



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 09:43 am BST

PDB ID : 3M30
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 : 1.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

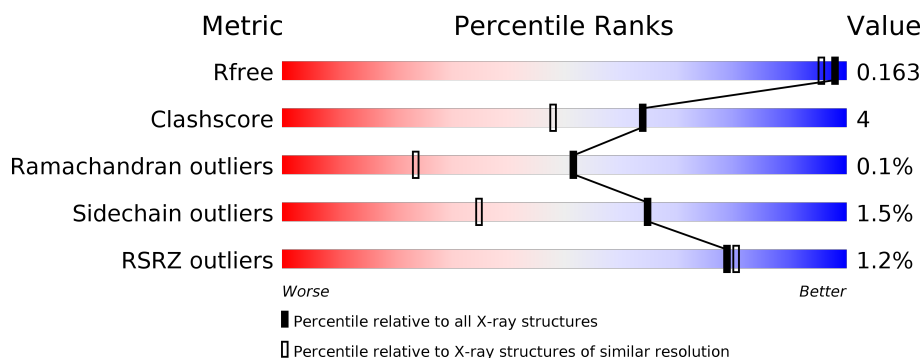
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	549	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>13%</div> <div>.</div> </div> </div>
1	D	549	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>12%</div> </div> </div>
2	B	442	<div> <div></div> <div> <div>85%</div> <div>14%</div> <div>.</div> </div> </div>
2	E	442	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>14%</div> <div>.</div> </div> </div>
3	C	248	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>..</div> </div> </div>
3	F	248	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>...</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	ACT	C	1	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 22789 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	33	0
			4469	2822	736	890	21			
1	D	548	Total	C	N	O	S	0	25	0
			4390	2787	722	861	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	30	0
			3505	2238	571	673	23			
2	E	442	Total	C	N	O	S	0	31	0
			3519	2241	573	682	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	10	0
			2050	1271	359	408	12			
3	F	246	Total	C	N	O	S	0	19	0
			2103	1304	367	420	12			

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

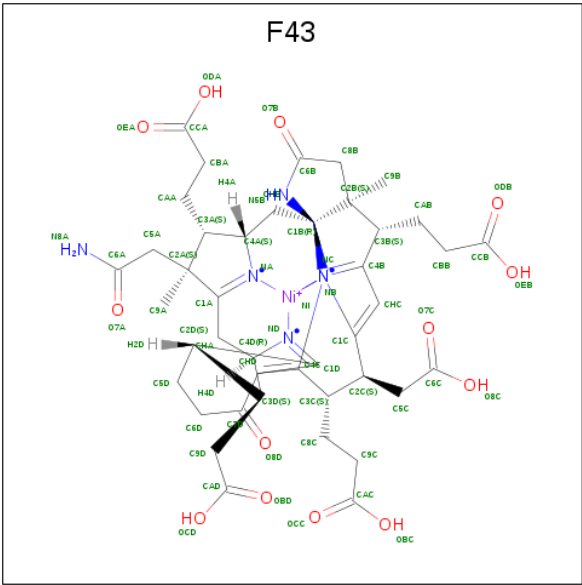
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total	Mg	0	0
			2	2		
4	E	1	Total	Mg	0	0
			1	1		
4	B	2	Total	Mg	0	0
			2	2		
4	C	1	Total	Mg	0	0
			1	1		

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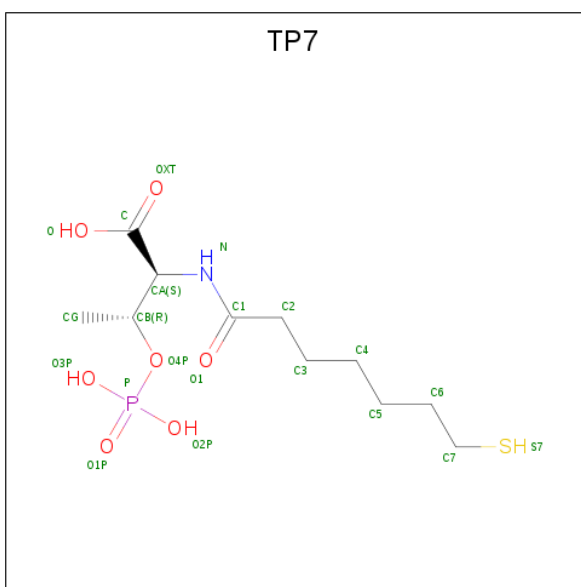
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	2
			2	2		
4	F	1	Total	Mg	0	0
			1	1		

- Molecule 5 is FACTOR 430 (three-letter code: F43) (formula: C₄₂H₅₁N₆NiO₁₃).



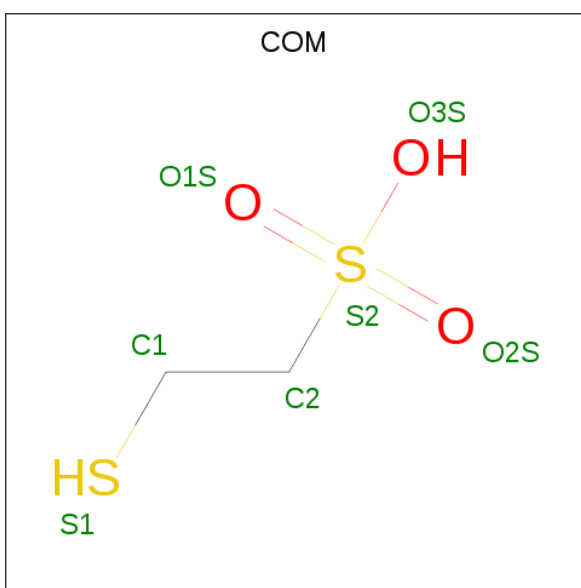
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		
5	D	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		

- Molecule 6 is Coenzyme B (three-letter code: TP7) (formula: C₁₁H₂₂NO₇PS).



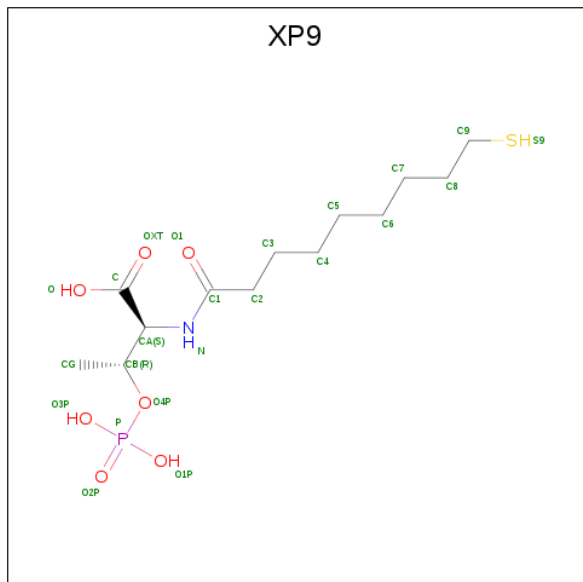
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	S	0	1
			21	11	1	7	1	1		
6	D	1	Total	C	N	O	P	S	0	1
			21	11	1	7	1	1		

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



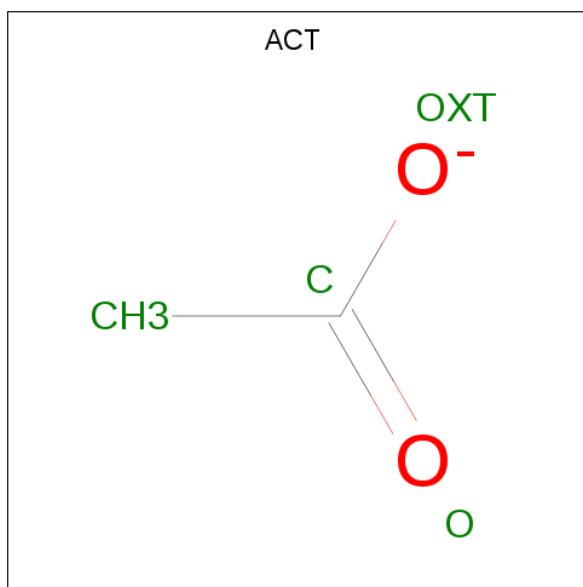
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	S	0	0
			7	2	3	2		
7	D	1	Total	C	O	S	0	0
			7	2	3	2		

- Molecule 8 is O-phosphono-N-(9-sulfanylnonanoyl)-L-threonine (three-letter code: XP9) (formula: $C_{13}H_{26}NO_7PS$).



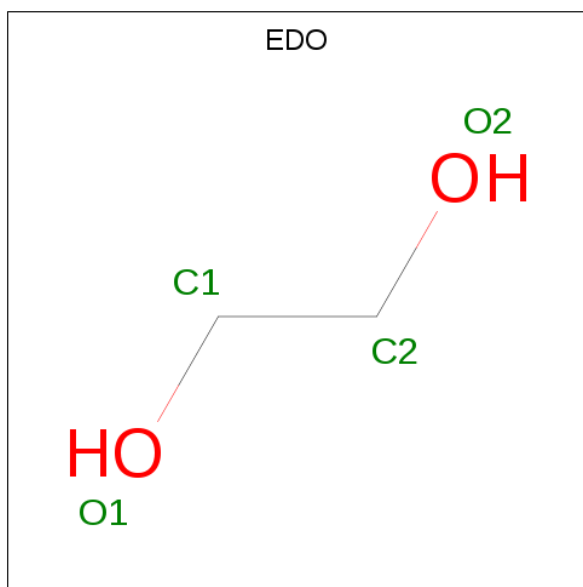
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	S	0	1
			46	26	2	14	2	2		
8	D	1	Total	C	N	O	P	S	0	1
			46	26	2	14	2	2		

- Molecule 9 is ACETATE ION (three-letter code: 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 (three-letter code: EDO) (formula: C₂H₆O₂).

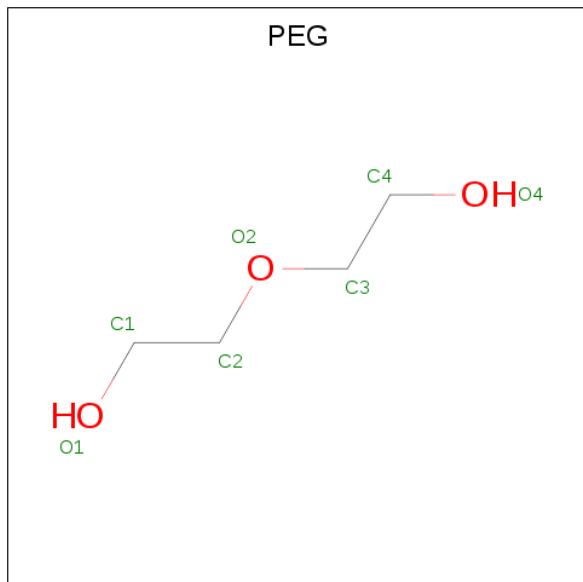


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			4	2	2		
10	B	1	Total	C	O	0	0
			4	2	2		
10	C	1	Total	C	O	0	0
			4	2	2		
10	D	1	Total	C	O	0	0
			4	2	2		
10	F	1	Total	C	O	0	0
			4	2	2		
10	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 12 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

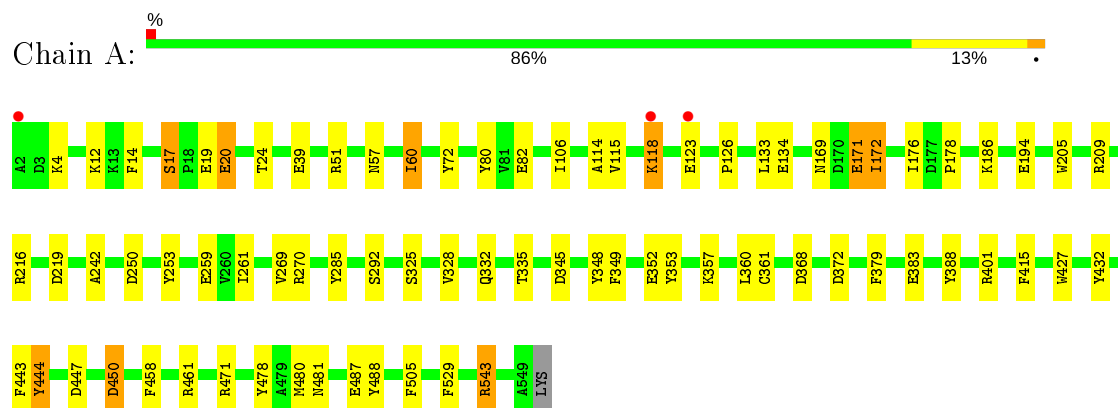
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	507	Total	O	0	30
			519	519		
13	B	451	Total	O	0	26
			472	472		
13	C	251	Total	O	0	11
			259	259		
13	D	502	Total	O	0	15
			511	511		
13	E	405	Total	O	0	15
			415	415		
13	F	252	Total	O	0	9
			256	256		

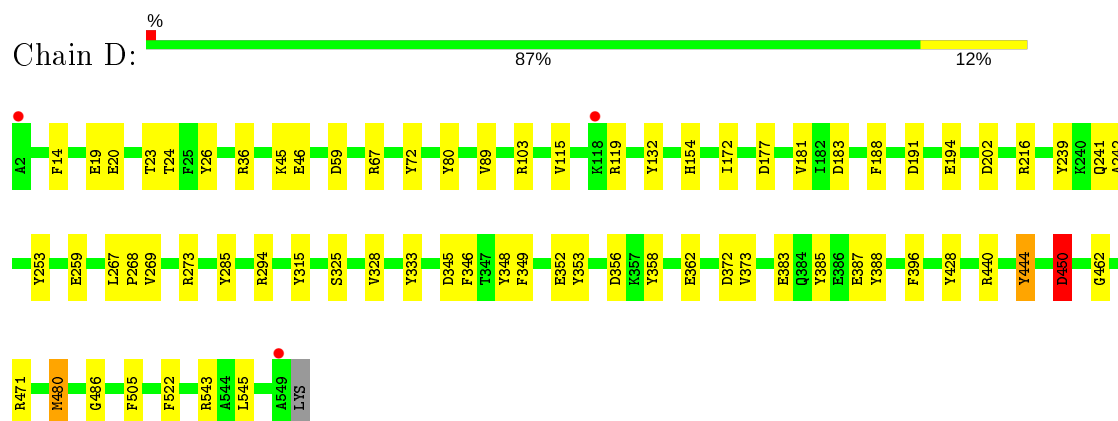
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

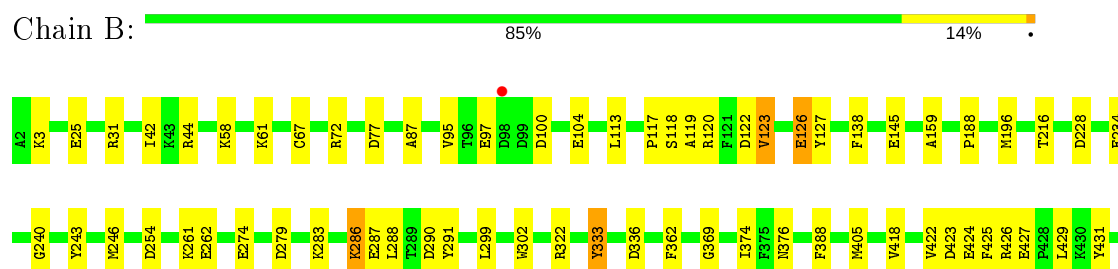
- Molecule 1: Methyl-coenzyme M reductase I subunit alpha



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



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





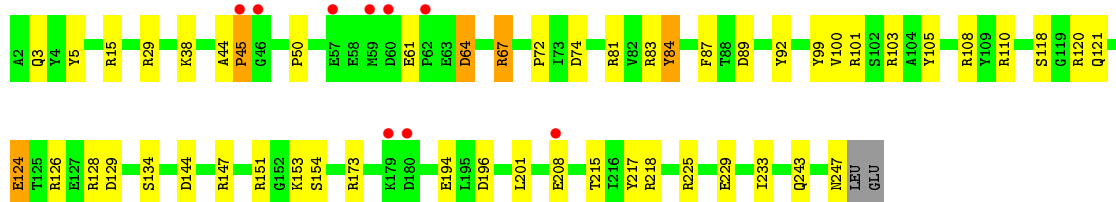
- Molecule 2: Methyl-coenzyme M reductase I subunit beta

Chain E: 85% 14%



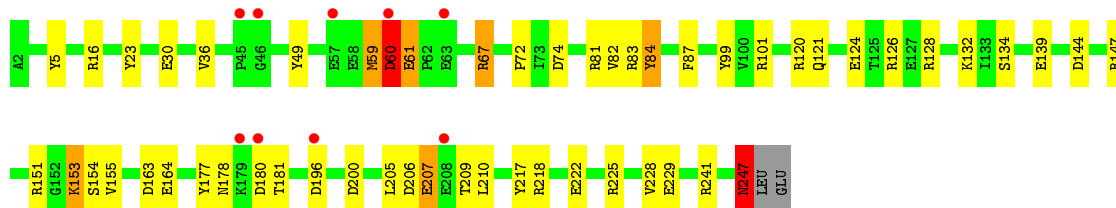
- Molecule 3: Methyl-coenzyme M reductase I subunit gamma

Chain C: 78% 19%



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

Chain F: 77% 19%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.02Å 118.26Å 122.39Å 90.00° 91.84° 90.00°	Depositor
Resolution (Å)	20.07 – 1.45 19.89 – 1.45	Depositor EDS
% Data completeness (in resolution range)	97.1 (20.07-1.45) 97.1 (19.89-1.45)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 1.45Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.136 , 0.164 0.135 , 0.163	Depositor DCC
R_{free} test set	20161 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	11.0	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.1	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 0.008 for -h,-l,-k 0.014 for h,-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	22789	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: ZN, PEG, SMC, ACT, MG, F43, MGN, TP7, XP9, AGM, EDO, GL3, COM, MHS

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.50	20/4572 (0.4%)	1.36	28/6206 (0.5%)
1	D	1.54	24/4505 (0.5%)	1.38	33/6116 (0.5%)
2	B	1.50	16/3628 (0.4%)	1.34	24/4904 (0.5%)
2	E	1.50	13/3633 (0.4%)	1.30	27/4910 (0.5%)
3	C	1.58	13/2109 (0.6%)	1.48	33/2841 (1.2%)
3	F	1.59	22/2179 (1.0%)	1.45	22/2933 (0.8%)
All	All	1.53	108/20626 (0.5%)	1.37	167/27910 (0.6%)

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	1
2	B	0	1
All	All	2	3

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	19	GLU	CD-OE1	9.52	1.36	1.25
3	F	139	GLU	CD-OE2	7.28	1.33	1.25
1	D	269	VAL	CA-CB	6.91	1.69	1.54
1	D	14	PHE	CD2-CE2	6.55	1.52	1.39
3	C	153	LYS	CE-NZ	6.43	1.65	1.49
1	A	292	SER	CB-OG	6.39	1.50	1.42
3	F	154	SER	CB-OG	6.30	1.50	1.42
1	A	269	VAL	CA-CB	6.29	1.68	1.54
3	F	218	ARG	CZ-NH1	6.29	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	543	ARG	CB-CG	6.26	1.69	1.52
3	F	87	PHE	CE2-CZ	6.22	1.49	1.37
3	F	222	GLU	CB-CG	6.18	1.63	1.52
1	A	72	TYR	CE2-CZ	6.16	1.46	1.38
3	C	124	GLU	CG-CD	6.07	1.61	1.51
2	B	274	GLU	CG-CD	6.05	1.61	1.51
2	B	117[A]	PRO	C-O	5.97	1.35	1.23
2	B	117[B]	PRO	C-O	5.97	1.35	1.23
2	B	25	GLU	CB-CG	5.95	1.63	1.52
3	F	124	GLU	CG-CD	5.95	1.60	1.51
2	B	145	GLU	CB-CG	5.93	1.63	1.52
3	F	84	TYR	CE1-CZ	5.92	1.46	1.38
1	A	401	ARG	CZ-NH1	5.90	1.40	1.33
3	C	3	GLN	CB-CG	-5.89	1.36	1.52
1	A	39	GLU	CD-OE2	-5.87	1.19	1.25
3	F	229	GLU	CD-OE1	-5.83	1.19	1.25
2	E	329	SER	CB-OG	5.80	1.49	1.42
3	F	49	TYR	CE2-CZ	5.80	1.46	1.38
2	B	87	ALA	CA-CB	5.78	1.64	1.52
3	F	177	TYR	CD1-CE1	5.78	1.48	1.39
2	E	353	GLU	CG-CD	5.77	1.60	1.51
3	F	99	TYR	CD2-CE2	5.76	1.48	1.39
2	E	11	TYR	CE1-CZ	5.75	1.46	1.38
1	D	46	GLU	CG-CD	5.75	1.60	1.51
3	F	155	VAL	CB-CG1	5.74	1.65	1.52
3	C	154	SER	CB-OG	5.74	1.49	1.42
1	D	20	GLU	CG-CD	5.73	1.60	1.51
3	C	105	TYR	CE1-CZ	5.72	1.46	1.38
3	F	36	VAL	N-CA	5.70	1.57	1.46
1	A	432	TYR	CG-CD1	5.69	1.46	1.39
1	A	134	GLU	CG-CD	5.69	1.60	1.51
3	C	87	PHE	CE2-CZ	5.69	1.48	1.37
2	B	302	TRP	CZ3-CH2	5.66	1.49	1.40
2	B	240	GLY	N-CA	5.63	1.54	1.46
2	E	305	TYR	CD1-CE1	5.62	1.47	1.39
2	B	138	PHE	CE1-CZ	5.62	1.48	1.37
1	A	348	TYR	CE1-CZ	5.60	1.45	1.38
1	A	259[A]	GLU	CD-OE1	-5.58	1.19	1.25
1	A	259[B]	GLU	CD-OE1	-5.58	1.19	1.25
2	E	5	GLU	CB-CG	5.58	1.62	1.52
1	D	396	PHE	CD2-CE2	5.58	1.50	1.39
2	E	407	SER	CB-OG	5.57	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	181	VAL	CB-CG1	5.54	1.64	1.52
3	C	38	LYS	CE-NZ	5.54	1.62	1.49
1	D	462	GLY	N-CA	5.53	1.54	1.46
2	E	321	ALA	CA-CB	5.51	1.64	1.52
2	B	431	TYR	CE2-CZ	5.49	1.45	1.38
3	F	84	TYR	CG-CD1	5.47	1.46	1.39
1	A	353	TYR	CE2-CZ	5.47	1.45	1.38
3	C	84	TYR	CD1-CE1	5.46	1.47	1.39
1	D	80	TYR	CE1-CZ	5.45	1.45	1.38
1	D	72	TYR	CG-CD2	5.43	1.46	1.39
1	A	82	GLU	CD-OE2	5.42	1.31	1.25
1	D	373	VAL	CB-CG2	5.42	1.64	1.52
1	A	458	PHE	CE1-CZ	5.41	1.47	1.37
2	B	427	GLU	CG-CD	5.37	1.60	1.51
1	D	253	TYR	CD2-CE2	5.36	1.47	1.39
1	D	349	PHE	CD1-CE1	5.36	1.50	1.39
3	F	164	GLU	CG-CD	5.34	1.59	1.51
1	D	486	GLY	CA-C	5.29	1.60	1.51
1	A	487	GLU	CD-OE2	5.28	1.31	1.25
3	C	134	SER	CB-OG	5.28	1.49	1.42
1	D	353	TYR	CE2-CZ	5.26	1.45	1.38
1	A	19	GLU	CD-OE1	5.24	1.31	1.25
3	C	218	ARG	CZ-NH1	5.23	1.39	1.33
3	F	30	GLU	CD-OE2	5.21	1.31	1.25
2	E	83	GLU	CG-CD	5.21	1.59	1.51
1	A	427	TRP	CD1-NE1	5.20	1.46	1.38
3	C	229	GLU	CB-CG	5.20	1.62	1.52
2	B	274	GLU	CD-OE1	5.20	1.31	1.25
3	F	217	TYR	CG-CD1	5.20	1.46	1.39
2	B	286	LYS	N-CA	5.19	1.56	1.46
3	F	247	ASN	CA-CB	5.17	1.66	1.53
1	D	259	GLU	CG-CD	5.16	1.59	1.51
1	D	294	ARG	CZ-NH1	5.14	1.39	1.33
1	A	134	GLU	CD-OE1	5.14	1.31	1.25
2	E	54	GLU	CD-OE1	-5.13	1.20	1.25
2	E	393	VAL	CB-CG2	5.13	1.63	1.52
1	A	388	TYR	CD2-CE2	5.12	1.47	1.39
2	E	305	TYR	CD2-CE2	5.12	1.47	1.39
3	F	134	SER	CB-OG	5.12	1.49	1.42
1	D	216	ARG	CZ-NH2	5.11	1.39	1.33
1	D	356[A]	ASP	CB-CG	5.11	1.62	1.51
1	D	356[B]	ASP	CB-CG	5.11	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	360	SER	CA-CB	5.11	1.60	1.52
2	B	426	ARG	CZ-NH2	5.10	1.39	1.33
1	D	26	TYR	CE1-CZ	5.09	1.45	1.38
3	F	23	TYR	CG-CD2	5.08	1.45	1.39
2	B	159	ALA	CA-CB	5.07	1.63	1.52
1	A	285	TYR	CE1-CZ	5.07	1.45	1.38
2	E	22	VAL	CB-CG2	5.05	1.63	1.52
3	C	118	SER	CB-OG	5.03	1.48	1.42
1	D	362	GLU	CD-OE2	5.03	1.31	1.25
2	B	216	THR	C-O	5.03	1.32	1.23
3	F	225	ARG	CZ-NH1	-5.01	1.26	1.33
1	D	444	TYR	CE2-CZ	-5.01	1.32	1.38
3	F	210	LEU	N-CA	5.01	1.56	1.46
3	C	243	GLN	CB-CG	-5.01	1.39	1.52
1	A	205	TRP	CG-CD1	5.00	1.43	1.36

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	147	ARG	NE-CZ-NH1	13.21	126.91	120.30
3	F	147	ARG	NE-CZ-NH1	12.33	126.47	120.30
2	B	44	ARG	NE-CZ-NH1	12.19	126.39	120.30
3	C	120	ARG	NE-CZ-NH1	9.91	125.25	120.30
3	F	147	ARG	NE-CZ-NH2	-8.87	115.87	120.30
2	B	31	ARG	NE-CZ-NH1	8.74	124.67	120.30
3	F	74	ASP	CB-CG-OD1	7.94	125.44	118.30
3	C	196	ASP	CB-CG-OD1	7.68	125.21	118.30
3	C	5	TYR	CB-CG-CD1	-7.60	116.44	121.00
2	E	353	GLU	OE1-CD-OE2	7.59	132.41	123.30
1	D	471	ARG	NE-CZ-NH2	-7.57	116.51	120.30
1	D	385	TYR	CB-CG-CD2	-7.42	116.55	121.00
3	F	120	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	A	543	ARG	NE-CZ-NH1	7.25	123.92	120.30
3	F	206	ASP	CB-CG-OD1	7.09	124.68	118.30
1	D	285	TYR	CB-CG-CD2	-7.04	116.77	121.00
3	C	151	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	A	471	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	A	209	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	D	444	TYR	CB-CG-CD2	-6.92	116.85	121.00
3	C	128	ARG	NE-CZ-NH2	-6.88	116.86	120.30
2	E	138	PHE	CB-CG-CD2	-6.75	116.08	120.80
2	B	44	ARG	NE-CZ-NH2	-6.73	116.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	59	MET	CG-SD-CE	-6.54	89.73	100.20
2	B	120[A]	ARG	NE-CZ-NH1	6.53	123.56	120.30
2	B	120[B]	ARG	NE-CZ-NH1	6.53	123.56	120.30
3	C	83	ARG	NE-CZ-NH1	6.51	123.55	120.30
2	B	426	ARG	NE-CZ-NH1	6.43	123.52	120.30
3	C	110	ARG	NE-CZ-NH1	6.36	123.48	120.30
3	C	147	ARG	NE-CZ-NH2	-6.34	117.13	120.30
2	B	333	TYR	CG-CD2-CE2	-6.33	116.23	121.30
2	B	279	ASP	CB-CG-OD1	6.33	124.00	118.30
1	D	67	ARG	NE-CZ-NH1	6.29	123.44	120.30
2	B	31	ARG	NE-CZ-NH2	-6.27	117.16	120.30
3	C	126	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	A	461	ARG	NE-CZ-NH2	-6.17	117.21	120.30
3	F	196	ASP	CB-CG-OD1	6.15	123.83	118.30
1	A	478	TYR	CB-CG-CD2	-6.14	117.32	121.00
1	A	450	ASP	CB-CA-C	6.13	122.66	110.40
2	B	228	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	A	20	GLU	OE1-CD-OE2	6.11	130.63	123.30
3	F	144	ASP	CB-CG-OD1	-6.09	112.82	118.30
3	F	128	ARG	NE-CZ-NH1	-6.07	117.27	120.30
3	C	29	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	D	440	ARG	NE-CZ-NH1	6.02	123.31	120.30
3	C	101	ARG	NE-CZ-NH2	-5.99	117.30	120.30
3	C	108	ARG	NE-CZ-NH2	-5.97	117.31	120.30
2	B	336	ASP	CB-CG-OD1	5.96	123.66	118.30
1	A	219	ASP	CB-CG-OD1	5.96	123.66	118.30
1	D	315	TYR	CB-CG-CD2	-5.95	117.43	121.00
1	A	379	PHE	CB-CG-CD1	5.94	124.96	120.80
3	C	144	ASP	CB-CG-OD2	5.92	123.63	118.30
3	F	101	ARG	NE-CZ-NH2	-5.92	117.34	120.30
2	B	77	ASP	CB-CG-OD2	-5.90	112.99	118.30
3	F	153[A]	LYS	CD-CE-NZ	-5.90	98.13	111.70
3	F	153[B]	LYS	CD-CE-NZ	-5.90	98.13	111.70
1	D	183	ASP	CB-CG-OD1	5.88	123.59	118.30
2	E	72	ARG	NE-CZ-NH1	5.86	123.23	120.30
2	E	425	PHE	CB-CG-CD2	-5.85	116.70	120.80
1	A	270	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	D	345	ASP	CB-CG-OD1	-5.84	113.04	118.30
2	E	44	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	401	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	A	133	LEU	CB-CG-CD1	-5.82	101.10	111.00
1	D	440	ARG	NE-CZ-NH2	-5.82	117.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	243	TYR	CB-CG-CD1	-5.82	117.51	121.00
1	D	202	ASP	CB-CG-OD1	5.78	123.51	118.30
1	A	216	ARG	NE-CZ-NH2	-5.78	117.41	120.30
3	C	129	ASP	CB-CG-OD1	-5.75	113.13	118.30
1	A	253	TYR	CB-CG-CD2	-5.74	117.56	121.00
2	E	322[A]	ARG	NE-CZ-NH1	5.67	123.14	120.30
2	E	322[B]	ARG	NE-CZ-NH1	5.67	123.14	120.30
2	B	100	ASP	CB-CG-OD2	-5.67	113.19	118.30
3	C	15	ARG	NE-CZ-NH2	-5.66	117.47	120.30
3	F	241	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	A	349	PHE	CB-CG-CD1	-5.65	116.85	120.80
1	D	333	TYR	CD1-CE1-CZ	-5.62	114.74	119.80
2	E	279	ASP	CB-CG-OD1	5.61	123.35	118.30
1	A	529	PHE	CB-CG-CD2	-5.61	116.88	120.80
1	A	80	TYR	CD1-CE1-CZ	-5.59	114.77	119.80
3	C	103	ARG	NE-CZ-NH1	5.59	123.10	120.30
2	B	72	ARG	NE-CZ-NH2	-5.58	117.51	120.30
2	E	388	PHE	CB-CG-CD1	-5.57	116.90	120.80
2	E	423	ASP	CB-CG-OD2	-5.57	113.28	118.30
1	A	444	TYR	CB-CG-CD2	-5.56	117.66	121.00
2	B	243	TYR	CB-CG-CD1	-5.56	117.67	121.00
1	D	349	PHE	CG-CD2-CE2	5.55	126.91	120.80
1	D	183	ASP	CB-CG-OD2	-5.54	113.32	118.30
2	E	279	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	505	PHE	CB-CG-CD2	-5.52	116.94	120.80
2	E	275	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	D	36	ARG	NE-CZ-NH1	5.50	123.05	120.30
2	B	388	PHE	CB-CG-CD1	-5.50	116.95	120.80
1	D	522	PHE	CB-CG-CD1	-5.50	116.95	120.80
1	A	450	ASP	N-CA-CB	5.48	120.47	110.60
3	C	225	ARG	NE-CZ-NH2	-5.48	117.56	120.30
3	C	92	TYR	CD1-CE1-CZ	-5.46	114.89	119.80
2	E	294	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	D	119	ARG	NE-CZ-NH2	-5.43	117.59	120.30
3	C	173	ARG	NE-CZ-NH1	-5.42	117.59	120.30
2	E	423	ASP	CB-CG-OD1	5.42	123.18	118.30
3	C	5	TYR	CZ-CE2-CD2	-5.42	114.92	119.80
1	D	59	ASP	CB-CG-OD1	5.42	123.17	118.30
1	A	447	ASP	CB-CG-OD1	5.41	123.17	118.30
2	E	329	SER	N-CA-CB	-5.39	102.42	110.50
3	F	144	ASP	CB-CG-OD2	5.39	123.15	118.30
3	F	163	ASP	CB-CG-OD2	-5.38	113.45	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	120[A]	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	E	120[B]	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	D	188	PHE	CB-CG-CD2	-5.38	117.04	120.80
1	A	345	ASP	CB-CG-OD1	-5.37	113.47	118.30
2	E	400	ASP	CB-CG-OD2	5.37	123.14	118.30
3	F	163	ASP	CB-CG-OD1	5.37	123.13	118.30
1	D	67	ARG	NE-CZ-NH2	-5.37	117.62	120.30
3	C	89	ASP	CB-CG-OD2	5.35	123.12	118.30
3	C	67[A]	ARG	NE-CZ-NH1	-5.33	117.63	120.30
3	C	67[B]	ARG	NE-CZ-NH1	-5.33	117.63	120.30
1	D	450	ASP	CB-CA-C	5.33	121.05	110.40
2	E	9	ASP	CB-CG-OD2	-5.32	113.52	118.30
1	A	14	PHE	CB-CG-CD2	-5.32	117.08	120.80
1	D	132	TYR	CZ-CE2-CD2	-5.30	115.03	119.80
1	D	103	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	D	103	ARG	NE-CZ-NH2	-5.29	117.65	120.30
3	C	99	TYR	CB-CG-CD1	-5.29	117.83	121.00
3	C	74	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	415	PHE	CB-CG-CD2	-5.28	117.11	120.80
2	E	279	ASP	OD1-CG-OD2	-5.26	113.30	123.30
2	E	225	GLU	OE1-CD-OE2	5.26	129.61	123.30
3	C	87	PHE	CB-CG-CD1	-5.25	117.12	120.80
2	E	127	TYR	CB-CG-CD2	-5.25	117.85	121.00
3	F	5	TYR	CZ-CE2-CD2	-5.25	115.08	119.80
3	F	126	ARG	NE-CZ-NH1	-5.23	117.68	120.30
1	D	26	TYR	CB-CG-CD2	5.23	124.14	121.00
2	E	147	ASP	CB-CG-OD1	5.23	123.01	118.30
1	D	89	VAL	CA-CB-CG2	-5.22	103.07	110.90
3	C	64[A]	ASP	CB-CG-OD2	-5.21	113.61	118.30
3	C	64[B]	ASP	CB-CG-OD2	-5.21	113.61	118.30
2	B	290	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	D	388	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	D	216	ARG	NE-CZ-NH2	-5.18	117.71	120.30
2	B	122[A]	ASP	CB-CG-OD1	5.17	122.96	118.30
2	B	122[B]	ASP	CB-CG-OD1	5.17	122.96	118.30
3	F	16	ARG	NE-CZ-NH1	5.17	122.89	120.30
3	C	103	ARG	NE-CZ-NH2	-5.16	117.72	120.30
3	F	81	ARG	NE-CZ-NH2	5.16	122.88	120.30
2	E	367	TYR	CB-CG-CD2	-5.14	117.91	121.00
3	F	120	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	488	TYR	CG-CD1-CE1	-5.13	117.19	121.30
3	C	217	TYR	CB-CG-CD1	-5.13	117.92	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	254	ASP	CB-CG-OD1	5.13	122.91	118.30
3	C	201	LEU	CB-CG-CD2	5.11	119.69	111.00
1	D	177	ASP	CB-CG-OD1	5.11	122.90	118.30
2	B	138	PHE	CB-CG-CD2	-5.10	117.23	120.80
1	D	385	TYR	CD1-CE1-CZ	-5.10	115.21	119.80
1	A	250	ASP	CB-CG-OD1	5.08	122.88	118.30
2	B	127	TYR	CZ-CE2-CD2	-5.08	115.22	119.80
1	D	346	PHE	CB-CG-CD2	-5.07	117.25	120.80
2	E	180	ASP	CB-CG-OD1	5.05	122.85	118.30
3	F	151	ARG	CG-CD-NE	-5.04	101.21	111.80
1	A	60	ILE	C-N-CA	-5.04	111.72	122.30
2	B	423	ASP	CB-CG-OD2	-5.03	113.77	118.30
1	D	450	ASP	N-CA-CB	5.02	119.64	110.60
3	C	126	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	D	23	THR	O-C-N	5.02	130.73	122.70
1	A	368	ASP	CB-CG-OD2	-5.01	113.79	118.30
2	E	367	TYR	CB-CG-CD1	5.01	124.00	121.00
2	B	291	TYR	CD1-CE1-CZ	-5.01	115.29	119.80

All (2) chirality outliers are listed below:

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

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	51	ARG	Sidechain
2	B	333	TYR	Sidechain
1	D	480	MET	Peptide

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4469	0	4240	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4390	0	4228	25	0
2	B	3505	0	3572	39	0
2	E	3519	0	3563	37	0
3	C	2050	0	1984	25	0
3	F	2103	0	2051	27	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	62	0	43	1	0
5	D	62	0	43	1	0
6	A	21	0	19	2	0
6	D	21	0	19	0	0
7	A	7	0	5	0	0
7	D	7	0	5	0	0
8	A	46	0	46	1	0
8	D	46	0	46	3	0
9	A	4	0	3	0	0
9	C	4	0	3	10	0
10	A	4	0	6	0	0
10	B	4	0	6	0	0
10	C	4	0	6	0	0
10	D	4	0	6	1	0
10	F	8	0	12	4	0
11	A	1	0	0	0	0
12	C	7	0	10	0	0
13	A	519	0	0	9	0
13	B	472	0	0	19	0
13	C	259	0	0	5	0
13	D	511	0	0	7	0
13	E	415	0	0	14	0
13	F	256	0	0	11	0
All	All	22789	0	19916	170	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (170) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:81:ARG:CG	9:C:1:ACT:H1	1.62	1.28
3:C:81:ARG:CD	9:C:1:ACT:H1	1.69	1.21
3:C:81:ARG:HD3	9:C:1:ACT:CH3	1.73	1.19
2:B:322[B]:ARG:NH2	3:C:67[B]:ARG:HG3	1.65	1.10
2:B:58[B]:LYS:HD2	13:B:3633:HOH:O	1.53	1.06
3:F:67[A]:ARG:HH11	3:F:67[A]:ARG:HG2	1.20	1.04
1:A:352[A]:GLU:HG2	13:A:4141:HOH:O	1.59	1.02
1:D:545:LEU:HD12	13:D:2591:HOH:O	1.64	0.97
3:C:81:ARG:HG2	9:C:1:ACT:H1	1.46	0.94
3:C:81:ARG:CG	9:C:1:ACT:CH3	2.50	0.90
1:A:24[A]:THR:HG23	13:C:3803:HOH:O	1.71	0.90
13:B:3688[A]:HOH:O	3:C:72[A]:PRO:HG3	1.71	0.89
3:F:207[B]:GLU:HG3	13:F:3759:HOH:O	1.72	0.89
3:C:81:ARG:HD3	9:C:1:ACT:H3	1.56	0.88
13:A:3768:HOH:O	1:D:545:LEU:HD11	1.75	0.86
3:C:81:ARG:HD3	9:C:1:ACT:H1	1.37	0.85
2:E:27:LEU:HD22	2:E:246[B]:MET:CE	2.07	0.84
3:F:207[A]:GLU:HG2	13:F:4112:HOH:O	1.77	0.84
1:D:383[B]:GLU:HG2	1:D:387[B]:GLU:OE2	1.79	0.83
3:C:124:GLU:HG3	13:C:4089:HOH:O	1.80	0.82
3:F:132[B]:LYS:NZ	10:F:252:EDO:H11	1.99	0.78
2:B:104[B]:GLU:HG2	13:B:3852:HOH:O	1.83	0.77
3:F:67[A]:ARG:NH1	3:F:67[A]:ARG:HG2	1.98	0.76
3:F:132[A]:LYS:HD2	13:F:1990:HOH:O	1.85	0.75
2:B:61[B]:LYS:CE	13:B:1223:HOH:O	2.34	0.75
1:D:348:TYR:O	1:D:352[A]:GLU:HG2	1.88	0.73
2:B:322[B]:ARG:HH21	3:C:67[B]:ARG:HG3	1.50	0.72
1:A:178[A]:PRO:HD3	13:A:1631:HOH:O	1.89	0.70
2:B:322[B]:ARG:CZ	3:C:67[B]:ARG:HG3	2.22	0.70
2:B:104[B]:GLU:CG	13:B:3852:HOH:O	2.37	0.70
3:F:207[B]:GLU:CG	13:F:3759:HOH:O	2.37	0.70
2:B:58[B]:LYS:HG3	13:B:859:HOH:O	1.92	0.69
2:B:196[B]:MET:CE	13:B:3731:HOH:O	2.40	0.69
3:F:67[A]:ARG:HH11	3:F:67[A]:ARG:CG	2.02	0.69
2:E:27:LEU:HD22	2:E:246[B]:MET:HE1	1.73	0.69
3:F:132[B]:LYS:HZ3	10:F:252:EDO:H11	1.56	0.68
2:B:118[B]:SER:HB3	13:B:1533:HOH:O	1.95	0.67
2:B:196[B]:MET:CE	13:B:574:HOH:O	2.42	0.66
1:D:545:LEU:CD1	13:D:2591:HOH:O	2.33	0.66
3:C:81:ARG:CD	9:C:1:ACT:CH3	2.41	0.66
2:E:27:LEU:CD2	2:E:246[B]:MET:CE	2.73	0.66
1:A:24[B]:THR:HG23	13:A:677:HOH:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24[A]:THR:HG23	13:F:1497:HOH:O	1.97	0.65
2:E:27:LEU:HD22	2:E:246[B]:MET:SD	2.37	0.65
1:A:123[B]:GLU:HG3	13:A:3785:HOH:O	1.97	0.64
1:D:239:TYR:HB2	1:D:241[B]:GLN:HE22	1.62	0.64
2:B:299:LEU:HD13	13:B:3737:HOH:O	1.97	0.64
2:E:122[B]:ASP:HB2	13:E:1158:HOH:O	1.96	0.64
2:E:27:LEU:CD2	2:E:246[B]:MET:HE1	2.28	0.64
2:E:58[B]:LYS:HE3	13:E:1433:HOH:O	1.97	0.63
2:E:118[B]:SER:HB3	13:E:2658:HOH:O	1.97	0.63
2:B:188:PRO:HD3	13:E:1304:HOH:O	1.99	0.63
3:C:194[B]:GLU:HG3	13:C:1318:HOH:O	2.00	0.62
1:A:194[B]:GLU:HG2	13:A:2095:HOH:O	1.99	0.62
2:B:322[B]:ARG:NH2	3:C:67[B]:ARG:CG	2.55	0.61
2:B:61[B]:LYS:HE2	13:B:1223:HOH:O	2.00	0.61
1:A:178[A]:PRO:HD2	13:A:1652:HOH:O	1.99	0.61
2:E:261:LYS:HE2	13:E:545:HOH:O	2.02	0.60
1:D:172[A]:ILE:HD12	13:D:2242:HOH:O	2.01	0.60
2:B:196[B]:MET:HE3	13:B:574:HOH:O	2.00	0.59
1:D:268:PRO:HB3	13:E:1668:HOH:O	2.02	0.59
2:B:196[B]:MET:HE1	13:B:3731:HOH:O	2.02	0.58
1:A:169[B]:ASN:OD1	1:A:171[B]:GLU:HB3	2.02	0.58
1:A:114:ALA:O	1:A:118:LYS:HD3	2.04	0.58
3:F:67[A]:ARG:NH1	3:F:67[A]:ARG:CG	2.64	0.58
2:B:95:VAL:HG21	2:B:119[B]:ALA:HB3	1.87	0.57
2:E:98[A]:ASP:HB2	13:E:3962:HOH:O	2.06	0.56
1:D:194[B]:GLU:HG2	13:D:3701:HOH:O	2.06	0.56
2:B:118[B]:SER:HB2	13:B:463:HOH:O	2.05	0.55
3:C:64[A]:ASP:HB3	3:C:67[A]:ARG:HB2	1.89	0.55
3:F:153[A]:LYS:NZ	13:F:1186:HOH:O	2.21	0.54
1:A:17[B]:SER:OG	1:A:20:GLU:HG3	2.08	0.54
1:A:4[A]:LYS:NZ	13:A:2253:HOH:O	2.32	0.54
2:B:299:LEU:HD21	13:C:1043:HOH:O	2.08	0.53
1:D:480:MET:O	8:D:555[B]:XP9:H7	2.08	0.53
3:F:132[B]:LYS:HZ2	10:F:252:EDO:H11	1.74	0.53
2:B:424[A]:GLU:HG3	13:B:3930:HOH:O	2.08	0.52
2:B:42[A]:ILE:HG13	2:B:425:PHE:CE1	2.44	0.52
1:A:481:ASN:HA	6:A:553[A]:TP7:S7	2.48	0.52
2:B:286:LYS:HE2	2:B:288:LEU:HD21	1.91	0.52
1:A:328:VAL:HB	5:D:552:F43:H9A1	1.90	0.52
2:E:61[B]:LYS:HE3	13:E:2370:HOH:O	2.09	0.52
3:C:44:ALA:HB1	3:C:45:PRO:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ALA:HB2	3:F:84:TYR:CE1	2.45	0.51
2:E:299:LEU:HD22	13:E:2973:HOH:O	2.11	0.51
2:E:322[A]:ARG:CZ	3:F:67[A]:ARG:HD2	2.40	0.50
3:C:84:TYR:CE1	1:D:242:ALA:HB2	2.46	0.50
13:B:3688[A]:HOH:O	3:C:72[A]:PRO:CG	2.42	0.50
2:E:322[A]:ARG:NH1	3:F:67[A]:ARG:HD2	2.28	0.49
2:E:95:VAL:HG21	2:E:119[B]:ALA:HB3	1.94	0.49
1:A:60:ILE:HD12	13:D:3878:HOH:O	2.13	0.49
3:C:50:PRO:HB2	9:C:1:ACT:H2	1.94	0.49
1:A:172:ILE:CG2	1:A:176[A]:ILE:HD11	2.43	0.48
2:B:196[B]:MET:SD	2:B:376:ASN:ND2	2.84	0.48
2:E:344[A]:LEU:HB3	2:E:345:PRO:HD2	1.95	0.48
2:E:97[A]:GLU:OE1	2:E:98[A]:ASP:OD1	2.32	0.48
2:B:123[B]:VAL:HG12	2:E:36:LYS:HA	1.96	0.48
3:F:132[A]:LYS:HE2	13:F:1692:HOH:O	2.14	0.48
2:B:58[B]:LYS:CD	13:B:3633:HOH:O	2.32	0.48
3:C:247:ASN:HB3	13:C:4090[B]:HOH:O	2.14	0.47
3:F:228:VAL:HG22	13:F:4164:HOH:O	2.14	0.47
5:A:1:F43:H9A1	1:D:328:VAL:HB	1.96	0.47
1:D:154:HIS:CE1	1:D:545:LEU:HD21	2.50	0.47
1:A:357:LYS:NZ	1:A:372[B]:ASP:OD1	2.32	0.47
10:F:251:EDO:C2	13:F:832:HOH:O	2.63	0.47
2:B:61[B]:LYS:NZ	13:B:1223:HOH:O	2.36	0.47
1:A:383[A]:GLU:HG3	13:A:2606:HOH:O	2.15	0.47
2:E:246[B]:MET:HE1	2:E:432:VAL:HG12	1.96	0.46
3:F:247:ASN:C	3:F:247:ASN:HD22	2.18	0.46
13:B:2205:HOH:O	2:E:188:PRO:HD3	2.14	0.46
2:B:405[A]:MET:HG3	1:D:115:VAL:HG22	1.98	0.46
2:B:246[A]:MET:CE	2:B:429:LEU:HD12	2.45	0.46
2:B:261[A]:LYS:HG2	2:B:262:GLU:HG3	1.98	0.46
1:D:358:TYR:OH	1:D:372[A]:ASP:OD2	2.25	0.46
1:A:186:LYS:NZ	1:A:186:LYS:HB2	2.31	0.45
1:A:172:ILE:HG22	1:A:176[A]:ILE:CD1	2.46	0.45
2:E:236[A]:MET:HG3	2:E:300:ALA:HA	1.97	0.45
1:D:191:ASP:HB2	13:D:3703:HOH:O	2.15	0.45
3:C:81:ARG:HG2	9:C:1:ACT:CH3	2.31	0.45
1:D:241[B]:GLN:HE21	1:D:241[B]:GLN:H	1.62	0.45
3:F:205:LEU:HD22	3:F:209:THR:HG21	1.98	0.45
1:A:115:VAL:HG22	2:E:405[B]:MET:SD	2.56	0.45
1:D:45[B]:LYS:NZ	13:D:2225:HOH:O	2.48	0.45
1:A:115:VAL:CG2	2:E:405[B]:MET:SD	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113[A]:LEU:HD13	2:B:418:VAL:HG13	1.99	0.44
1:D:267:LEU:HD12	1:D:273:ARG:HB2	2.00	0.44
2:E:122[B]:ASP:CB	13:E:1158:HOH:O	2.62	0.44
2:E:214:LEU:HB2	2:E:428:PRO:HG3	1.99	0.44
1:D:428:TYR:HD1	1:D:450:ASP:HB3	1.83	0.44
3:F:180[B]:ASP:O	3:F:181[B]:THR:CG2	2.66	0.44
3:F:61:GLU:HB2	3:F:67[A]:ARG:NH2	2.32	0.44
1:A:480:MET:O	8:A:555[B]:XP9:H7	2.18	0.43
1:A:172:ILE:CD1	1:A:172:ILE:N	2.81	0.43
2:E:299:LEU:CD2	13:E:2973:HOH:O	2.66	0.43
2:B:362:PHE:O	2:B:369:GLY:HA3	2.19	0.43
1:D:348:TYR:CZ	10:D:556:EDO:H11	2.54	0.43
1:A:360:LEU:O	1:A:361[B]:CYS:HB2	2.19	0.43
2:B:434:GLU:O	2:B:438[B]:GLU:HG3	2.18	0.43
3:F:200[A]:ASP:HB2	13:F:1920:HOH:O	2.18	0.43
2:E:39:VAL:HG21	2:E:221:THR:HG21	2.01	0.43
2:E:17:LEU:HD21	2:E:20[A]:GLU:HG3	2.01	0.42
3:F:59:MET:O	3:F:60:ASP:C	2.56	0.42
2:E:113[A]:LEU:HD13	2:E:418:VAL:HG13	2.00	0.42
2:E:61[B]:LYS:CE	13:E:2444:HOH:O	2.66	0.42
13:E:3631[A]:HOH:O	3:F:72:PRO:HG3	2.18	0.42
2:B:322[B]:ARG:HH21	3:C:67[B]:ARG:CG	2.22	0.42
1:A:115:VAL:HG22	2:E:405[A]:MET:HG3	2.02	0.42
2:B:422:VAL:HB	2:B:425:PHE:CD2	2.55	0.42
1:A:169[A]:ASN:ND2	1:A:172:ILE:HD13	2.35	0.41
2:B:67:CYS:HB3	1:D:505:PHE:CE1	2.54	0.41
3:F:180[B]:ASP:O	3:F:181[B]:THR:HG22	2.20	0.41
2:B:196[B]:MET:SD	2:B:374:ILE:O	2.79	0.41
1:D:239:TYR:CB	1:D:241[B]:GLN:HE22	2.31	0.41
1:A:57:ASN:HB3	1:A:60:ILE:HG12	2.02	0.41
1:A:169[B]:ASN:OD1	1:A:172:ILE:HD13	2.21	0.41
3:F:82:VAL:O	3:F:83:ARG:HD2	2.20	0.41
3:C:100:VAL:HG21	3:C:215:THR:HB	2.03	0.41
1:A:443:PHE:CZ	6:A:553[A]:TP7:S7	3.13	0.41
2:E:424[A]:GLU:HG2	13:E:3642:HOH:O	2.20	0.41
2:E:246[A]:MET:CE	2:E:429:LEU:HD12	2.51	0.41
2:B:126:GLU:HB3	2:E:126:GLU:HB3	2.03	0.41
2:E:261:LYS:HG2	13:F:3664:HOH:O	2.20	0.41
8:D:555[B]:XP9:H7A	2:E:361:PHE:HE2	1.85	0.41
1:A:106:ILE:HB	1:A:261:ILE:HB	2.04	0.40
1:A:332:GLN:HA	1:A:335:THR:OG1	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:555[B]:XP9:H7A	2:E:361:PHE:CE2	2.55	0.40
2:B:3:LYS:HE2	2:B:234:GLU:OE1	2.22	0.40
3:C:233:ILE:HA	3:C:233:ILE:HD13	1.88	0.40
3:F:178[B]:ASN:HB3	3:F:181[B]:THR:OG1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	574/549 (105%)	556 (97%)	17 (3%)	1 (0%)	47	22
1	D	566/549 (103%)	549 (97%)	16 (3%)	1 (0%)	47	22
2	B	471/442 (107%)	461 (98%)	10 (2%)	0	100	100
2	E	472/442 (107%)	462 (98%)	10 (2%)	0	100	100
3	C	254/248 (102%)	246 (97%)	8 (3%)	0	100	100
3	F	263/248 (106%)	254 (97%)	8 (3%)	1 (0%)	34	13
All	All	2600/2478 (105%)	2528 (97%)	69 (3%)	3 (0%)	51	24

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	60	ASP
1	D	325	SER
1	A	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	466/434 (107%)	454 (97%)	12 (3%)	46	13
1	D	458/434 (106%)	456 (100%)	2 (0%)	91	80
2	B	371/341 (109%)	365 (98%)	6 (2%)	62	31
2	E	372/341 (109%)	365 (98%)	7 (2%)	57	23
3	C	224/216 (104%)	220 (98%)	4 (2%)	59	26
3	F	232/216 (107%)	224 (97%)	8 (3%)	37	6
All	All	2123/1982 (107%)	2084 (98%)	39 (2%)	65	26

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12[A]	LYS
1	A	12[B]	LYS
1	A	17[A]	SER
1	A	17[B]	SER
1	A	118	LYS
1	A	126	PRO
1	A	171[A]	GLU
1	A	171[B]	GLU
1	A	172	ILE
1	A	444	TYR
1	A	450	ASP
1	A	543	ARG
2	B	97	GLU
2	B	123[A]	VAL
2	B	123[B]	VAL
2	B	126	GLU
2	B	283	LYS
2	B	287	GLU
3	C	45	PRO
3	C	61	GLU
3	C	121	GLN
3	C	208	GLU
1	D	444	TYR
1	D	450	ASP
2	E	126	GLU
2	E	236[A]	MET

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Mol	Chain	Res	Type
2	E	236[B]	MET
2	E	236[C]	MET
2	E	283	LYS
2	E	438[A]	GLU
2	E	438[B]	GLU
3	F	60	ASP
3	F	61	GLU
3	F	67[A]	ARG
3	F	67[B]	ARG
3	F	121	GLN
3	F	207[A]	GLU
3	F	207[B]	GLU
3	F	247	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	241	GLN
3	C	121	GLN
2	E	21	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	SMC	A	452	1	5,6,7	1.23	0	2,6,8	2.27	1 (50%)
1	MHS	A	257	1	7,11,12	2.13	2 (28%)	6,14,16	4.28	3 (50%)
1	GL3	A	445	1	2,3,4	2.44	1 (50%)	1,2,4	0.20	0
1	GL3	D	445	1	2,3,4	2.43	1 (50%)	1,2,4	0.36	0
1	MHS	D	257	1	7,11,12	1.52	1 (14%)	6,14,16	3.81	3 (50%)
1	SMC	D	452	1	5,6,7	1.23	1 (20%)	2,6,8	1.99	1 (50%)
1	MGN	A	400	1	6,9,10	1.07	0	5,12,14	0.60	0
1	MGN	D	400	1	6,9,10	1.43	1 (16%)	5,12,14	0.43	0
1	AGM	D	271	1	10,11,12	1.78	1 (10%)	6,13,15	1.45	1 (16%)
1	AGM	A	271	1	10,11,12	1.33	2 (20%)	6,13,15	1.99	2 (33%)

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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	271	AGM	CB-CA	4.25	1.59	1.53
1	A	257	MHS	CE1-NE2	4.06	1.44	1.34
1	A	445	GL3	C-S	-3.46	1.68	1.80
1	D	445	GL3	C-S	-3.42	1.68	1.80
1	D	257	MHS	CE1-NE2	3.20	1.42	1.34
1	D	400	MGN	O-C	2.66	1.28	1.19
1	A	257	MHS	CB-CA	2.46	1.59	1.53
1	A	271	AGM	O-C	2.39	1.29	1.19
1	A	271	AGM	CZ-NH2	2.22	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	452	SMC	CB-SG	2.02	1.83	1.80

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	MHS	NE2-CE1-ND1	-9.49	98.17	112.26
1	D	257	MHS	NE2-CE1-ND1	-7.21	101.55	112.26
1	D	257	MHS	CM-ND1-CG	4.15	129.96	124.44
1	A	257	MHS	CD2-NE2-CE1	3.63	111.44	105.78
1	D	257	MHS	CD2-NE2-CE1	3.49	111.23	105.78
1	A	271	AGM	NE1-CZ-NH2	-3.38	114.70	120.59
1	A	452	SMC	CA-CB-SG	-3.19	108.89	114.04
1	A	271	AGM	NH1-CZ-NE1	2.76	125.72	119.55
1	D	452	SMC	CA-CB-SG	-2.49	110.01	114.04
1	D	271	AGM	NE1-CZ-NH2	-2.48	116.26	120.59
1	A	257	MHS	CB-CA-C	-2.03	107.67	111.47

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	D	271	AGM	CE2-CD-NE1-CZ
1	A	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 10 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	C	251	-	3,3,3	0.56	0	2,2,2	0.50	0
5	F43	D	552	1,7	46,71,71	3.07	12 (26%)	48,118,118	2.18	14 (29%)
10	EDO	D	556	-	3,3,3	0.48	0	2,2,2	0.58	0
9	ACT	C	1	-	1,3,3	1.65	0	0,3,3	0.00	-
8	XP9	A	555[C]	-	18,22,22	0.77	0	20,28,28	0.91	1 (5%)
10	EDO	F	252	-	3,3,3	0.76	0	2,2,2	0.23	0
7	COM	A	554	5	6,6,6	1.39	1 (16%)	7,8,8	1.85	3 (42%)
8	XP9	A	555[B]	-	18,22,22	0.82	0	20,28,28	1.25	2 (10%)
8	XP9	D	555[B]	-	18,22,22	0.78	1 (5%)	20,28,28	1.13	2 (10%)
6	TP7	D	553[A]	-	16,20,20	1.02	1 (6%)	18,26,26	1.02	2 (11%)
8	XP9	D	555[C]	-	18,22,22	0.80	1 (5%)	20,28,28	0.92	1 (5%)
6	TP7	A	553[A]	-	16,20,20	1.08	1 (6%)	18,26,26	1.04	1 (5%)
9	ACT	A	556[B]	4	1,3,3	1.04	0	0,3,3	0.00	-
10	EDO	F	251	-	3,3,3	0.64	0	2,2,2	0.58	0
10	EDO	B	446	-	3,3,3	0.53	0	2,2,2	0.31	0
12	PEG	C	252	-	6,6,6	0.57	0	5,5,5	0.94	0
7	COM	D	554	5	6,6,6	0.83	0	7,8,8	1.21	1 (14%)
10	EDO	A	557	-	3,3,3	0.79	0	2,2,2	0.70	0
5	F43	A	1	1,7	46,71,71	3.01	10 (21%)	48,118,118	1.62	11 (22%)

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	C	251	-	-	0/1/1/1	-
5	F43	D	552	1,7	-	1/18/185/185	-
10	EDO	D	556	-	-	1/1/1/1	-
5	F43	A	1	1,7	-	1/18/185/185	-
8	XP9	A	555[C]	-	-	3/22/26/26	-
10	EDO	F	252	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	COM	A	554	5	-	0/4/4/4	-
8	XP9	A	555[B]	-	-	3/22/26/26	-
8	XP9	D	555[B]	-	-	4/22/26/26	-
6	TP7	D	553[A]	-	-	1/20/24/24	-
8	XP9	D	555[C]	-	-	1/22/26/26	-
6	TP7	A	553[A]	-	-	2/20/24/24	-
10	EDO	A	557	-	-	1/1/1/1	-
10	EDO	F	251	-	-	1/1/1/1	-
10	EDO	B	446	-	-	1/1/1/1	-
7	COM	D	554	5	-	0/4/4/4	-
12	PEG	C	252	-	-	1/4/4/4	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1	F43	NI-NB	11.01	2.13	1.89
5	D	552	F43	NI-NA	10.57	2.12	1.89
5	A	1	F43	NI-NA	10.49	2.12	1.89
5	D	552	F43	NI-NB	10.19	2.11	1.89
5	A	1	F43	NI-ND	8.77	2.08	1.89
5	D	552	F43	NI-ND	8.09	2.07	1.89
5	D	552	F43	CHD-C1D	5.28	1.50	1.43
5	D	552	F43	CHB-C1B	4.95	1.56	1.53
5	D	552	F43	C3C-C4C	4.24	1.57	1.50
5	A	1	F43	CHC-C4B	4.05	1.50	1.39
5	A	1	F43	C3C-C4C	3.88	1.56	1.50
5	A	1	F43	CHA-C4D	3.78	1.56	1.53
5	D	552	F43	O8D-C7D	3.46	1.30	1.23
5	A	1	F43	C8B-C6B	3.13	1.56	1.50
5	D	552	F43	C1C-NC	2.85	1.43	1.37
7	A	554	COM	C2-S2	2.85	1.81	1.77
5	A	1	F43	C4A-NA	2.79	1.53	1.49
6	D	553[A]	TP7	P-O4P	2.74	1.64	1.59
5	A	1	F43	C5C-C2C	-2.62	1.49	1.54
5	D	552	F43	CHC-C4B	2.49	1.46	1.39
5	A	1	F43	C9B-C2B	2.48	1.59	1.54
5	D	552	F43	C5C-C2C	2.45	1.58	1.54
5	D	552	F43	CAA-C3A	2.44	1.58	1.53
8	D	555[C]	XP9	P-O4P	2.33	1.63	1.59
8	D	555[B]	XP9	P-O4P	2.32	1.63	1.59
6	A	553[A]	TP7	P-O4P	2.11	1.63	1.59
5	D	552	F43	C2A-C3A	-2.00	1.51	1.54

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	552	F43	O8D-C7D-C6D	-6.98	109.42	120.86
5	D	552	F43	C4B-CHC-C1C	5.63	135.06	125.84
5	D	552	F43	C6D-C7D-CHD	5.09	126.53	116.95
5	D	552	F43	C5D-C2D-C1D	3.92	115.72	110.45
5	A	1	F43	O8D-C7D-C6D	-3.90	114.48	120.86
8	A	555[B]	XP9	C7-C8-C9	3.76	119.77	113.09
5	D	552	F43	C2D-C1D-CHD	-3.54	117.31	121.85
5	D	552	F43	C9A-C2A-C3A	3.48	118.12	112.98
5	D	552	F43	C3D-C2D-C1D	-3.35	97.01	102.69
7	A	554	COM	O1S-S2-C2	-3.06	103.23	106.92
5	A	1	F43	C1B-C2B-C3B	3.03	105.99	101.51
5	A	1	F43	CAB-C3B-C2B	-3.01	112.73	119.09
5	A	1	F43	C9A-C2A-C3A	2.87	117.22	112.98
6	A	553[A]	TP7	CB-CA-N	2.85	117.74	111.38
5	D	552	F43	C1D-CHD-C4C	-2.78	117.41	125.31
5	A	1	F43	C4A-NA-C1A	-2.67	105.73	108.97
5	D	552	F43	CAB-C3B-C2B	-2.66	113.45	119.09
5	A	1	F43	C8C-C9C-CAC	-2.66	107.87	113.59
5	A	1	F43	C9B-C2B-C8B	-2.63	103.80	110.45
8	A	555[B]	XP9	CB-CA-N	2.58	117.14	111.38
5	D	552	F43	CAB-CBB-CCB	-2.58	108.05	113.59
7	A	554	COM	O3S-S2-O1S	2.54	117.47	111.27
5	A	1	F43	CAA-CBA-CCA	-2.53	108.14	113.59
6	D	553[A]	TP7	CB-CA-N	2.49	116.95	111.38
8	D	555[B]	XP9	C7-C8-C9	2.49	117.51	113.09
8	A	555[C]	XP9	CB-CA-N	2.46	116.88	111.38
5	D	552	F43	C2B-C1B-NB	2.45	105.50	101.84
8	D	555[B]	XP9	CB-CA-N	2.40	116.74	111.38
5	D	552	F43	C3C-C4C-NC	2.24	113.50	110.05
5	D	552	F43	O7B-C6B-C8B	-2.18	123.94	126.59
5	D	552	F43	C7D-CHD-C4C	2.17	126.18	121.61
8	D	555[C]	XP9	CB-CA-N	2.17	116.22	111.38
5	A	1	F43	C5D-C2D-C1D	2.15	113.35	110.45
7	A	554	COM	O3S-S2-O2S	-2.09	106.16	111.27
7	D	554	COM	O2S-S2-C2	2.05	109.39	106.92
5	A	1	F43	O7B-C6B-C8B	-2.05	124.09	126.59
5	A	1	F43	C3B-C4B-CHC	-2.03	118.94	123.32
6	D	553[A]	TP7	O4P-P-O1P	-2.03	101.57	109.39

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	553[A]	TP7	CB-O4P-P-O3P
5	D	552	F43	C3A-CAA-CBA-CCA
5	A	1	F43	C3A-CAA-CBA-CCA
8	A	555[B]	XP9	C6-C7-C8-C9
8	A	555[B]	XP9	C3-C4-C5-C6
10	D	556	EDO	O1-C1-C2-O2
10	F	252	EDO	O1-C1-C2-O2
8	D	555[B]	XP9	C4-C5-C6-C7
8	D	555[B]	XP9	C6-C7-C8-C9
10	B	446	EDO	O1-C1-C2-O2
8	D	555[B]	XP9	C2-C3-C4-C5
10	F	251	EDO	O1-C1-C2-O2
10	A	557	EDO	O1-C1-C2-O2
8	A	555[C]	XP9	CB-O4P-P-O3P
8	A	555[B]	XP9	CB-O4P-P-O3P
8	D	555[B]	XP9	CB-O4P-P-O3P
8	A	555[C]	XP9	C7-C8-C9-S9
8	D	555[C]	XP9	C7-C8-C9-S9
8	A	555[C]	XP9	C2-C3-C4-C5
6	D	553[A]	TP7	CB-O4P-P-O3P
12	C	252	PEG	O2-C3-C4-O4
6	A	553[A]	TP7	C2-C3-C4-C5

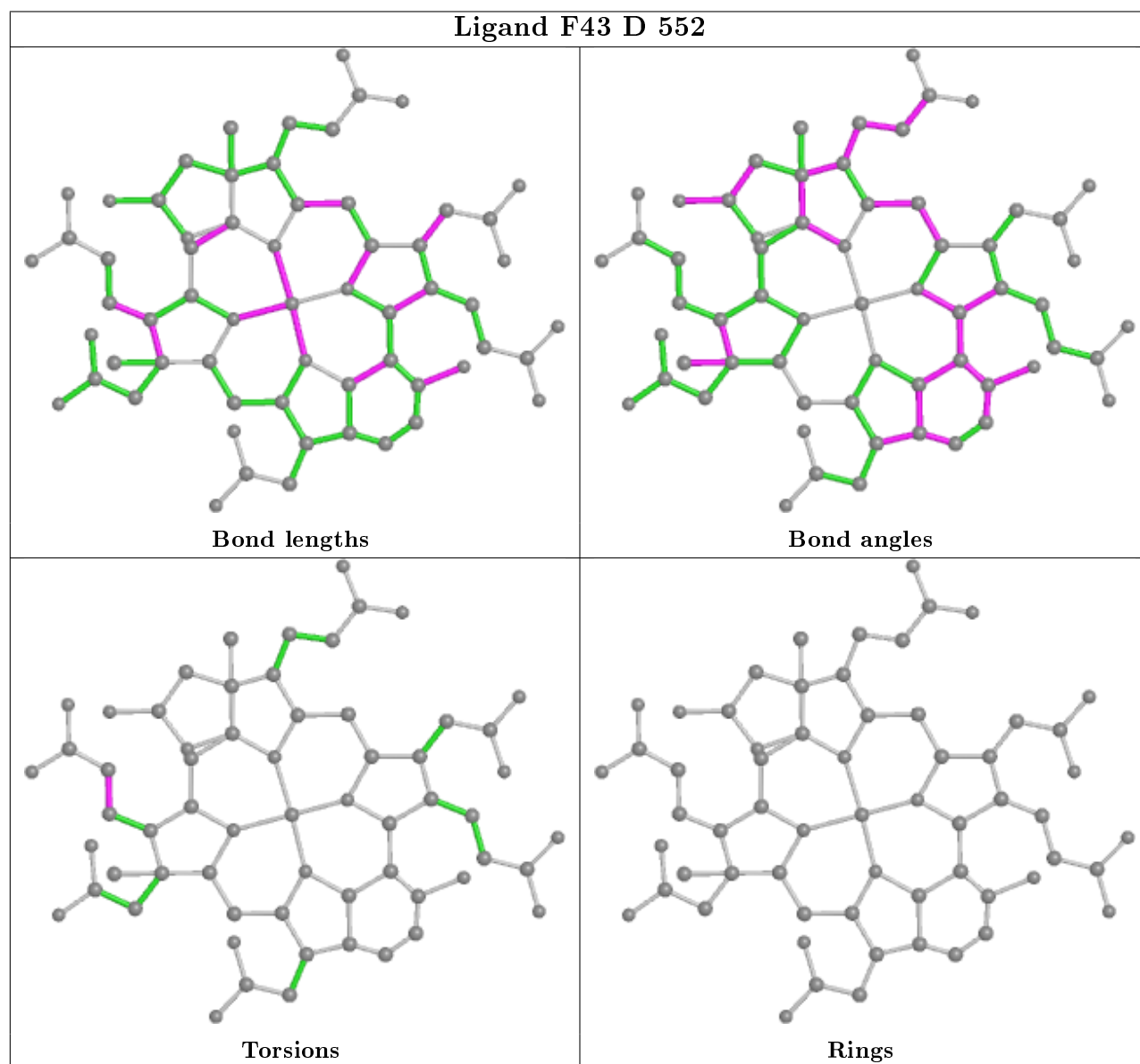
There are no ring outliers.

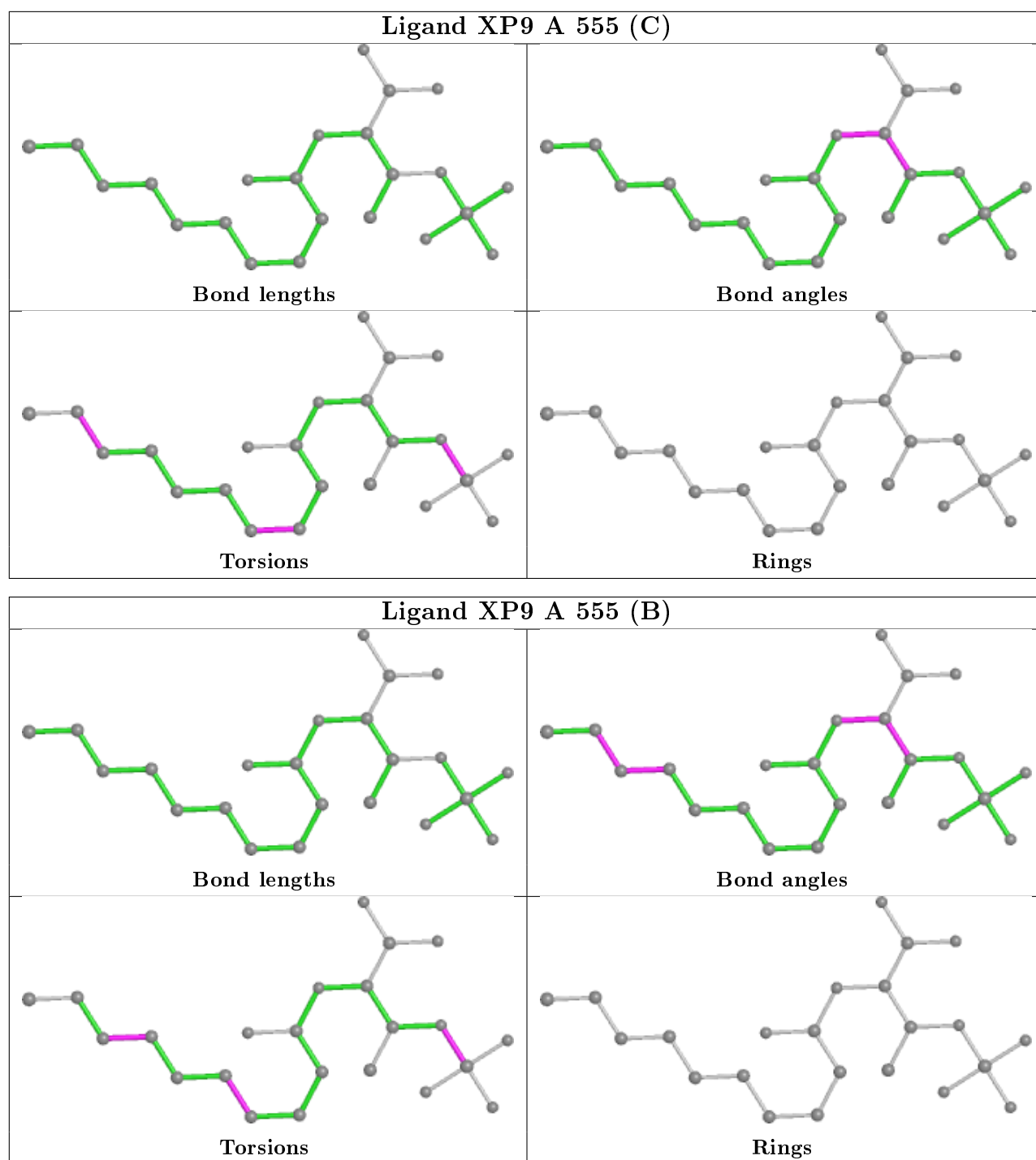
9 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	552	F43	1	0
10	D	556	EDO	1	0
9	C	1	ACT	10	0
10	F	252	EDO	3	0
8	A	555[B]	XP9	1	0
8	D	555[B]	XP9	3	0
6	A	553[A]	TP7	2	0
10	F	251	EDO	1	0
5	A	1	F43	1	0

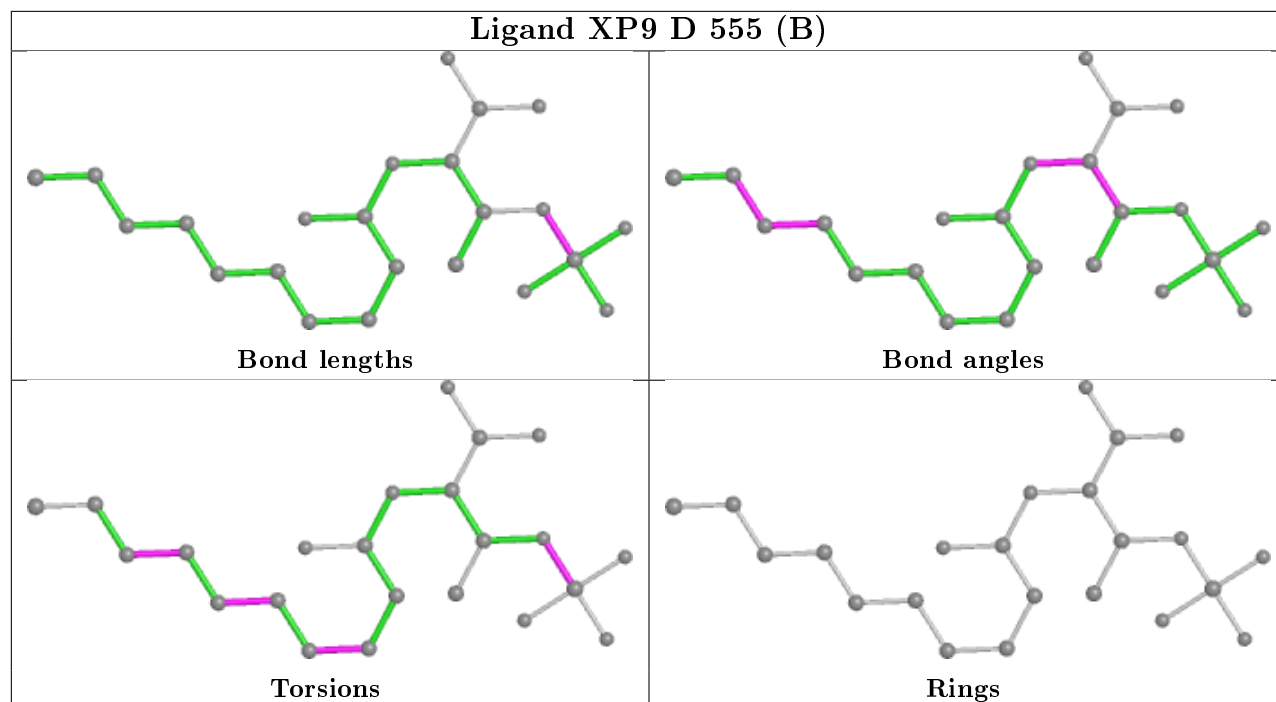
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

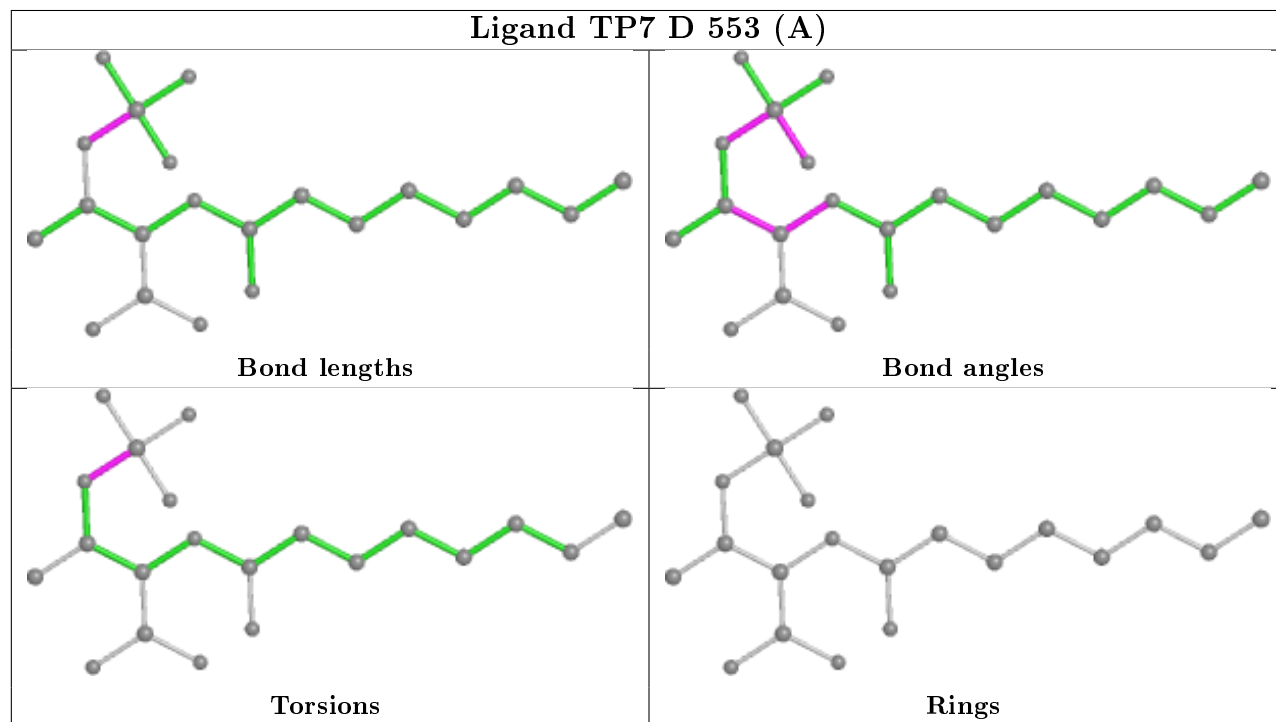




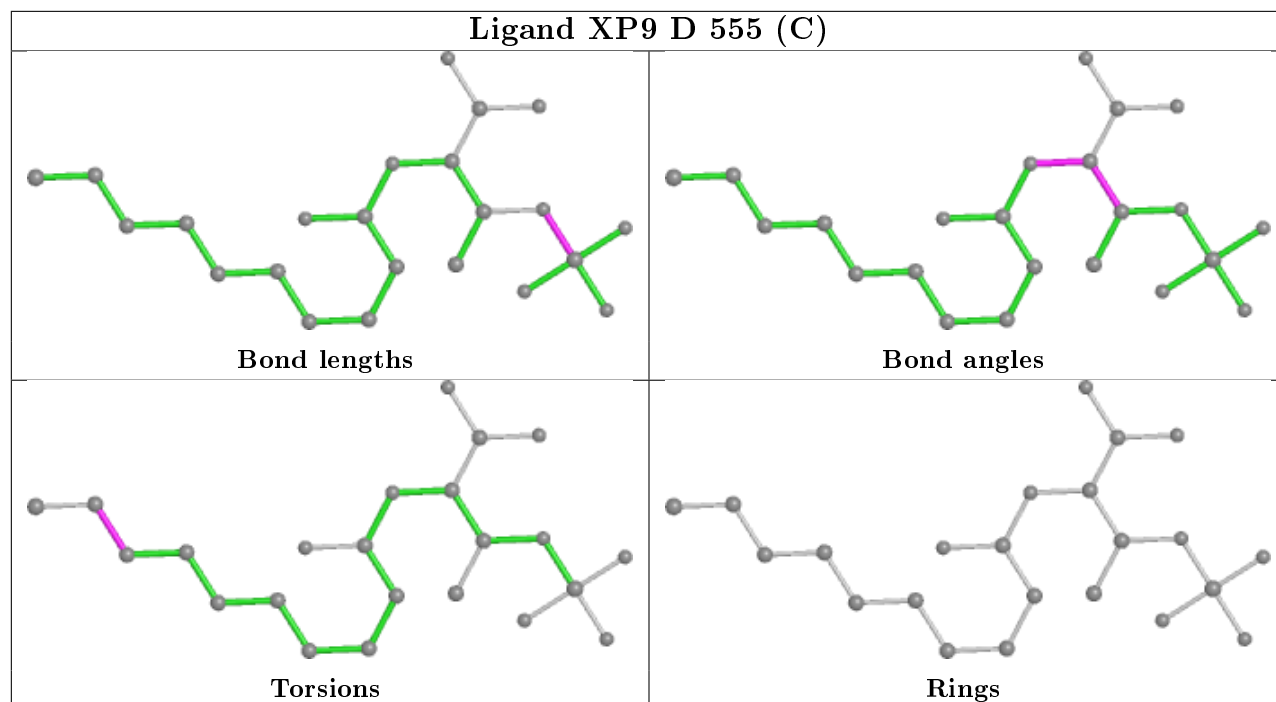
Ligand XP9 D 555 (B)



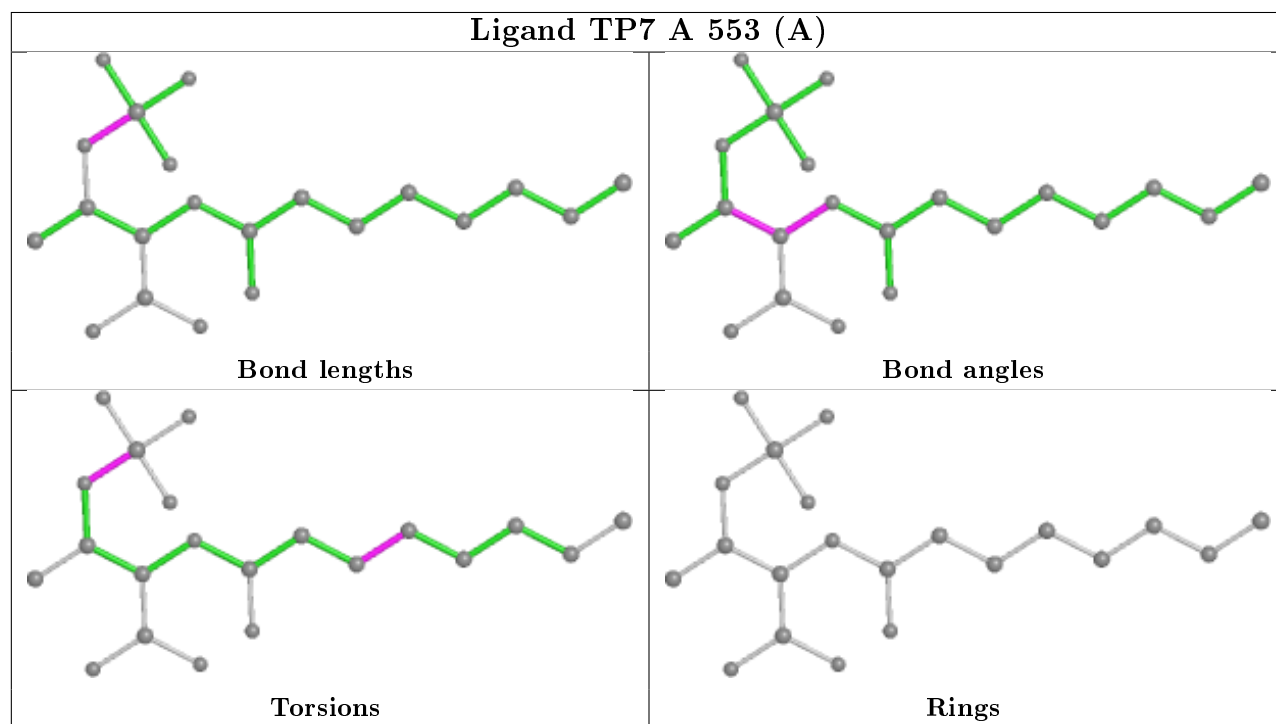
Ligand TP7 D 553 (A)

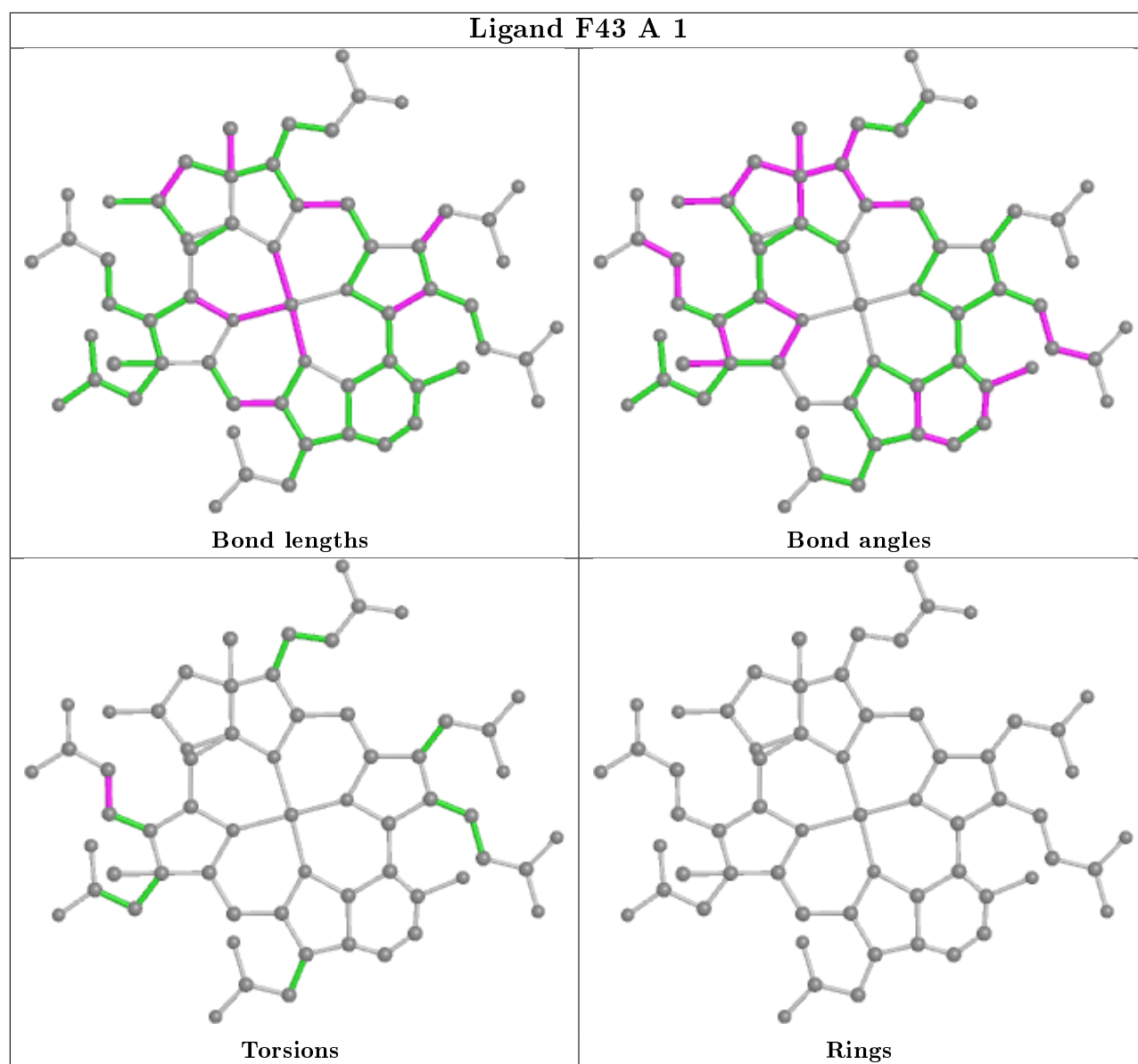


Ligand XP9 D 555 (C)



Ligand TP7 A 553 (A)





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	543/549 (98%)	-0.68	3 (0%) 89 91	5, 9, 20, 34	0
1	D	543/549 (98%)	-0.68	3 (0%) 89 91	5, 9, 20, 38	0
2	B	442/442 (100%)	-0.69	1 (0%) 95 95	6, 11, 20, 39	0
2	E	442/442 (100%)	-0.61	4 (0%) 84 86	7, 12, 24, 42	0
3	C	246/248 (99%)	-0.45	9 (3%) 41 44	8, 13, 30, 49	0
3	F	246/248 (99%)	-0.38	9 (3%) 41 44	8, 14, 30, 53	0
All	All	2462/2478 (99%)	-0.62	29 (1%) 79 80	5, 11, 23, 53	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	60	ASP	5.4
3	C	60	ASP	5.2
3	F	45	PRO	4.8
3	C	45	PRO	4.8
1	D	549	ALA	4.7
3	F	180[A]	ASP	3.7
2	E	441	ASN	3.6
3	C	180	ASP	3.1
2	B	98	ASP	3.1
3	F	179[A]	LYS	3.1
3	F	57	GLU	2.8
3	F	63	GLU	2.7
2	E	297	ASP	2.7
3	F	46	GLY	2.6
3	C	59	MET	2.6
3	C	57	GLU	2.6
3	C	62	PRO	2.5
1	D	2	ALA	2.5
3	F	196	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	118	LYS	2.4
3	C	208	GLU	2.2
2	E	442	GLU	2.2
2	E	98[A]	ASP	2.2
1	D	118	LYS	2.1
1	A	123[A]	GLU	2.1
3	F	208	GLU	2.1
3	C	179	LYS	2.0
3	C	46	GLY	2.0
1	A	2	ALA	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	AGM	D	271	12/13	0.97	0.06	5,6,7,9	0
1	MHS	D	257	11/12	0.98	0.05	8,10,12,13	0
1	MGN	A	400	10/11	0.98	0.05	5,7,8,8	0
1	MGN	D	400	10/11	0.98	0.05	6,7,8,8	0
1	MHS	A	257	11/12	0.98	0.04	9,11,13,18	0
1	AGM	A	271	12/13	0.98	0.05	5,6,7,8	0
1	SMC	A	452	7/8	0.99	0.06	6,7,8,10	0
1	SMC	D	452	7/8	0.99	0.05	7,7,10,11	0
1	GL3	A	445	4/5	0.99	0.06	5,6,7,7	0
1	GL3	D	445	4/5	1.00	0.06	5,6,6,7	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

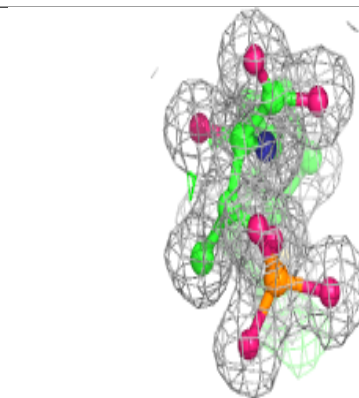
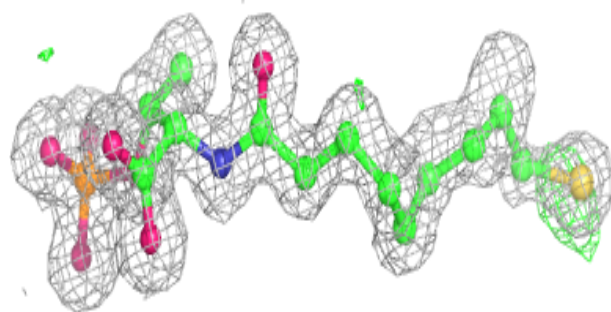
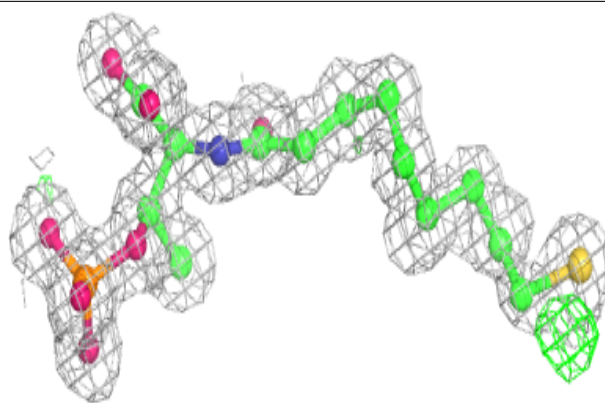
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	EDO	A	557	4/4	0.76	0.11	35,35,36,43	0
12	PEG	C	252	7/7	0.83	0.12	37,38,44,44	0
10	EDO	F	252	4/4	0.84	0.15	35,39,40,44	0
9	ACT	C	1	4/4	0.87	0.20	27,29,30,33	4
10	EDO	C	251	4/4	0.87	0.13	36,39,40,43	0
10	EDO	F	251	4/4	0.88	0.11	34,34,36,39	0
10	EDO	D	556	4/4	0.90	0.09	33,36,41,41	0
10	EDO	B	446	4/4	0.93	0.09	42,42,43,44	0
4	MG	B	444	1/1	0.96	0.14	26,26,26,26	0
4	MG	A	551[A]	1/1	0.97	0.21	20,20,20,20	1
4	MG	B	445	1/1	0.97	0.32	34,34,34,34	0
4	MG	F	250	1/1	0.97	0.07	15,15,15,15	0
8	XP9	A	555[C]	23/23	0.98	0.06	5,8,8,10	23
8	XP9	A	555[B]	23/23	0.98	0.06	6,7,9,11	23
6	TP7	D	553[A]	21/21	0.98	0.06	7,8,9,12	21
4	MG	C	250	1/1	0.98	0.08	15,15,15,15	0
6	TP7	A	553[A]	21/21	0.98	0.05	7,8,10,13	21
9	ACT	A	556[B]	4/4	0.98	0.07	13,15,16,17	4
8	XP9	D	555[B]	23/23	0.98	0.07	6,7,10,12	23
8	XP9	D	555[C]	23/23	0.98	0.07	6,8,9,11	23
4	MG	A	552[B]	1/1	0.98	0.10	12,12,12,12	1
4	MG	D	1	1/1	0.98	0.14	21,21,21,21	0
4	MG	D	551	1/1	0.99	0.24	24,24,24,24	0
4	MG	E	444	1/1	0.99	0.18	21,21,21,21	0
5	F43	D	552	62/62	0.99	0.05	4,7,9,12	0
5	F43	A	1	62/62	0.99	0.05	5,7,10,13	0
7	COM	D	554	7/7	0.99	0.06	9,10,12,13	0
7	COM	A	554	7/7	0.99	0.04	9,9,12,12	7
11	ZN	A	558	1/1	1.00	0.03	10,10,10,10	1

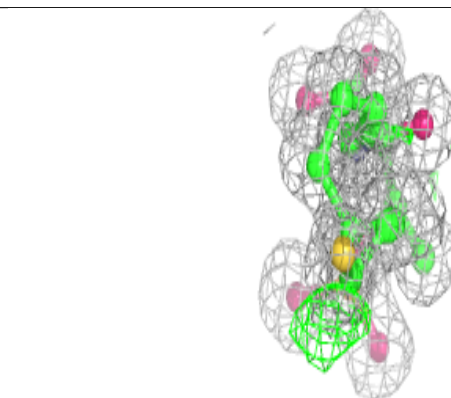
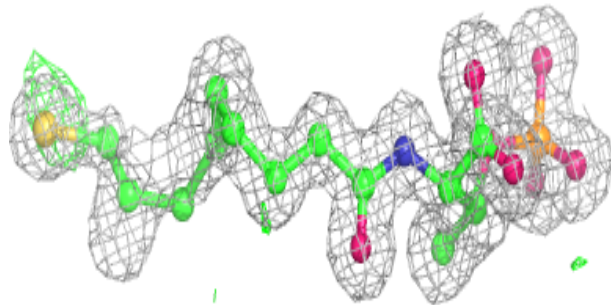
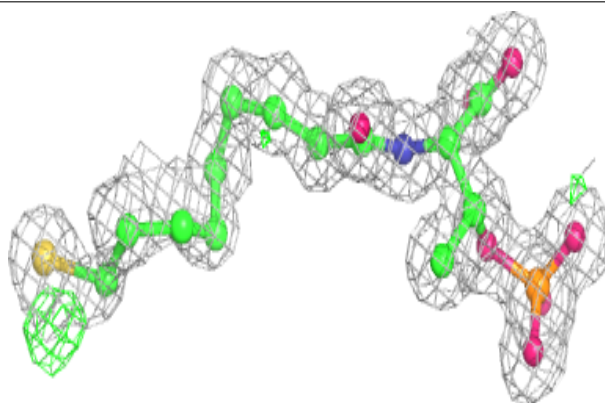
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around XP9 A 555 (C):

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

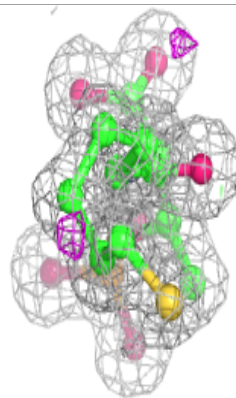
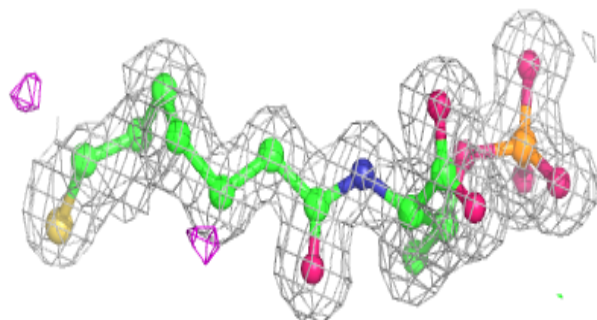
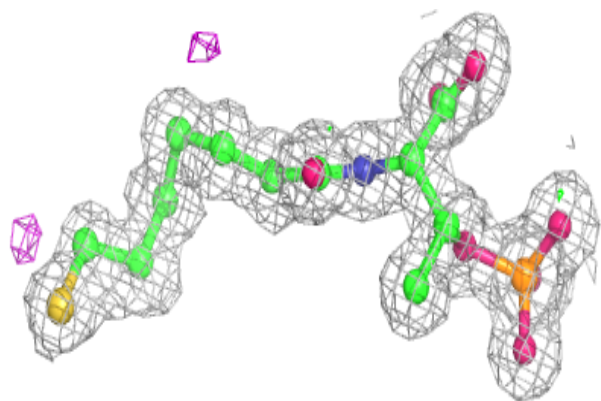
**Electron density around XP9 A 555 (B):**

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

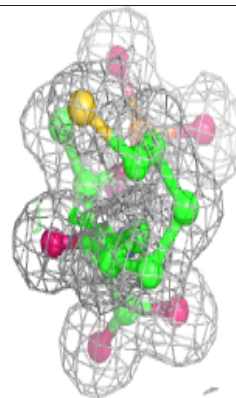
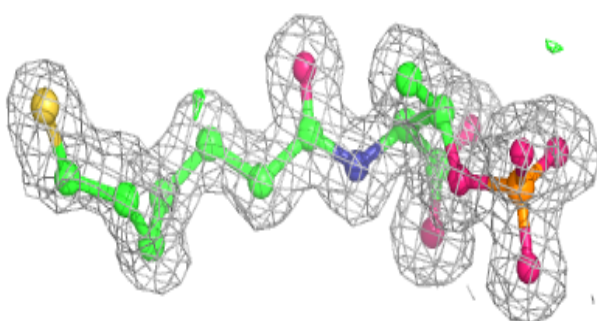
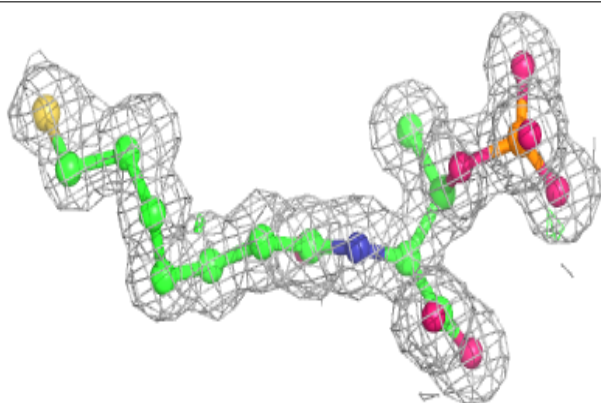


Electron density around TP7 D 553 (A):

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

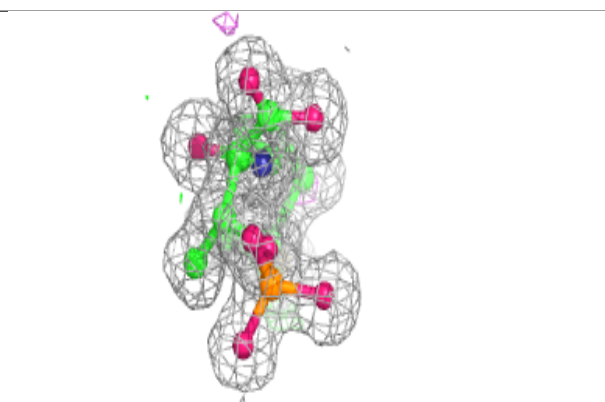
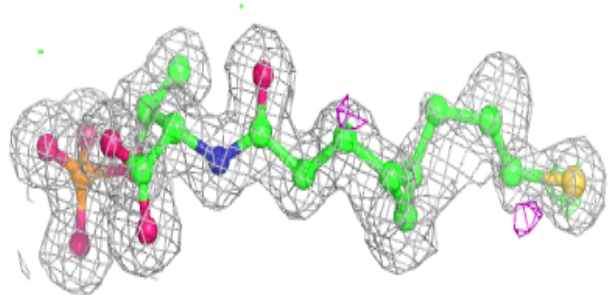
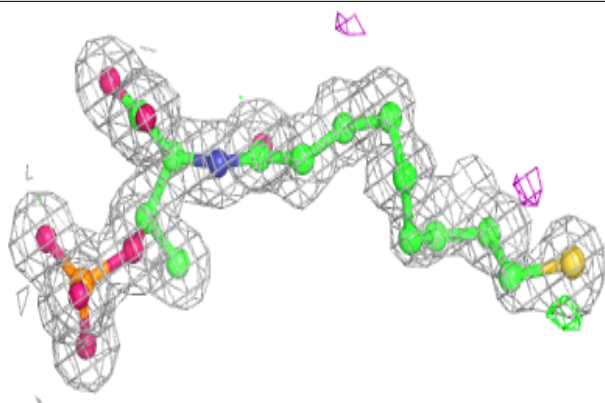
**Electron density around TP7 A 553 (A):**

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

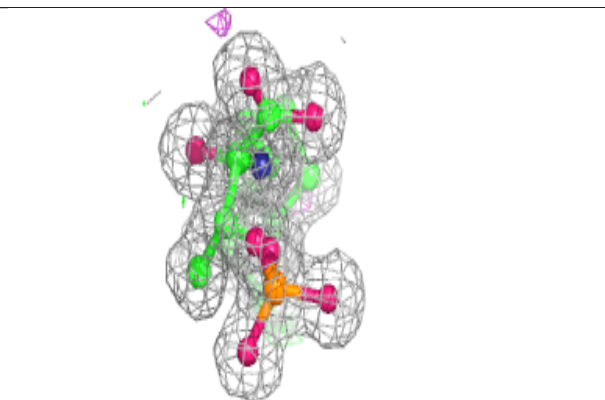
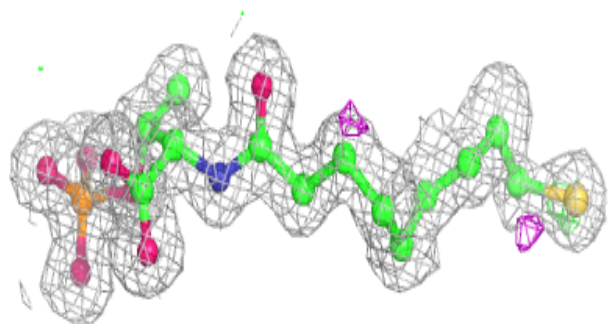
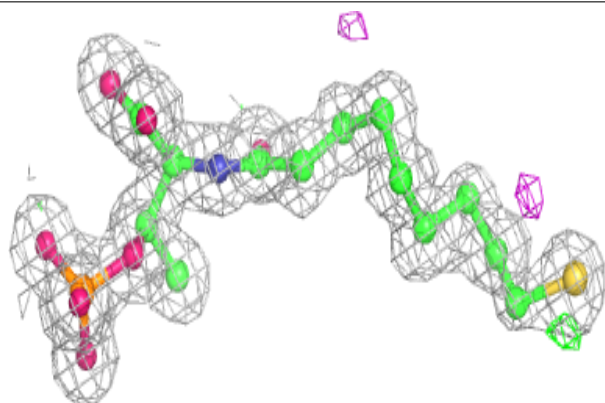


Electron density around XP9 D 555 (B):

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

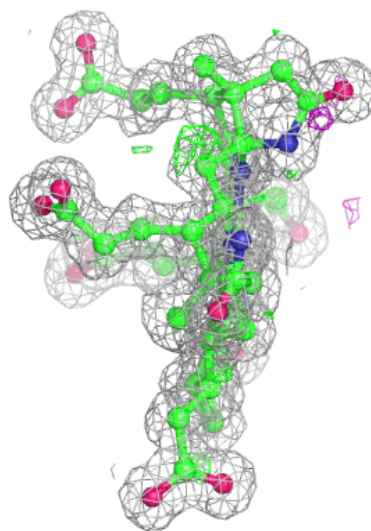
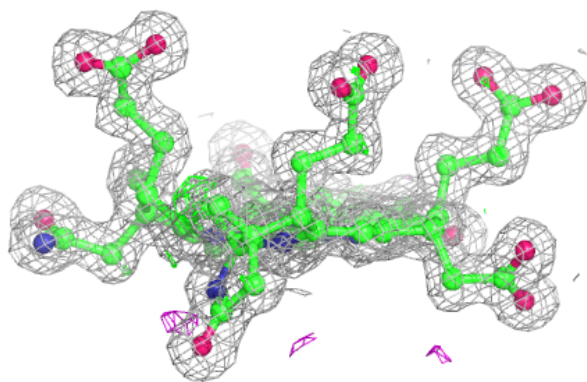
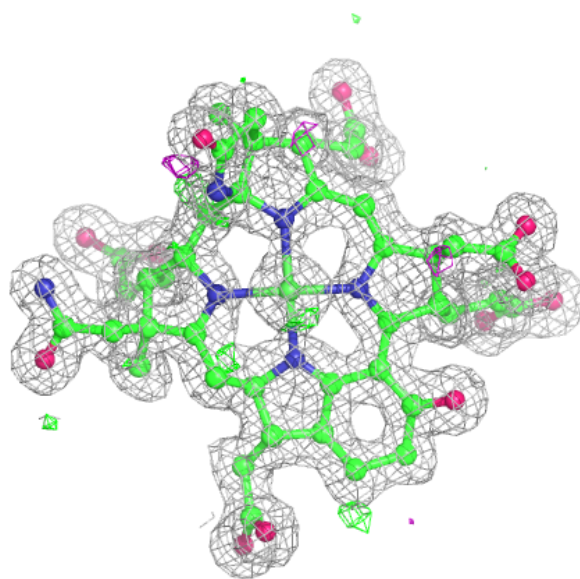
**Electron density around XP9 D 555 (C):**

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



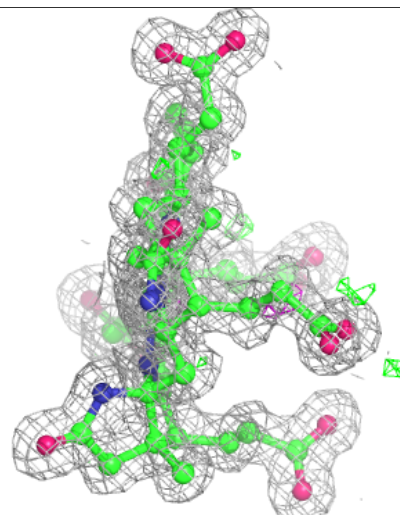
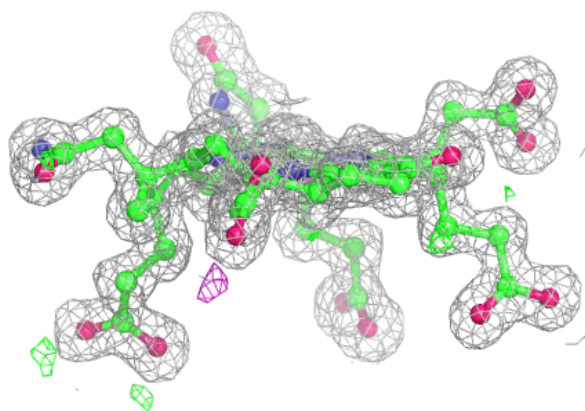
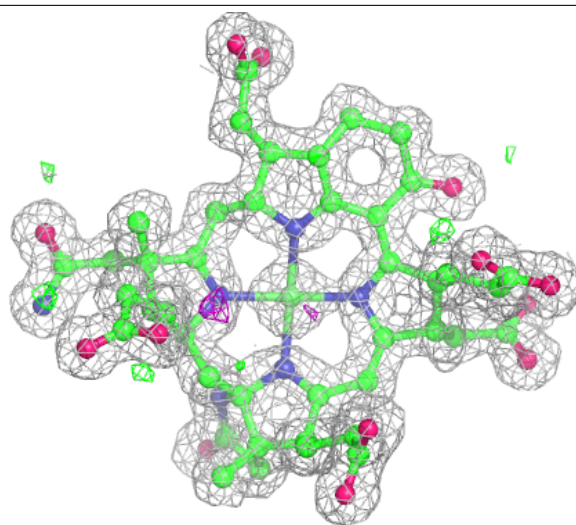
Electron density around F43 D 552:

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



Electron density around 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.