Full wwPDB X-ray Structure Validation Report (i)

Oct 1, 2023 – 12:19 AM EDT

PDB ID	:	3M2U
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

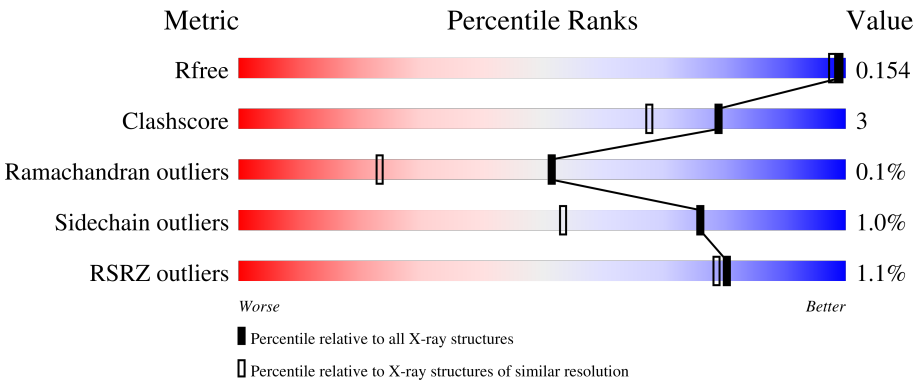
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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}	130704	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (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 <=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	84% 13% •
1	D	549	% 85% 14% •
2	B	442	86% 14% •
2	E	442	% 83% 16% •
3	C	248	3% 81% 17% • •

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Mol	Chain	Length	Quality of chain
3	F	248	4% 81% 16%

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
			Total	C	N	O	S			
1	A	548	4446	2817	734	874	21	0	31	0
1	D	548	4410	2799	724	867	20	0	28	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	442	3464	2212	563	666	23	0	24	0
2	E	442	3527	2250	571	683	23	0	34	0

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

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

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

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

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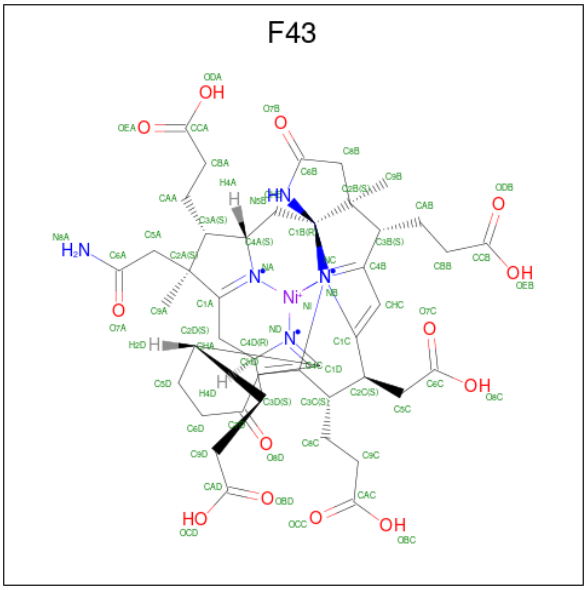
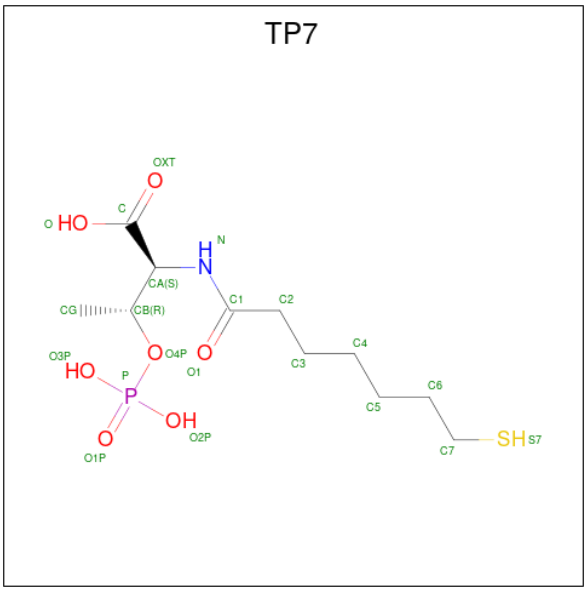
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	E	2	2	2	0	1
			Total	Mg		
4	F	1	1	1	0	0

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



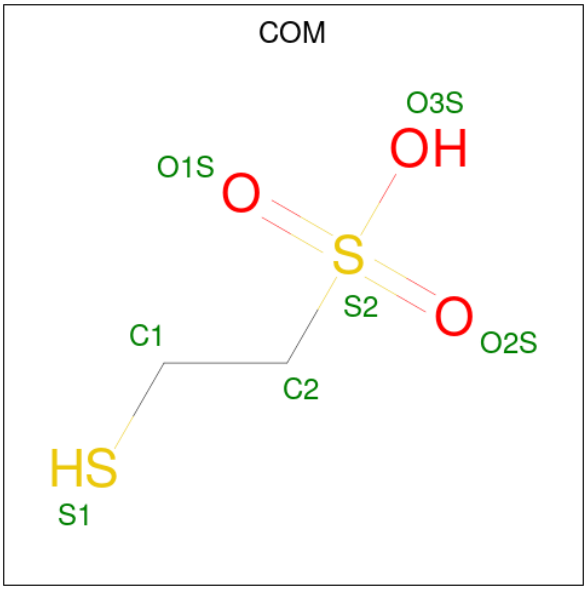
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	Ni	O		
5	A	1	62	42	6	1	13	0	0
			Total	C	N	Ni	O		
5	D	1	62	42	6	1	13	0	0

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



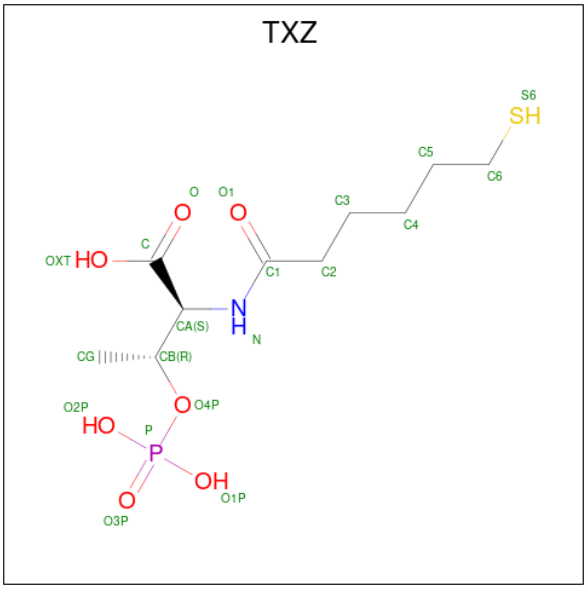
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
6	A	1	21	11	1	7	1	1	0	1
			Total	C	N	O	P	S		
6	D	1	21	11	1	7	1	1	0	1

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



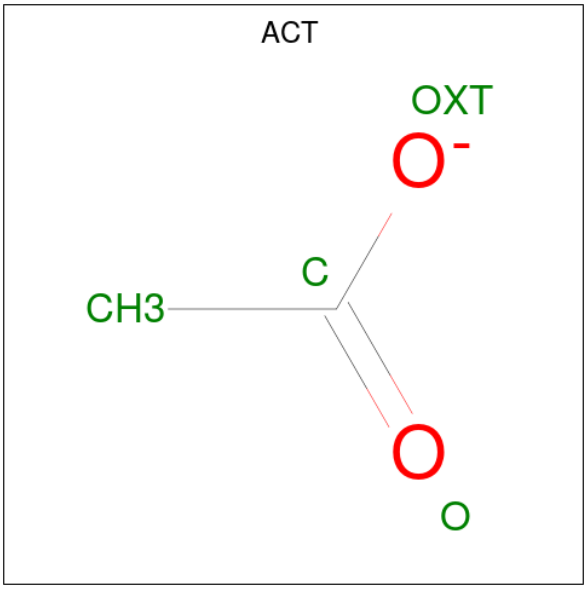
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
7	A	1	7	2	3	2	0	1
			Total	C	O	S		
7	D	1	7	2	3	2	0	1

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



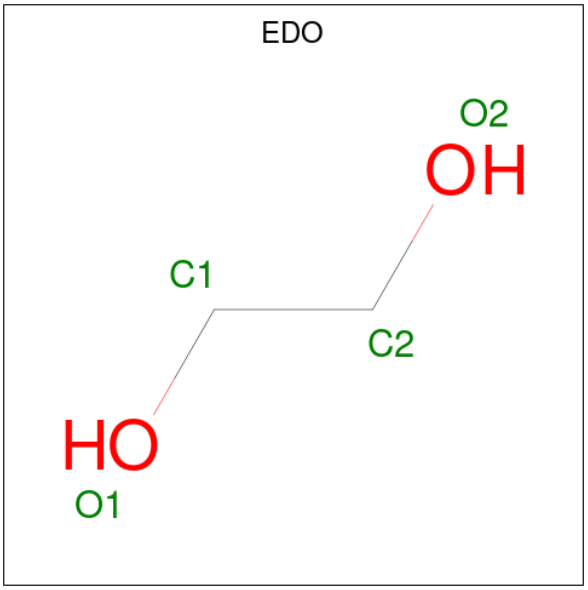
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
8	A	1	20	10	1	7	1	1	0	1
			Total	C	N	O	P	S		
8	D	1	20	10	1	7	1	1	0	1

- Molecule 9 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



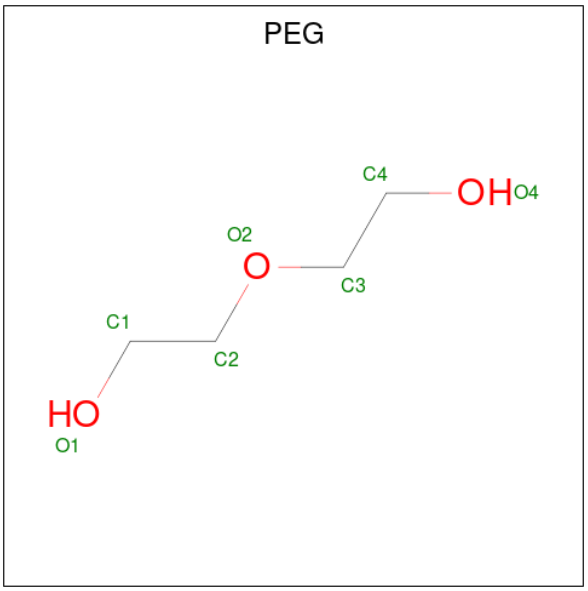
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	A	1	4	2	2	0	1
			Total	C	O		
9	C	1	4	2	2	0	0

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 11 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 13 is water.

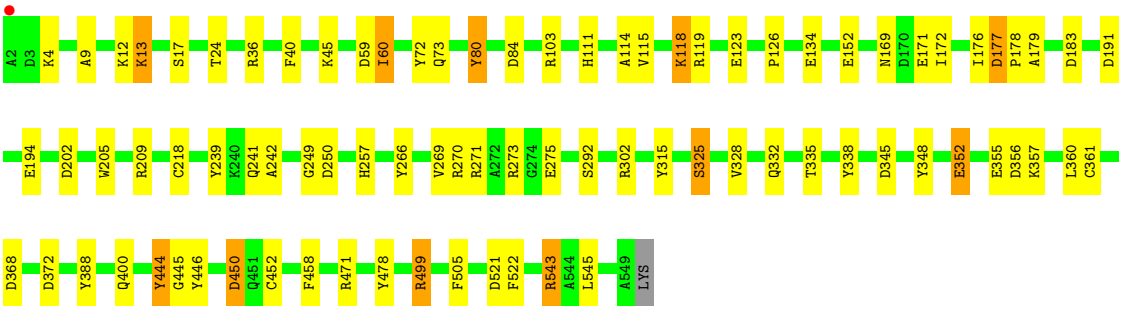
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	482	Total O 491 491	0	24
13	B	436	Total O 454 454	0	26
13	C	245	Total O 255 255	0	15
13	D	488	Total O 502 502	0	23
13	E	393	Total O 400 400	0	11
13	F	246	Total O 250 250	0	10

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.

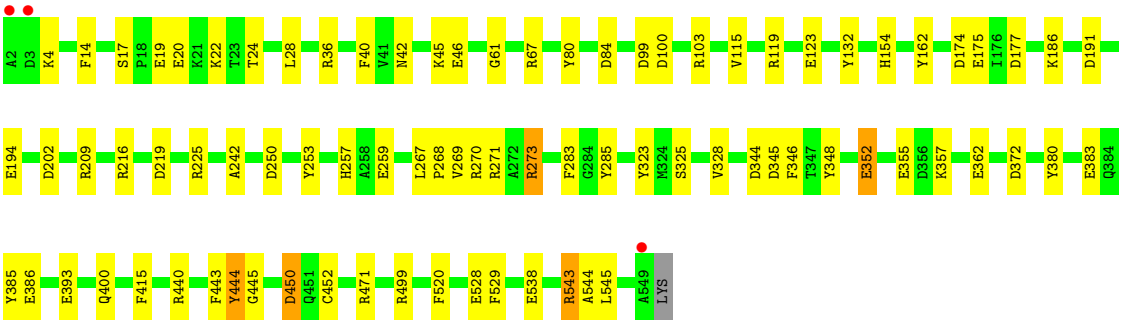
• Molecule 1: Methyl-coenzyme M reductase I subunit alpha

Chain A: 84% 13% •



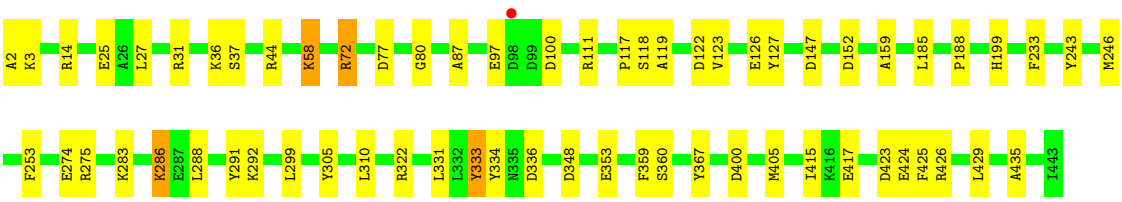
• Molecule 1: Methyl-coenzyme M reductase I subunit alpha

Chain D: % 85% 14% •



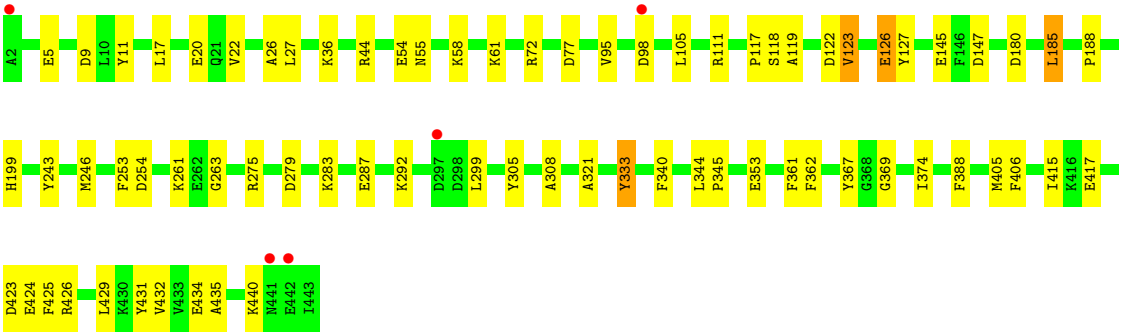
• Molecule 2: Methyl-coenzyme M reductase I subunit beta

Chain B: 86% 14% •



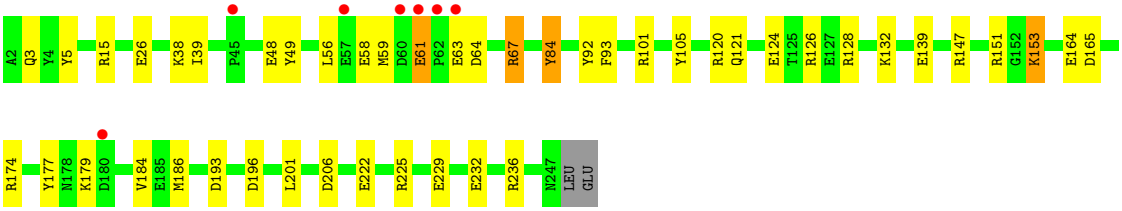
• Molecule 2: Methyl-coenzyme M reductase I subunit beta

Chain E:



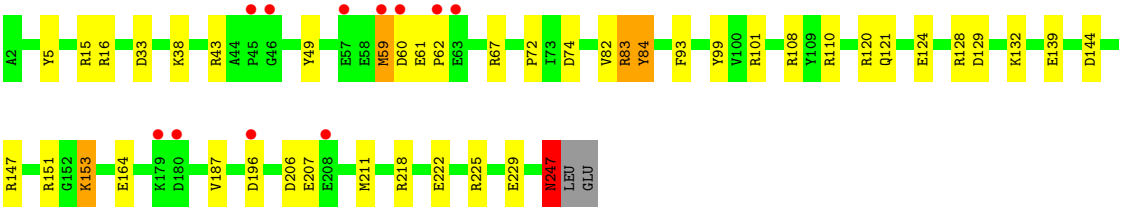
• Molecule 3: Methyl-coenzyme M reductase I subunit gamma

Chain C:



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

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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) 98.6 (19.89-1.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.01%)	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 , 51.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	1.60	28/4555 (0.6%)	1.38	44/6181 (0.7%)
1	D	1.61	27/4531 (0.6%)	1.43	49/6148 (0.8%)
2	B	1.58	28/3580 (0.8%)	1.38	24/4841 (0.5%)
2	E	1.61	31/3656 (0.8%)	1.40	26/4943 (0.5%)
3	C	1.64	20/2143 (0.9%)	1.52	28/2885 (1.0%)
3	F	1.67	14/2105 (0.7%)	1.53	32/2833 (1.1%)
All	All	1.61	148/20570 (0.7%)	1.43	203/27831 (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	1
1	D	1	0
2	B	0	2
2	E	0	1
All	All	2	4

All (148) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	134	GLU	CD-OE1	9.96	1.36	1.25
2	B	3	LYS	CD-CE	-9.19	1.28	1.51
3	C	153	LYS	CE-NZ	8.90	1.71	1.49
2	B	58	LYS	CB-CG	-8.75	1.28	1.52
1	A	171	GLU	CB-CG	7.69	1.66	1.52
3	C	177	TYR	CE2-CZ	-7.44	1.28	1.38
3	F	139	GLU	CD-OE2	7.28	1.33	1.25
1	D	259[A]	GLU	CG-CD	7.25	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	259[B]	GLU	CG-CD	7.25	1.62	1.51
1	A	134	GLU	CG-CD	7.16	1.62	1.51
1	D	123	GLU	CD-OE1	-7.16	1.17	1.25
3	C	124	GLU	CG-CD	7.09	1.62	1.51
2	E	434	GLU	CG-CD	6.99	1.62	1.51
1	A	205	TRP	CG-CD1	6.98	1.46	1.36
1	A	444	TYR	CZ-OH	6.87	1.49	1.37
2	E	353	GLU	CG-CD	6.80	1.62	1.51
2	B	274	GLU	CG-CD	6.78	1.62	1.51
3	C	229	GLU	CD-OE2	6.75	1.33	1.25
1	D	444	TYR	CD1-CE1	6.70	1.49	1.39
1	A	352[A]	GLU	CB-CG	6.55	1.64	1.52
1	A	352[B]	GLU	CB-CG	6.55	1.64	1.52
3	F	218	ARG	CZ-NH1	6.49	1.41	1.33
3	F	124	GLU	CG-CD	6.49	1.61	1.51
2	E	321	ALA	CA-CB	6.49	1.66	1.52
2	E	5	GLU	CG-CD	6.48	1.61	1.51
2	E	305	TYR	CD2-CE2	6.44	1.49	1.39
1	A	123	GLU	CD-OE2	6.39	1.32	1.25
3	C	38	LYS	CE-NZ	6.37	1.65	1.49
3	C	3	GLN	CG-CD	6.35	1.65	1.51
2	E	253	PHE	CD1-CE1	6.34	1.51	1.39
3	C	84	TYR	CD1-CE1	6.33	1.48	1.39
1	D	269	VAL	CA-CB	6.31	1.68	1.54
2	B	417	GLU	CD-OE2	6.27	1.32	1.25
3	C	84	TYR	CE2-CZ	-6.24	1.30	1.38
2	B	360	SER	CB-OG	6.23	1.50	1.42
1	D	543	ARG	CB-CG	6.18	1.69	1.52
3	F	49	TYR	CE2-CZ	6.18	1.46	1.38
2	B	87	ALA	CA-CB	6.12	1.65	1.52
1	D	444	TYR	CE2-CZ	-6.08	1.30	1.38
3	C	139	GLU	CD-OE2	6.07	1.32	1.25
1	A	338	TYR	CE1-CZ	6.07	1.46	1.38
1	A	269	VAL	CA-CB	6.03	1.67	1.54
3	F	67	ARG	CZ-NH2	6.02	1.40	1.33
1	A	123	GLU	CG-CD	6.01	1.60	1.51
1	A	292	SER	CB-OG	5.98	1.50	1.42
1	D	162	TYR	CG-CD2	5.97	1.47	1.39
1	D	4	LYS	CG-CD	-5.96	1.32	1.52
1	D	538	GLU	CD-OE1	5.95	1.32	1.25
2	B	333	TYR	CG-CD2	5.94	1.46	1.39
3	F	222	GLU	CB-CG	5.92	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	383[A]	GLU	CB-CG	-5.90	1.41	1.52
1	D	383[B]	GLU	CB-CG	-5.90	1.41	1.52
3	F	164	GLU	CD-OE2	5.85	1.32	1.25
2	B	159	ALA	CA-CB	5.85	1.64	1.52
2	E	117[A]	PRO	C-O	5.84	1.34	1.23
2	E	117[B]	PRO	C-O	5.84	1.34	1.23
2	E	434	GLU	CB-CG	5.83	1.63	1.52
1	D	386	GLU	CD-OE1	5.82	1.32	1.25
2	B	435	ALA	CA-CB	5.79	1.64	1.52
2	E	123[A]	VAL	CB-CG2	-5.79	1.40	1.52
2	E	123[B]	VAL	CB-CG2	-5.79	1.40	1.52
3	C	222	GLU	CB-CG	5.76	1.63	1.52
1	D	123	GLU	CG-CD	5.75	1.60	1.51
2	E	22	VAL	CB-CG2	5.74	1.65	1.52
3	F	84	TYR	CE1-CZ	5.74	1.46	1.38
1	A	471	ARG	CZ-NH2	5.74	1.40	1.33
2	E	126	GLU	CD-OE2	5.73	1.31	1.25
2	E	435	ALA	CA-CB	5.72	1.64	1.52
1	A	60	ILE	C-N	-5.72	1.22	1.33
1	D	4	LYS	CE-NZ	-5.72	1.34	1.49
1	D	14	PHE	CD2-CE2	5.71	1.50	1.39
1	D	175	GLU	CD-OE2	-5.70	1.19	1.25
2	E	54	GLU	CD-OE1	-5.70	1.19	1.25
2	E	54	GLU	CB-CG	5.66	1.62	1.52
1	A	36	ARG	CZ-NH1	5.66	1.40	1.33
1	D	19	GLU	CD-OE1	5.65	1.31	1.25
2	E	406	PHE	CE2-CZ	5.64	1.48	1.37
1	A	119	ARG	CB-CG	-5.62	1.37	1.52
1	A	72	TYR	CE2-CZ	5.62	1.45	1.38
1	A	152	GLU	CG-CD	5.58	1.60	1.51
2	B	2	ALA	N-CA	5.58	1.57	1.46
2	E	243	TYR	CD2-CE2	5.57	1.47	1.39
2	E	292	LYS	CD-CE	5.56	1.65	1.51
2	E	431	TYR	CD2-CE2	5.55	1.47	1.39
1	D	119	ARG	CG-CD	5.55	1.65	1.51
2	B	322[A]	ARG	CZ-NH1	5.51	1.40	1.33
2	B	322[B]	ARG	CZ-NH1	5.51	1.40	1.33
1	D	362	GLU	CD-OE2	5.50	1.31	1.25
2	B	118	SER	CA-CB	5.50	1.61	1.52
1	D	543	ARG	CG-CD	-5.49	1.38	1.51
3	F	225	ARG	CZ-NH1	-5.44	1.25	1.33
1	D	61	GLY	N-CA	5.43	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	544	ALA	CA-CB	5.42	1.63	1.52
2	E	26	ALA	CA-CB	5.42	1.63	1.52
2	E	11	TYR	CE1-CZ	5.42	1.45	1.38
3	F	187	VAL	CB-CG1	5.37	1.64	1.52
2	B	253	PHE	CD1-CE1	5.36	1.50	1.39
1	A	239	TYR	CE2-CZ	5.36	1.45	1.38
2	B	367	TYR	CG-CD1	5.34	1.46	1.39
3	C	124	GLU	CD-OE1	-5.34	1.19	1.25
1	D	132	TYR	CD2-CE2	5.33	1.47	1.39
2	B	286	LYS	N-CA	5.32	1.56	1.46
2	E	145	GLU	CD-OE2	5.32	1.31	1.25
2	B	274	GLU	CD-OE1	5.30	1.31	1.25
2	B	117	PRO	C-O	5.29	1.33	1.23
2	B	44	ARG	CZ-NH2	5.29	1.40	1.33
2	B	127	TYR	CE1-CZ	5.27	1.45	1.38
2	E	340	PHE	CG-CD1	5.26	1.46	1.38
1	A	325	SER	CA-CB	5.26	1.60	1.52
3	F	164	GLU	CG-CD	5.26	1.59	1.51
2	B	243	TYR	CZ-OH	5.26	1.46	1.37
2	E	367	TYR	CD2-CE2	5.25	1.47	1.39
3	C	184	VAL	CB-CG1	5.23	1.63	1.52
2	E	417	GLU	CD-OE2	5.23	1.31	1.25
1	D	393	GLU	CG-CD	5.23	1.59	1.51
3	C	48	GLU	CB-CG	5.22	1.62	1.52
2	B	58	LYS	CE-NZ	5.20	1.62	1.49
1	A	355	GLU	CD-OE2	5.19	1.31	1.25
3	C	229	GLU	CD-OE1	-5.19	1.20	1.25
2	E	367	TYR	CE2-CZ	-5.19	1.31	1.38
1	A	239	TYR	CG-CD1	5.17	1.45	1.39
2	B	334	TYR	CD2-CE2	5.17	1.47	1.39
3	C	120	ARG	CZ-NH1	5.16	1.39	1.33
3	C	49	TYR	CG-CD1	5.15	1.45	1.39
3	C	193	ASP	CB-CG	5.15	1.62	1.51
2	B	80	GLY	N-CA	5.13	1.53	1.46
2	E	308	ALA	CA-CB	5.13	1.63	1.52
2	E	287	GLU	CD-OE1	5.13	1.31	1.25
2	B	233[A]	PHE	CD2-CE2	5.13	1.49	1.39
2	B	233[B]	PHE	CD2-CE2	5.13	1.49	1.39
3	C	26	GLU	CB-CG	5.13	1.61	1.52
1	D	380	TYR	CG-CD1	5.13	1.45	1.39
1	A	123	GLU	CD-OE1	5.12	1.31	1.25
2	B	305	TYR	CZ-OH	5.10	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	353	GLU	CD-OE1	-5.10	1.20	1.25
2	E	263	GLY	N-CA	5.09	1.53	1.46
3	F	229	GLU	CD-OE2	5.08	1.31	1.25
3	C	58	GLU	CB-CG	-5.08	1.42	1.52
1	A	275	GLU	CD-OE2	5.07	1.31	1.25
3	C	26	GLU	CG-CD	-5.07	1.44	1.51
3	F	38	LYS	CE-NZ	5.06	1.61	1.49
1	A	315	TYR	CD1-CE1	5.05	1.47	1.39
2	E	406	PHE	CG-CD1	5.05	1.46	1.38
1	A	446	TYR	CE2-CZ	5.04	1.45	1.38
1	D	19	GLU	CG-CD	5.03	1.59	1.51
1	A	178[A]	PRO	CA-C	5.00	1.62	1.52
1	A	178[B]	PRO	CA-C	5.00	1.62	1.52
3	F	247	ASN	CA-CB	5.00	1.66	1.53

All (203) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	147	ARG	NE-CZ-NH1	18.90	129.75	120.30
2	B	44	ARG	NE-CZ-NH1	14.68	127.64	120.30
3	F	147	ARG	NE-CZ-NH1	13.93	127.26	120.30
2	E	353	GLU	OE1-CD-OE2	13.62	139.64	123.30
3	C	147	ARG	NE-CZ-NH2	-11.91	114.34	120.30
1	A	471	ARG	NE-CZ-NH1	10.58	125.59	120.30
3	F	101	ARG	NE-CZ-NH2	-10.44	115.08	120.30
3	C	101	ARG	NE-CZ-NH2	-10.03	115.28	120.30
3	F	59	MET	CG-SD-CE	-9.91	84.33	100.20
3	F	5	TYR	CB-CG-CD1	-9.58	115.25	121.00
1	A	444	TYR	CB-CG-CD2	-9.46	115.32	121.00
2	E	275	ARG	NE-CZ-NH2	-8.99	115.81	120.30
2	E	44	ARG	NE-CZ-NH1	8.89	124.75	120.30
3	F	225	ARG	NE-CZ-NH2	-8.71	115.95	120.30
1	A	471	ARG	NE-CZ-NH2	-8.64	115.98	120.30
2	B	31	ARG	NE-CZ-NH1	8.62	124.61	120.30
3	C	196	ASP	CB-CG-OD1	8.59	126.03	118.30
3	F	67	ARG	NE-CZ-NH2	-8.55	116.02	120.30
3	C	5	TYR	CZ-CE2-CD2	-8.52	112.13	119.80
1	A	356	ASP	CB-CG-OD1	-8.34	110.79	118.30
2	B	100	ASP	CB-CG-OD2	-8.27	110.86	118.30
3	C	206	ASP	CB-CG-OD1	8.19	125.67	118.30
1	D	216	ARG	NE-CZ-NH1	8.17	124.39	120.30
1	D	119	ARG	NE-CZ-NH2	-8.04	116.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	353	GLU	OE1-CD-OE2	8.02	132.92	123.30
3	F	206	ASP	CB-CG-OD1	7.84	125.36	118.30
1	D	40	PHE	CB-CG-CD2	-7.81	115.33	120.80
3	C	120	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	D	216	ARG	NE-CZ-NH2	-7.74	116.43	120.30
3	F	144	ASP	CB-CG-OD2	7.72	125.25	118.30
2	B	426	ARG	NE-CZ-NH1	7.68	124.14	120.30
2	B	77	ASP	CB-CG-OD2	-7.65	111.41	118.30
1	D	444	TYR	CB-CG-CD2	-7.64	116.41	121.00
2	E	185	LEU	CB-CG-CD1	7.64	123.99	111.00
2	E	9	ASP	CB-CG-OD2	-7.60	111.46	118.30
1	D	209	ARG	NE-CZ-NH1	7.57	124.08	120.30
3	F	144	ASP	CB-CG-OD1	-7.51	111.54	118.30
3	C	105	TYR	CB-CG-CD1	7.38	125.43	121.00
1	A	543	ARG	NE-CZ-NH1	7.34	123.97	120.30
3	F	147	ARG	NE-CZ-NH2	-7.32	116.64	120.30
3	F	196	ASP	CB-CG-OD1	7.26	124.83	118.30
1	D	386	GLU	OE1-CD-OE2	-7.23	114.62	123.30
1	A	40	PHE	CB-CG-CD2	-7.19	115.77	120.80
1	D	202	ASP	CB-CG-OD1	7.05	124.65	118.30
3	F	128	ARG	NE-CZ-NH1	-7.04	116.78	120.30
1	A	36	ARG	NE-CZ-NH2	6.98	123.79	120.30
3	C	105	TYR	CB-CG-CD2	-6.96	116.82	121.00
1	A	522	PHE	CB-CG-CD1	-6.95	115.93	120.80
2	E	333	TYR	CB-CG-CD1	-6.93	116.84	121.00
2	E	9	ASP	CB-CG-OD1	6.91	124.52	118.30
3	C	67[A]	ARG	NE-CZ-NH1	-6.85	116.87	120.30
3	C	67[B]	ARG	NE-CZ-NH1	-6.85	116.87	120.30
1	D	471	ARG	NE-CZ-NH2	-6.85	116.87	120.30
1	A	273	ARG	NE-CZ-NH1	6.78	123.69	120.30
3	F	151	ARG	CG-CD-NE	-6.78	97.56	111.80
3	F	83	ARG	NE-CZ-NH2	-6.77	116.91	120.30
3	F	16	ARG	NE-CZ-NH2	-6.71	116.95	120.30
2	E	243	TYR	CB-CG-CD1	-6.68	116.99	121.00
3	C	15	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	D	346	PHE	CB-CG-CD1	6.55	125.39	120.80
2	B	72	ARG	NE-CZ-NH1	6.54	123.57	120.30
3	C	236	ARG	NE-CZ-NH1	-6.53	117.04	120.30
1	D	177	ASP	CB-CG-OD1	6.53	124.17	118.30
1	D	346	PHE	CB-CG-CD2	-6.50	116.25	120.80
3	C	120	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	270	ARG	NE-CZ-NH1	6.48	123.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	291	TYR	CD1-CE1-CZ	-6.43	114.01	119.80
1	A	444	TYR	CD1-CE1-CZ	-6.42	114.02	119.80
1	D	67	ARG	NE-CZ-NH1	6.38	123.49	120.30
3	C	225	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	A	266	TYR	CB-CG-CD2	-6.37	117.18	121.00
1	D	345	ASP	CB-CG-OD1	-6.36	112.58	118.30
2	E	279	ASP	CB-CG-OD1	6.34	124.01	118.30
2	B	152	ASP	CB-CG-OD2	-6.34	112.60	118.30
3	C	126	ARG	NE-CZ-NH1	6.33	123.46	120.30
2	B	25	GLU	OE1-CD-OE2	6.33	130.89	123.30
1	D	344	ASP	CB-CG-OD1	-6.32	112.61	118.30
1	D	14	PHE	CB-CG-CD2	-6.29	116.40	120.80
1	A	499	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	D	528	GLU	OE1-CD-OE2	-6.27	115.78	123.30
1	D	250	ASP	CB-CG-OD2	-6.27	112.66	118.30
3	F	16	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	A	103	ARG	NE-CZ-NH1	6.26	123.43	120.30
2	B	111	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	A	345	ASP	CB-CG-OD1	-6.22	112.70	118.30
2	E	180	ASP	CB-CG-OD1	6.22	123.90	118.30
2	B	291	TYR	CB-CG-CD1	-6.18	117.29	121.00
1	A	239	TYR	CD1-CE1-CZ	6.16	125.34	119.80
3	C	128	ARG	NE-CZ-NH1	-6.15	117.22	120.30
1	D	543	ARG	NE-CZ-NH2	-6.11	117.24	120.30
1	A	60	ILE	C-N-CA	-6.11	109.47	122.30
2	B	185	LEU	CB-CG-CD1	6.06	121.30	111.00
3	F	110	ARG	NE-CZ-NH1	-6.03	117.28	120.30
1	A	45	LYS	CD-CE-NZ	-6.02	97.85	111.70
2	E	423	ASP	CB-CG-OD1	6.01	123.71	118.30
2	B	359	PHE	CB-CG-CD1	6.00	125.00	120.80
3	F	120	ARG	NE-CZ-NH1	5.98	123.29	120.30
3	C	92	TYR	CD1-CE1-CZ	-5.96	114.43	119.80
1	A	250	ASP	CB-CG-OD1	5.96	123.67	118.30
2	E	361	PHE	CB-CG-CD2	-5.96	116.63	120.80
1	A	80	TYR	CB-CG-CD2	-5.91	117.45	121.00
3	F	93	PHE	CB-CG-CD1	-5.91	116.67	120.80
1	A	505	PHE	CB-CG-CD2	-5.89	116.68	120.80
2	E	111	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	D	283	PHE	CB-CG-CD2	-5.87	116.69	120.80
1	A	450	ASP	CB-CA-C	5.86	122.12	110.40
1	D	100	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	A	478	TYR	CB-CG-CD2	-5.85	117.49	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	15	ARG	NE-CZ-NH2	-5.84	117.38	120.30
2	E	353	GLU	CG-CD-OE2	-5.83	106.65	118.30
3	C	165	ASP	CB-CG-OD1	-5.77	113.11	118.30
1	A	458	PHE	CB-CG-CD2	-5.74	116.78	120.80
1	D	36	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	D	225	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	348	TYR	CB-CG-CD2	-5.74	117.56	121.00
1	A	388	TYR	CZ-CE2-CD2	-5.73	114.64	119.80
1	A	209	ARG	NE-CZ-NH2	-5.70	117.45	120.30
3	F	124	GLU	OE1-CD-OE2	5.70	130.13	123.30
1	D	36	ARG	NE-CZ-NH1	-5.67	117.46	120.30
2	E	426	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	D	348	TYR	CB-CG-CD1	-5.63	117.62	121.00
1	A	368	ASP	CB-CG-OD2	-5.63	113.24	118.30
2	E	254	ASP	CB-CG-OD2	-5.59	113.27	118.30
2	E	147	ASP	CB-CG-OD1	5.58	123.32	118.30
3	F	153[A]	LYS	CD-CE-NZ	-5.58	98.87	111.70
3	F	153[B]	LYS	CD-CE-NZ	-5.58	98.87	111.70
2	B	348	ASP	CB-CG-OD1	5.57	123.32	118.30
1	A	183	ASP	CB-CG-OD2	-5.57	113.29	118.30
3	C	174	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	D	174	ASP	CB-CG-OD1	5.55	123.29	118.30
1	D	28	LEU	CB-CG-CD2	-5.55	101.57	111.00
1	A	177[A]	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	177[B]	ASP	CB-CG-OD1	5.52	123.27	118.30
3	F	74	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	A	521	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	D	253	TYR	CZ-CE2-CD2	-5.50	114.85	119.80
1	D	520	PHE	CB-CG-CD2	-5.49	116.95	120.80
1	D	273	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	D	450	ASP	N-CA-CB	5.46	120.43	110.60
3	F	43	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	D	219	ASP	CB-CG-OD1	5.45	123.20	118.30
3	F	33	ASP	CB-CG-OD1	5.45	123.20	118.30
2	E	72	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	13[A]	LYS	CB-CA-C	-5.43	99.54	110.40
1	A	13[B]	LYS	CB-CA-C	-5.43	99.54	110.40
1	A	545	LEU	CB-CG-CD2	-5.42	101.78	111.00
1	D	175	GLU	OE1-CD-OE2	5.42	129.80	123.30
1	D	499	ARG	NE-CZ-NH2	-5.41	117.59	120.30
2	B	36	LYS	CD-CE-NZ	-5.41	99.27	111.70
3	F	108	ARG	NE-CZ-NH2	-5.40	117.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	93	PHE	CB-CG-CD1	-5.40	117.02	120.80
2	B	425	PHE	CB-CG-CD2	-5.39	117.03	120.80
2	E	105	LEU	CB-CG-CD1	-5.38	101.86	111.00
1	D	529	PHE	CB-CG-CD2	-5.37	117.04	120.80
2	E	243	TYR	CZ-CE2-CD2	-5.37	114.97	119.80
1	D	270	ARG	NE-CZ-NH2	-5.36	117.62	120.30
2	E	388	PHE	CB-CG-CD2	5.36	124.55	120.80
2	B	336	ASP	CB-CG-OD1	5.34	123.11	118.30
1	A	84	ASP	CB-CG-OD1	-5.34	113.49	118.30
2	B	147	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	521	ASP	CB-CG-OD1	5.32	123.08	118.30
1	A	40	PHE	CB-CG-CD1	5.32	124.52	120.80
3	C	151	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	302	ARG	NE-CZ-NH2	-5.31	117.65	120.30
2	E	425	PHE	CB-CG-CD2	-5.31	117.09	120.80
2	E	77	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	A	444	TYR	CB-CG-CD1	5.29	124.17	121.00
1	A	103	ARG	NE-CZ-NH2	-5.28	117.66	120.30
3	C	92	TYR	CG-CD1-CE1	5.26	125.51	121.30
3	F	74	ASP	CB-CG-OD1	5.25	123.03	118.30
1	D	415	PHE	CB-CG-CD2	-5.25	117.12	120.80
1	D	285	TYR	CB-CG-CD2	-5.25	117.85	121.00
2	B	423	ASP	CB-CG-OD2	-5.24	113.58	118.30
2	E	279	ASP	OD1-CG-OD2	-5.24	113.34	123.30
3	F	99	TYR	CB-CG-CD1	-5.21	117.87	121.00
3	F	225	ARG	NH1-CZ-NH2	5.20	125.12	119.40
1	D	99	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	202	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	A	209	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	D	80	TYR	CB-CG-CD2	-5.20	117.88	121.00
1	D	443	PHE	CB-CG-CD2	-5.20	117.16	120.80
3	F	129	ASP	CB-CG-OD2	5.19	122.97	118.30
1	D	385	TYR	CD1-CE1-CZ	-5.16	115.16	119.80
3	C	232	GLU	OE1-CD-OE2	5.15	129.48	123.30
3	F	129	ASP	CB-CG-OD1	-5.15	113.66	118.30
2	B	305	TYR	CE1-CZ-CE2	5.15	128.04	119.80
2	B	400	ASP	CB-CG-OD2	5.15	122.93	118.30
1	D	103	ARG	NE-CZ-NH2	-5.14	117.73	120.30
2	B	292	LYS	CD-CE-NZ	-5.10	99.96	111.70
3	C	124	GLU	OE1-CD-OE2	5.10	129.42	123.30
1	D	84	ASP	CB-CG-OD2	5.10	122.89	118.30
3	C	151	ARG	NE-CZ-NH2	5.09	122.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	126	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	D	543	ARG	NE-CZ-NH1	5.07	122.83	120.30
2	E	423	ASP	CB-CG-OD2	-5.07	113.74	118.30
2	B	275	ARG	NE-CZ-NH2	-5.05	117.77	120.30
3	C	84	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	D	440	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	59	ASP	CB-CG-OD2	-5.03	113.78	118.30
1	D	543	ARG	CA-CB-CG	5.03	124.46	113.40
2	E	127	TYR	CG-CD1-CE1	-5.03	117.28	121.30
1	D	450	ASP	CB-CA-C	5.02	120.44	110.40
1	D	415	PHE	CB-CG-CD1	5.01	124.30	120.80

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
2	E	333	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4446	0	4259	24	0
1	D	4410	0	4244	22	0
2	B	3464	0	3524	17	0
2	E	3527	0	3584	28	0
3	C	2072	0	2014	14	0
3	F	2041	0	1991	14	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	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	7	0
13	B	454	0	0	4	0
13	C	255	0	0	5	0
13	D	502	0	0	7	0
13	E	400	0	0	11	0
13	F	250	0	0	5	0
All	All	22594	0	19852	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
1:A:352[B]:GLU:HG2	13:A:4123:HOH:O	1.56	1.04
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
3:C:186[B]:MET:HE2	3:C:201:LEU:HD11	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:A:554[A]:COM:S1	13:A:4190:HOH:O	2.45	0.74
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: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
2:E:27:LEU:HD22	2:E:246[B]:MET:HE1	1.71	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
3:C:186[B]:MET:HE1	3:C:201:LEU:HD11	1.76	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
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
2:E:27:LEU:CD2	2:E:246[B]:MET:HE1	2.31	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
2:E:27:LEU:CD2	2:E:246[B]:MET:CE	2.80	0.60
1:D:22:LYS:HZ1	10:D:558:EDO:H12	1.66	0.59
3:F:153[A]:LYS:NZ	13:F:1186:HOH:O	2.22	0.59
3:C:132:LYS:HD2	13:C:4122[B]:HOH:O	2.02	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
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
2:B:246[A]:MET:HE3	2:B:429:LEU:HD12	1.87	0.56
3:C:64[A]:ASP:HB3	3:C:67[A]:ARG:HB2	1.87	0.56
2:B:246[A]:MET:CE	2:B:429:LEU:HD12	2.36	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
1:D:46[B]:GLU:HG3	13:D:700:HOH:O	2.08	0.54
3:F:59:MET:O	3:F:60:ASP:C	2.46	0.53
2:E:95:VAL:HG21	2:E:119[B]:ALA:HB3	1.91	0.53
2:E:98[A]:ASP:HB2	13:E:3962:HOH:O	2.07	0.52
2:E:246[B]:MET:HE1	2:E:432:VAL:HG12	1.91	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:177[B]:ASP:C	1:A:179:ALA:N	2.69	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:61:GLU:CB	3:F:62:PRO:CD	2.90	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: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
2:B:37:SER:OG	2:B:424[B]:GLU:OE1	2.25	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
3:F:247:ASN:C	3:F:247:ASN:HD22	2.22	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: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
2:E:374:ILE:HD12	2:E:374:ILE:C	2.41	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 (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	572/549 (104%)	553 (97%)	18 (3%)	1 (0%)	47 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	569/549 (104%)	555 (98%)	13 (2%)	1 (0%)	47	21
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%)	51	23

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	463/434 (107%)	455 (98%)	8 (2%)	60	31
1	D	460/434 (106%)	455 (99%)	5 (1%)	73	50
2	B	366/341 (107%)	364 (100%)	2 (0%)	88	74
2	E	375/341 (110%)	372 (99%)	3 (1%)	81	62
3	C	228/216 (106%)	226 (99%)	2 (1%)	78	58
3	F	224/216 (104%)	222 (99%)	2 (1%)	78	58
All	All	2116/1982 (107%)	2094 (99%)	22 (1%)	76	53

All (22) 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

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Mol	Chain	Res	Type
1	A	126	PRO
1	A	444	TYR
1	A	450	ASP
1	A	543	ARG
2	B	97	GLU
2	B	283	LYS
3	C	61	GLU
3	C	121	GLN
1	D	352[A]	GLU
1	D	352[B]	GLU
1	D	444	TYR
1	D	450	ASP
1	D	543	ARG
2	E	185	LEU
2	E	283	LYS
2	E	440	LYS
3	F	121	GLN
3	F	247	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	AGM	D	271	1	10,11,12	1.54	2 (20%)	6,13,15	0.53	0
1	SMC	A	452	1	5,6,7	1.42	1 (20%)	2,6,8	1.88	1 (50%)
1	MHS	A	257	1	7,11,12	1.41	1 (14%)	6,14,16	3.45	3 (50%)
1	GL3	A	445	1	2,3,4	2.54	1 (50%)	1,2,4	0.32	0
1	AGM	A	271	1	10,11,12	1.34	1 (10%)	6,13,15	1.73	2 (33%)
1	MGN	A	400	1	6,9,10	1.11	1 (16%)	5,12,14	0.92	0
1	MHS	D	257	1	7,11,12	1.39	1 (14%)	6,14,16	3.70	5 (83%)
1	MGN	D	400	1	6,9,10	1.87	2 (33%)	5,12,14	0.53	0
1	SMC	D	452	1	5,6,7	0.68	0	2,6,8	1.95	1 (50%)
1	GL3	D	445	1	2,3,4	2.27	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	AGM	D	271	1	-	1/10/11/13	-
1	SMC	A	452	1	-	1/3/5/7	-
1	MHS	A	257	1	-	0/5/6/8	0/1/1/1
1	GL3	A	445	1	-	0/1/1/2	-
1	AGM	A	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	MGN	D	400	1	-	0/7/9/12	-
1	SMC	D	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	445	GL3	C-S	-3.59	1.68	1.80
1	D	445	GL3	C-S	-3.20	1.69	1.80
1	D	400	MGN	O-C	3.17	1.30	1.19
1	D	271	AGM	CG-CD	3.06	1.58	1.53
1	D	400	MGN	CB1-CG	2.80	1.59	1.53
1	A	452	SMC	CB-SG	2.56	1.84	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	271	AGM	CB-CA	2.31	1.56	1.53
1	A	400	MGN	O-C	2.24	1.27	1.19
1	D	257	MHS	O-C	2.12	1.28	1.19
1	A	271	AGM	CZ-NE1	2.05	1.36	1.33
1	A	257	MHS	CB-CG	2.02	1.53	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	257	MHS	NE2-CE1-ND1	-6.50	102.61	112.26
1	D	257	MHS	NE2-CE1-ND1	-6.36	102.82	112.26
1	D	257	MHS	CD2-NE2-CE1	4.27	112.44	105.78
1	A	257	MHS	CM-ND1-CG	3.91	129.64	124.44
1	D	257	MHS	CM-ND1-CG	3.57	129.19	124.44
1	A	257	MHS	CD2-NE2-CE1	2.74	110.06	105.78
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
1	A	271	AGM	NH1-CZ-NE1	2.49	125.11	119.55
1	D	257	MHS	CG-CD2-NE2	-2.12	104.86	108.80
1	A	271	AGM	CE2-CD-NE1	-2.09	104.92	110.37
1	D	257	MHS	CB-CA-C	-2.06	107.61	111.47

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	452	SMC	CA-CB-SG-CS
1	D	452	SMC	CA-CB-SG-CS
1	D	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 monosaccharides 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	$\#\|Z\| > 2$
10	EDO	A	557	-	3,3,3	0.38	0	2,2,2	0.10	0
8	TXZ	D	556[B]	-	18,19,19	1.19	1 (5%)	23,25,25	1.13	0
11	PEG	C	252	-	6,6,6	0.59	0	5,5,5	0.80	0
9	ACT	C	1	-	3,3,3	1.16	0	3,3,3	1.69	1 (33%)
7	COM	D	555[A]	5	6,6,6	2.56	3 (50%)	7,8,8	0.48	0
5	F43	D	553	1,13,7	61,71,71	2.68	14 (22%)	64,118,118	1.82	18 (28%)
5	F43	A	1	1,13,7	61,71,71	2.71	17 (27%)	64,118,118	1.80	15 (23%)
6	TP7	D	554[A]	-	19,20,20	1.09	1 (5%)	24,26,26	1.56	4 (16%)
10	EDO	D	558	-	3,3,3	0.65	0	2,2,2	0.67	0
10	EDO	D	557	-	3,3,3	0.62	0	2,2,2	0.11	0
7	COM	A	554[A]	5	6,6,6	1.92	2 (33%)	7,8,8	1.97	2 (28%)
10	EDO	A	558	-	3,3,3	0.51	0	2,2,2	0.80	0
10	EDO	F	251	-	3,3,3	0.55	0	2,2,2	0.50	0
9	ACT	A	556[A]	4	3,3,3	0.83	0	3,3,3	1.56	1 (33%)
11	PEG	A	559	-	6,6,6	0.94	0	5,5,5	2.11	2 (40%)
10	EDO	F	252	-	3,3,3	0.55	0	2,2,2	0.40	0
6	TP7	A	553[A]	-	19,20,20	1.26	1 (5%)	24,26,26	1.26	1 (4%)
10	EDO	C	251	-	3,3,3	0.35	0	2,2,2	0.71	0
8	TXZ	A	555[B]	-	18,19,19	1.28	3 (16%)	23,25,25	1.13	1 (4%)

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	F	251	-	-	1/1/1/1	-
10	EDO	D	557	-	-	1/1/1/1	-
7	COM	D	555[A]	5	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	EDO	C	251	-	-	1/1/1/1	-
11	PEG	A	559	-	-	2/4/4/4	-
10	EDO	A	557	-	-	1/1/1/1	-
5	F43	D	553	1,13,7	-	9/28/185/185	-
5	F43	A	1	1,13,7	-	9/28/185/185	-
6	TP7	D	554[A]	-	-	0/24/24/24	-
8	TXZ	D	556[B]	-	-	2/23/23/23	-
6	TP7	A	553[A]	-	-	2/24/24/24	-
10	EDO	F	252	-	-	1/1/1/1	-
10	EDO	D	558	-	-	1/1/1/1	-
11	PEG	C	252	-	-	0/4/4/4	-
10	EDO	A	558	-	-	1/1/1/1	-
7	COM	A	554[A]	5	-	0/4/4/4	-
8	TXZ	A	555[B]	-	-	2/23/23/23	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	553	F43	NI-NB	11.32	2.13	1.89
5	D	553	F43	NI-NA	10.71	2.12	1.89
5	A	1	F43	NI-NA	10.25	2.11	1.89
5	A	1	F43	NI-NB	9.37	2.09	1.89
5	D	553	F43	NI-ND	8.04	2.06	1.89
5	A	1	F43	NI-ND	7.84	2.06	1.89
5	A	1	F43	CHA-C4D	5.55	1.58	1.53
5	A	1	F43	CHB-C1B	5.08	1.56	1.53
7	D	555[A]	COM	O1S-S2	-4.24	1.32	1.45
5	A	1	F43	C4C-NC	4.12	1.41	1.35
5	A	1	F43	C3C-C4C	3.77	1.56	1.50
5	D	553	F43	C3C-C4C	3.57	1.56	1.50
5	D	553	F43	CHD-C1D	3.46	1.48	1.43
7	D	555[A]	COM	O3S-S2	3.25	1.59	1.47
5	A	1	F43	C4A-NA	3.11	1.54	1.49
5	A	1	F43	CHC-C4B	3.10	1.48	1.39
7	A	554[A]	COM	C2-S2	-3.09	1.73	1.77
5	A	1	F43	C1C-NC	3.01	1.43	1.37
5	A	1	F43	O8D-C7D	2.99	1.29	1.23
5	A	1	F43	OEB-CCB	-2.97	1.20	1.30
5	A	1	F43	OCC-CAC	2.74	1.31	1.22
5	D	553	F43	O8D-C7D	2.69	1.28	1.23
7	A	554[A]	COM	C1-C2	-2.61	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	553[A]	TP7	OXT-C	2.54	1.29	1.22
5	A	1	F43	CAA-CBA	2.54	1.60	1.52
8	A	555[B]	TXZ	O-C	2.53	1.29	1.22
5	D	553	F43	OBD-CAD	2.49	1.30	1.22
5	D	553	F43	C3A-C4A	2.34	1.57	1.53
5	D	553	F43	C4A-NA	2.29	1.52	1.49
5	A	1	F43	O8C-C6C	-2.24	1.23	1.30
5	D	553	F43	CAA-C3A	2.23	1.57	1.53
5	D	553	F43	CHC-C4B	2.22	1.45	1.39
5	D	553	F43	CAA-CBA	2.21	1.59	1.52
5	D	553	F43	C5C-C2C	2.21	1.57	1.53
8	A	555[B]	TXZ	CA-N	2.19	1.50	1.45
5	A	1	F43	OBD-CAD	2.18	1.29	1.22
6	D	554[A]	TP7	C7-S7	-2.10	1.73	1.80
5	D	553	F43	C1C-NC	2.09	1.41	1.37
5	A	1	F43	OCD-CAD	-2.09	1.23	1.30
7	D	555[A]	COM	C1-C2	-2.08	1.46	1.51
8	D	556[B]	TXZ	C3-C2	2.06	1.59	1.52
8	A	555[B]	TXZ	CG-CB	2.02	1.56	1.51

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	553	F43	O8D-C7D-C6D	-6.00	111.03	120.86
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	120.86
5	A	1	F43	C4A-NA-C1A	-4.56	103.44	108.97
5	D	553	F43	C6D-C7D-CHD	3.96	124.39	116.95
5	A	1	F43	C2B-C1B-NB	3.75	107.45	101.84
5	A	1	F43	OBC-CAC-C9C	3.67	125.83	114.03
7	A	554[A]	COM	O2S-S2-C2	3.66	111.32	106.92
11	A	559	PEG	O4-C4-C3	3.65	132.97	111.81
5	A	1	F43	C6D-C7D-CHD	3.46	123.46	116.95
5	A	1	F43	C3D-C4D-ND	3.43	107.68	102.34
5	D	553	F43	CAB-C3B-C2B	-3.21	112.29	119.09
5	A	1	F43	O7C-C6C-C5C	-3.20	112.53	122.80
5	D	553	F43	OBC-CAC-C9C	3.17	124.23	114.03
5	D	553	F43	C2D-C1D-CHD	-2.91	118.12	121.85
5	A	1	F43	C5D-C2D-C1D	2.87	114.31	110.45
5	D	553	F43	C1D-CHD-C4C	-2.84	117.24	125.31
5	A	1	F43	OBD-CAD-C9D	-2.78	113.87	122.80
5	D	553	F43	C9A-C2A-C3A	2.77	117.07	112.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1	F43	OCC-CAC-C9C	-2.69	114.43	123.08
6	A	553[A]	TP7	O1-C1-C2	-2.69	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	-2.64	104.81	111.27
5	D	553	F43	C3D-C2D-C1D	-2.58	98.32	102.69
5	D	553	F43	C3D-C4D-ND	2.56	106.32	102.34
5	D	553	F43	C2C-C5C-C6C	-2.50	109.06	114.04
5	D	553	F43	O7B-C6B-N5B	-2.46	121.93	125.13
6	D	554[A]	TP7	CB-CA-N	2.45	116.86	111.38
5	A	1	F43	C3B-C4B-CHC	-2.45	118.03	123.32
5	D	553	F43	OCD-CAD-C9D	2.40	121.78	114.07
5	D	553	F43	OCC-CAC-C9C	-2.40	115.37	123.08
11	A	559	PEG	C3-O2-C2	2.39	123.65	113.29
5	A	1	F43	C3C-C4C-NC	2.39	113.73	110.05
5	A	1	F43	C9B-C2B-C8B	-2.37	104.47	110.45
5	D	553	F43	C1B-C2B-C3B	2.35	104.99	101.51
6	D	554[A]	TP7	O1-C1-N	2.33	126.89	122.95
5	D	553	F43	C4B-CHC-C1C	2.32	129.63	125.84
5	D	553	F43	C3C-C4C-NC	2.29	113.58	110.05
5	A	1	F43	CAB-C3B-C2B	-2.25	114.34	119.09
6	D	554[A]	TP7	O4P-P-O1P	-2.22	100.84	109.39
9	A	556[A]	ACT	OXT-C-CH3	2.17	124.13	115.18
9	C	1	ACT	OXT-C-O	-2.17	114.07	122.05
5	D	553	F43	C5D-C2D-C1D	2.15	113.34	110.45
5	A	1	F43	OCD-CAD-C9D	2.11	120.83	114.07
5	D	553	F43	C5C-C2C-C3C	-2.07	109.64	114.94

There are no chirality outliers.

All (34) 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
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	557	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

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Mol	Chain	Res	Type	Atoms
8	D	556[B]	TXZ	C2-C3-C4-C5
6	A	553[A]	TP7	CB-O4P-P-O3P
11	A	559	PEG	C4-C3-O2-C2
8	D	556[B]	TXZ	C3-C4-C5-C6
5	A	1	F43	C2C-C5C-C6C-O8C
6	A	553[A]	TP7	C4-C5-C6-C7
5	D	553	F43	C2C-C5C-C6C-O7C
5	A	1	F43	CAA-CBA-CCA-OEA
10	F	251	EDO	O1-C1-C2-O2
5	D	553	F43	CAA-CBA-CCA-OEA
5	D	553	F43	C8C-C9C-CAC-OBC
5	A	1	F43	CAA-CBA-CCA-ODA
5	D	553	F43	CAA-CBA-CCA-ODA
10	C	251	EDO	O1-C1-C2-O2
5	A	1	F43	C2C-C5C-C6C-O7C
5	A	1	F43	CAB-CBB-CCB-OEB
5	D	553	F43	CAB-CBB-CCB-OEB
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-O8C
5	A	1	F43	CAB-CBB-CCB-ODB
5	D	553	F43	C8C-C9C-CAC-OCC

There are no ring outliers.

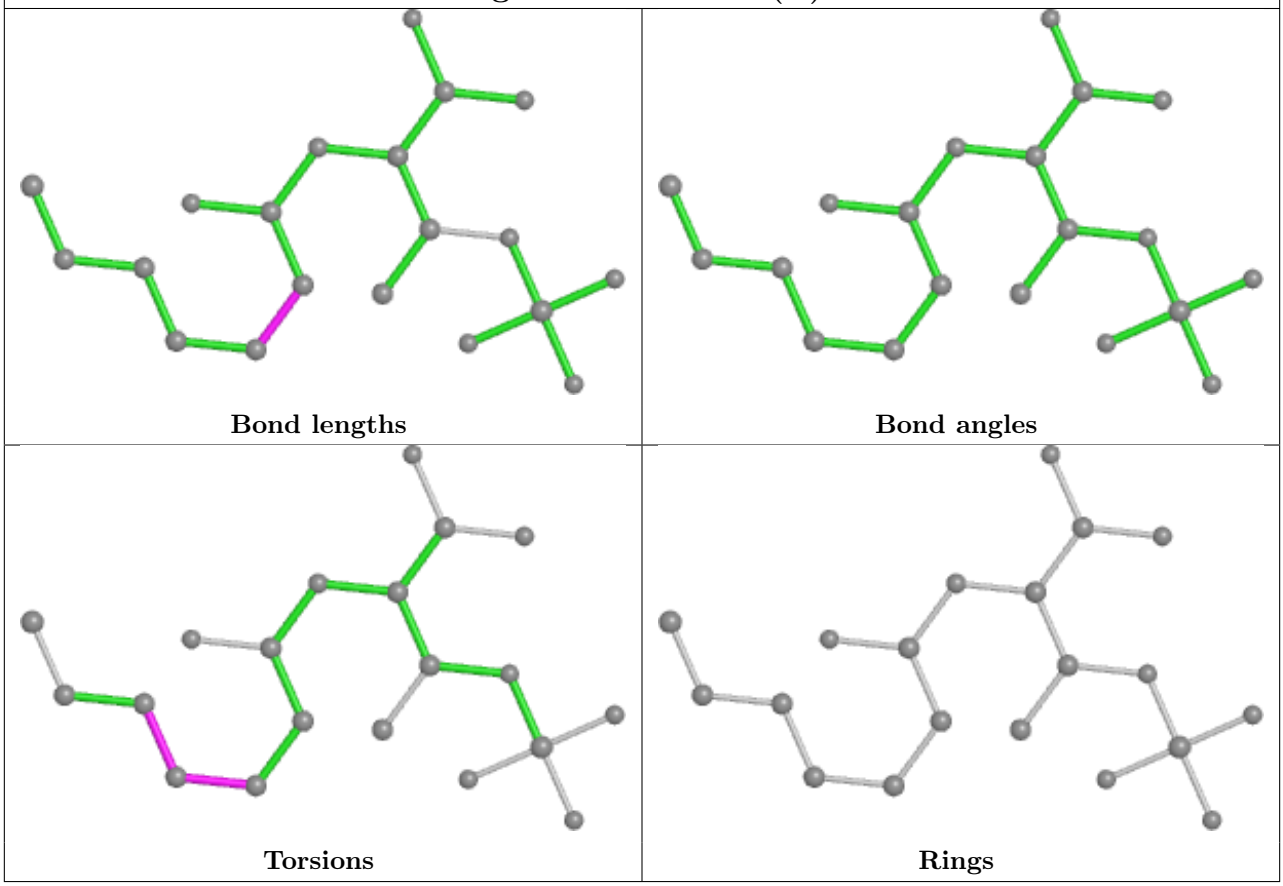
5 monomers are involved in 6 short contacts:

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
7	A	554[A]	COM	1	0
10	A	558	EDO	1	0

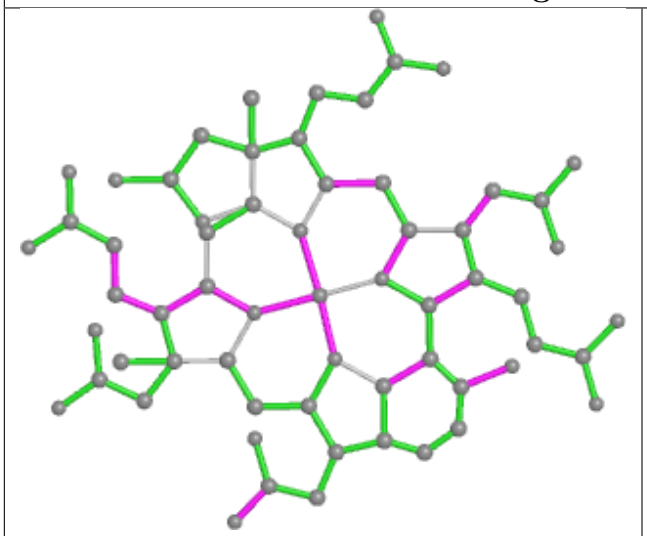
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

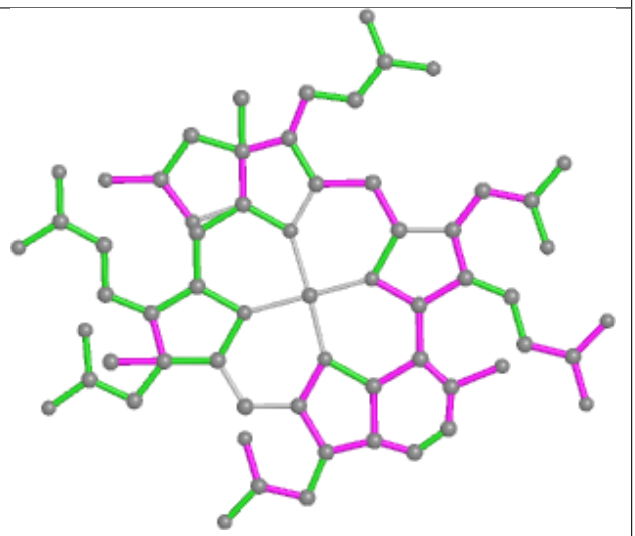
Ligand TXZ D 556 (B)



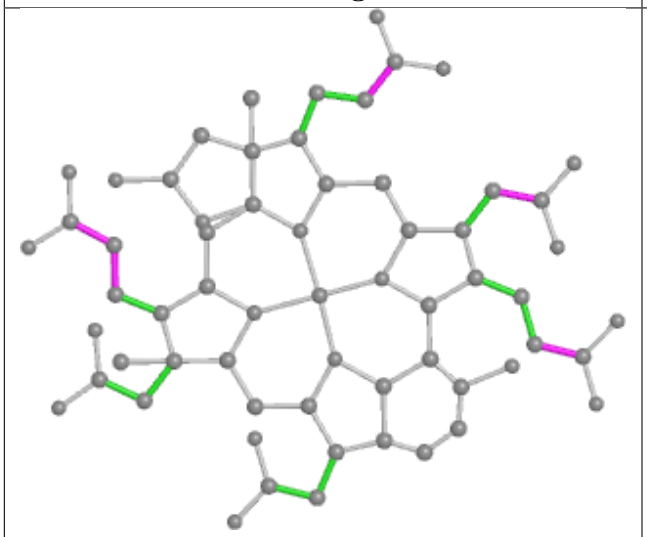
Ligand F43 D 553



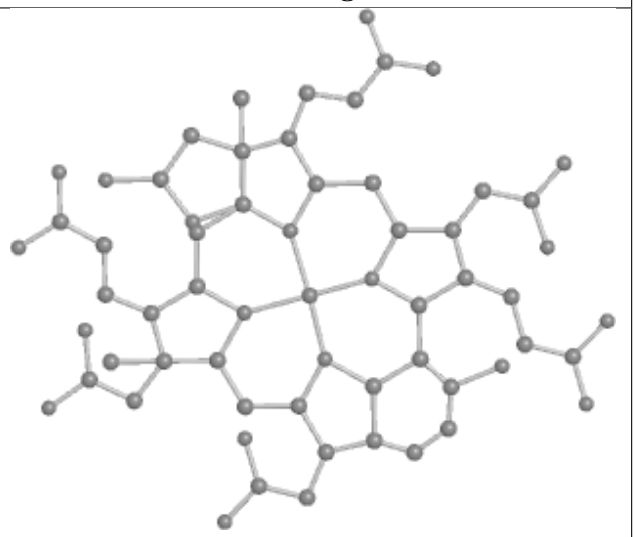
Bond lengths



Bond angles

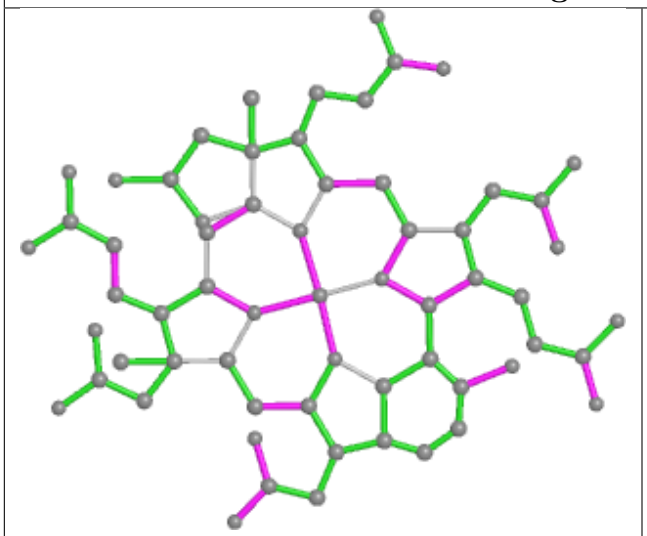


Torsions

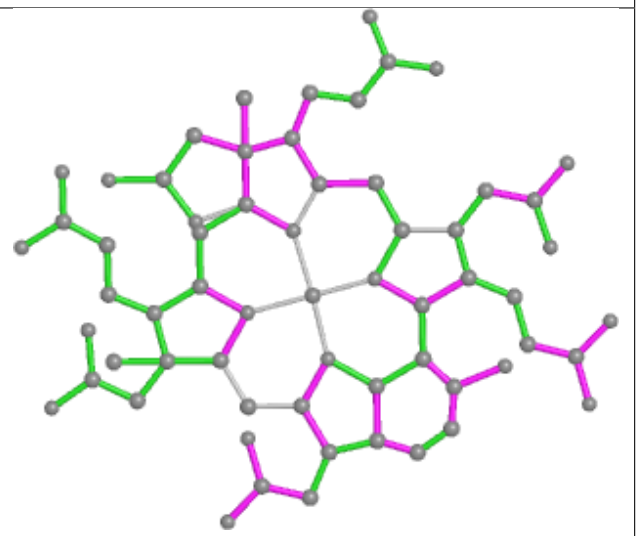


Rings

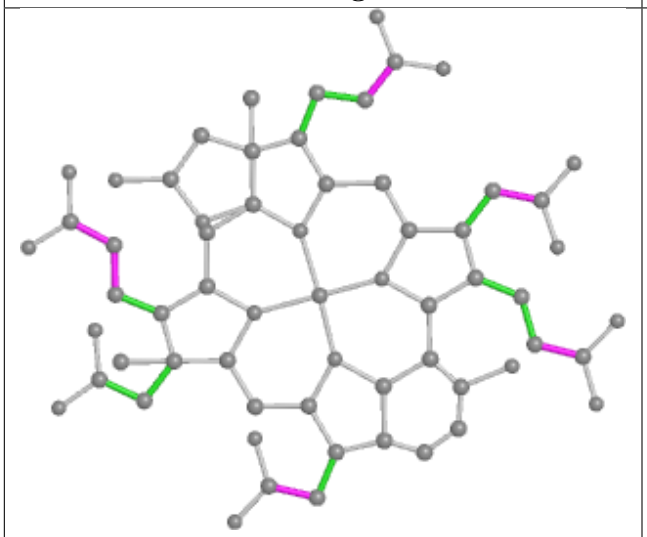
Ligand F43 A 1



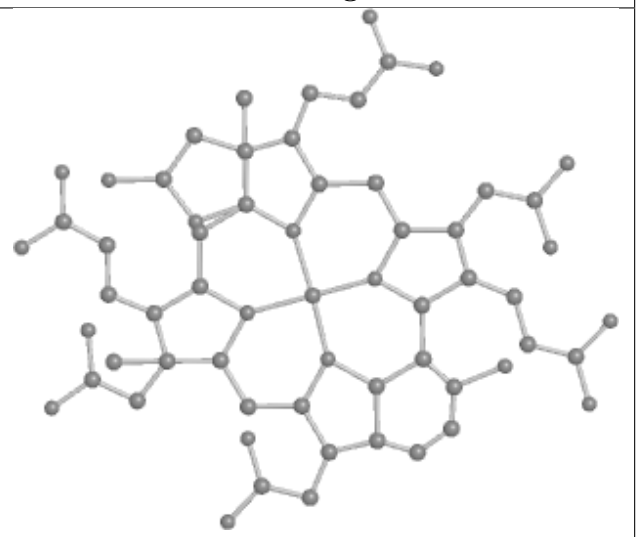
Bond lengths



Bond angles

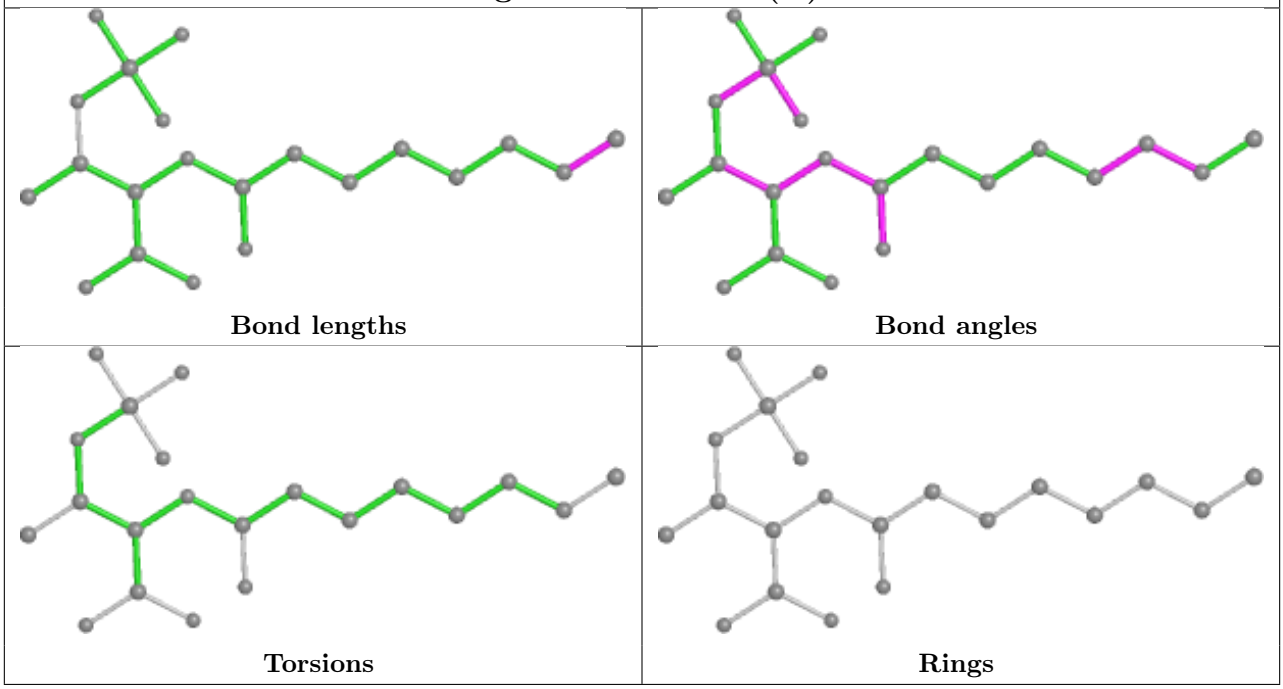


Torsions

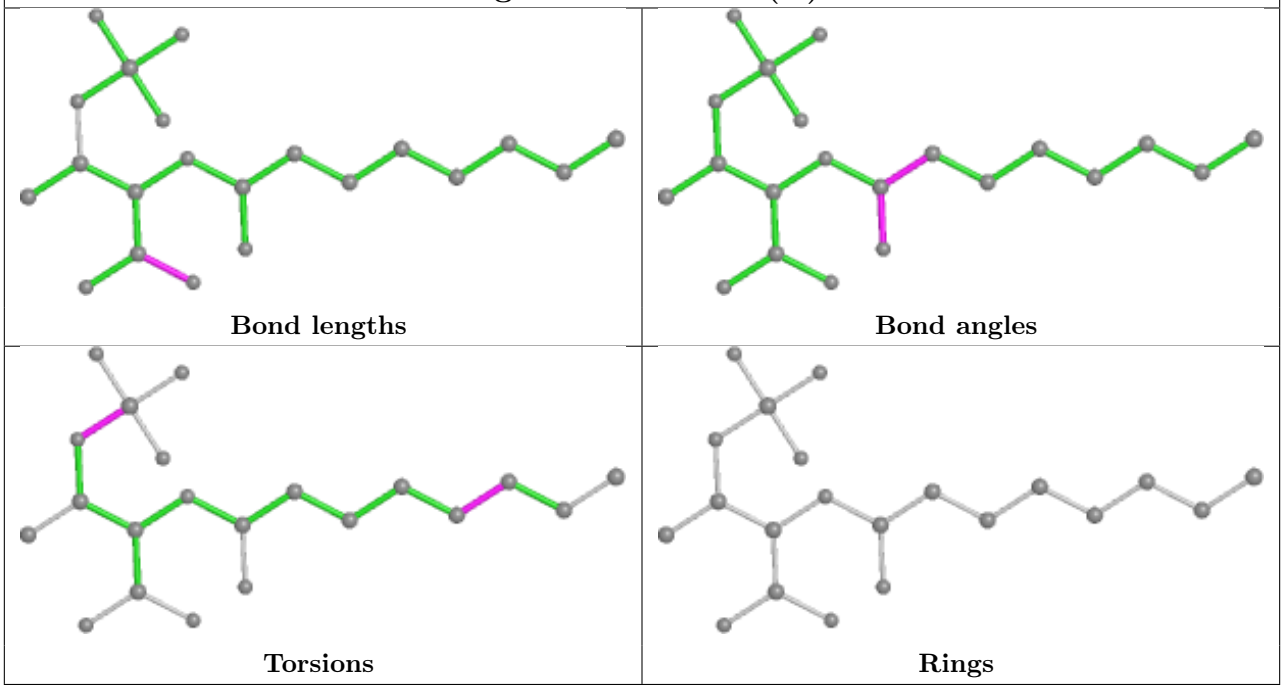


Rings

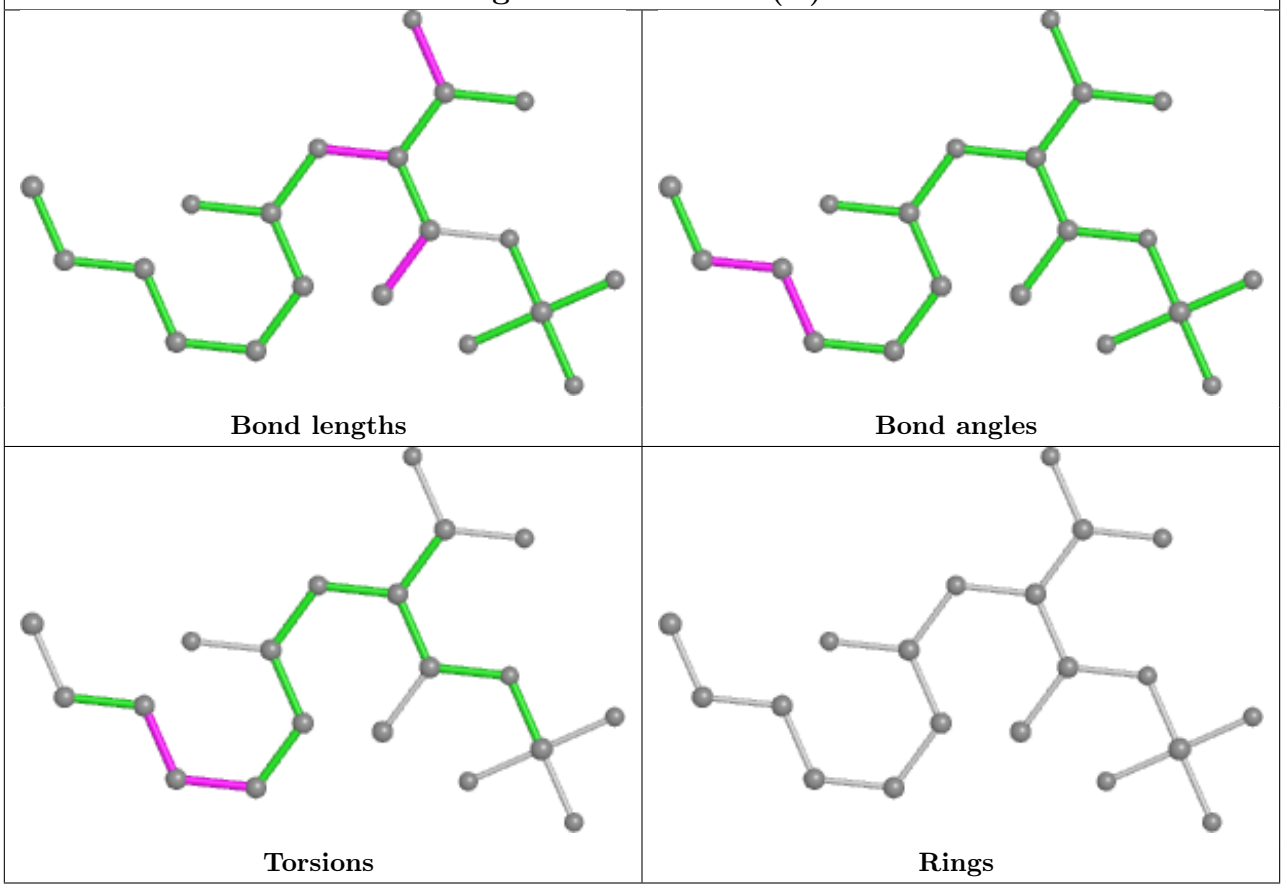
Ligand TP7 D 554 (A)



Ligand TP7 A 553 (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%)	-0.69	1 (0%)	95	93	7, 10, 20, 32	0
1	D	543/549 (98%)	-0.70	3 (0%)	89	88	7, 10, 20, 43	0
2	B	442/442 (100%)	-0.69	1 (0%)	95	93	7, 12, 21, 38	0
2	E	442/442 (100%)	-0.60	5 (1%)	80	79	8, 13, 25, 44	0
3	C	246/248 (99%)	-0.50	7 (2%)	53	52	9, 13, 29, 52	0
3	F	246/248 (99%)	-0.41	11 (4%)	33	33	9, 14, 32, 57	0
All	All	2462/2478 (99%)	-0.63	28 (1%)	80	79	7, 12, 23, 57	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	60	ASP	7.0
3	C	60	ASP	6.5
1	D	549	ALA	5.0
3	C	62	PRO	5.0
2	B	98	ASP	3.7
1	D	2	ALA	3.5
3	F	62	PRO	3.5
2	E	441	ASN	3.1
3	F	45	PRO	3.1
3	F	57	GLU	2.9
3	C	180	ASP	2.9
2	E	98[A]	ASP	2.9
3	F	180	ASP	2.8
3	C	45	PRO	2.8
1	A	2	ALA	2.6
3	C	63	GLU	2.6
3	F	63	GLU	2.6
2	E	297[A]	ASP	2.6
3	C	57	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
3	F	208	GLU	2.4
3	C	61	GLU	2.4
3	F	196	ASP	2.4
3	F	59	MET	2.3
2	E	442	GLU	2.2
2	E	2	ALA	2.1
1	D	3	ASP	2.1
3	F	179	LYS	2.1
3	F	46	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	0.05	9,11,14,15	0
1	MHS	D	257	11/12	0.97	0.05	8,10,13,14	0
1	MGN	A	400	10/11	0.98	0.05	6,8,9,9	0
1	AGM	A	271	12/13	0.98	0.05	5,7,7,8	0
1	AGM	D	271	12/13	0.98	0.06	6,7,8,9	0
1	MGN	D	400	10/11	0.98	0.04	6,8,9,9	0
1	SMC	A	452	7/8	0.99	0.05	7,7,9,11	0
1	SMC	D	452	7/8	0.99	0.05	8,9,10,12	0
1	GL3	D	445	4/5	1.00	0.04	7,7,7,8	0
1	GL3	A	445	4/5	1.00	0.06	6,7,8,8	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

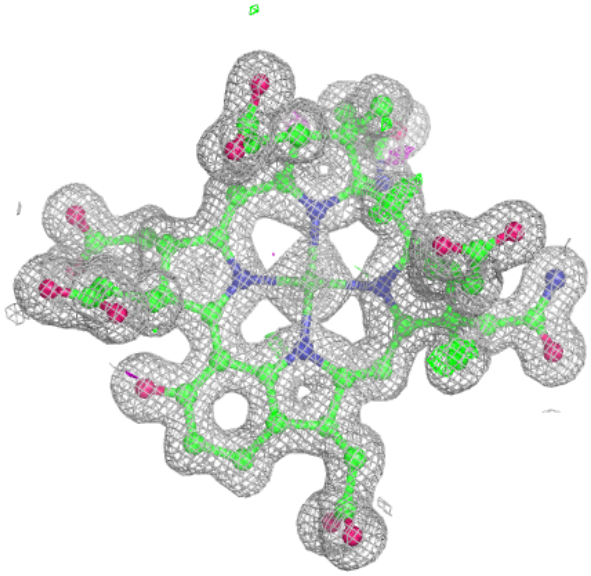
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

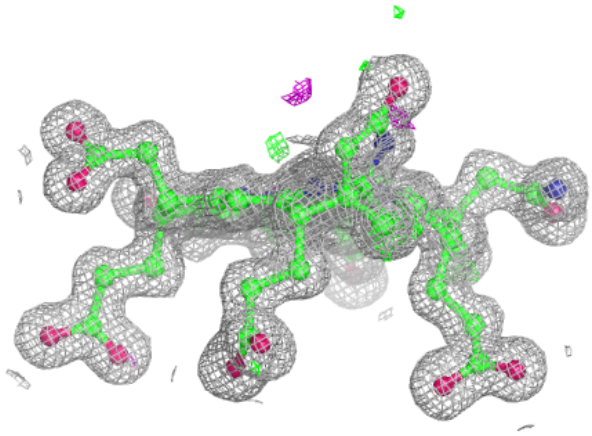
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	EDO	A	558	4/4	0.75	0.20	48,50,50,51	0
11	PEG	C	252	7/7	0.79	0.14	35,38,45,47	0
10	EDO	A	557	4/4	0.82	0.09	40,46,46,48	0
10	EDO	D	557	4/4	0.83	0.11	43,43,45,48	0
10	EDO	F	251	4/4	0.86	0.09	36,42,45,46	0
10	EDO	F	252	4/4	0.87	0.09	35,36,44,44	0
11	PEG	A	559	7/7	0.89	0.10	21,36,45,45	0
9	ACT	C	1	4/4	0.90	0.16	35,36,36,38	0
10	EDO	D	558	4/4	0.91	0.09	24,33,38,39	0
4	MG	B	444	1/1	0.93	0.20	29,29,29,29	0
10	EDO	C	251	4/4	0.93	0.09	40,42,44,44	0
4	MG	D	1	1/1	0.94	0.12	23,23,23,23	1
4	MG	D	552	1/1	0.96	0.23	20,20,20,20	1
7	COM	D	555[A]	7/7	0.96	0.11	6,10,11,14	7
4	MG	A	552[B]	1/1	0.96	0.18	20,20,20,20	1
7	COM	A	554[A]	7/7	0.97	0.09	9,10,13,14	7
4	MG	B	445[A]	1/1	0.97	0.25	20,20,20,20	1
4	MG	E	445[B]	1/1	0.97	0.14	20,20,20,20	1
4	MG	F	250	1/1	0.98	0.09	15,15,15,15	0
9	ACT	A	556[A]	4/4	0.98	0.07	14,15,16,16	4
4	MG	D	551	1/1	0.98	0.13	18,18,18,18	1
5	F43	D	553	62/62	0.99	0.05	6,8,10,12	0
6	TP7	A	553[A]	21/21	0.99	0.05	8,9,12,15	21
6	TP7	D	554[A]	21/21	0.99	0.05	7,8,11,12	21
4	MG	E	444	1/1	0.99	0.22	21,21,21,21	0
4	MG	C	250	1/1	0.99	0.07	16,16,16,16	0
8	TXZ	A	555[B]	20/20	0.99	0.05	5,8,10,12	20
8	TXZ	D	556[B]	20/20	0.99	0.05	7,8,10,11	20
4	MG	A	551[A]	1/1	0.99	0.21	17,17,17,17	1
5	F43	A	1	62/62	0.99	0.05	7,8,11,13	0
12	ZN	A	560	1/1	1.00	0.03	11,11,11,11	1

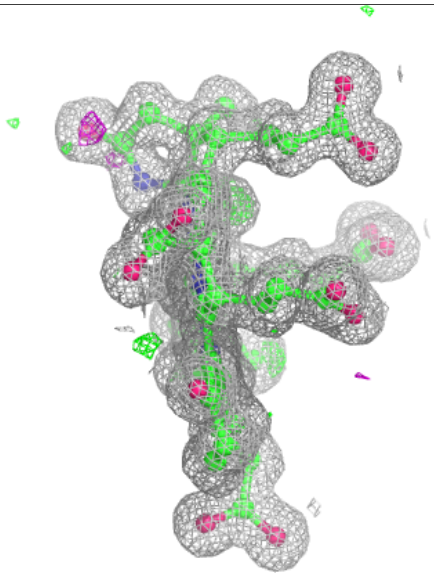
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

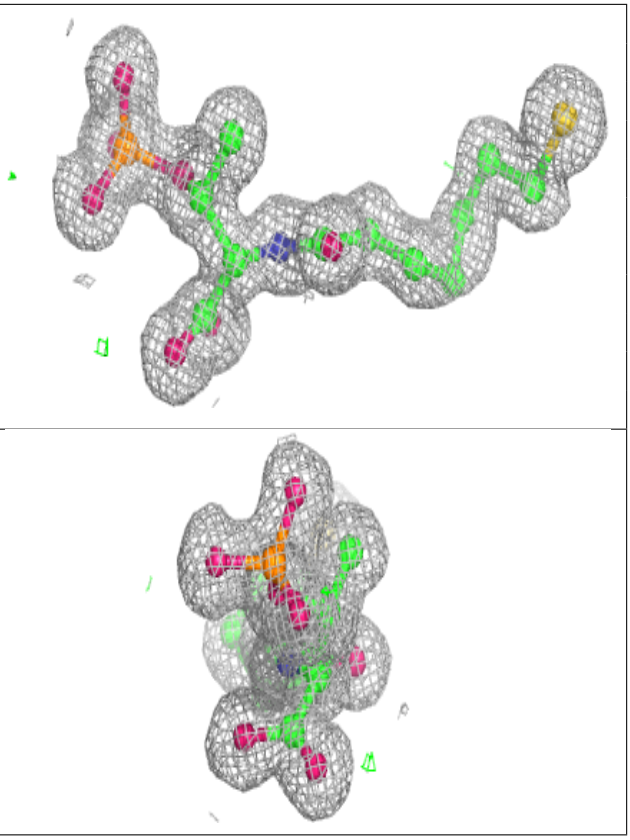






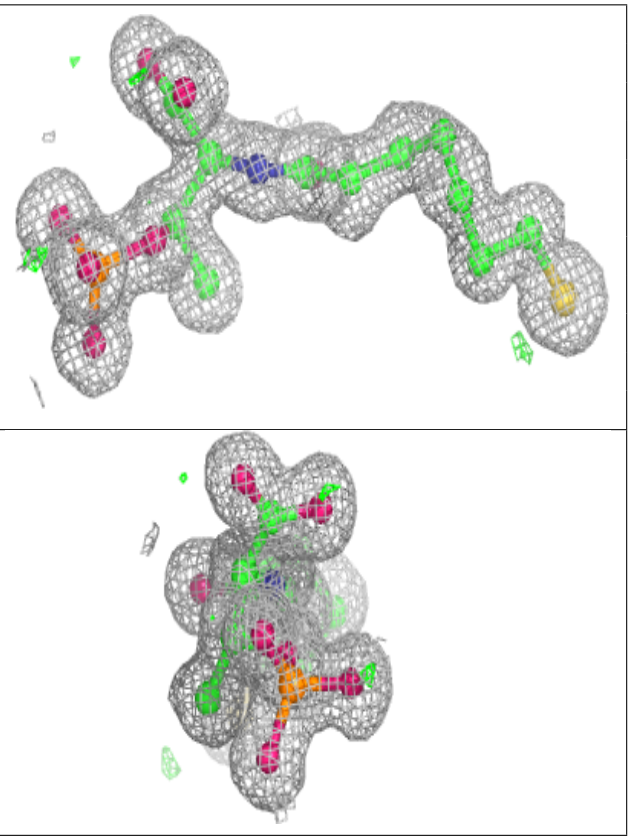
Electron density around TP7 A 553 (A):

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



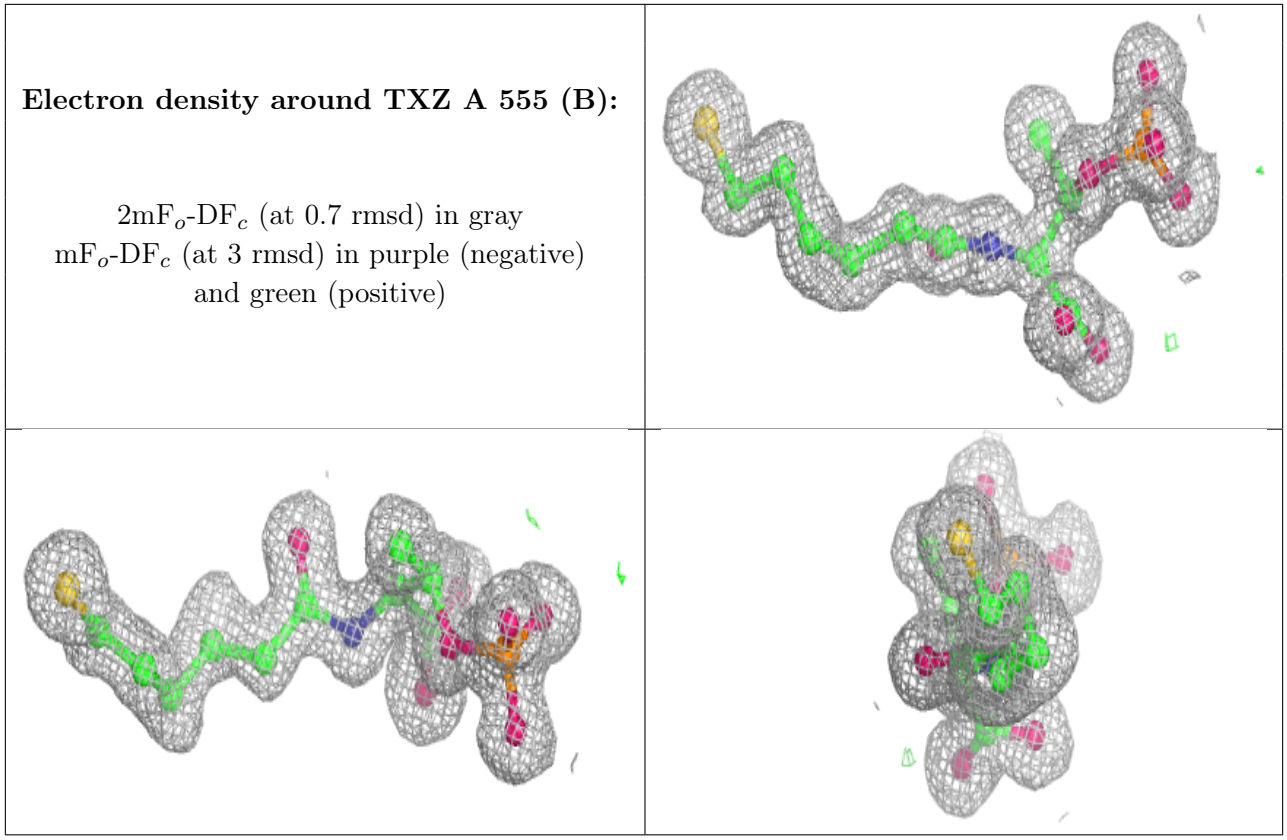
Electron density around TP7 D 554 (A):

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



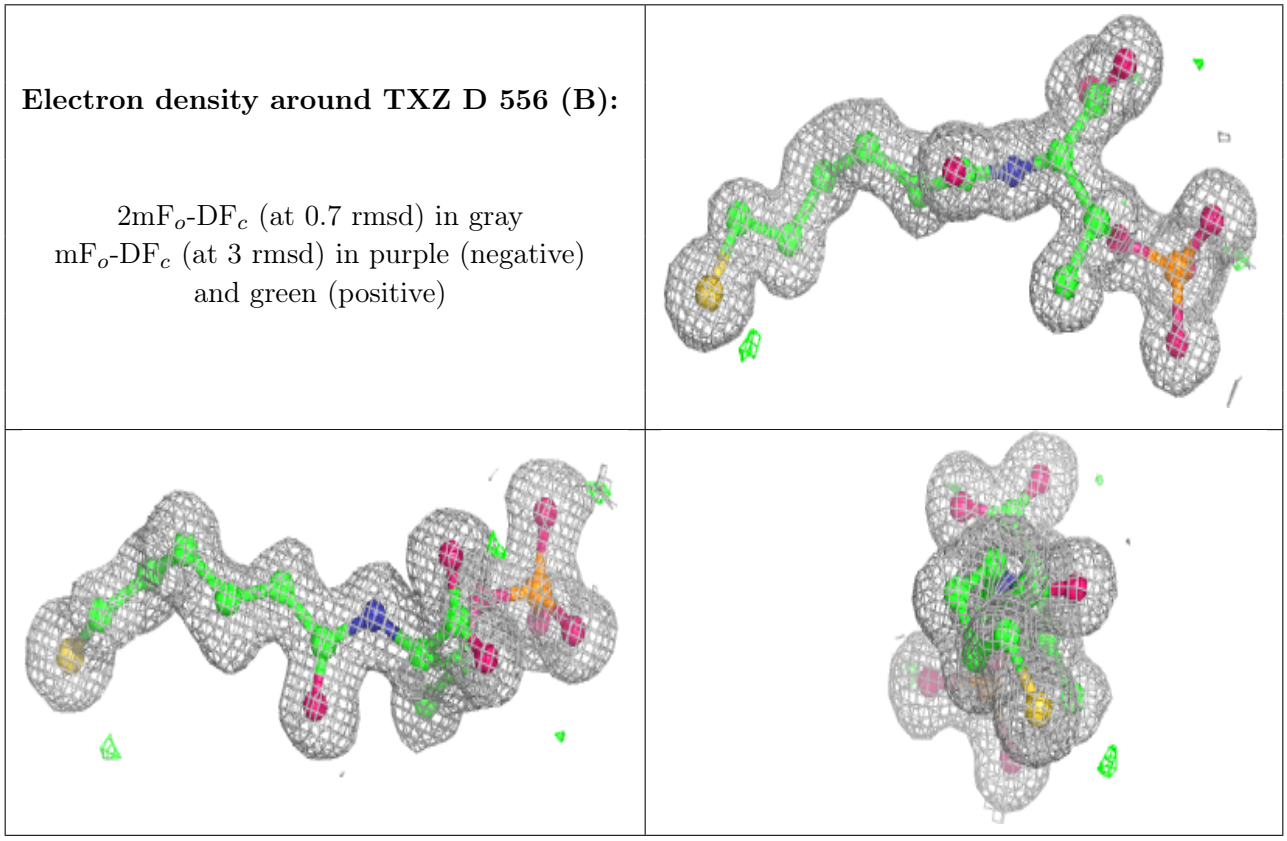
Electron density around TXZ A 555 (B):

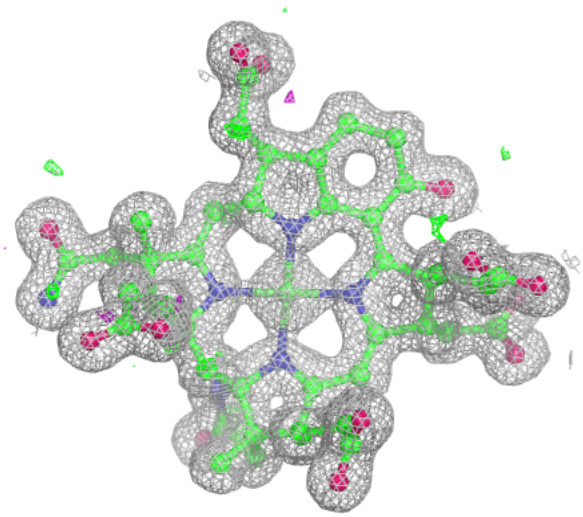
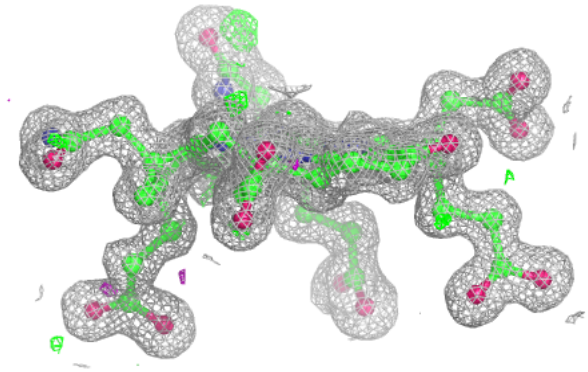
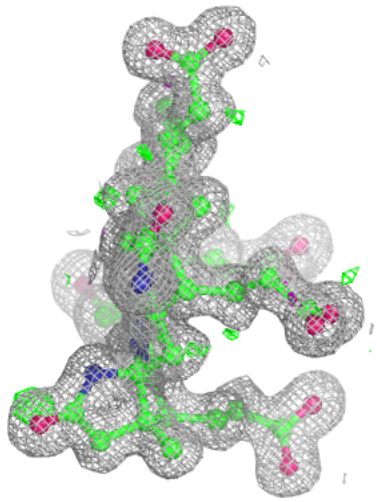
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)	
	

6.5 Other polymers (i)

There are no such residues in this entry.