]	TXZ	C2-C3-C4-C5
11	A	559	PEG	C4-C3-O2-C2
8	D	556[B]	TXZ	C3-C4-C5-C6
6	A	553[A]	TP7	C4-C5-C6-C7
5	D	553	F43	CAA-CBA-CCA-OEA
5	A	1	F43	CAA-CBA-CCA-OEA
5	A	1	F43	C2C-C5C-C6C-O8C
5	A	1	F43	CAB-CBB-CCB-OEB
5	D	553	F43	CAB-CBB-CCB-OEB
5	D	553	F43	C8C-C9C-CAC-OBC
5	A	1	F43	CAA-CBA-CCA-ODA

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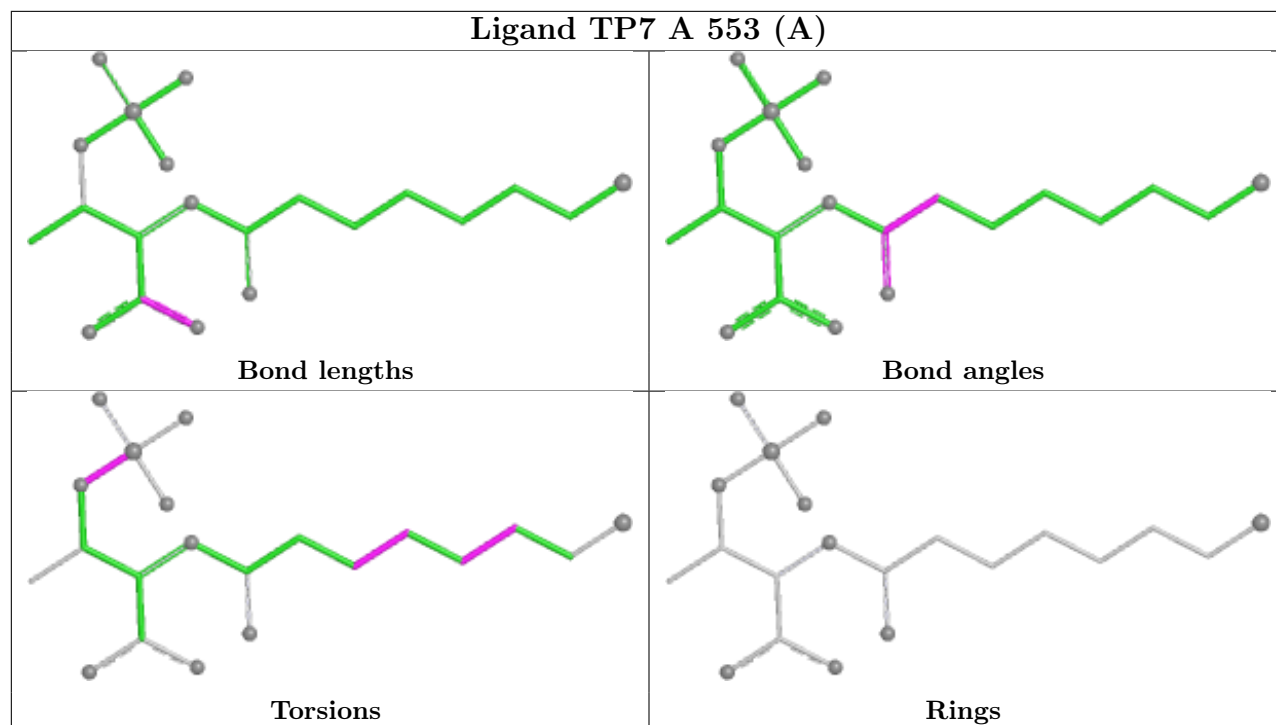
Mol	Chain	Res	Type	Atoms
10	F	251	EDO	O1-C1-C2-O2
5	D	553	F43	CAA-CBA-CCA-ODA
5	A	1	F43	C8C-C9C-CAC-OCC
5	D	553	F43	CAB-CBB-CCB-ODB
5	A	1	F43	C3D-C9D-CAD-OCD
5	D	553	F43	C2C-C5C-C6C-O7C
10	C	251	EDO	O1-C1-C2-O2
5	A	1	F43	CAB-CBB-CCB-ODB
6	A	553[A]	TP7	CB-O4P-P-O3P
5	A	1	F43	C2C-C5C-C6C-O7C
5	D	553	F43	C8C-C9C-CAC-OCC
5	D	553	F43	C3D-C9D-CAD-OB
5	D	553	F43	C2C-C5C-C6C-O8C
6	A	553[A]	TP7	C2-C3-C4-C5

There are no ring outliers.

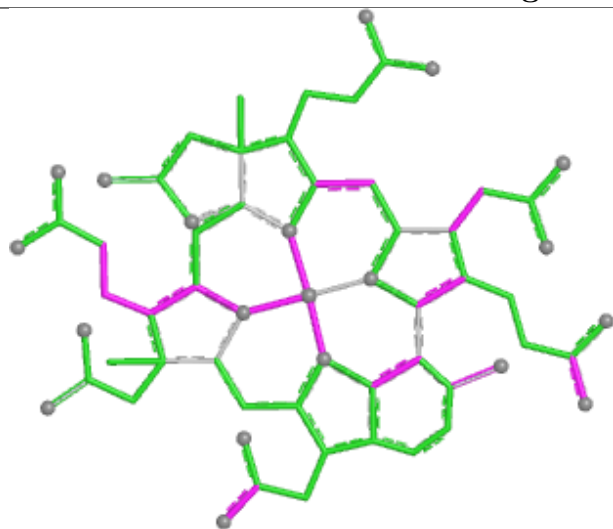
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	553	F43	1	0
5	A	1	F43	1	0
10	D	558	EDO	2	0
10	A	558	EDO	1	0

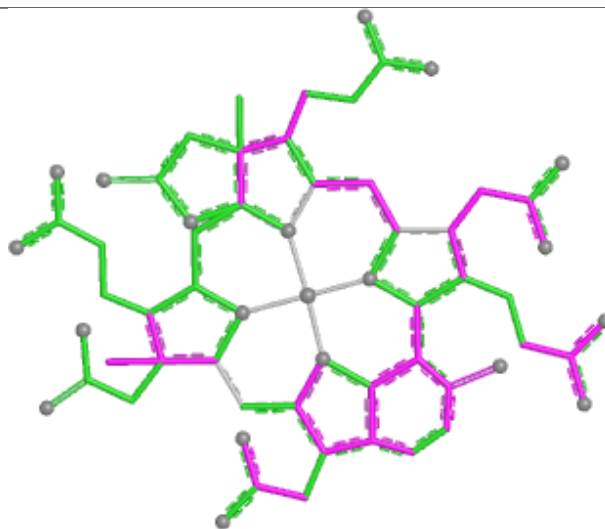
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



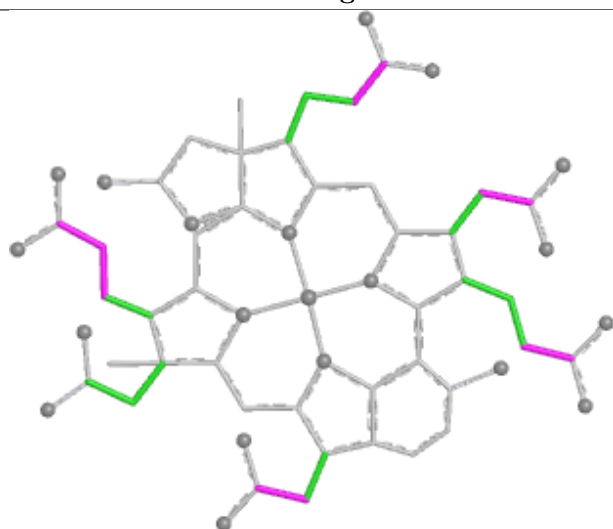
Ligand F43 D 553



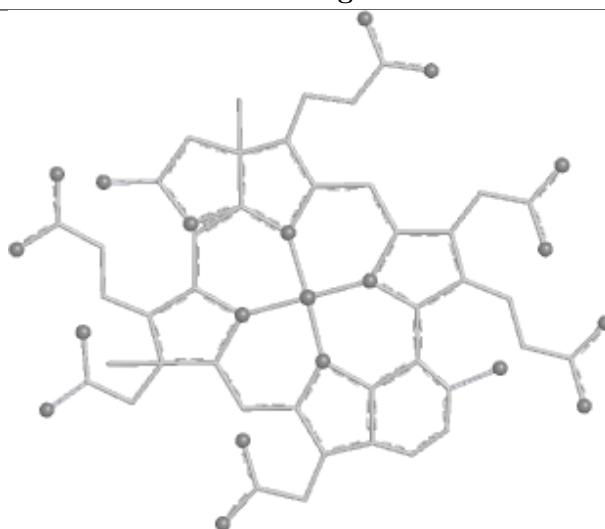
Bond lengths



Bond angles

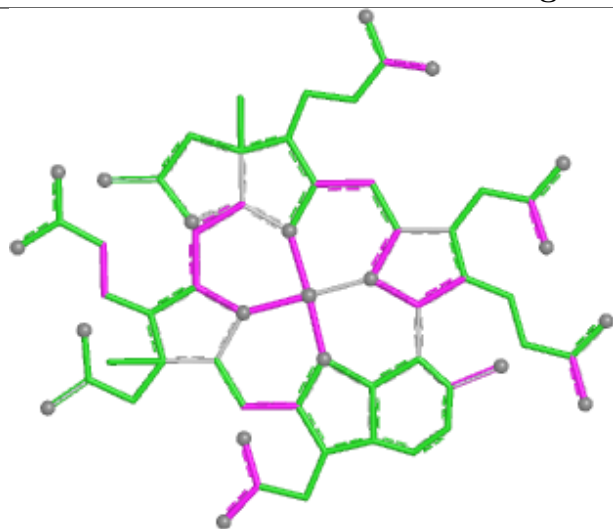


Torsions

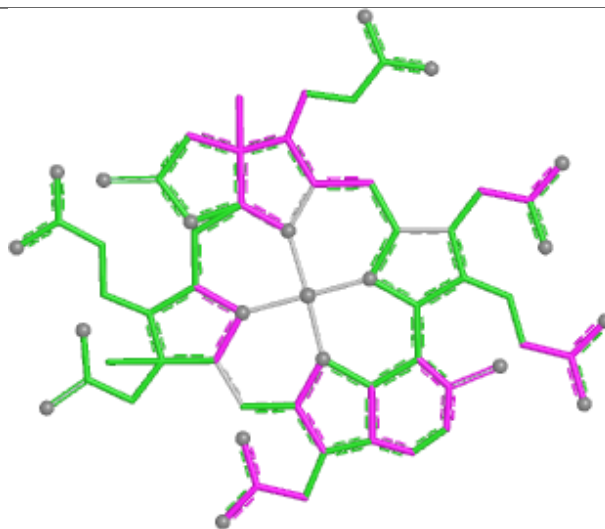


Rings

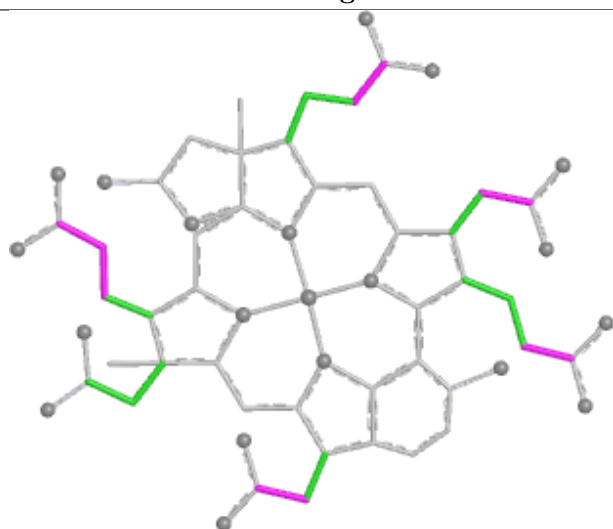
Ligand F43 A 1



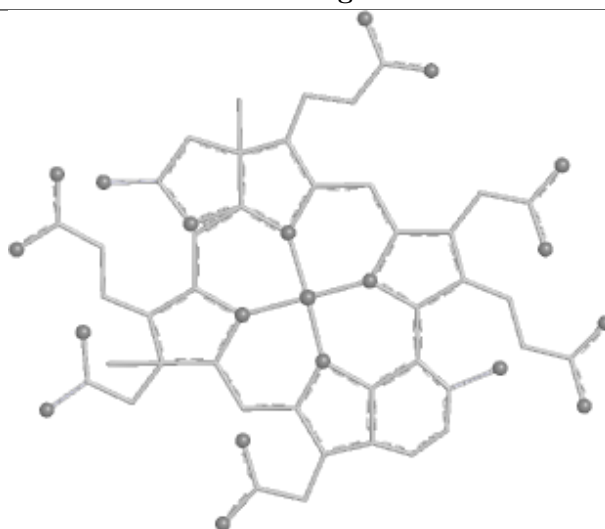
Bond lengths



Bond angles

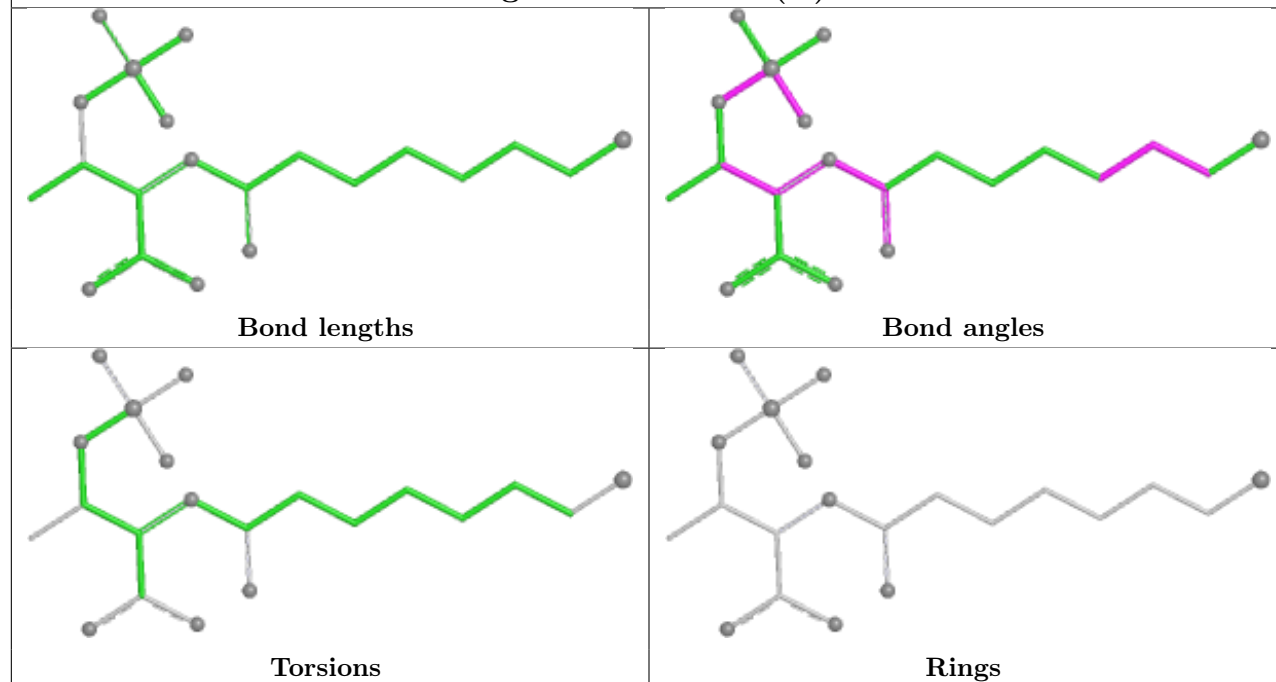


Torsions

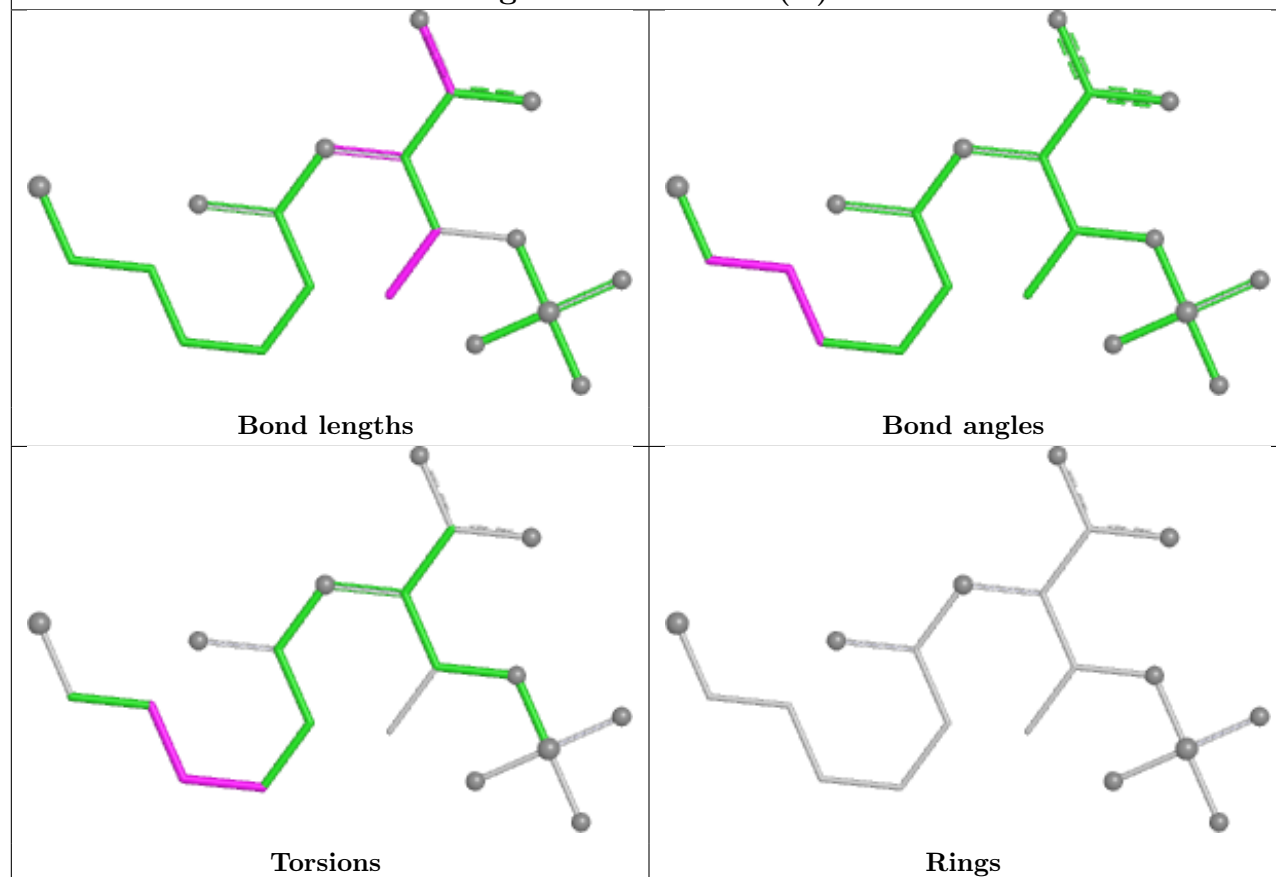


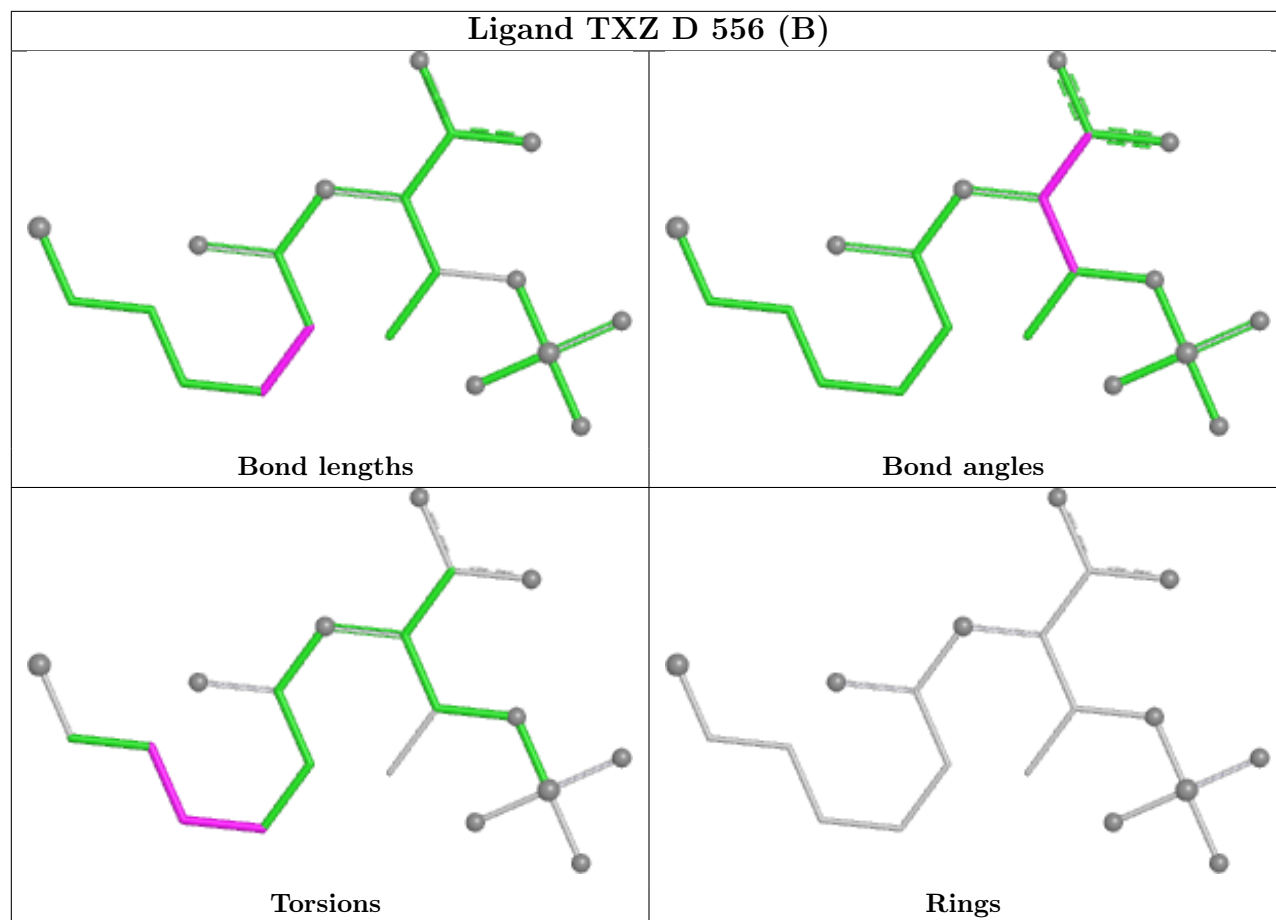
Rings

Ligand TP7 D 554 (A)



Ligand TXZ A 555 (B)





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	543/549 (98%)	-0.85	0 100 100	4, 10, 20, 32	30 (5%)
1	D	543/549 (98%)	-0.84	1 (0%) 91 93	4, 10, 20, 43	28 (5%)
2	B	442/442 (100%)	-0.76	0 100 100	5, 12, 20, 38	24 (5%)
2	E	442/442 (100%)	-0.66	0 100 100	6, 12, 24, 44	34 (7%)
3	C	246/248 (99%)	-0.65	2 (0%) 82 85	5, 13, 29, 52	14 (5%)
3	F	246/248 (99%)	-0.54	2 (0%) 82 85	6, 14, 32, 57	10 (4%)
All	All	2462/2478 (99%)	-0.75	5 (0%) 91 93	4, 11, 22, 57	140 (5%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	62	PRO	2.8
3	C	62	PRO	2.7
3	F	60	ASP	2.7
3	C	60	ASP	2.6
1	D	2	ALA	2.5

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	0.05	9,11,14,15	0
1	MHS	D	257	11/12	0.97	0.04	8,10,13,14	0
1	MGN	A	400	10/11	0.98	0.04	6,8,9,9	0
1	AGM	A	271	12/13	0.98	0.03	5,7,7,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	AGM	D	271	12/13	0.98	0.04	6,7,8,9	0
1	SMC	A	452	7/8	0.99	0.04	7,7,9,11	0
1	MGN	D	400	10/11	0.99	0.03	6,8,9,9	0
1	SMC	D	452	7/8	0.99	0.04	8,9,10,12	0
1	GL3	D	445	4/5	1.00	0.02	7,7,7,8	0
1	GL3	A	445	4/5	1.00	0.03	6,7,8,8	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($\text{\AA}^2$)	Q<0.9
9	ACT	C	1	4/4	0.80	0.11	35,36,36,38	0
10	EDO	A	558	4/4	0.81	0.13	48,50,50,51	0
10	EDO	F	252	4/4	0.84	0.12	35,36,44,44	0
10	EDO	C	251	4/4	0.87	0.10	40,42,44,44	0
11	PEG	C	252	7/7	0.87	0.11	35,38,45,47	0
10	EDO	A	557	4/4	0.88	0.10	40,46,46,48	0
10	EDO	D	558	4/4	0.89	0.10	24,33,38,39	0
10	EDO	D	557	4/4	0.90	0.11	43,43,45,48	0
11	PEG	A	559	7/7	0.90	0.10	21,36,45,45	0
10	EDO	F	251	4/4	0.90	0.10	36,42,45,46	0
4	MG	D	552	1/1	0.93	0.09	20,20,20,20	1
4	MG	A	552[B]	1/1	0.95	0.08	20,20,20,20	1
7	COM	D	555[A]	7/7	0.95	0.08	6,10,11,14	7
4	MG	B	444	1/1	0.95	0.11	29,29,29,29	0
4	MG	D	1	1/1	0.95	0.10	23,23,23,23	1
7	COM	A	554[A]	7/7	0.96	0.09	9,10,13,14	7
4	MG	B	445[A]	1/1	0.96	0.10	20,20,20,20	1
4	MG	E	445[B]	1/1	0.96	0.04	20,20,20,20	1
4	MG	D	551	1/1	0.98	0.04	18,18,18,18	1
9	ACT	A	556[A]	4/4	0.98	0.04	14,15,16,16	4
4	MG	F	250	1/1	0.98	0.06	15,15,15,15	0
4	MG	E	444	1/1	0.98	0.15	21,21,21,21	0

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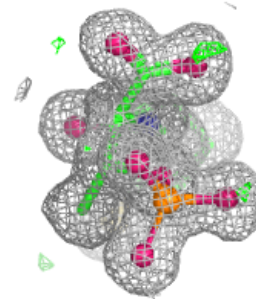
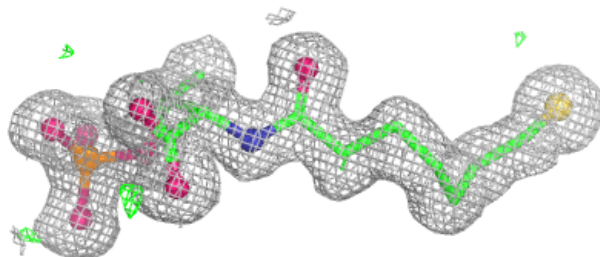
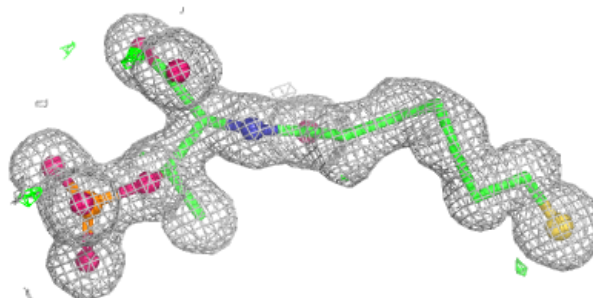
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	TP7	D	554[A]	21/21	0.99	0.04	7,8,11,12	21
4	MG	A	551[A]	1/1	0.99	0.10	17,17,17,17	1
4	MG	C	250	1/1	0.99	0.05	16,16,16,16	0
8	TXZ	A	555[B]	20/20	0.99	0.03	5,8,10,12	20
8	TXZ	D	556[B]	20/20	0.99	0.04	7,8,10,11	20
5	F43	A	1	62/62	0.99	0.03	7,8,11,13	0
5	F43	D	553	62/62	0.99	0.03	6,8,10,12	0
6	TP7	A	553[A]	21/21	0.99	0.04	8,9,12,15	21
12	ZN	A	560	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.

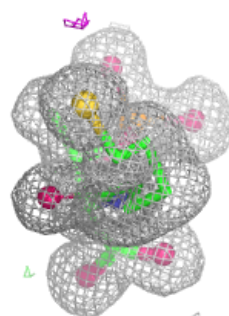
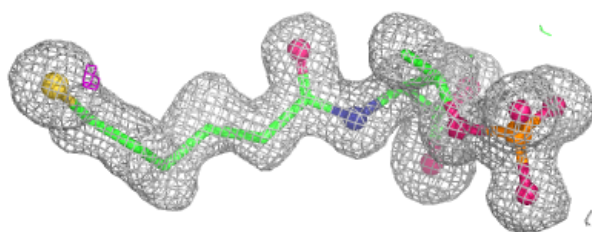
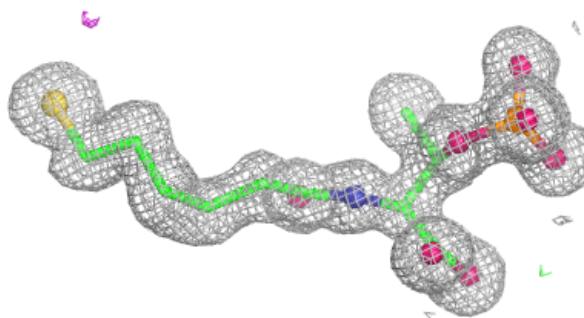
Electron density around TP7 D 554 (A):

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

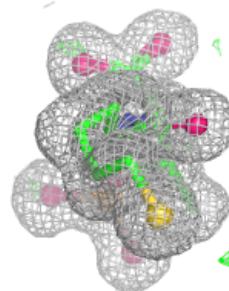
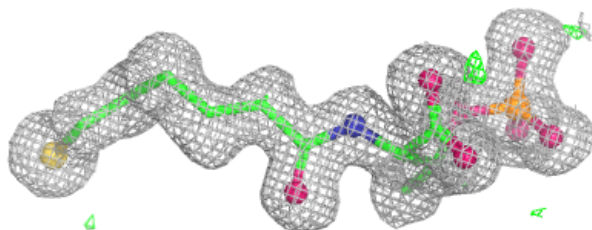
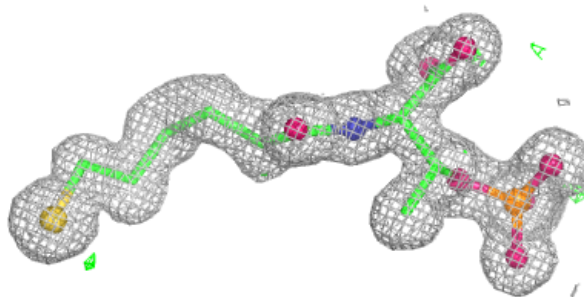


Electron density around TXZ A 555 (B):

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

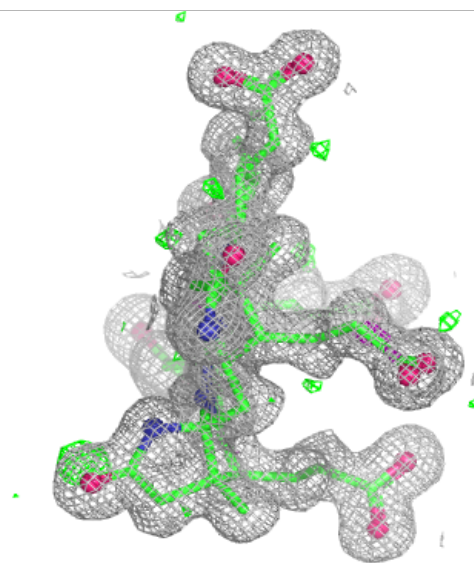
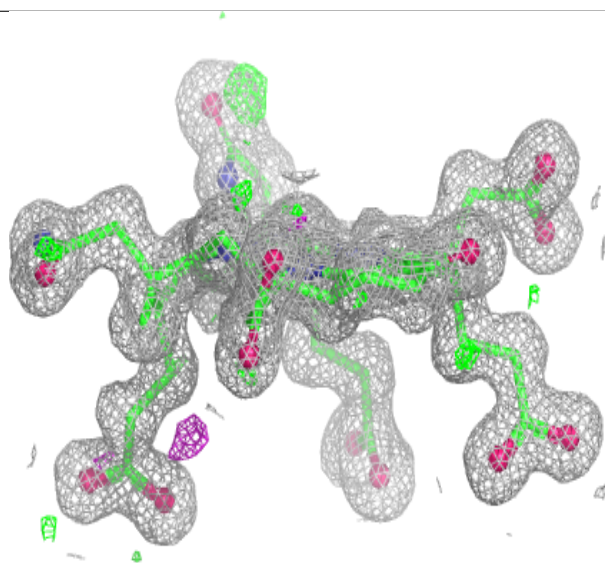
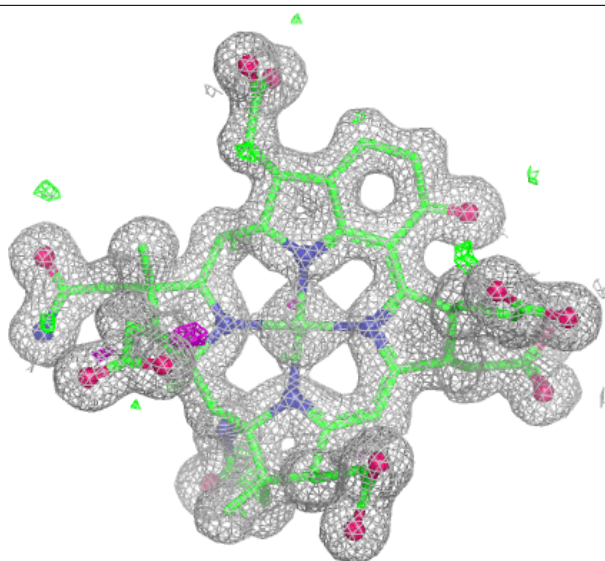
**Electron density around TXZ D 556 (B):**

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



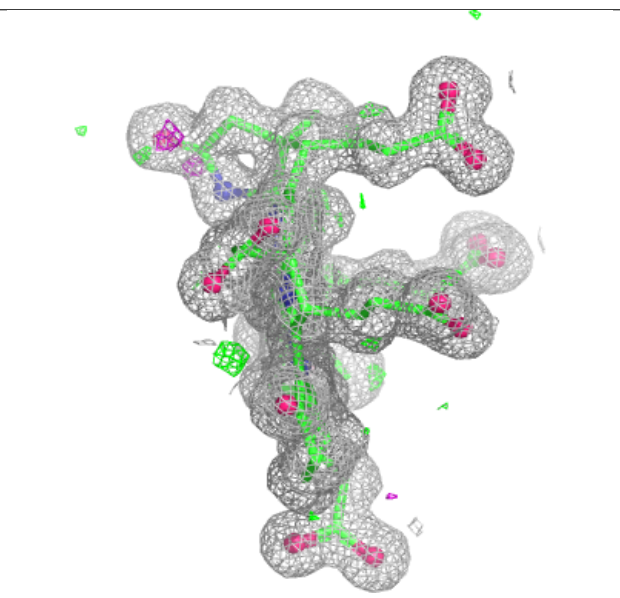
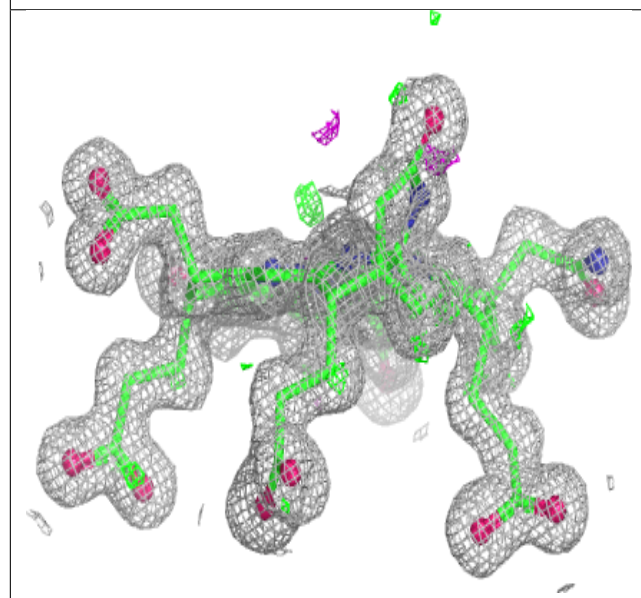
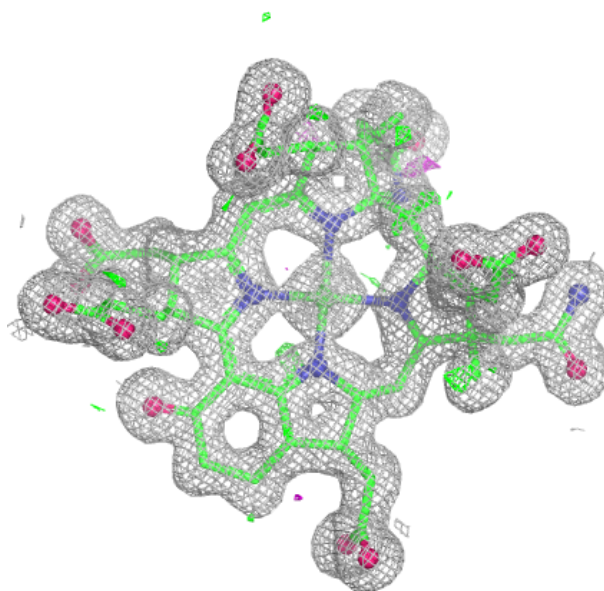
Electron density around F43 A 1:

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



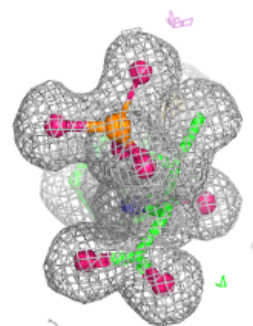
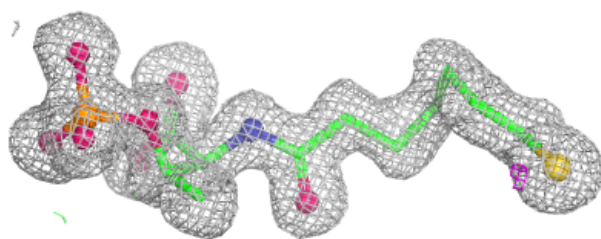
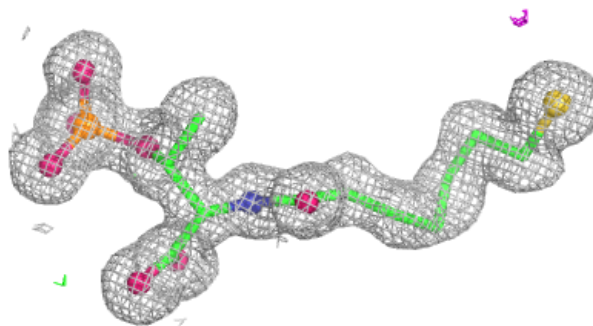
Electron density around F43 D 553:

$2mF_o-DF_c$ (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)



6.5 Other polymers ⓘ

There are no such residues in this entry.